NOTES ON NUMERICAL FLUID MECHANICS AND MULTIDISCIPLINARY DESIGN · VOLUME 100

100 Volumes of 'Notes on Numerical Fluid Mechanics'

40 Years of Numerical Fluid Mechanics and Aerodynamics in Retrospect

Ernst Heinrich Hirschel
Egon Krause (Eds.)

Springer

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Ernst Heinrich Hirschel
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(Editors)

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Preface I

Aircraft concepts are always driven by the requirements of the desired mission. A different purpose for the use of the aircraft consequently results in a different design. Therefore, depending on the intended outcome, conflicting requirements need to be fulfilled, for example, efficient cruise speed and greater cargo capabilities, in combination with short take-off and landing field lengths, or high speed and agility combined with variable payload demands. Due to the highly complex, non-linear physical environment in which aircraft operate, this task demands that the most advanced methods and tools are employed, to gain the necessary understanding of flow phenomena, and to exploit the flow physics to achieve maximum aircraft efficiency.

In the natural sciences, researchers try to create and extend human knowledge by understanding and explaining the mechanisms of physical processes. In engineering, a designer is limited by certain requirements, and in order to fulfil these requirements the necessary technical tools need to be designed. In general, for a given problem the corresponding scientific or technical solution is sought. In order to successfully advance from a problem towards a solution, three main methods may be used. The two classical methods include theory and experiment, which are now being complemented by a third method, described as numerical simulation. The experimental approach is based on physical observation, measurement of relevant values, and methodical variation of the subject matter. For example, such experiments are used to gain a physical understanding as well as to validate and investigate design alternatives. In aerodynamics, experimental research is carried out by wind tunnel and flight testing. However, in the theoretical approach, certain correlations between physical observation and mathematical principles are hypothesized, and a corresponding mathematical formulation is developed, which describes the main mechanisms of the observed phenomena. A typical example of theoretical design methods is the Lifting-Line-Theory, developed by Ludwig Prandtl in 1918, which is itself based on potential theory.

With the progressive innovations in computer technology over the past decades, accompanied by corresponding algorithmic developments, numerical

simulation has matured from a scientific peculiarity to a tool applicable to the broad spectrum, from scientific investigations to product-oriented engineering design. Numerical simulation emulates physical processes by solving systems of differential equations, and can be interpreted as a complementary element to experimentation and theoretical consideration. Furthermore, as it involves elements of both experimentation and theoretical consideration, it may be regarded as the bridge between experiment and theory.

Numerical simulation is inherently interdisciplinary, as physics, mathematics, and informatics are all equally concerned. In 1755, Leonhard Euler proposed a set of non-linear partial differential equations, which describe the conservation of mass and momentum for an inviscid fluid. More than 50 years later, Claude Navier in 1822, and George Stokes in 1845, independently introduced viscous transport into these equations. This was subsequently extended to include the energy equation. After being cast into the so-called conservation form to capture flow discontinuities, the differential equations proposed now form the basis of numerical simulation in fluid dynamics today.

A direct solution of these differential equations is not generally feasible, and analytical solutions can only be obtained in unique cases, which are of limited practical interest. Essentially, there are two major routes that are followed to solve these equations: Either the equations will be further simplified, so that solutions are easier to obtain, which for example, resulted in the establishment of the potential theory of aerodynamics. Or the original exact equations will be solved only approximately by establishing and solving a corresponding set of discrete algebraic equations, which is numerical flow simulation. This process has been termed "Numerical Fluid Mechanics," respectively "Computational Fluid Dynamics" (CFD), since the solution of the algebraic system of equations requires the use of high performance computers.

For aerodynamics, the development of Computational Fluid Dynamics is particularly driven by an interest in transonic flows, which evolved in the early days of commercial jet aviation when the transonic drag rise phenomenon received particular attention. The solution of the Euler equations was essential for CFD research in the 1980s. This is comparable to the 1990s, which was the decade instrumental to solving the Navier-Stokes equations. A project for the development and validation of a reliable and efficient numerical tool for the aerodynamic simulation of a complete aircraft was initiated under the leadership of the German Aerospace Center (DLR) which would meet industrial implementation requirements. A software system titled MEGAFLOW was developed, and incorporated the block-structured Navier-Stokes code FLOWer, and the unstructured Navier-Stokes code TAU. Both codes have reached a high level of maturity and in cooperation with the DLR are intensively used by the German Aerospace Industry and its European partners in the design processes of new aircraft.

Numerical simulation has identified two challenges for future research and development. The first challenge is to extend the range of applicability of CFD methods. Furthermore, the second challenge is directly concerned with

the cost of applying CFD methods in the design process within multidisciplinary numerical simulation and optimization tools. For instance, in order to determine the static and dynamic loads required for structural design, hundreds of thousands of aerodynamic load cases need to be evaluated.

The tremendous progress achieved in numerical simulation over the past decades would not have been possible without the substantial increase in computational power. Therefore, in addition to the other notable theories of numerical simulation, the so-called Moore's Law developed in the 1960s by Gordon Moore, describes the continuum of increasing computational power. More specifically the theory hypothesizes that within 30 years computational power would increase by a factor of 33,000; and a computational job, which today would require 30 years, will in the future take only 8 hours to process. To further meet the challenges of numerical simulations, as hypothesized by Moore, there will be opportunities to make use of the upcoming greater computational capabilities. If efficiently implemented, this may open up the possibility to "flight-test" a simulated aircraft with all of its multidisciplinary interactions in a virtual environment. This would help to increase performance, reduce risk and to promote cost effectiveness in aircraft design processes by not only compiling all the data required for development and certification with a guaranteed accuracy, but also in a significantly reduced time frame. Thus, within the framework of numerical simulation and the methods of aircraft conceptual design, development and detailed design, the capabilities will be revolutionized.

There has been dramatic progress over more than 30 years in developing and applying numerical methods successfully in research and development. This success has been accompanied, stimulated and documented not only by appropriate working groups, workshops and international conferences but also by initiating in 1978 the book series "Notes on Numerical Fluid Mechanics." This series, as well as earlier the GAMM Committee on Numerical Fluid Mechanics with its conferences and workshops, originated at the DLR (at that time DFVLR) in Cologne-Porz. The present volume, produced 30 years after the series' first publication, underlines the capabilities of todays methods and tools and provides an impressive display of the expansive range of applications for science, engineering and particularly for aircraft research, design and development.

Cologne
October 2008

Prof. Dr. Joachim Szodruch
Member of the Executive Board
DLR German Aerospace Center

Preface II

Over the last three decades, Computational Science and Engineering evolved into a "third pillar" of scientific research alongside theory and experiment. The discipline of Computational Science, on the one hand, enhances scientific investigation by enabling theorists and practitioners to build and test models of complex phenomena, yielding new information, innovation and fresh insight into the research process that is not available through other means. On the other hand, it is a discipline sui generis that unlocks new areas of research, e. g., where experiments are impossible, too dangerous or forbidden. Essential contributions from Computational Science can be expected in a variety of fields of interest. They will lead to major advances in scientific research, leading to important industrial innovation and having a high societal impact.

The interplay between mathematical modeling and algorithm development/implementation is the driving force for Computational Science and Engineering. The availability of sophisticated numerical methods like Computational Fluid Dynamics is crucial to enhance the usability of modern supercomputers as for example the massively parallel IBM BlueGene systems. It's one of the aims of the Jülich Supercomputing Centre to cooperate with all scientific communities to enable important new simulation software for supercomputing.

The acceleration in the development of parallel supercomputers together with the advancing requirements of computational scientists and engineers with respect to application, memory, data storage, and data transfer capabilities, makes it increasingly difficult for single institutions to provide continual funding for latest top-ranked systems in ever shorter periods. A possible solution is the creation of networks or alliances which agree on close collaboration and internal innovation cycles. With the creation of the Gauß Centre for Supercomputing in 2006, Germany created a new and powerful structure for its three national supercomputing centers, the Leibniz Supercomputing Centre at Garching/München, the Supercomputing Centre Jülich, and the High Performance Computing Center Stuttgart, to take a leading role in Europe. The Gauss Centre for Supercomputing represents Germany as a single legal entity

in the European supercomputing infrastructure initiative PRACE (Partnership for Advanced Computing in Europe) which aims at the creation and sustained operation of a pan-European Tier-0 supercomputing service and its full integration into the European HPC ecosystem from 2010 on, as one of the list items of the European Strategy Forum on Research Infrastructures, ESFRI. Within the framework of PRACE, Germany's Forschungszentrum Jülich aspires to host the first European supercomputing centre with $Petaflop/s$ capability in 2009/2010.

The potential of CFD applications on high-end HPC systems can be illustrated using a computation performed recently by CERFACS (Toulouse, France) on an IBM BlueGene/L machine as reported in the "Scientific Case for European Petascale Computing" by the HPC in Europe Taskforce. This simulation of the ignition of a helicopter gas turbine (about 20 millions numerical cells) is one of the most complex large eddy simulations in turbulent combustion and took 60,000 CPU hours on 1024 processors (about 2.5 days of wall clock time). In order to reach a steady state regime, 100 to 200,000 additional CPU hours are required which can only be achieved on Petaflop systems.

The Notes on Numerical Fluid Mechanics and Multidisciplinary Design have been a most faithful companion of the field in the past. The Gauss Centre for Supercomputing is convinced that the NNFM will be a complete success in the forthcoming Petaflop Era as well.

Jülich
October 2008

Prof. Dr. Achim Bachem
Gauß Centre for Supercomputing,
Chairman of the Board of Directors
of the Research Centre Jülich

Foreword of the Volumes' Editors

Volume 100 of the series "Notes on Numerical Fluid Mechanics and Multidisciplinary Design" is dedicated to an overview of the origins and the development of the series, but also of the breathtaking development the field of numerical fluid mechanics has undergone over the past 40 years. This development holds also for other fields, like numerical engineering, physics, et cetera.

It is the intention of the book, to show in short contributions developments of the field as such, to illustrate applications in the aerospace sector, in engineering and physics, and finally developments in algorithms, computer sciences, and computer hardware. It was, however, not intended to present a stringent history of the development of numerical fluid mechanics.

It is a pleasure to acknowledge that the co-editors of the series and so many colleagues from the field of numerical fluid mechanics, but also from other fields followed the invitation to contribute to the volume. We have therefore a collection of outstanding contributions, both informative and entertaining.

The contributions were taken in their original form. In order to achieve a certain conformity of the layout, appropriate changes were made. Misprints were tacitly corrected.

The book in this form was only possible because of the generous support by the German Aerospace Center (DLR), the Leibniz Supercomputing Center (LRZ) at Garching/München, the Supercomputing Center Jülich (JCS), and the High Performance Computing Center Stuttgart (HLRS). This highly appreciated help made it possible to achieve the broad spectrum of the book.

Finally many thanks are due to the publisher of the NNFM series, the Springer-Verlag and there especially to Th. Ditzinger, who very effectively helped to publish this jubilee volume.

The first co-editor of this book retires with this volume as general editor of the series. The new general editor is W. Schröder, Aachen. Good luck to him and the series!

Zorneding and Aachen — E.H. Hirschel
January 2009 — E. Krause

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Introduction

Numerical fluid mechanics and aerodynamics, or if one likes, computational fluid dynamics, evolved since the mid 1960s, in a time span a little longer than a human generation, from a mere toy into a powerful and accepted tool of science and engineering.

The driving factors were initially sheer curiosity and enthusiasm, later, when the potential became manifest, it were the application needs, first mainly of the aerospace sector, later also of other sectors. This happened and happens with any new development: it spawns its own needs and applications. A very important factor was, luckily, the evolving computer power. It really took off with some time lag compared to the codes, but then, since the mid 1980s, computer power rose dramatically, and still rises.

The contributors to this volume as well as the editors of it, had the privilege not only to witness the evolution of numerical fluid mechanics and aerodynamics, but also, to different degrees, to help to develop and shape it. With this Volume 100 of the book series "Notes on Numerical Fluid Mechanics and Multidisciplinary Design" a retrospection at the evolution of the field is tried.

1 Some Historical Observations

It can be asked, why *numerical fluid mechanics* did evolve and not *numerical structure mechanics*, or some other field. Of course, structure mechanics basically is linear. But this holds also for classical aerodynamics. Once, however, viscous effects come in or one enters the transonic and then the supersonic/hypersonic domain, one has to deal with non-linear phenomena.

It is interesting to observe that one finds in a publication celebrating 50 years of the Society for Applied Mathematics and Mechanics (GAMM), [1], a note that the Association of German Engineers (VDI) organized meetings in the years 1919/1920 about the topics "Numerical integration of differential equations" and "Finite-difference computation and is application to technical problems".

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In Germany the mathematician Felix Klein (1849-1925) was pushing the application of mathematics in practice. Basically his idea was the "mathematization" of empirical sciences. In order to further his ideas, he got D. Hilbert in 1895 to come to the University Göttingen, H. Minkowski in 1902, and in 1904 C. Runge and L. Prandtl. Prandtl founded together with R. von Mises in 1922 GAMM. Most importantly, he created, after some steps in between since 1907, the Aerodynamische Versuchsanstalt (AVA) Göttingen, see, e. g., [2]. Under his leadership the "Göttingen school of fluid mechanics" evolved.

In our context important is, that L. Prandtl formulated in 1945 in the Betz commemorative publication, [3]: "*Already for a long time it is a central idea of the Göttingen fluid mechanics research to render, by suitable experiment-supported theories, future experiments superfluous*".

This certainly does not mean, that he was referring exclusively to numerical methods, but, nevertheless, he was actively involved in numerical fluid mechanics. L. Collatz notes in [4], that he heard at the beginning of the 1930s in Göttigen a lecture of L. Prandtl, where he treated, to Collatz's astonishment, numerical methods for difficult hydrodynamic problems. Prandtl developed together with A. Busemann the method of characteristics for the solution of the Euler equations for supersonic flow[1], [5], he also worked on a "continuation method" for the solution of the boundary-layer equations (1938).

One can imagine that the motivation for this was, regarding the first topic, his work since 1905 on flow problems of steam turbines (Prandtl-Meyer expansion, 1908) and, since the early 1920s, the beginning work on compressibility effects in aerodynamics. Aircraft at that time were not flying that fast, but propeller tips were reaching the speed of sound, see also [2]. Regarding the second topic, the restrictions of analytical solution methods for his boundary-layer equations (1904) asked for more general solution methods than the similarity method of Blasius and the integral method of von Kármán-Pohlhausen. Both topics, compressible flow and boundary-layer flow, are non-linear topics.

Very remarkable is, that Göttingen in the 1920s was the cradle of the famous Courant-Friedrichs-Lewy (CFL) condition (1928), [6], which is indispensable for any numerical scheme, see also the contribution of A. Rizzi and E. H. Hirschel in Part II of this book. Again a line goes back to F. Klein: R. Courant was a doctoral student of D. Hilbert, K. O. Friedrichs and H. Lewy were Courant's doctoral students.

Was there a connection to Prandtl's work? The method of characteristics theoretically fulfills exactly the CFL condition. If one looks at the two papers, no trace of a mutual recognition can be found. After all, the authors were together in Göttingen and most of them were even at the same university. Maybe after the death of F. Klein in 1925 his goal to bring together theory and practice was no more heeded in Göttingen.

[1] The method of characteristics, see also the contribution by A. Rizzi and E. H. Hirschel in Part II of this book, originally is a graphical method. However, it can rightfully be considered as a *numerical* method.

Anyway, after 1945 fluid mechanics and aerodynamics went fully into the non-linear domain. The advent of turbo-jet and of rocket propulsion extended flight speed into the transonic, the supersonic, and the hypersonic domain. The restrictions of ground-facility simulation were a strong motivation to search for other simulation means and this were the discrete numerical methods. However, it was not Germany, where Prandtl's tradition could well have been followed, but it was the USA, and to a degree the Soviet Union, where first the topic was taken up at large. Rising computer power and algorithm development, the latter, following Prandtl's example, first pursued mainly by fluid mechanicists, were pushing the methods towards a now well established research and engineering tool besides analytical methods and experiment.

2 Development of Computer Power and Algorithms

When the editors of this volume worked in the last quarter of the 1960s at the DVL/DFVLR Institute of Applied Gas Dynamics in Cologne-Porz on numerical solutions of the three-dimensional boundary-layer equations et cetera, they had available first a Zuse Z22 digital vacuum tube computer[2]. It had a core memory of 256 words (mid 1960s), a magnetic drum memory of 8192 words, and was programmed with either the assembly-like programming language "Freiburger Code", or with ALGOL. Soon the Telefunken TR440 and other machines followed.

Computer power since has grown steadily[3]. The microprocessor, emerging in the early 1970, changed all, see the contribution of A. Bode and C. Trinitis in Part V of this book. However, even at the beginning of the 1980s the chip performance was very small, and accordingly computer power, Figs. 1 and 2 (both figures are from the end of the 1990s). The, compared to today, very small power obviously was no obstacle for the people working on codes and applying them to fluid mechanical and aerodynamic problems. The volumes of the NNFM series give testimony in this regard.

Programming initially was cumbersome. The spread of FORTRAN 66 (still called FORTRAN IV) in the second half of the 1960s was a real boon for the code developer and user. The punched tape and the punch card were, quite for a time, the store of both the code and the input and control data. Wall-clock times were incredibly long, even for problems which take almost no time on today's computers. The new computer architectures, the vector computer, becoming widely available around 1980, and the parallel computer, available a couple of years later – for both architectures see the contribution of T. Watanabe and M. Nomura in Part V – posed new problems in programming and use.

[2] At that time the question "analog computer" or "digital computer" was not yet fully decided in favor of the latter.

[3] We define computer power loosely as a kind of sum of computer speed and storage.

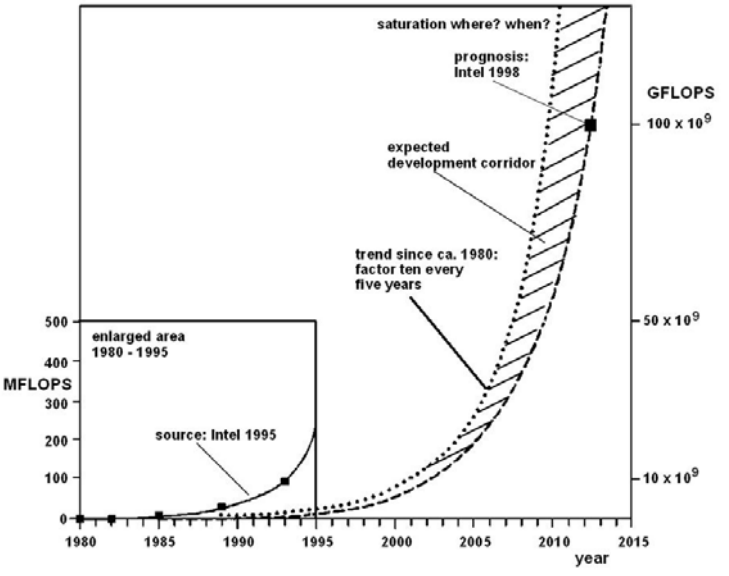

Fig. 1. Development of chip performance since the 1980s, [7].

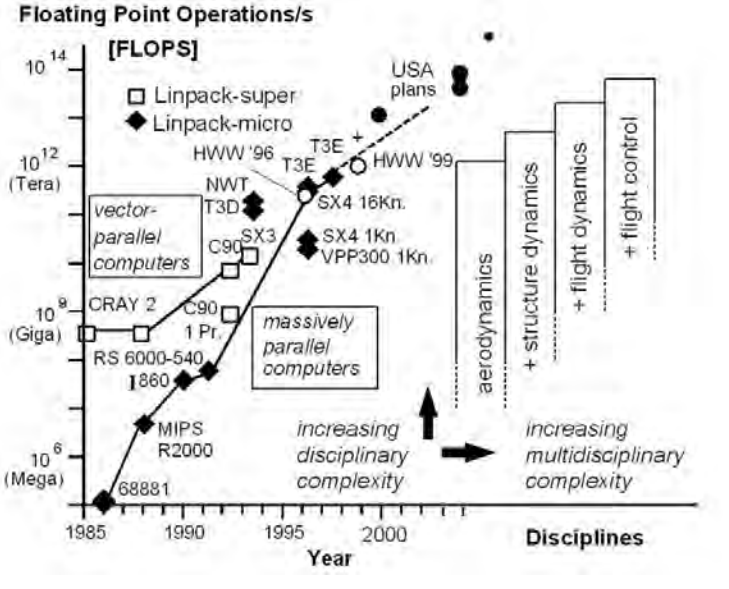

Fig. 2. Development of computer performance since the second half of the 1980s and – schematically – increasing disciplinary and multidisciplinary complexity, [7].

General problems initially were not only small computer speed and storage, but also the for a long time weak capabilities in grid generation, and, after the finished computation, data reduction and visualization. Of concern was, how far a given solution is grid-independent, whether it really has converged et cetera. These questions are still valid today, but much easier to answer.

Computer power development was a deciding element in the evolution of numerical methods, the other was algorithm development. Early codes of course made use of a host of different solution techniques for the algebraic systems which result from the discretization of the systems of partial differential equations describing fluid flow. The catchword for a long time was convergence acceleration. Algorithm development and computer science, see, e. g., the contributions by U. Trottenberg and T. Clees, and by H.-J. Bungartz, M. Mehl, and Ch. Zenger in Part V, brought – in particular in view of the new computer architectures – enormous gains, which however cannot be graphically illustrated in a simple way like the growth of computer power.

3 About Conceptions and Misconceptions

An initial misconception about numerical methods in fluid mechanics, certainly due to the unabating enthusiasm of some early pioneers, was that these methods would solve by themselves so far unsolved fluid mechanical or aerodynamical problems. It is necessary to conceive that numerical methods, first of all, have "only" tool character. Today one speaks of the three pillars of fluid mechanics and aerodynamics, viz. analytic methods, experimental simulation, i. e. ground-facility experimentation, and numerical simulation. In this sense numerical simulation has now also "method" character.

Research often is done in tool- or method-oriented ways, in contrast to problem-oriented ways. In the early days, usually codes were developed in order to compute – and, of course, investigate – a particular flow problem. Today, one may have access to a suite of programmes, whose use is supported by best-of-practice rules.

Industrial use of flow or aerodynamic codes, first of all is problem-oriented. Also here basic misconceptions existed and still exist. Different departments, with different tools, may perceive mutually unwanted competition. Universities and research establishments need to understand how and to what end aerodynamic codes are employed and what this means for present and future research.

Fig. 3 shows a schematic of tasks and tools of aerodynamics as an industrial discipline, [7], see also [8], which, of course acts always in concert with a host of other disciplines[4]. Numerical aerodynamics, besides other methods, has a major role in the aerodynamic *shape definition* of a flight vehicle. This

[4] The different product phases like pre-design, design et cetera, see, e. g., [8], are not distinguished.

holds also for the *design verification* of the (final) design in view of the performance guaranteed to the customer. Here the wind tunnel has an important role, too, especially since the mid 1990s the European Transonic Wind Tunnel, [9]. The ETW is a cryogenic facility which permits true Mach number and Reynolds number (as well as dynamic pressure) simulation in real flight parameter ranges. This allows for natural laminar-turbulent transition (not yet matched by numerical aerodynamics) and of, for instance, true simulation of shock/boundary layer interaction. Of course, in some cases only flight tests will allow the final verification.

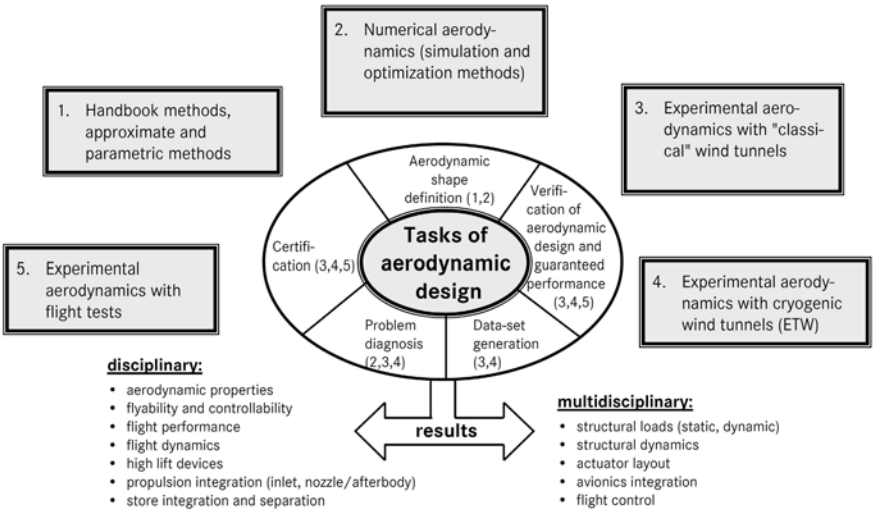

Fig. 3. Schematic of tasks and tools of industrial aerodynamics, [7].

The next task then is *data-set generation*, needed for the assembly of the so called aerodynamic model of the flight vehicle. This is, and will be for quite some time, the task of the wind tunnel, however, for reasons, which cannot be discussed here, not yet that of the ETW. Modern wind tunnels have such a high productivity, that, even if model manufacturing and instrumentation is taken into account, numerical aerodynamics cannot beat them. However, this does not hold, with very few exceptions, see, e. g., the discussion in [10], for the high supersonic and hypersonic flight domain.

Then it comes *problem diagnosis*. Diagnosis is needed in order to clarify why a given shape does have a certain aerodynamic performance or not. More important usually is the latter question, therefore *problem diagnosis*. The appropriate tool for this task clearly is numerical aerodynamics, although, if flow-physics modelling is critical, one has to go to the ETW or to flight

tests, the fifth tool. Finally for *certification* of the new flight vehicle one or several of the tools will be needed.

This all is an ideal picture. In reality it may look different to different degrees. Very important is, that this picture is the result of a paradigm change, which happened in the last decade. This change was due to the advances of numerical aerodynamics. In future the picture will change further in favor of numerical aerodynamics. However, this will only be effective, if, in particular, flow-physics modelling is drastically improved, see the next section.

It was elaborated, that a basic understanding of, for instance, industrial practice in aerodynamic design, is necessary in order to avoid misconceptions. It appears, however, that the implications of the advancement of numerical methods, see, e. g., [11], [8], at least in the aerospace sector are not understood to the needed degree on all concerned organization levels nor thematized sufficiently, for instance by the professional organizations. This, however, is necessary in order to shape most effectively the future national and international research and development efforts especially in view of the ecological and economical challenges, which are becoming more and more apparent.

4 Future Developments and Needs

The history of the development of numerical methods of fluid mechanics and aerodynamics is so far marked by the efforts to make the codes more fast, exact, and robust. This is a matter of algorithm development, which certainly will not go away for a while, although the matter of convergence speed may become secondary, because of the still growing computer performance.

To prepare for a numerical simulation, geometry preparation, usually from a CAD model and grid generation are necessary. The generation of, for instance, a structured multi-block grid for a whole aircraft configuration takes almost as much time as the manufacturing of a wind tunnel model. Unstructured grids and hybrid-Cartesian grids, both with the feature of self-adaptation or self-organization during the convergence process, appear to be the solution of the problem.

Flow-physics and thermo-chemical modelling are now addressed, the latter being a topic primarily of supersonic and hypersonic flight. The former concerns laminar-turbulent transition as well as turbulent shock/boundary-layer and other strong interactions, and especially separated and vortical flows. The latter concerns high-temperature real-gas effects of all kinds, which are not consider further here. Unfortunately it was not possible to give larger room to flow-physics modelling in this book.

For the determination of boundary-layer instability, also in view of natural and hybrid laminar wing flow (drag reduction), so-called stability methods are in use. Actual transition prediction is made today with the help of semi-empirical methods, with large uncertainty and unreliability. This is acceptable, if a design is transition insensitive. However, in view of the topic of transition

control for drag reduction and to match the capabilities of the ETW, this is not acceptable.

Numerical methods were early-on applied to study boundary-layer instability and transition, mostly by direct numerical simulation (DNS) also in order to validate and extend the above mentioned methods. At this time, these methods cannot, due to the sheer computer power needed, replace the above methods. Developments like non-local and non-linear methods, in the form of non-linear parabolized stability equation (PSE) methods, are presently not pursued to the needed degree (receptivity modelling problem, see below), although their potential has amply been demonstrated.

Turbulence modelling relies on statistical models, whose development was spurred by the evolution of the numerical methods. These models fail in some cases, for instance if separation has to be simulated. Modelling approaches like large eddy simulation (LES) with a lot of variants, up to hybrid approaches, are tried, with partly spectacular results, but actually without a real breakthrough so far.

Almost fully missing so far are receptivity models for both transition and turbulence models of all kinds. Real-life free stream fluctuations and noise, as well as real-life surface impurities (roughness, holes, joints of all kinds, steps, et cetera) affect laminar-turbulent transition and turbulent transport phenomena (skin friction, thermal loads). In this context it is mentioned that high aerodynamic shape fidelity and surface quality is needed at certain airframe portions (leading edges of wings, of trim, control and stabilization surfaces, slats, flaps, et cetera), but not necessarily everywhere at the airframe. Manufacturing costs and airframe weight could be reduced, if demands are relaxed, based on directed simulations with appropriate receptivity models.

With regard to the implications of the advancement of numerical methods the remark has to be made, that flow-physics modelling does not receive the attention which actually is needed. Compared to the efforts spent on the algorithmic development of numerical aerodynamic simulation methods, see for Europe the contribution by C.-C. Rossow and L. Cambier in Part III of this book[5], the efforts spent on flow-physics modelling are inadequate. It is urgently necessary to create and shape medium and long term national[6] and international research and development efforts also for this topic in view of the present and future ecological and economical challenges.

Regarding block-building and validation data for flow-physics modelling one should be aware, that low Reynolds number experiments on strong interaction and separation can be deceptive[7]. In such cases – which first of all must

[5] The development of the German numerical simulation system MEGAFLOW is now underway for almost 15 years.

[6] In Germany the German Research Foundation DFG sponsored corresponding efforts, as also the EU in Europe. In any case, they never reached the breadth and duration as had and has algorithm development.

[7] It is, for instance, since long known that separation topology can strongly depend on the Reynolds number (also the Mach number) and that, for instance, the

be identified – experiments must be made in realistic Reynolds and Mach number intervals, which would mean – in view of transonic flight – experiments in the ETW and even free-flight experiments, as was made regarding transition and transition control for drag reduction in several German national and European research and development programmes, see, e. g., [12].

Last but not least, because multi-disciplinary simulation and optimization is one of the next big challenges for numerical methods, flow-physics modelling, but in particular structure-physics modelling, will belong to the deciding factors. For the latter see the contribution by E. H. Hirschel and C. Weiland in Part III of this book.

5 Scope and Content of the Volume

This book, Volume 100 of the series "Notes on Numerical Fluid Mechanics and Multidisciplinary Design", is devoted to an overview of the development of the series, which reflects the development of numerical fluid mechanics from the beginnings, about 40 years ago, up to now. Considered too are applications in the aerospace field, as well as developments and applications in other fields, and also algorithms and hardware technology. The book consists of five major parts and an appendix. An introduction is given to each of the major parts.

Part I describes the series and its origins. It was initially closely related to the former GAMM-Committee for Numerical Methods in Fluid Mechanics. Details are given, also about the environment especially in Germany, where the series originated. In their forum, Part II, the co-editors of the series present short overviews of the developments in their countries, with different emphasis regarding the topics.

The series was from the beginning to a certain degree dominated by topics of numerical aerodynamics. Therefore current applications, predominantly from the aerospace field, are discussed in Part III, whereas Part IV is devoted to discussions of numerical solutions in other fields of engineering and physics in general. Finally, in Part V, the foundation of numerical fluid mechanics and aerodynamics is considered, viz. algorithms, computer science, et cetera, and finally the computer hardware.

In the appendix, Part VI, all 100 volumes are listed, also some forerunner volumes, as well as new and forthcoming volumes.

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The NNFM Series

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Summary The book series "Notes on Numerical Fluid Mechanics and Multidisciplinary Design" is portrayed. It originally was conceived as publication organ of the GAMM-Committee for Numerical Methods in Fluid Mechanics, but soon its scope was extended. In three sections it is sketched how the series came into being, how its aim developed, and how it evolved from the first to the present volume. The general editors and the co-editors of the series are listed and their duties are outlined. Finally acknowledgements are expressed to the publishing houses of the series, first Vieweg, then the Springer-Verlag, and especially to the persons directly involved in the publication of the series.

1 Introduction

In 1978 E. Krause was visited by A. Schubert from the German publishing house Vieweg, who invited him to write a book on numerical methods – see the contribution of E. Krause in this part of the book. Krause declined, but suggested, in view of the 1974 established GAMM-Committee for Numerical Methods in Fluid Mechanics – see the following contribution by C. Weiland and E. H. Hirschel – to initiate a book series on numerical methods. The idea was that always the newest solution methods and the latest results should be published without delay. K. Förster, and K. Roesner, both representing the GAMM-Committee, and A. Schubert discussed in Karlsruhe the idea further. The outcome was the proposal to initiate such a book series.

On the occasion of the annual meeting (Jahrestagung) of GAMM in Brussels, the GAMM-Committee for Numerical Methods in Fluid Mechanics met, too, on March 27, 1978. At that time K. Roesner was the chairman. One of the main topics of this meeting was the decision to start, with Vieweg, the new book series, which got the name "Notes on Numerical Fluid Mechanics". The proceedings of the biennial GAMM-Conferences on Numerical Methods in Fluid Mechanics and of the GAMM-Workshops were to be published in this series. K. Förster was elected to be the editor of the series.

E.H. Hirschel et al. (Eds.): 100 Vol. of 'Notes on Num. Fluid Mech.', NNFM 100, pp. 13–18.
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2 The Aim of the Series

On the back cover of the volumes one finds the statement:

"The aim of this series is to publish promptly and in a detailed form new material from the field of Numerical Fluid Mechanics including the use of advanced computer systems. Reports are published on specialized conferences, workshops, research programs, and monographs".

Even if originally the aim of the series was the publication of the proceedings of the GAMM-committee's conferences and workshops, it was opened very soon for other publications from the field of numerical methods in fluid mechanics. Table 1 gives an overview over the different topics of the volumes of the series from Volume 1 to Volume 100. The volumes[1] originated in Germany, in many European countries, Japan, and Russia.

Table 1. Topics of the NNFM volumes from No. 1 to No. 100.

Topic	Number of volumes
Proceedings of the committee's conferences	7
Results of the committee's workshops	12
Results of other GAMM-workshops and seminars	14
Results of other workshops	7
Proceedings of STAB/DGLR symposia	6
Proceedings of other conferences and meetings	16
Proceedings of Euromech Colloquia	2
Monographs	5
Results of DFG - Priority Research Programmes	7
Results of a DFG - Collaborative Research Programme	1
Results of a joint DFG/CNRS Programme	3
Results of programmes supported by the European Commission	16
Others	4

[1] For the volume's titles, editors, authors, and bibliographical data see the list in the Appendix on the pages 493 to 503.

3 Evolution of the Series

In the first volume of the series the results of the first GAMM-Workshop on Numerical Methods in Fluid Mechanics were published. The title of the workshop was "Boundary Algorithms for Multidimensional Inviscid Hyperbolic Flows", the organizer of the workshop and editor of the volume was K. Förster. The volumes front cover is shown in Fig. 1.

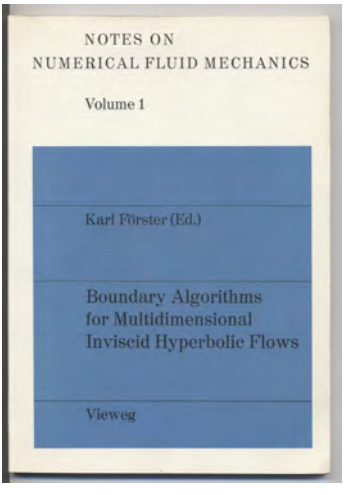


Fig. 1. Front cover of Volume 1.

Volume 2 contained the proceedings of the Third GAMM-Conference on Numerical Methods in Fluid Mechanics, DFVLR Porz/Cologne, October 10 to 12, 1979. The proceedings of the first two conferences were published as internal publication of the DFVLR Institute für Angewandte Gasdynamik, Porz-Wahn, Germany, see the list of the forerunner volumes on the pages 493 and 494 of the Appendix.

After editing the first six volumes, K. Förster had to give up the editorship of the series. In 1984 E. H. Hirschel took over. He asked several members of the GAMM-Committee to join him as co-editors, see the next section.

The number of volumes per year increased after the series became better known, Fig. 2, with some fluctuations over the years.

Early on plans evolved to publish also monographs in the series. Volume 4 by E. H. Hirschel and W. Kordulla was the first one[2]. Other monographs

[2] The topic of Volume 4 did not find much interest, especially in (West-) Germany. In 1987, however, a slightly extended version was published by the Russian MIR publishing house. Y. I. Sokin communicated in 2008, that it was translated by Ms. L. V. Sokolovskaya, edited by V. P. Shidlovskii, the total number of copies printed was 3,500, and it was used as university text book.

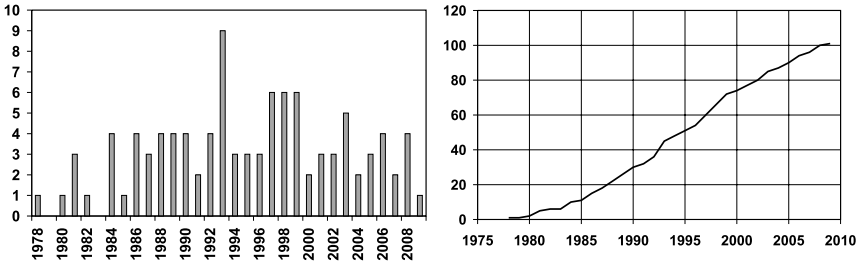


Fig. 2. Numbers of volumes published per year since 1978 (left) and accumulated numbers (right).

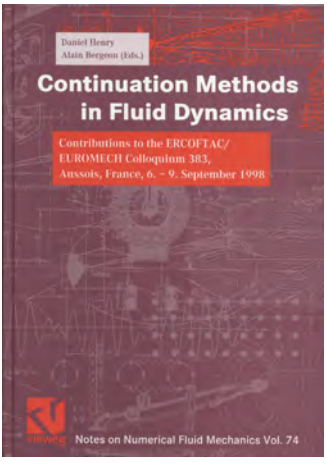
followed, but after Volume 34, appearing in 1992, it was decided, to pursue monographs not further. It was felt, that the series was too specialized and Vieweg was not enough present outside of Germany and Europe.

1988 Vieweg had become a subsidiary company of the Bertelsmann publishing group, later Bertelsmann Professional Information, and finally Bertelsmann/Springer. Since 1990, with Volume 27, the volumes appeared with a hard cover. With that volume also the logo "NNFM" was introduced. In 2000, with Volume 73, the layout of the cover was changed. Only two volumes appeared with that cover. The front cover of the second one is shown in Fig. 3(a), which is that of the last volume, Volume 74, of the series appearing with Vieweg.

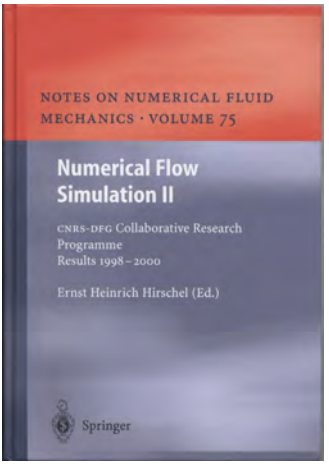
The series passed in 2001 from Vieweg to the Springer-Verlag, which was at that time part of the BertelsmannSpringer Science and Business Media group. The volumes got a new cover layout. The – new – front cover of Volume 75, the first one to appear with the Springer-Verlag, is shown in Fig. 3(b). In 2002, beginning with Volume 79 the series' title was changed to "Notes on Numerical Fluid Mechanics and Multidisciplinary Design", because it was felt that the emerging partial move of numerical fluid mechanics away from monodisciplinary to multidisciplinary topics should be reflected in the title of the series.

4 The General Editors and the Co-Editors

The first (general) editor of the series was K. Förster from the University Stuttgart. He built up the series, but had to retire in 1984. His successor, E. H. Hirschel, from MBB Military Aircraft, Ottobrunn/München, and, at that time, Technical University München, now retired, asked several members of the GAMM-Committee to serve as co-editors in order to promote the series more effectively especially outside of Germany. Since 2008 W. Schröder, RWTH Aachen, is the general editor of the series.



(a)



(b)

Fig. 3. Front cover of the volumes: (a) last volume, Volume 74, with Vieweg, (b) first volume, Volume 75, with the Springer-Verlag.

The co-editors are and have been:

– M. Pandolfi, Politecnico di Torino, Italy, since 1984,
– A. Rizzi, KTH, Royal Institute of Technology, Stockholm, Sweden, since 1984,
– B. Roux, Institute de Méchanique des Fluides, Marseille, France, since 1984,
– E. M. Murman, Massachusetts Institute of Technology (M.I.T.), Cambridge, USA, from 1987 to 1990,
– K. W. Morton, Oxford University, Oxford, Great Britain, from 1987 to 1995,
– K. Fujii, The Institute of Space and Astronautical Science (ISAS), Tokyo/ Kanagawa, Japan, since 1988,
– B. van Leer, The University of Michigan, Ann Arbor, USA, since 1990,
– M. Leschziner, UMIST, Manchester, Great Britain, now Imperial College of Science, Technology and Medicine, London, since 1996,
– W. Haase, Dasa Military Aircraft, Ottobrunn/München, now retired, since 1998,
– J. Periaux, Dassault Aviation, Paris/St. Cloud, France, now retired, since 2001,
– Y. I. Shokin, Institute of Computational Technologies of the Sibirian Branch of the Russian Academy of Sciences, Novosibirsk, Russia, since 2005,
– W. Schröder, RWTH Aachen, Germany, co-editor and designated general editor since 2007, general editor since 2008.

The duties of the co-editors are, besides the promotion of the series also the acquisition of new volumes. The general editor then makes contact with the

prospective volume editor(s), collects, checks and prepares the manuscript, and finally sends it to the publishing house for production. The commercial side of a volume's publication is handled by the publishing house.

General editors and co-editors were and are also active as volume editors or co-editors, or, up to Volume 34, as volume authors or co-authors, all even before being on the board. For the volumes published so far one finds – see the List of Volumes in the Appendix: K. Förster: 1 volume, K. Fujii: 3 volumes, W. Haase: 5 volumes, E. H. Hirschel: 11 volumes, B. van Leer: 1 volume, M. A. Leschziner: 3 volumes, M. Pandolfi: 1 volume, J. Periaux: 7 volumes, A. Rizzi: 4 volumes, B. Roux: 1 volume, Y. I. Shokin: 4 volumes.

5 And Last, But Not Least ...

Last, but not least thanks are due to all who have helped to run the series and to make it a success. This was first the publishing house Vieweg, which decided to take the risk and to set up the series, and where the volumes of the series appeared from 1978 until 2001, and then the Springer-Verlag, who took it over in 2001 and publishes it since then.

At Vieweg the person, who first did the actual publication work, was Alfred Schubert, together with Minna Hübner (Volumes 1 to 6). Then Björn Gondesen took over (Volumes 7 to 38). He was also in charge of the cooperation with the MIR publishing house for the Russian edition of Volume 4. Since 1993, beginning with Volume 39, Wolfgang Schwarz was responsible for the series. His lady assistants were first Minna Hübner and then Carola Brusberg, Frauke Schindler and Walburga Hummel.

At the Springer-Verlag, beginning with Vol. 75 in 2001, Thomas Ditzinger is in charge, assisted by Heather King. Helping the general editor in the change from paper handling to electronic handling of the manuscripts was Frank Holzwarth.

All of them sincere thanks for the trustful, competent and effective cooperation.

With pleasure acknowledged are the efforts of K. Förster in setting up the series and the always very pleasant and helpful cooperation with the co-editors. Finally thanks are due to the volume authors and editors, who trusted the series and who with their volumes established it and its reputation.

The Origin of the Series in the GAMM-Committee for Numerical Methods in Fluid Mechanics

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Summary The NNFM series originated as publication organ of the GAMM-Committee for Numerical Methods in Fluid Mechanics. This committee was founded in (West-) Germany in 1974 and existed until 1992. Its development and the main activities – the organization of GAMM-Workshops and GAMM-Conferences on Numerical Methods in Fluid Mechanics – are sketched in this contribution.

1 Introduction

Up to the 1960s the scientific work on fluid dynamics and aerodynamics traditionally was based mainly on analytical and experimental tools. Experimental facilities (water tunnels, wind tunnels, et cetera), semi-empirical relations and analytical solutions of reduced forms of the governing equations were the methods of choice during that time. At the end of the 1960s and the beginning of the 1970s there were some first activities – beyond the academic work at the universities and research establishments – to apply numerical methods for solving derivatives of the Navier-Stokes equations (boundary layer equations, potential equations, et cetera) for application problems.

The commencements were modest and the researchers had to fight with stability and convergence queries, in particular for the convective part of the equations, with lack of accuracy of the solution and with problems conducting the transformation from Cartesian to arbitrary curvilinear coordinates while preserving the conservation properties of the governing equations.

Over the years there were, besides others, two key events in the development of the numerical methods.

E.H. Hirschel et al. (Eds.): 100 Vol. of 'Notes on Num. Fluid Mech.', NNFM 100, pp. 19–28.
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The first one was the publication of H. Viviand [1], where the conservative transformation from Cartesian to arbitrary curvilinear coordinates was described (without using extensively the tensor calculus).

The second one has dealt with the use of elements of the theory of characteristics for the discretisation of the convective operator of the governing equations. The key papers are the ones of Godunov [2], van Leer [3], Roe [4] and Chakravarthy et al. [5].

These ideas have advanced the numerical methods to such an extent that today three-dimensional solutions of the steady and unsteady Navier-Stokes equations around configurationally complex airplanes and space vehicles are possible[1]. But in the beginning of the 1970s such a capability of the numerical methods was only far on the horizon.

1.1 The GAMM-Committee for Numerical Methods in Fluid Mechanics

Despite the fact that in the beginning of the 1970s the capacity of the numerical methods was rather small, some young researchers at the DFVLR in Cologne-Porz, Germany (E. Krause and E. H. Hirschel), who believed in the possible great potential of numerical methods, have founded in October 1971 the "Arbeitsgruppe für numerische Methoden in der Strömungsmechanik[2]". At that time, work on numerical methods in fluid mechanics was widely considered to be a topic not worth of much support.

The working group was composed of people from universities, research institutes and industry. They worked on the topics:

- flow past blunt bodies in the supersonic flight regime,
- flow with chemical reactions,
- application of "Mehrstellenverfahren" for the solution of the boundary-layer equations,
- three-dimensional boundary layers,
- subsonic flow past 2-D and 3-D configurations with separation,
- shock-boundary layer interaction.

For these topics so-called problem groups were established. We have a glance at two of them. The one on the first topic, established in 1972, was founded and headed by K. Roesner, University Freiburg. Members were K. Förster, University Stuttgart, D. Rues, DFVLR Aachen (later Göttingen), and C. Weiland, RWTH Aachen (later DFVLR Cologne-Porz). In the frame of the

[1] Of course this does not mean that today the problems of physical modelling are satisfactorily solved, which regards turbulence, transition, catalytic wall boundary conditions, et cetera.

[2] "Working Group for Numerical Methods in Fluid Mechanics". This group was at the same time a working party in the frame of the "European Research Programme on Viscous Flows (Eurovisc)", see, e. g., [6].

German ART programme (Association for Re-Entry Technologies) work in this group was sponsored, and contacts were established to industry (Dornier, ERNO, MBB). The group on the second topic was founded and headed by N. Peters, RWTH Aachen (1973).

The Arbeitsgruppe communicated its results in the so-called Profiles, which were informal publications of collections of short work descriptions. An attempt by E. Krause in 1971 to get a sponsoring of the group by the DFG was not successful. Since December 1972 E. H. Hirschel has acted as the executive chairman of the Arbeitsgruppe.

The Arbeitsgruppe became known, and, due to the direct contact of K. Roesner to H. Görtler the latter proposed at the annual meeting of GAMM in 1972 to establish the "GAMM-Fachausschuss für Numerische Methoden in der Strömungsmechanik[3]", which in effect changed the Arbeitsgruppe into a GAMM committee.

The committee was called into being at the inaugural meeting on April 3, 1974, which was organized by K. Roesner, under participation of the following founding members:

K. Förster, Th. Herbert, E. H. Hirschel, E. Krause, K. Roesner, W. Schönauer, B. Schmidt, J. Smolderen and H. J. Wirz.

The above mentioned change was then executed during the committee meeting on October 18, 1974, where also the GAMM president at that time, E. Becker, Technische Hochschule Darmstadt, took part.

The committee members[4] elected E. H. Hirschel to be its first chairman. The committee aimed from the beginning to be international. It also established contacts to other fields like meteorology, process engineering, et cetera. Being of large importance were considered close contacts to applied mathematics.

The committee's tasks and functions were fully developed within the course of approximately one year. By April 1975 they were mainly:

- the exchange and discussion of results, problems and initiation of research on and using numerical methods,
- the organization and execution of a biennial international conference on numerical methods[5],
- the initiation and performance of workshops[6] with respect to specific research items.

[3] GAMM-Committee for Numerical Methods in Fluid Mechanics.

[4] The committee members at that time didn't coincide completely with the founding members. They were: Th. Herbert, E. H. Hirschel, E. Krause, K. Nickel, N. Peters, R. Rautmann, K. Roesner, W. Schönauer, J. Smolderen, W. Wesseling and H. J. Wirz.

[5] The "GAMM-Conferences on Numerical Methods in Fluid Mechanics", see below.

[6] The "GAMM-Workshops on Numerical Methods in Fluid Mechanics", see also below.

The influence of the committee's work was supported and strengthened by the establishment of the publication series "Notes on Numerical Fluid Mechanics" (NNFM) in 1978. The publisher was the German Vieweg Verlag, Wiesbaden, see the preceding contribution.

Chairmen of the committee were:

Oct. 1974	– Feb. 1976	E. H. Hirschel,
Feb. 1976	– May 1979	K. Roesner,
May 1978	– Oct. 1982	N. Peters,
Oct. 1982	– Oct. 1987	U. Schumann,
Oct. 1987	– end of 1992	W. Kordulla[7].

Over the lifetime of the committee of more than 18 years, as usual, the members of the committee changed, some persons did retire while others were added. The list, in alphabetic order, of the persons who were members of the committee during its lifetime time, is:

M. Deville, Belgium	K. Förster, Germany
B. Gampert, Germany	Th. Herbert, Germany
E. H. Hirschel, Germany	W. Kordulla, Germany
E. Krause, Germany	Y. Morchoisne, France
K. Morgan, Great Britain	K. Nickel, Germany
N. Peters, Germany	M. Pandolfi, Italy
R. Piva, Italy	W. Prosnak, Poland
R. Rautmann, Germany	A. Rizzi, Sweden
K. Roesner, Germany	B. Roux, France
D. Rues, Germany	V. V Rusanow, Russia
I. L. Ryhming, Switzerland	J. Smolderen, Belgium
W. Schönauer, Germany	U. Schumann, Germany
Y. Shokin, Russia	H. Viviand, France
C. Weiland, Germany	P. Wesseling, The Netherlands
W. Wesseling, The Netherlands	H. J. Wirz, Belgium

2 The Book Series "Notes on Numerical Fluid Mechanics"

In 1974 the new committee of course discussed the matter of publications. A possible dedicated book series was not considered. The events took their course, when E. Krause was contacted by the publisher Vieweg, however not

[7] The committee was no longer active acting beyond the year 1992, mainly due to the Europeanisation of the "GAMM-Conferences on Numerical Methods in Fluid Mechanics" into the conferences of the "European Committee on Computational Methods in Applied Sciences" (ECCOMAS), see below.

regarding a book series. In the preceding contribution details about the history of the series can be found.

The now 30 years of the series have seen a dramatic evolution of numerical methods with respect to the quality of the methods: accuracy, stability and convergence behavior. Similarly the application to very complex geometrical configurations with the capacity of a sufficient degree of flow resolution has obtained a very high level.

The key points addressed in the introduction to this contribution are today part of every modern CFD code, and a lot of further work in this regard was published in the series since then, some of them also by the authors mentioned in the introduction.

3 The GAMM-Conferences on Numerical Methods in Fluid Mechanics

During the initial meetings of the GAMM-Committee it was planned to keep the yearly informal meetings of the Arbeitsgruppe. The first announcement of the October 1975 meeting, dated December 16, 1974, spoke of a conference on "Numerical Methods in Fluid Mechanics". At the meeting on April 1, 1975, the committee finally agreed on the "GAMM-Conferences on Numerical Methods in Fluid Mechanics" as biennial conferences on numerical methods, alternating with the "International Conference on Numerical Methods in Fluid Dynamics".

The first of the conferences was organized by E. H. Hirschel and W. Geller at the DFVLR in Cologne-Porz, October 8 to 10, 1975. It was attended by approximately 100 persons from seven countries. 30 papers were presented on topics from aerodynamics, environmental sciences, hydrodynamics, medicine, meteorology, and nuclear energy. Besides V. V. Rusanow from the USSR Academy of Science, some more persons from the Soviet Union could participate thanks to the efforts of K. Roesner to acquire funding for them. He was able to secure this kind of support at least for the second and the third conference, which were held also at the DFVLR in Cologne-Porz.

Several mathematicians attended the conference, true to the goal of the committee, to establish close contacts between the fields of numerical fluid mechanics and applied mathematics. The organizers of the conference, who also published the proceedings as internal report[8], noted in the preface the *"different languages these people speak"*, but were confident, that a "convergence" finally can be reached.

With the years the conference was getting more and more international and was held, besides in Germany, in the European countries France, Italy,

[8] See the list of forerunner volumes of the NNFM series on the pages 493 and 494 of the Appendix.

Belgium, The Netherland and Switzerland. Nine GAMM-Conferences were organized, the last one 1991 in Lausanne, Switzerland.

After having installed the publication medium "Notes on Numerical Fluid Mechanics" in 1978, the conference proceedings, first that of the third conference, were issued in this series, see Table 1.

Table 1. GAMM-Conferences organized and the proceedings' volumes published in the NNFM series.

No	Location	Date	Chairmen	Number of Papers	NNFM
I	Cologne, Germany	8. - 10.10. 1975	E.H. Hirschel W. Geller	30	forerunner publication
II	Cologne, Germany	11. - 13.10. 1977	E.H. Hirschel W. Geller	34	forerunner publication
III	Cologne, Germany	10. - 12.10. 1979	E.H. Hirschel	32	Vol. 2
IV	Paris, France	7. - 9.10. 1981	H. Viviand A. Rizzi	32	Vol. 5
V	Rome, Italy	5. - 7.10. 1983	M. Pandolfi R. Piva	45	Vol. 7
VI	Göttingen, Germany	25. - 27.9. 1985	D. Rues W. Kordulla	51	Vol. 13
VII	Louvain-La-Neuve, Belgium	9. - 11.9. 1987	M. Deville	55	Vol. 20
VIII	Delft, Netherland	27. - 29.9. 1989	P. Wesseling	60	Vol. 29
IX	Lausanne, Switzerland	25. - 27.9. 1991	I.L. Ryhming J. Vos	54	Vol. 35

At the end of the second half of the 1980s, E. H. Hirschel, since 1980 with MBB, but no more a member of the GAMM-Committee, thought it to be necessary to unite in an appropriate way the in Europe existing groups and committees on numerical fluid mechanics. He proposed to create a "Federation of European Numerical Fluid Mechanics Groups (FENFMG)" and contacted the chairman of the GAMM-Committee, then W. Kordulla, and also chairmen of other groups. W. Kordulla took a first step in inviting to a discussion during a meeting of the committee in Delft, April 1989. FENFMG was to strengthen the development of numerical methods in fluid mechanics and to channel the scientific events in Europe. Its activities were proposed to be patterned basically after those of the committee.

The events got their own dynamics and at the beginning of the 1990s the "European Conference on Computational Methods in Applied Sciences (ECCOMAS)" was born. The GAMM-Conferences were merged after the ninth conference in Lausanne, Switzerland in September 1991 into the ECCOMAS-Conferences. The first ECCOMAS conference took place under the chairmanship of C. Hirsch in Brussels, Belgium, from September 7 to 11, 1992. After the GAMM-Conferences ceased to exist also the GAMM-Committee did.

4 GAMM-Workshops on Numerical Methods in Fluid Mechanics

At the meeting of the GAMM-committee on October 10, 1975, one day before the beginning of the first GAMM-Conference on Numerical Methods in Fluid Mechanics, E. H. Hirschel proposed the introduction of "GAMM-Workshops on Numerical Methods in Fluid Mechanics" as activities complementary to the GAMM-Conferences and Euromech colloquia.

He defined their scope as: *"Extensive informal discussion on a high professional level of the mathematical and numerical aspects of very sharply defined topics in order to disseminate knowledge, to provoke direct comparisons of methods, to foster cooperation, and to stimulate new work".*

Participants were to be people active on the topic in question, who have made already several contributions, no observers, no beginners, number of participants 10, at most 15, duration of a workshop 1 day, 2 at maximum.

Fig. 1. Participants of the first GAMM-Workshop in Stuttgart. From left to right. First row: K. Förster, G. Moretti, L. Zannetti, M. Pandolfi, L. Karlson. Second row: T. deNeef, K. Roesner, C, Weiland, L. Theilemann, H. H. Frühauf.

There is no doubt that one reason for the successful work of the GAMM-Committee was the organization and performance of the GAMM-Workshops, which were the blueprint for coming similar activities worldwide. Mostly the organizers of these workshops were committee members. The first one, organized by K. Förster, had the title "Boundary Algorithms for Multidimensional Inviscid Hyperbolic Flows" and was held in Stuttgart, Germany. The photograph, Fig. 1, shows the participants of this workshop.

In total 17 workshops were held and the results obtained were published mostly in the "Notes on Numerical Fluid Mechanics". Table 2 gives on overview over the titles, the chairmen, the dates and the NNFM volumes of the proceedings of all the workshops performed.

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Table 2. GAMM-Workshops organized and the proceedings' volumes published in the NNFM series.

No	Title	Date	Location	Chairmen	NNFM
1	Boundary Algorithms for Multidimensional Inviscid Hyperbolic Flows	28.2. - 1.3. 1977	Stuttgart, Germany	K. Foerster	Vol. 1 1978
2	Fast Solution Methods for the Discretized Poisson Equations	3. - 4.3. 1977	Karlsruhe, Germany	U. Schumann	–
3	Finite Element and Finite Volume Methods for Hyperbolic and Mixed-Type PDE's	22.8. 1978	Friedrichs-hafen, Germany	W. Schmidt F. G. Sator	–
4	Numerical Methods for the Computation of Inviscid Transonic Flows with Shock Waves	18. - 19.9. 1979	Stockholm, Sweden	A. Rizzi H. Viviand	Vol. 3 1981
5	Spectral Methods	23. -24.10. 1980	Louvain-La-Neuve, Belgium	M. Deville	–
6	Numerical Methods in Laminar Flame Propagation	12. - 14.10. 1981	Aachen, Germany	N. Peters J. Warnatz	Vol. 6 1982
7	Lehrveranstaltungen auf dem Gebiet der numerischen Methoden der Strömungsmechanik	25. - 26.2. 1982	Essen, Germany	B. Gampert	–
8	Laminar Flow Over a Backward Facing Step	Jan. 1983	Bievres, France	K. Morgan J. Periaux F. Thomasset	Vol. 9 1984
9	Numerical Calculation of Nonequilibrium Diffusion Flamelet Structures	1. - 3.12. 1983	Heidelberg, Germany	N. Peters J. Warnatz	–
10	The Efficient Use of Vector Computers with Emphasis on Computational Fluid Dynamics	13. - 15.3. 1985	Karlsruhe, Germany	W. Schönauer W. Gentzsch	Vol. 12 1986
11	Numerical Simulation of Compressible Navier-Stokes Flows	4. - 6.12. 1985	Sophia-Antipolis, France	M. O. Bristeau R. Glowinski J. Periaux H. Viviand	Vol. 18 1987
12	Direct and Large-Eddy Simulation of Turbulent Flows also as EUROMECH 199	30.9. - 1.10. 1985	München, Germany	R. Friedrich U. Schumann	Vol. 15 1986

GAMM-Workshops organized and the proceedings' volumes published in the NNFM series, (Table 1.1. continued).

No	Title	Date	Location	Chairmen	NNFM
13	Numerical Simulation of Compressible Euler Flows	10. - 13.6. 1986	Rocquencourt, France	A. Dervieux B. van Leer J. Periaux A. Rizzi	Vol. 26 1989
14	Numerical Simulation of Oscillatory Convection in Low Prandtl Number Fluids	12. - 14.10. 1988	Marseille, France	B. Roux	Vol. 27 1990
15	3-D Computation of Incompressible Internal Flows	14. - 15.9. 1989	Lausanne, France	I. L. Ryhming G. Sottas	Vol. 39 1993
16	Numerical Simulation of 3-D Incompressible Unsteady Vicous Laminar Flows	22. - 24.5. 1991	Paris, France	M. Deville T.H. Le Y. Morchoisne	Vol. 36 1992

The Environment of the Series in the Initial Phase

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Summary This article reviews some of the work carried out on numerical methods in fluid mechanics in Germany during the past four decades: Early investigations in the sixties dealt with the extension of already existing solutions for two-dimensional flow problems to those of three-dimensional flows. In the following decades international short courses and conferences were established, and cooperation between scientists of various research centers and universities was successfully initiated and built up. The German Research Foundation generously sponsored these activities in two priority programs and in a third cooperative research program co-sponsored by the French Centre National Recherche et Scientific. In the nineties the German Science Council proposed a recommendation to the Federal Government to establish high-performance computing in Germany on an internationally competitive basis, which finally resulted in the foundation of the German Gauss Center for Supercomputing.

1 Introduction

In January 2007 the Research Center Jülich and the Rheinisch-Westfälische Technische Hochschule Aachen announced the foundation of a *German Research School for Simulation Sciences* (GRS). The school was introduced by the German Minister for Education and Research as a model for a new form of university education in Germany. The GRS is set up as a graduate and postgraduate school, leading the students to a master's and doctor's degrees in the simulation sciences. This new field comprises the mathematical simulation of natural and technical processes with the aid of high-performance computers, as for example complex biological, chemical, physical, and medical processes, and assists in the realization of engineering projects, which otherwise would not have a chance to be materialized, as for example the design of advanced, highly fuel-efficient aircraft.

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springerlink.com

The foundation of the GRS took place forty years after the author had published his first paper in what is now called numerical fluid mechanics. The paper was entitled *Numerical solution of the boundary-layer equations*. It appeared in the Journal of the American Institute of Aeronautics and Astronautics (AIAA). Although the investigation dealt with the construction of an implicit numerical solution of Prandtl's equations and not so much with the fluid mechanical aspects, it had to be published in the AIAA-Journal, as a corresponding journal for simulation sciences did not exist at that time. Publications on numerical methods were often greeted with skepticism, to say the least, and even thirty years later the question, whether numerical simulations with high-performance computers were at all necessary, was often raised in decision-making committee meetings. The remark Max Planck made in 1948 on the acceptance of new scientific achievements also seemed to apply to the simulation sciences (in the translation): *A new scientific truth usually does not make its way in the sense, that its opponents are persuaded and declare themselves as enlightened, but rather that the opponents become extinct and that the rising generation was made familiar with the truth from the very beginning.* But now, eventually, the simulation sciences are a new form of university education.

Recently, the computational potential in Germany was consolidated: In autumn 2006 at the inauguration of the SGI system Altix 4700 at the Leibniz Computing Center of the Bavarian Academy of Sciences in Munich (LRZ) the German Minister for Education and Research announced a new national strategy in high-performance computing: The three national high-performance computing centers, the High-Performance Computing Center Stuttgart (HLRS), the John von Neumann Institute for Computing in Jülich (NIC), and the LRZ in Munich, merged into the Gauss Center for Supercomputing. The alliance of the three centers represents one of the largest and most powerful supercomputer infrastructure in Europe [1]. It took more than half a century to arrive at this goal, counting from the very beginning of computing in the fifties of the last century.

Upon request of the general editor of the *Notes on Numerical Fluid Mechanics*, Professor E. H. Hirschel, some of the developments the author was involved in during the past four decades will briefly be reviewed in the following. The author also takes this opportunity to thank the editor of this series for his continuous effort to make such an outstanding success of the *Notes*. The publication of the hundredth volume is indeed the best proof of the quality of the investigations published in the series since its foundation.

2 Early Investigations

In the sixties, the author was involved in developing algorithms for numerical solutions of the boundary-layer equations. The first investigations were focussed on the implementation of the boundary conditions and the

reduction of the computational effort, as the computational speed was still rather limited. The problems studied comprised the influence of distorted profiles of the tangential velocity component on the wall shear-stress distribution, of pressure gradients on suction in hypersonic boundary layers, and of tangential slot injection on the mixing and combustion process in supersonic boundary layers, and others.

With increase of the storage capacity algorithms could be designed for the solution of the boundary-layer equations for three-dimensional flows [2]. The step into the third dimension necessitated the introduction of suitable finite-difference schemes, in order to be able to satisfy the numerical domain of dependence condition, the concept of which was already introduced by R. Courant, K. O. Friedrichs, and H. Lewy as early as 1928, long before actual computational work was started [3]. Of the schemes introduced, the *zick-zack-scheme* became rather popular; it offered the largest numerical domain of dependence for the smallest amount of computational effort with second-order accuracy. The storage problem was circumnavigated by employing three magnetic tapes to store the initial and boundary conditions and the newly computed data. Calculation times were extremely long and could only be managed during weekends.

Several three-dimensional boundary-layer problems were investigated with the solution developed: For example the influence of normal injection and suction on the downstream flow development, of locally heated wall surface elements, and of perturbed inflow conditions. The development of three-dimensional boundary layers on swept wings was studied with various closure assumptions for the Reynolds stresses in subsequent investigations.

Also in the sixties, together with colleagues of New York University an algorithm was constructed for the numerical solution of the Poisson equation on a staggered Cartesian grid [4]. This was one of the first solutions with which the lift of a wing section in a two-dimensional non-uniform stream could numerically be simulated.

In the following years the work on the development of algorithms followed two different directions. One was motivated by the 1968 Stanford Conference on Computation of Turbulent Boundary Layers: More or less all the numerical solutions presented failed to predict the experimental data to which they were to be compared. In order to be able to decide on the accuracy of the closure models for the Reynolds stresses, the numerical accuracy of the solutions had to be improved. This was attempted by reducing the truncation error in the finite-difference form of the boundary-layer equations with the aid of the Mehrstellen-method, earlier developed by L. Collatz [5] and others [6].

The second line of investigations was initiated by the need for a better understanding of flows with strong rotation, as they occur in gas centrifuges for isotope separation. Scientists of the Nuclear Research Center Jülich had repeatedly encouraged studies of such flows with numerical techniques; experimental techniques were difficult to use, as probes intruded into the flow would immediately disturb the flow pattern so much that results could barely be

interpreted. First numerically simulated flows with strong rotation, obtained with a solution of the Navier-Stokes equations, were discussed at a colloquium on flow-processes in gas centrifuges, held at the DFVLR Research Center in Cologne in 1970 [7]. This colloquium was the start of a long cooperation with the Nuclear Research Center Jülich and the associated industry.

In the following years, the numerical solutions of the Navier-Stokes equations were continuously refined and improved, and the experience gained in constructing and applying numerical solutions of the conservation equations soon led to the initiation of introductory courses, lectures, conferences, and also to the introduction of this series.

3 Spreading the News

As regular scientific meetings on flow computations were not yet established, small informal meetings were held at the DFVLR in Cologne and elsewhere in Germany (Arbeitsgruppe für Numerische Methoden in der Strömungsmechanik - Working Group for Numerical Methods in Fluid Mechanics, see the preceding contribution by C. Weiland). Among the participants were Professors K. Förster of the University of Stuttgart, E. H. Hirschel, and D. Rues of the DFVLR, and K. Roesner, at that time at the Max Planck-Institut für Strömungsforschung in Göttingen. These meetings served to exchange information about the ongoing work and the machine capabilities available at the various research centers and universities.

It was quite a surprise when an International Conference on Numerical Methods in Fluid Dynamics was announced for September 1970, proposed to be organized by Professor Maurice Holt of the University of California at Berkeley. According to the announcement it was the second of a new series, but little or nothing was known about the first. Rumors had it, that it was initiated in 1969 in Akademgorodok in Siberia by a member of the Russian Academy of Sciences, Professor N.N. Yanenko. The relatively sparse scientific contacts between East and West in those days of the Cold War made it hard to believe that such a step was at all possible.

Yanenko's idea to initiate a series of conferences for the new branch of fluid mechanics on a worldwide basis was greeted with great enthusiasm, and the second conference became a great success. Altogether 65 papers were presented by scientists from Australia, Canada, France, Germany, The Netherlands, UK, the USA, and the USSR. The conference was a sound scientific affair, the participants had the impression, that it was just one of a well-established series. The third conference followed two years later in Paris.

In 1971 Professor J. Smolderen, at that time the director of the Von Kármán Institute for Fluid Dynamics (VKI) in Rhode Saint Genèse, Belgium, invited the author to lecture in the short course program of the institute. The first series of lectures was given in February 1972 [8]. The lectures were well attended, perhaps also due to the fact, that Professor Smolderen had managed to

have applied mathematicians – among them Professor L. Collatz of Hamburg University - lecture on numerical problems to an audience, which had mainly engineering background. This proved to be a useful approach for advancing the new field of computational fluid dynamics. The lectures were continued in the following years, some of them even in the frame of the AGARD lecture series program. When the author was appointed professor at the RWTH Aachen in 1972, he initiated a course on mathematical fluid dynamics. The course was based on the lectures given at the VKI: Numerical solution techniques for the Euler equations, Prandtl's boundary-layer equations, and the Navier-Stokes equations were taught on an introductory level to students of the faculty of mechanical engineering.

Within the "Arbeitsgruppe für Numerische Methoden in der Strömungsmechanik" K. Roesner set up a "problem group" on "Flow Past Blunt Bodies in the Supersonic Flight Regime", see the preceding contribution, proposed a program of work, and meetings were held with K. Förster, D. Rues, C. Weiland of the Aerodynamisches Institut of the RWTH Aachen, and scientists from ERNO industries every month at Freiburg University. V. V. Rusanov's solution of the Euler equations was the first object of study, and it was possible to improve the rate of convergence for low supersonic free-stream conditions. First results obtained for the blunt-body problem were presented at the Fourth International Conference on Numerical Methods in Fluid Dynamics organized in Boulder, Colorado, USA, already in the same year, in 1974 [9].

As described by C. Weiland in the preceding contribution, through contacts of K. Roesner, Professor H. Goertler of Freiburg University in 1974 suggested to set up a working party for numerical methods in fluid mechanics within the Gesellschaft für Angewandte Mathematik und Mechanik (GAMM). From the Arbeitsgruppe für Numerische Methoden in der Strömungsmechanik originated such the GAMM-Fachausschusss für Numerische Methoden in der Strömungsmechanik (GAMM-Committee for Numerical Methods in Fluid Mechanics).

Also in 1974 first contacts were established with Russian scientists. Academician Y.I. Shokin visited the author at the Aerodynamisches Institut in Aachen. It so happened that Dr. P. Kutler, one of the leading scientists of NASA Ames Research Center in California was also visiting Aachen, and a workshop was organized, in which also members of the GAMM-Committee for Numerical Methods in Fluid Mechanics participated.

The GAMM-Committee was accepted without hesitation by the engineering community working in fluid mechanics and also by applied mathematicians. With Professor Goertler's consent it was proposed to organize a series of GAMM-Conferences on Numerical Methods in Fluid Mechanics. The first was held one year later, in 1975, at the DFVLR in Cologne, where 30 papers were presented. It was organized by E.H. Hirschel. In the following years the conference was extended to other European countries and became very much in demand as a platform for communication in computational fluid dynamics.

After Professor W. Schneider of the Vienna University of Technology had published his book "Mathematische Methoden der Strömungsmechanik" with the Vieweg Verlag in 1978, a representative of the Verlag approached the author and invited him to write a companion book on numerical methods. Although the offer was very tempting, the chances of success seemed to be limited because of the rapid development of the field. There was some fear that the book might already be out of date before it went into print. The author therefore suggested to initiate a series of books on numerical methods so that always the newest methods of solutions and the latest results could be published without delay. This proposal was accepted at the GAMM-Committee during the GAMM Annual Meeting in Brussels in 1978 and also by the Vieweg Verlag. To indicate the rapid progress and the preliminary nature of the results the title of the series, which celebrates its hundredth publication with this volume, was chosen to be *Notes on Numerical Fluid Mechanics.* The first volume was published by K. Förster in 1978 under the title *Boundary Algorithms for Multidimensional Inviscid Flows.*

Four years later, in June 1982, the Eighth International Conference on Numerical Methods in Fluid Dynamics was held at the RWTH Aachen, organized by the staff of the Aerodynamisches Institut. Over two hundred scientists attended. The topics discussed included problems of computational aerodynamics, numerical computations of gas explosions, predictions of two-dimensional separated flows and wall-bounded turbulent shear flows, descriptions of shock-wave structures by capturing and fitting techniques, and others. The ninth conference was held in France in 1984. The GAMM-Conferences toured Europe: France in 1981, Italy in 1983, Germany in 1985, Belgium in 1987, The Netherlands in 1989, and finally Switzerland in 1991. It was only after the European Community on Computational Methods in Applied Sciences (ECCOMAS) was founded in 1993 and began to organize the ECCOMAS Conferences, that the GAMM Conferences were terminated. The International Conferences on Numerical Methods in Fluid Dynamics continued to be organized on a world-wide basis every other year. Within three decades scientific communication in computational fluid mechanics was well established, and the *Notes on Numerical Fluid Mechanics* became an indispensable tool to establish the bounds.

4 The DFG-Priority Programs

After encouraging progress was made in the development of numerical tools for solving flow problems, the author submitted a proposal to the German Research Foundation (DFG) for funding the further development in the frame of a priority program in 1982. As successfully practiced at the VKI in the lecture series, it was suggested that applied mathematicians should also be invited to participate in order to improve the theoretical basis for the methods of solution to be developed.

A priority program with a funding period of six years seemed to be the appropriate one of the research programs offered by the DFG, as it required a nationwide cooperation between its participants and as it was expected to produce particular scientific gain. The program proposed was focussed on the construction of numerical solutions of the conservation equations for inviscid and viscous flows, including boundary layers, wakes, jets, internal flows, for transitional and turbulent flows, and for diffusion processes. The cooperation with applied mathematicians was expected to bring improvement of the rate of convergence, in the construction of grids, the development of discretization procedures, and in the analysis of the solution properties. After several round-table discussions with representatives of applied mathematics and fluid mechanics and the prospective reviewers, the Senate of the DFG approved the proposal under the title *Finite Approximations in Fluid Mechanics*. Funding began in 1983.

The various projects of the program were worked out by scientists of the universities in Aachen, Berlin, Bochum, Darmstadt, Erlangen-Nürnberg, Hamburg, Heidelberg, Kaiserslautern, Karlsruhe, Kiel, München, Paderborn, and Stuttgart, and of the research centers DFVLR Göttingen and Oberpfaffenhofen, IBM Heidelberg, and GMD St. Augustin. One third of the projects was submitted by applied mathematicians. First results were presented at a colloquium at the DFG in Bonn in 1985. The contributions were published by E. H. Hirschel in the *Notes* in volume 14 in 1986 [10]. The individual projects were reviewed by a group of external reviewers.

In the following year a colloquium was organized in Bonn, to which representatives of the industry were invited. Fifteen papers were presented, dealing with applications of numerical methods in aircraft design, in aerodynamic problems of the automotive industry, in the design of turbomachinery, heat exchangers and furnaces, in reactor technology, and in problems of atmospheric circulation. Because of a rather favorable response a second colloquium was organized in April 1989, at which the final results of the priority program were presented to an audience, in part invited from industry.

The discussion between the scientists participating in the program, in particular between applied mathematicians and engineers was successfully stimulated in two workshops in 1987 and 1988. Both workshops were well attended and progress of work could persuasively be demonstrated. The presentations were centered on the topics of application of the multigrid method and problems of numerical damping. The results were again published by E. H. Hirschel in the *Notes* in volume 25 [11].

By the end of 1988 the performance of computing machines had substantially advanced, and the author was encouraged to submit a proposal under the title *Flow Simulation on Supercomputers,* which the Senate of the DFG readily approved. The new supercomputers required the algorithms to be geared to the architecture of the machines, in particular for massive-parallel machines, and as a consequence, more than one third of the projects proposed, dealt with problems of parallelization. The proposals were submitted by scientists of the

universities in Aachen, Berlin, Braunschweig, Cottbus, Dresden, Duisburg, Erlangen-Nürnberg, Essen, Freiburg, Hamburg, Hannover, Heidelberg, Karlsruhe, Kaiserslautern, Kiel, Magdeburg, München, Osnabrück, Paderborn, Stuttgart, and Zurich, and the research centers DLR Cologne, Göttingen, and Oberpfaffenhofen, IBM Heidelberg, and FZ Karlsruhe. Cooperation between the various projects was again stimulated by internal colloquia, organized in 1990 and 1991at the RWTH Aachen, and a third at the DFG in Bonn in 1992.

A new era began, when in 1992 cooperation with scientists of the Groupment de Recherche Méchanique des Fluides Numérique of the French Centre National Recherche et Scientific (CNRS) was initiated at a jointly organized workshop on *Parallel Computing in Fluid Mechanics* at the Institut National de Recherche en Informatique et en Automatique in Sofia Antipolis in France. The problems studied comprised developments of solution techniques and applications as well. The work on parallelization included development of time and space multi-grid methods, of parallel finite element methods for the solution of the Navier-Stokes equations, performance enhancement of parallelized algorithms, adaptive operator techniques, and parallel interactive and integrated visualization techniques. The applications of parallelized algorithms dealt with simulations of turbulent flow, of various viscous incompressible flows, of unsteady flows in turbomachinery, of chemically reacting flow, and of aerodynamic flows.

The work on other solution techniques included approximations in high-order norms, low Mach number solutions based on asymptotic analysis, solutions based on the artificial compressibility concept, and on higher-order upwind schemes on unstructured grids. The applications included simulation of aerodynamic and of hypersonic flows, of flows in turbomachinery and complex internal flows. The investigations of transitional and turbulent flows were aimed at direct simulation of internal compressible turbulent flows and of separated flows; at large-eddy simulation of near-wall turbulence, of turbulent flows in curved pipes, and of turbulent boundary-layer flow over a hemisphere. First results were published in volume 38 of the *Notes* in 1993 [12].

The emphasis of work on parallel algorithms also stimulated cooperation at the RWTH Aachen and the Research Center in Jülich. In 1991 Professors K. Indermark of the Chair for Informatics II, F. Hoßfeld of the Central Institute for Applied Mathematics of the Research Center Jülich, and the author set up a working party for the development of parallel algorithms in technical and scientific applications. One year later, Professor U. Trottenberg of the Institute for Methodic Fundamentals of the Society for Mathematics and Data Processing (GMD) and Professor A. Bachem of the Institute of Mathematics of Cologne University joined the party. It is still in existence, and seminars and cooperative ventures are still being carried out on various subjects.

The cooperation with the Groupment de Recherche Méchanique des Fluides Numérique of the CNRS mentioned above was continued. A second joint workshop was held in May 1993 in Lambrecht (Pfalz) on the topic *Three-Dimensional Flow - Alternative Formulations and Solution of the Conservation*

Equations. At this workshop representatives of the CNRS and the DFG under the chairmanship of the vice president of the DFG, Professor S. Wittig discussed possibilities of cooperation. Agreement was reached on the following points: Cooperation in l0 joint projects within the frame of existing programs; participation of a French representative in the meetings of the German reviewing board and vice versa; organization of a joint meeting in Sophia-Antipolis at the end of 1994 with the aim of preparing a joint CNRS-DFG research program on computational fluid dynamics.

A third CNRS-DFG workshop was organized in December 1993 at Stuttgart University under the topic *Computational Fluid Dynamics on Parallel Systems.* The contributions were published in volume 50 of the *Notes.* They were edited by Professor S. Wagner of Stuttgart University [13]. The fourth workshop was held in Sophia-Antipolis in November 1994. As proposed in Lambrecht, 20 projects for a prospective joint program were discussed in the presence of representatives of the CNRS and the DFG. A joint French-German committee formulated a general proposal, which then was simultaneously submitted to the CNRS and the DFG in March 1995 under the title *Joint French - German Research Program: Numerical Flow Simulation.* The 26 proposals submitted were reviewed by a French - German reviewing group in November 1995, and 20 proposals were recommended for funding over a period of two years beginning in April 1996, and submitted for final decision to the CNRS and the DFG.

The DFG Priority Research Program *Flow Simulation on High-Performance Computers* substantially stimulated and fostered research in numerical fluid mechanics over a period of six years. It initiated and supported work on paralellization. It brought together engineers and applied mathematicians in fruitful cooperation. The program helped to maintain international competitiveness in flow research and markedly fastened the ties to the corresponding French program. The final results were published in volume 52 of the *Notes* in 1996 [14].

5 The CNRS-DFG Venture

Soon after the joint French-German committee had formulated the proposal for a joint research program and had submitted it to the CNRS and the DFG in March 1995, the Directeur Général of the CNRS, Professor G. Aubert, and the President of the DFG, Professor W. Frühwald, welcomed the initiative and agreed on providing financial support necessary for carrying out research in the various projects. After the Senate of the DFG had recommended a special frame for the support, both the CNRS and the DFG announced the program. The individual projects relied on the cooperation of a French and a German partner. The proposals of the following French – German partner – projects were approved for funding:

1.: ACCESS Aachen – CNRS St. Martin d'Heres; 2. and 3.: RWTH Aachen – CNRS Saint Etienne du Rouvray, (2 partmer groups); 4.: RWTH Aachen – INP de Grenoble; 5.: FU Berlin – Univ. d' Aix-Marseille; 6.: TU Berlin – Ecole Centrale de Lyon; 7.: Univ. Bonn – Ecole Normale Superieure Paris; 8.: TU Dresden – Ecole Normale Superieure de Lyon; 9.: Univ. – Duisburg – INRIA Sophia Antipolis; 10.: Univ. Erlangen-Nürnberg – Univ. d' Aix-Marseille; 11.: Univ. Freiburg – INSA Toulouse; 12.: TU Hamburg-Harburg – Ecole Centrale de Nantes; 13.: Univ. Karlsruhe – Ecole Centrale de Lyon; 14.: Univ. Kaiserslautern – INRIA Le Chesnay; 15.: Univ. Kiel – Ecole Centrale de Lyon; 16.: TU München – Ecole Centrale de Nantes; 17.: Univ. d. B. München – Univ. d' Aix-Marseille; 18.: Univ. Paderborn – Univ. de Nice-Sophia Antipolis, 19.: Univ. Stuttgart – Univ. de Valenciennes; 20.: Univ. Stuttgart – Univ. Piere et Marie Curie, Paris.

As in the previous priority programs the strengthening of the cooperation between engineers and applied mathematicians was a second important goal of the program: The algorithms to be developed should now be geared to the fast changes in the architecture of high-performance computers. Relevant topics of fluid dynamics referred to turbulence, combustion, convection and interface problems.

First results of the program were discussed at the fifth CNRS-DFG workshop on the *Simulation of Three-Dimensional Turbulent and Vortical Flows*, organized by Professors R. Friedrich of the TU Munich and P. Bontoux of the Université d' Aix-Marseille in December 1996 in Munich [15], and one year later, in November 1997, all results of the program were presented at the sixth CNRS-DFG workshop in Marseille [16]. Both organizations, the CNRS and the DFG had signalized that the program could be continued, provided the French-German reviewing board would recommend further funding of the program. For this reason the board also convened at the workshop in Marseille, evaluated the work carried out until then, and examined the new proposals. The overall reaction of the board was positive, and the program was recommended for another two years of funding, with the projects to be continued under the previous headings *Development of Solution Techniques*, *Crystal Growth and Melts*, *Flows of Reacting Gases*, *and Turbulent Flows*. It was also proposed that a further CNRS-DFG workshop should be held in 1998 on turbulent flows, to be organized by Professor W. Rodi in Karlsruhe.

A culminating point of the program was the eighth workshop, organized in November 1999 in Berlin in the Magnus-House, made available by the German Physical Society. Joseph Louis de Lagrange lived in the Magnus-House from 1766 to 1787, after Friedrich II had appointed him Director of Physics and Mathematics at the Academy. Professors I. Hertel, Secretary of State of the Senate of the City of Berlin, O. Mahrenholtz, representative of the President of the DFG, and T. Alziary de Roquefort, representative of the CNRS held the introductory lectures. The participants of the colloquium then impressively demonstrated the success of the partner projects. The results presented could not have been obtained without the funding in the joint program, and

a large number of investigations received international recognition. By then ten former participants of the program had been appointed professor, among them a French scientist at a German university, and vice versa, a German at a French university. The reviewers recommended the program to be extended for another two years. A new approach to further cooperation should then be discussed. The results of this period of the program were published in 2001 in [17].

The very last workshop of the program was held October 2001 at the Laboratoire J.A. Dieudonné of the Université de Nice-Sophia Antipolis. It was organized by Professors R. Peyret of the Université de Nice-Sophia Antipolis and P. Bontoux of the Université d' Aix-Marseille About 90 French and German scientists participated. Grouped into four main topics the twenty partner projects were aimed at developing advanced numerical solutions of the Navier-Stokes equations, and investigating the numerical solutions developed, and at solving the flow problems mentioned before. The topics signalize, that the problems posed were not selected from traditional hydro- and aerodynamics, but mainly from technical physics, including chemical processes, as they occur in melts and flows of reacting gases, in addition to constructing and testing numerical solutions to be implemented on high-performance computers, and to simulating turbulent flows.

The reviewing group included members of several disciplines, mathematicians, mechanicians, thermodynamicists, and engineers: Professors T. Alziary de Roquefort of the Laboratoire de Etudes Aerodynamiques des CNRS in Poitiers, H. Buggisch of the University Karlsruhe, T. Gallouet of the Université d' Aix-Marseille, P. Huerre of the Ecole Polytechnique in Palaiseau, W. Kordulla of the DLR Göttingen, A. Lerat of ENSAM Paris, R. Rannacher of the University of Heidelberg, and G. Warnecke of Magdeburg University. The third jointly published volume of the *Notes* gave an overview over the state of the investigations carried out until then [18].

The last workshop in Nice demonstrated, that by long-term planning and combining the scientific potentials in France and Germany the international competitiveness in numerical flow simulation could successfully be maintained. Extension of the initiative to other countries seems possible, if certain rules, securing the success of international and interdisciplinary cooperation are obeyed.

The CNRS-DFG program would not have been as successful as it was, had it had not found strong administrative support. In recognition of his outstanding administrative management of the program the Directrice Générale of CNRS, Dr. G. Berger, awarded Dr. W. Lachenmeier the CNRS-Medal, officially given to him by Professor S. Candel, Ecole Centrale and Académie des Sciences de Paris, during the reception of the 26th of October 2002 in Nice. The award was also extended to Professor O. Mahrenholtz, representative of the President of the DFG, to Professor E.H. Hirschel, for editing the *Notes on Numerical in Fluid Mechanics*, and to the author, for promoting the French-German

Collaboration since 1991 and chairing the DFG-CNRS Program on Numerical flow Simulation from 1996 to 2002.

6 High Performance Computing

Early in 1995 the author was invited by the Wissenschaftsrat (German Science Council, WR) to serve in an advisory group *High-Performance Computers*, which had the task to work out a recommendation for the provision of high-performance computing capacity, its regional distribution, and usage for science and research. After several meetings the recommendation was published in July 1995 [19]. The group arrived at the conclusion, that, in view of the rapid international technological development and the growing importance of high-performance computing, the government should impetuously establish two to four high-performance computing centers of highest computing capacity, in order not to loose the accession to modern computational technology. The proper use of high-performancc computers should be guaranteed by institutionalizing a suitable organizational body, directed by a steering committee, and assisted by a reviewing board for evaluation of the projects submitted.

A proposal for a high-performance computing center was already submitted by the Land Baden-Württemberg in 1992. Since installation of the machines proposed to be purchased was scheduled for summer 1996, the Ministry for Science and Research of the Land Baden-Württemberg commissioned an advisory group to formulate the guidance principles for the organization, operation and use of the High-Performance Computing Center Stuttgart (HLRS) in 1995. The deliberations, in which the author participated, resulted in recommendations for the overall organizational form of the HLRS, cooperative ventures with industry, definition of tasks of the center, structure of the steering committee, institutionalization of centers of competence, usage and operation, distribution of resources and contingents, recompenzations, admission to the HLRS, standards, operational modes, safety, and user support.

The steering committee was proposed to consist of twelve members, six nominated by the DFG, and six by the Conference of the Rectors of the Land Baden-Württemberg. The committee was appointed by the Minister for Science and Research, and representatives of the ministry participated as consultants in the meetings. The following tasks were defined: Advise the center in general, and in particular decide on the user profile, lay down rules for the distribution of computing capacity, decide on projects proposals, assist in the selection of hard- and software, approve financial settlements, define operational modes, formulate rules for usage and operation, comment on the statement of accounts and on the annual report of the centers of competence, and if necessary, commission sub-committees.

The High-Performance Computing Center Stuttgart was inaugurated in July 1996. The first meeting of the steering committee was held July 14,

1996. Professor W. Jäger of Heidelberg University was elected vice chairman, and the author chairman. He held this position until the fall 2004.

Since 1996 scientists from universities and research institutions from all over in Germany and research teams from industry had access to the facilities of the HLRS, at that time the massively-parallel system CRAY T3E/512 and the vector-parallel system NEC SX4/32. After two years of operation a first review and results workshop was organized in January 1998. Some 80 projects were processed on the T3E, dealing with numerical simulations of problems in theoretical physics (45%), fluid mechanics (20%), chemistry (l3%), solid-state physics (about l0%), and climate studies (about 9%). The rest of the problems was originating in bio-informatics, structural mechanics, electrical engineering, informatics, and combustion processes. About 90 projects, processed on the SX4, dealt with the simulation of problems in fluid mechanics (66%), solid-state physics (20%), chemistry (7%), theoretical physics (4%), prediction of flames (3%), and electrical engineering. All projects were evaluated by external reviewers and members of the steering committee.

A selection of close to 40 contributions was published in the first issue of the series *High Performance Computing in Science and Engineering,* established with the Springer Verlag in 1998 [20], in order to document the vast field of applications of high-performance computing in science and engineering, ranging, for example, from numerical simulations of complex flow phenomena to modeling of earthquakes or the dynamics of amorphous silica. The series has been continued over the years, the last issue containing the transactions of 2006, edited by W. E. Nagel, W. Jäger, and M. Resch [21]. The Leibniz Computing Center of the Bavarian Academy of Sciences in Munich adopted the workshop reviews and transactions and published its first transactions in 2003 [22].

In 1999 the German Science Council convened an advisory group, which was asked to review all aspects of the 1995 recommendation for the provision of high-performance computing capacity for science and research. The group, to which the author was also invited, investigated the entire spectrum of problems associated with the operation and usage of high-performance computers. It organized several hearings with close to twenty experts, including those responsible for financial aspects and scientific administration. The recommendation was published in 2000 [23]. In addition to more detailed recommendations, extracted from the experience gained with the existing high-performance computing centers in Germany during the past five years, the main conclusion of the deliberations was, that the 1995 recommendation was confirmed in its basic structure. It was emphasized again, that at least one computer of the highest capacity should always be available in one of the high-performance centers in Germany.

In another recommendation of the year 2003 the Science Council recommended the installation of a high-performance computer at Stuttgart University [24]. The inauguration of the new building of the High-Performance

Computing Center Stuttgart and of the new high-performance computer NEC SX-8 took place July 21 2005.

One of the last activities the author participated in was the foundation of the German-Russian Center for Computational Technologies and High-Performance Computing. The center was established in 2003 during a visit in Akademgorodok by Academician Professor Y.I Shokin, director of the Institute of Computational Technology of the Siberian Branch of the Russian Academy of Sciences in Novosibirsk, Professor M. Resch, director of the High Performance Computing Center of the University of Stuttgart in Germany, and the author. The main goal of the center is to discuss results in the various branches of the computational sciences, as for example computational fluid dynamics, to present mathematical methods for the development of new materials, construct prediction methods for the solution of environmental problems, and, above all, initiate cooperation between Russian and German scientists in the development of algorithms, soft- and hardware support for high-performance computation, and of visualization techniques for numerical simulations.

A first *Russian-German Advanced Research Workshop on Computational Science and High Performance Computing* was held at the Institute of Computational Technologies in Akademgorodok, September 30 to October 2, 2003. The workshop was organized by Y. I. Shokin, and M. Resch; participation was by invitation only. Scientists of 15 universities and research centers followed the invitation extended by the Institute of Computational Technologies in Akademgorodok and the High Performance Computing Center of the University of Stuttgart. The proceedings were published in volume 88 of the *Notes* [25]. A second workshop was organized two years later in Stuttgart in March 2005, and the proceedings were published in volume 91 of the *Notes* [26].

Upon Y. I. Shokin's suggestion scientists of the al-Farabi Kazakh National University participated in the second workshop in Stuttgart. As the Kazakh scientists showed great interest in developing a cooperation with the HLRS, it was agreed on to organize a workshop in Kazakhstan. Already in October 2005 scientists of the Institute of Mathematics and Mechanics and the Institute of Mathematics of the al-Farabi Kazakh National University in Almaty, of the HLRS and the Institute of Aerodynamics and Gasdynamics of the University of Stuttgart, the Institute of Aerodynamics of the RWTH Aachen, the Institute of Applied Mathematics of the University of Freiburg, the Institute of Technical Thermodynamics of the University of Karlsruhe (TH), the Institute of Computational Technologies, and of the Sobolev Institute of Mathematics in Novosibirsk got together in Almaty for the workshop proposed, and the proceedings of which were published in volume 93 of the *Notes* [27].

7 Concluding Remarks

During the various phases of work on numerical methods in fluid mechanics the author was given the opportunity to work together with many scientists and engineers. Their cooperative enthusiasm is gratefully acknowledged. In particular to be mentioned is the young generation, with new ideas and endurance establishing solutions to important problems of our time. The discussion with the young generation was of particular excitement. It is one of the driving forces in our field.

The continued support of the various agencies cannot be left out in this summary. Mentioned are the ministries of the Länder, their universities, and in particular, the Deutsche Forschungsgemeinschaft. Special mention is made of the Land Baden-Württemberg, which over many years promoted high-performance computing with extraordinary support. Many of the projects processed on the machines of the High Performance Computing Center Stuttgart could not have been brought to a successful end, had the Land not availed the support.

Grateful acknowledgement is also due to the Springer Verlag for publishing this series and helping to deliver the results of investigations in numerical fluid mechanics to the international science community. It is hoped that the *Notes* will continue to contribute to the global promotion of high performance scientific computing.

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German and EU High-Performance Computation Centers

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Summary A short historical background about the usage of digital computers in Germany since 1956 is presented. Soon after the beginning, the demand on computing capacity increased, so that computing centers were founded at universities, research establishments and in industry. Later on the foundation of federal high-performance supercomputing centers was started supported by the government. The development of these centers is described as well as the access to them by the costumers. In addition, a high-performance computing supply pyramid was created with different levels of computing power. On this basis Germany started to participate in the construction of a European high performance supercomputing infrastructure, that is described including the goals and the proposed tasks.

1 Introduction

Computational science (CS) and scientific-based engineering science (SBES) have certainly brought new methodologies and ideas into mainstream science and engineering. CS, fuelled by top-level supercomputers, has become a third pillar of the scientific methodology alongside theory and experiment [1], but is also increasingly an important instrument to gain scientific knowledge in all disciplines. Simulations with High-Performance Computing (HPC) are also getting more and more important in economy and industry since top industrial products can often only be designed using numerical simulation [2]. However, the necessary IT-infrastructure is often so expensive that a single institution cannot afford the procurement and the operating cost of so-called Capability Systems. Capability computing is characterized by simulations using a large number of processors, sometimes with an enormous requirement in very high processor performance, in a cooperative mode. Often large amounts of memory and the ability to process extensive data sets are required. Such simulations

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are dependent on a high bandwidth, low-latency communication fabric that connects the individual processors. These capabilities imply a single parallel computer that no loosely coupled distributed computing infrastructure can provide [1]. In contrary to that capacity computing has the goal to maximize the throughput of a large number of program runs of small or medium size, on different data sets. This style of computing can be dealt with in a cost effective manner, by providing adequate capacity at the regional or national level by upcoming grid-based computing methods.

Already in the 1950s digital computers were installed at universities, research institutions and in industry. Though these machines had nothing to do with capability computing since they had a performance comparable to that of a PC nowadays. Still, they were expensive enough so that only a few digital computers could be purchased. However, a relatively large community could use them. In this respect, they were comparable with capability systems at present.

2 Historical Background

When the author of this article started his studies as mechanical engineer at the Technical University of Munich in fall 1956 he noticed that a remarkable event had taken place just a few months before. On May 8, 1956 the PERM (Programmgesteuerte elektronische Rechenmaschine München) was put into operation, a computer that was designed and built under the guidance of Hans Piloty and Robert Sauer, both professors of the Technical University of Munich and Members of the Bavarian Academy of Sciences. Piloty and Sauer very soon recognized that on the one hand electronic data processing rapidly gained very high importance and that on the other hand the computing power of the PERM was comparably too low. Therefore, on March 7, 1962 an Academy-Commission for Electronic Computing was founded upon the suggestion of these two scientists. This commission got in 1975 the new name "Commission for Information Processing" and got finally the name "Commission for Computer Sciences" in 1990 [3]. The last commission decided to found a computing center, the later LRZ (Leibniz Computing Center) with the help of the Free State of Bavaria.

During the early 1960s many computing centers were established at universities, research institutes and other institutions. First of all the "Deutsche Rechenzentrum" (German Computing Center) with an IBM 7090 was established in Darmstadt where FORTRAN courses were offered to members of universities and research institutes and where the possibility was given to use the IBM 7090. This was a great opportunity at that time.

In the meanwhile numerical fluid Dynamics (CFD) became an important issue besides theory and experiment in research of fluid mechanical problems. In recognition of this fact, Professor Krause initiated two priority programs of the Deutsche Forschungsgemeinschaft, DFG (German Research Foundation)

with funding periods of six years [4]. The first program was entitled "Finite Approximations in Fluid Mechanics" with funding starting in 1983. The second program was entitled "Flow Simulation on Supercomputers". It already indicates the usage of these high-performance machines that had substantially advanced in performance and storage capacity. But also parallel computing was a theme within this program. The author realized that a meaningful usage of these parallel machines would be too difficult for him as an engineer. Therefore, he tried to find a partner from the computer sciences to get acquainted with this new type of machines. Fortunately, he could start cooperation with Professor Bode form the Technical University of Munich who had two parallel computers, namely the Alliant FX/2800 and Intel iPSC/860. The cooperation was very fruitful [5], [6]. Funding of two projects by the DFG started in 1988. High performance computers were already available at several universities and research institutes, e. g. at the Universities of Berlin, Hannover, Karlsruhe, and Stuttgart, at the Academy of Sciences in Munich, at the Institute for Plasma Physics in Garching and the Neumann Institute for Computing (NIC) in Jülich. In 1991 the author and his group got access to an improved parallel computer, the Intel Paragon. Shortly after this experience he and his team could use a cluster with 5 IBM RS/6000 workstations with which they reached a performance comparable to the vector computer CRAY II [7].

Later on the author initiated the DFG Verbund-Schwerpunktprogramm "Transition" [8] a cooperative priority research program of universities, research establishments and industry in Germany. This DFG program was launched in April 1996 and was to run for six years with the aim to explore laminar-turbulent transition by a coordinated use, development and validation of advanced experimental techniques, theoretical methods and especially numerical simulation methods, binding together all the appropriate resources available in Germany [9]. This program is mentioned here because two special features of CFD were applied. The first one is DNS (Direct Numerical Simulation) where the full unsteady Navier-Stokes equations are solved without applying any turbulence model. The second one is the usage of fourth-order finite differences [10] or even 6th-order compact differences [11] in space. The time integration is performed by the classical fourth-order Runge-Kutta scheme. At that time an accuracy of second order was usually applied by scientists and orders of accuracy higher than two were an extreme exception.

3 Foundation of Federal High-Performance Supercomputing Centers

3.1 Jülich Supercomputing Center of the Forschungszentrum (Research Center) Jülich

In 1987 the first German federal High-Performance Computing Center was founded at the Forschungszentrum (Research Center) Jülich that is now one

of the three Federal High-Performance Supercomputing Centers in Germany. In October 2007, a 16-rack Blue Gene/P system with 65,536 processors was installed. This system was mainly financed by the Helmholtz Association and the State of North Rhine Westphalia. With its peak performance of 222.8 TFlop/s and a measured LINPACK computing power of 167.3 TFlop/s Jülich's Blue Gene/P - dubbed JUGENE - was ranked second in the TOP500 list of the fastest computers in the world which was released in November 2007 in Reno, USA. At present it is the top supercomputer in Jülich and in Germany.

In 1995 the Wissenschaftsrat, WR (German Science Council) established an advisory group "High-Performance Computers" [4] that worked out a recommendation for the disposition of high-performance computing capacity, its regional distribution, and its usage for science and research. A final recommendation was published in July 1995 [3] and [12]. The definition of HPC systems regards high-performance supercomputers as a unit with many processors, with a relatively large storage and with a highly capable internal, tightly coupled communication network [13]. The importance of simulations with HPC systems was recognised by the WR only in the 1990s. In 1995 [14] and 1996 [12] first recommendations were presented to supply science and research with HPC capacity. There was an additional statement that there are advantages in contests of the scientific and economic range if high capacity computers are available.

3.2 Höchstleistungsrechenzentrum Stuttgart, HLRS (High-Performance Supercomputing Center Stuttgart)

The Universitätsrechenzentrum Stuttgart, URS (University Computing Center Stuttgart) exists since 1978. A proposal for a high-performance computing center was submitted by the Land of Baden-Württemberg in 1992 [4]. The Federal High-Performance Supercomputing Center Stuttgart (HLRS) was inaugurated in July 1996. The Ministry for Science and Research of the Land Baden-Württemberg commissioned a Lenkungsausschuss (advisory group) to define the guidance principles for the organization, operation and use of the HLRS. The first meeting of this steering committee was held July 14, 1996. The author is member of this committee. At that time the HLRS as Federal High-Performance Supercomputing Center had essentially two machines, the vector-parallel computer NEC SX-4/32 and the massively-parallel Computer CRAY T3E/512. Scientists from all universities and research institutions in Germany as well as from industry could use these machines after their application for computing time was approved by the steering committee. The top computer of HLRS at present is a NEC SX-8/576M72 Vector-Supercomputer with 576 CPUs and peak performance of 12.67 TFlop/s. It was installed in spring 2005.

The WR [14] demanded in a "Recommendation for a Provision of Science and Research with High-Performance Computing Capacity" that approximately three Federal High-Performance Supercomputing Centers should

be established in Germany that should procure high-performance computers in a timely staggered manner and that should be as high as possible in the Top500 listing of the world high performance computers. In order to do the relevant planning and to evaluate applications of computing centers to become Federal High-Performance Supercomputing Centers the WR established the committee "Nationaler Koordinierungsausschuss zur Beschaffung und Nutzung von Höchstleistungsrechnern", NKAH (National Coordinating Committee for the Procurement and Utilization of High-Performance Computers). After Jülich and Stuttgart had already been established as federal High-Performance Supercomputing Centers the State of Bavaria with LRZ Munich and the so called northern German Computer Compound Arrangement with Hannover and Berlin as local computing centers applied for the third federal High-Performance Supercomputing Center. After a careful evaluation of the proposals, the NKAH Committee recommended that the new Federal High-Performance Supercomputing Center should be established at the LRZ in Bavaria.

3.3 Höchstleistungsrechenzentrum Bayern, HLRB (High-Performance Supercomputing Center Bavaria)

The Leibniz-Rechenzentrum, LRZ (Leibniz Computing Center) of the Bavarian Academy of Sciences already existed since 1964. The HLRB was installed on March 1, 2000 at LRZ. Access to the supercomputers of HLRB is also managed by a steering committee that exists since May 2000. The author is chairperson of this committee. The main users of high-performance computing, members of the steering committee and the computer experts of LRZ choose after a careful selection process the Hitachi SR800-F1 as the new high performance computer for HLRB. The Hitachi SR800-F1 in its final stage had 168 nodes with 1344 processors and a peak performance 2.016 TFlop/s. In June 2006 the Hitachi SR800-F1 was replaced by an Altix 4700-System of SGI with 4096 Intel Itanium2-processors and a peak performance of 26.2 TFlop/s and a sustained performance of 7 TFlop/s in the first installation stage. In December 2007 the system was extended with twice as many CPUs and has a peak performance of approximately 68 TFlop/s and a sustained performance of 13 Flop/s.

It is interesting to note that the State of Bavaria represented by the Ministry of Science and Art had sponsored a research project named FORTWIHR (Forschungsverbund für Technisch-Wissenschaftliches Höchstleistungsrechnen) in 1992 that means before the HLRB was installed. The program had a volume of 10 Million Deutsche Marks and ran for 3 years. It sponsored research projects and was indeed an excellent preparation for the application of HLRB. This project was extended twice (FORTWIHR II and FORTWIHR III). In 2000 the Ministry of Science and Art established a new Competence Network KONWIHR that sponsored research projects and consultation services for the HLRB customers.

In 2000, the WR had recommended a special procedure for the usage of high-performance computers [2], [15]:

- The importance of high-performance computing as an unalterable tool for natural sciences and engineering sciences as well as for the development of many products in industry was stated.
- The federal high-performance supercomputing centers should stand on top of the supply pyramid for data processing.
- Usage of HPC should only be allowed based on scientific judgement.
- No charges should be demanded.
- The WR recommended that the top federal high-performance supercomputers should be procured according to a so-called supply spiral.
- A national coordinating committee for federal high-performance computers should be installed starting in 2001.
- New HPC competence networks should be established, new groups of users should be disclosed.
- New corresponding courses of study should be initiated.

4 Participation of Germany in European High-Performance Supercomputing

In November 2004 the National Coordinating Committee for the Procurement and Utilization of High-Performance Computers and accordingly the WR recommended that the "Bundesministerium für Bildung und Wissenschaft, BMBF" (German Federal Ministry of Culture and Science) should apply for a European High-Performance Supercomputing Center [16]. An HPC infrastructure should be established that put on top of the existing three supply levels in Germany (Fig. 1) a Tier-0 level as a European supply level.

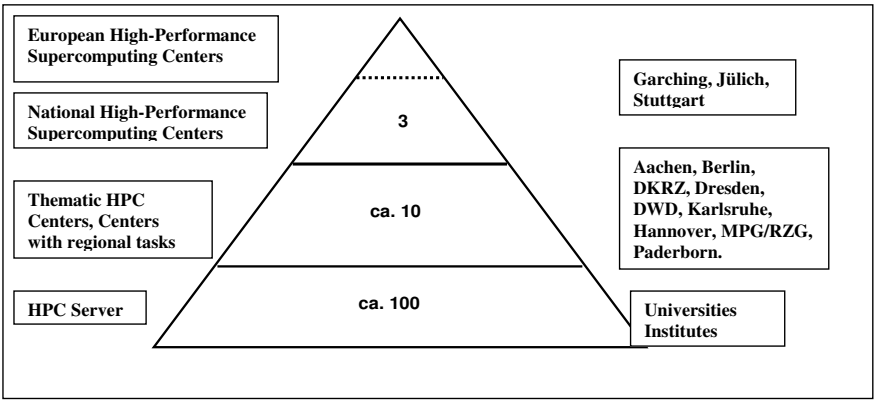

Fig. 1. HPC-Supply Pyramid [2].

In the computational science (CS) and scientific-based engineering science (SBES) community, it was very clear from the very beginning that the HPC-computing centers in the total HPC-supplying concept had to be supplemented by HPC-Software and user oriented competence networks as well as a broader HPC specific education [2]. A series of important HPC competence networks with regional importance were established, e. g. BremHLR (Bremen), hkz-bw und WiR (Baden-Württemberg), IWR (Heidelberg), KONWIHR (Bayern), Munich Computational Science Centre MCSC (München), NIC compound arrangement (DESY, FZJ, GSI), north German compound arrangement, PC2 (Paderborn), SCAI (FhG). In addition, corresponding Bachelor and Master Courses of study in Computational Sciences, Computational Engineering were established on several universities, e. g. in Aachen, Bochum, Braunschweig, Darmstadt, Erlangen, München, Rostock und Stuttgart. In order to coordinate these courses of study, a working group of Computational Engineering was founded in 2005. The recommendations of the WR mentioned above led to intensified discussions in Germany, but also in Europe concerning the handling of HPC in the future. Soon it became very clear that a national HPC concept would be urgent. Four arguments for such a concept were frequently cited that H.-G. Hegering summarized in his presentation [2]:

1. Scientific computing and HPC must nationally be promoted in order to protect the advantages of German HPC positions. It must come to a boosting of an informed political opinion to sponsor HPC in Germany.
2. The quick built-up and the lasting protection of the HPC supply pyramid must be guaranteed by a) including all supply levels, b) an adequate network and grid structures to all accesses of resources, c) sponsoring the necessary development of algorithms and software developments, d) support of more appropriate broad education, e) sponsoring of competence networks, f) coordinating and long lasting planning of finances and procuring.
3. Strengthening of the position of Germany at all European HPC activities. Creation of an organizing structure within the BRD that acts as a representative for Germany in Europe and that at the same time considers the problems of the federal structure of Germany.
4. At least one European Supercomputing Center (a so-called Tier-0-Center) must exist in Germany.

In the meanwhile, several preparatory meetings had taken place in Europe to do some planning towards a European High-Performance Supercomputer. Parallel to these events the States of Bavaria and Baden-Württemberg of Germany published a common study towards a European Supercomputer in May 2006 [13]. Parallel to this action, the Bundesministerium für Bildung und Wissenschaft, BMBF (Federal Ministry of Culture and Science) initiated the so-called Reuter-Committee that is named after the Chairman of the working group, Professor Reuter (European Media Laboratory LtD, Heidelberg). In this Reuter Committee, the heads of all German High-Performance Supercomputing Centers and High-Performance Computing Centers could present

their opinions about a future structuring of HPC in a common strategy paper [17].

In addition, the directors of the three High-Performance Supercomputing Centers in Garching (in the vicinity of Munich), Jülich and Stuttgart agreed upon in an obligatory manner to act as Gauss Centre for Supercomputing in the future and to combine the previous cooperation in an organizing frame [18]. Professor Bachem, Director of the Research Center Jülich was nominated the first representative. This will lead to a first step of a common representation of the three centers. Furthermore, the ideas towards a European Supercomputing Center were extended towards statements for the further development of HPC in Germany, including the role of the computing centers that are positioned directly below the three federal High-Performance Supercomputing Centers in the supply pyramid. On November 9, 2006, a meeting of the four corresponding ministries of the Federal Government, the States of Bavaria, Baden-Württemberg and North Rhine Westphalia took place to clarify the legal organization.

In preparing the activities towards the seventh Frame Program of the EU Professors Bode, Lippert and Hildebrand prepared a "Scientific Use Case for a European High-Performance Computer" [19].

5 Development of High-Performance Supercomputing in Europe

Between August 2005 and April 2006, an international scientific panel, put together by cooperation between Finland, France, Germany, the Netherlands and the United Kingdom, produced the scientific case for high-end scientific computing in Europe [1]. The basis of this idea was the recognition of the strategic role of High Performance Computing (HPC) at the leading edge, so-called "Leadership-Class Supercomputing", for European Science and Economy. It is clear that isolated European countries would not be able to provide their researchers and engineers with resources competitive on the world stage. However, it is necessary to have regional, national and European HPC concepts that coordinate the necessary steps based on the situation in the education and the development sector and that make possible the payment of investment and the operation of a HPC infrastructure in Europe. In focusing on the requirements for the successful exploitation of Leadership-Class Supercomputing - the provision of the order of 1 PetaFlop/s peak performance around 2009 - the panel mentioned above demanded the exploitation of such a resource that is based on an associated computational infrastructure. The panel envisaged:

one or more general purpose Pflops-class machines operating at the apex of a wide pyramid of computational resources that embrace national, regional and thematic centres, accessible through a data network or grid, with appro-

priate use support organizations dedicated to ensuring maximum exploitation throughout the entire European community.

The panel emphasized that Europe has been very successful in establishing a remarkable number of elements of this resource and performance pyramid, notably through the GEANT2 network and its high throughput optical interconnections, and with the DEISA supercomputer grid. Thus, the panel came to the important conclusion that providing scientists and engineers with access to capability computers of leadership-class must be recognized as an essential strategic priority in Europe. In addition, the panel stated that such resources are likely to be extremely expensive and require significant expertise to procure, deploy and utilize efficiently; some fields would even require research for specialized and optimized hardware. The panel stresses furthermore that these resources should be reserved for the most exigent computational tasks of high potential value. This would require organizing an appropriate process to screen proposals, and to run the resources as permanent research infrastructure.

Based on the recommendations of the WR [16] German representatives started in 2005 various conversations with HPC partners in Europe, e.g. within the frame of DEISA (Distributed European Infrastructure for Supercomputing Applications), that is a European HPC and grid project between eleven Supercomputing-Centers. In addition, the BMBF started contacts to the European initiatives ESFRI (European Strategy Forum on Research Infrastructure) und HPC-EUR (a group of European HPC experts) [2]. In 2006, HPC-EUR brought out the study "Scientific Cases for a European HPC-Initiative" [1] that should substantiate the need for a European HPC-Supercomputer of the Petaflop Class. The EU organized in March 2006 a hearing entitled "The need for an HPC infrastructure service provisioning model in Europe" by which the preparatory work of ESFRI and e-IRG (e-Infrastructure Reflection Group) should be supplemented and should be helpful for a planned HPC-relevant invitation of tenders within the 7th frame program of the EU.

The HPC European Task Force (HET) pursued the same goal. All EU-Nations with interest in HPC were represented within the HET consortium, Germany was represented by the BMBF and by the Gauß Center of Supercomputing, GCS that was already planned at that time. Three elaborations were formulated [20]:

- "Towards a Sustainable HPC Ecosystem through Enabling Petaflop Computing in Europe".
- "HET Peer Review Process Proposal for Tier-0 Applications".
- "A Sustainable High Performance Computing Ecosystem for Europe".

Finally, the "European HPC Service" was included into the ESFRI listing of infrastructure projects that are entitled to be supported and which is a prerequisite for a sponsoring within the 7th EU research program. Only one European consortium was entitled to apply for this HPC project. This HPC-project

proposal should lead to a creation of a European HPC-Infrastructure with two phases (a preparatory phase, and an implementation phase).

6 The Gauß Center of Supercomputing, GCS

Beginning with the year 2005 it became clear in Germany that Germany should be represented with one "voice" in all the European activities with respect to HPC. First of all a study [19] commissioned by the BMBF about the scientific need of Petaflop-Computing was initiated in August 2005. The States of Bavaria and Baden-Württemberg established a working group in addition to that in January 2006 that produced the study "Konzept für Einrichtung und Betrieb eines Deutsch-Europäischen Zentrums für Höchstleistungsrechnen" [13]. Commissioned by the BMBF, the so-called "Reuter Committee" created the document "High Performance Computing in Deutschland - Argumente zur Gründung einer strategischen Allianz" [17] with the beginning of May 2006. On July 13, 2006 the MBF published a press release entitled "Schavan: Strategische Allianz schafft größten europäischen Rechnerverbund" that announced the creation of an appropriate organizing merger of the three German Supercomputing Centers. Indeed, the three heads of which had regular meetings since July 2006 in order to deliberate about ways of cooperation. The name "Gauss Centre for Supercomputing" (GCS) was chosen and Prof. Bachem (Forschungszentrum Jülich, FZJ) was appointed first representative.

On February 1, 2007 a "Memorandum of Understanding with respect to the Gauss Centre for Supercomputing" [22] was signed and was published in the common GCS web portal. After that, the rules of a non-profit-making registered organization "Gauss Centre for Supercomputing (GCS) e.V." were developed. On April 13, 2007, the organization was finally founded. Its foundation members are the representatives of the three national computing centers, their heads and the chairpersons of their steering committees.

The goals and tasks of the new organization are the following [2]:

- Sponsoring of science and research by winning new technical findings and experiences in the field of scientific supercomputing, especially by concentrating the supercomputer resources in the ranges high-performance computing and capability computing, also within the European frame.
- GCS serves as a basis for the coordination of the three national supercomputing centers. This concerns also the inter-operability between the HPC centers, the optimization of computer architectures and their procurement. This means also the creation of rules for a common policy of usage and admittance.
- GCS is willing to guarantee the supply of the computer based science in Germany and Europe with HPC-capacity of the highest performance class (Capability Computing). This is level Tier-0 and Tier-1 of the European and German, respectively, supply pyramid (Fig. 1).

- Closest Cooperation with HPC-supply level 2 (Fig. 1). Active involvement during the foundation of the HPC-Allianz (HPC Alliance) that includes the Tier-2 computing centers.

The foundation of GCS led to a boostening of the national ability to act in Europe. Only four days after the foundation of GCS, the contract with the EU, the PRACE-MoU, could be signed by the GCS-Chairperson, Professor Bachem.

7 The Association PRACE: Partnership for Advanced Computing in Europe

A prerequisite to submit EU-Proposals to the FP7-Call is the formation of a European association and the existence of a corresponding arrangement of the association. This arrangement was signed as "Memorandum of Understanding Concerning the Establishment of a European Tier-0 High Performance Computing Service" at the BMBF in Berlin on April 17, 2007 by the PRACE association that was formed by 14 partner nations, namely France, Germany, The Netherlands, Spain and The United Kingdom, as well as Austria, Finland, Greece, Italy, Norway, Poland, Portugal, Sweden, Switzerland. The five countries on top of this series are so-called Principal Partners (PP), the rest are General Partners (GP). Germany is represented by the GCS. The PPs are qualified applicants for a European Tier-0 Center.

From an organizing point of view, a Principal Partner Committee (PPC) contains all Principal Partners with right to vote as well as an additional observing member of the General Partners that changes on a regular basis [21]. The PPC is the essential decision panel since the Principal Partners de facto bear by far most of the costs for the European Tier-0 Infrastructure. The Management Board (MB) is the general assembly of all partners, the MB decides according to the PRACE MoU.

8 Construction of a European Supercomputer Infrastructure

The goal of the PRACE proposal focuses first of all on the first phase of two years, the "Preparatory Phase" in the years 2008 and 2009. The goal is to successfully reach the "Implementation Phase" 2009/2010. Several accompanying tasks must be elaborated [2]:

- A legal and an organizing structure in which all questions of performance and partnership as well as the relationship to the EU Commission or the relation to the scientific users must be clarified.
- Financing and using models as well as corresponding contracts have to be worked out to guarantee a long lasting permanent European HPC service.

- Definition of a Peer Review Process and of a centralized procedure of access to the supercomputer
- Definition of a consistent operating model of all Tier-0 centers.
- Putting up, optimizing and "Petascaling" of selected applications.

9 Concluding Remarks

A strong commitment to maintaining a competitive advantage can be observed looking at the explicit plans put in place in the USA to regain world leadership after the Earth Simulator was installed in Japan. Current plans in the USA are extremely ambitious to develop and deliver supercomputers in the range of multiple Petaflop/s by 2011. It is therefore hoped that European and national politicians as well as the EU will maintain the necessary effort to establish a European Supercomputing Infrastructure in order to prevent that the competitiveness of European science and industry is jeopardized.

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General Developments of Numerical Fluid Mechanics Until the Middle of the 20th Century

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Summary. Today's computational methods are built upon physical and numerical models. Thus it is important to have an appreciation of the reasoning and thought processes that established our current understanding of the mechanics of fluids, all put in place before the age of numerical solutions. A brief sketch is given of the evolution of the ideas that led to the formulation of the equations governing fluid flow, the problems to which the equations were applied, and the efforts to solve them before computers were available. After the historical origins of the fluid-flow models are in place, the last section traces the transition undergone during the 20th Century, starting with analytical means to solve the mathematical problems that successively evolved into numerical approaches to solving them, thus leading up to the present time of the computational era.

1 Introduction

The histories of the exact sciences usually show an easily recognized pattern. Initially there is a period of unguided and unrelated experimentation when the simpler and more striking facts are discovered, often in a dramatic or unexpected fashion. At this stage the experimenters are working in the dark and any theories which may be formulated are necessarily speculative and, as often as not, utterly wrong. This period is generally followed by an era of consolidation, particularly on the experimental side, with results becoming more precise and numerical, if less spectacular, than before and a definite technique of experimentation begins to emerge. This stage is almost always characterized by an abundance of empirical formulae which have been invented, in default of a general theory, as a convenient way of summarizing results and as

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guides for future work. The science reaches maturity when the experimental probings have gone deep enough to reveal the true theoretical basis of the subject; the empirical formulae give place to exact mathematical theorems, which may ultimately attain the status of *natural laws*, the truth of which is accepted without question by all concerned.

Fluid mechanics, of which aerodynamics is a part, has not entirely followed this familiar pattern of development. In mechanics and astronomy, and later in electricity and magnetism, optics, heat and thermodynamics, and other branches of mathematical physics, the calculus of Newton and Leibniz opened the way of swift and sure progress with theory and observation only rarely in conflict. In the 18th century Euler and Bernoulli applied the calculus to problems of fluid motion and so founded the classical hydrodynamics, which deals with motion in a hypothetical medium called an *ideal fluid*. The classical hydrodynamics became a subject of immense attraction to mathematicians who made it so highly abstract as almost to deserve the name of *pure* mathematics. To engineers it had considerably less appeal, for they found its results either unintelligible or completely at variance with reality when applied to real fluids. In the 18th and 19th centuries the classical hydrodynamics, following its aim of producing a logical and consistent theory capable of yielding exact solutions of idealized problems, became a largely academic study and as such made little effective contribution to the problem of flight until it was realized that viscosity played an important role in very thin layers close to the wing surface, called boundary layers. If the places where these layers separate from the surface could be determined from some external criteria, the idealized theory of hydrodynamics supplemented, e.g. by the Kutta condition at a sharp trailing edge, could then become very practical indeed.

Today's computational methods are built upon models, both physical and numerical ones, so it is important to have an appreciation of the reasoning and thought processes that established our current understanding of the mechanics of fluids, all before the age of numerical solutions.

2 From Antiquity to the Renaissance

The study of fluids can be traced back to antiquity when Archimedes founded hydrostatics. The earliest analysis of the motion of a projectile in flight occurs in the Physica of Aristotle (384-322 B.C.) as a part of his proof of the impossibility of a vacuum. The 'proof' that led to his *medium theory* is a vivid illustration of the gulf which sometimes lies between the ancient Greek mind and our own in the domain of physical science.

Briefly, Aristotle argues that a body such as an arrow can continue in motion only as long as force is continually applied to it and that any withdrawal of the force would immediately cause the body to stop. Further, since it was held to be impossible to conceive of anything in the nature of action at a distance, the force required some material medium in contact with the body

for its transmission. Thus a projectile could not move in a vacuum, which is absurd, and hence a vacuum cannot exist.

The argument clearly requires that the air sustains the projectile in its flight, but Aristotle did not linger over this, to us the real problem. He suggested that the atmosphere might push the arrow along by rushing to fill the vacuum in its rear, or (rather more obscurely) that motion, once started, would be maintained by the air as a consequence of its *fluidity*. In both cases the air sustained and did not retard the flight of the arrow.

In these arguments lie the characteristic features of the strength and the weakness of ancient Greek science. The strength lies in the power of conceiving a philosophical problem as an abstraction from a material phenomenon, a process which is still an essential feature of all mathematical physics. The whole argument, however, collapses and proves nothing because its premises are at variance with the essential physical facts, and this because of the absence of experimental data from Greek science. Such, however, was the authority of the Aristotelian doctrines that these views held sway, or were given serious consideration, right up to the middle ages of European culture.

The centuries which lie between Aristotle and the birth of modern science with Galileo and Newton hold little of interest for aerodynamics until we come to Leonardo da Vinci (1452-1519) who discarded the central concept of the Aristotelian scheme, that the air assisted the motion, and instead considered the atmosphere as a resisting medium [1]. This is the essential step, without which all aerodynamic theory would be in vain. Leonardo's concept is that of making a surface support a weight by the application of power to the resistance of the air, but he went wrong in his subsequent development of the idea. He supposed that the flapping motion of the wing of a bird causes the air in contact with it to *condense* and behave as a rigid body on which the bird is supported, the motion of the wing being sufficiently rapid to ensure that the stroke is completed before the local *condensation* is passed on to other layers of air. Soaring flight, in which the wings are held nearly motionless, Leonardo explained on the same hypothesis by saying (quite correctly) that what mattered was the relative motion of the air and the wing so that, given a favourable wind, the bird can soar without beating its wings.

A *condensation* process resembling that envisaged by Leonardo does occur in nature, but becomes appreciable only at very high speeds. What Leonardo did not know was that to attain any noticeable amount of local compression in a free atmosphere it would be necessary for the wings to be moving through the air at extremely high speed, so that his explanation could not possibly apply to, say, the flight of an eagle or any other bird which uses slow powerful wing beats. On the other hand his conception of the bird being able to fly because, and only because, the air offers resistance is essentially correct and marks a great step forward on the Aristotelian doctrine. He effectively posed that the fundamental problem for a theory is to explain quantitatively the details of resistance to motion.

In the later Middle Ages machines came into use in small manufacturing, public works, and mining. During the Renaissance the clock was perfected, proved useful for astronomy and navigation, and quickly was taken as a model of the universe. Machines in general then led to theoretical mechanics and to the scientific study of motion and of change. Galileo Galilei (1565-1642) advanced the theory of hydrodynamics further by introducing the concepts of inertia and momentum and laid the foundation for the study of the dynamics of bodies [2]. Above all we owe to Galileo, more than to any other man of his period, the spirit of modern science based on the interplay of experiment and theory, with stress on the intensive use of mathematics. He knew that a rolling ball experiences both friction and especially air resistance which he tried to understand but incorrectly conjectured to be proportional to velocity. He did succeed in proving experimentally that a body floats, not because of it shape as Aristotle believed, but because of its density relative to the density of the fluid in which it is immersed.

Galilei also showed that the effect of force was not to produce motion, but to change motion, that is to produce acceleration. But it was Sir Isaac Newton (1642-1727) who later gave this conclusion the mathematical form of his famous Second Law upon which all branches of dynamics including hydrodynamics could grow on a sound philosophical basis. Blaise Pascal (1623-1662) developed these ideas further into a coherent theory of hydrostatics by establishing the basic laws for water at rest. He proved that the pressure at any point within a fluid is the same in all directions and depends only on the depth. Earlier investigators all held the hypothesis of simple proportionality between resistance and velocity until Christian Huyghens (1629-1695) found the proportionality of the resistance to the square of the velocity to be more in accord with his experiments. Newton later derived this law, which Huyghens discovered experimentally, by deduction for certain special flow conditions. It is usually referred to as Newtonian theory.

3 The Enlightenment: the Age of Reason

Newton began his study by stating that resistance depends on three factors: the density of the fluid, its velocity, and the shape of the body in motion. He observed also that different phenomena contribute to resistance. One is due to inertia and varies with the density of the fluid, but a second results from the viscosity of the fluid itself, and the third from the friction between the body and the fluid. Both these latter parts, Newton reasoned, could only be very small especially at high velocities and therefore could be neglected in the first analysis. But resistance coming from the inertia of matter must always be accounted for because it constitutes the essential mechanical property of matter. Thus began classical work on the understanding of ideal inviscid fluids, and as far as the description of drag is concerned led to the paradox of d'Alembert (1717-1783).

Mathematical productivity in the eighteenth century concentrated on the calculus and its applications to mechanics. The major figures in this activity were Leibniz, the Bernoulli brothers, Euler, Lagrange, and Laplace and others all closely connected with the philosophers of the Enlightenment. Scientific activity usually centered around academies, and not universities, of which those at Paris, Berlin, and St. Petersburg were outstanding. It was a period in which enlightened rulers like Louis XIV, Frederick the Great, and Catherine the Great surrounded themselves with learned men.

3.1 Leonhard Euler

Up to this time the development of fluid mechanics rested heavily on experimental observations. This changed with Leonhard Euler (1707-1783), the great mathematical architect and founder of fluid mechanics as a true analytical science. He is the key figure in 18th century mathematics and the dominant theoretical physicist of the century. He published more than 500 books and papers during his life-time, and it has been estimated that during his adult life he averaged writing about 800 pages a year [3].

In 1741 Frederick the Great invited him to join the Berlin Academy and it was there that he did his greatest work, including infinite processes of analysis, the function concept, infinite series, calculus of variations, differential equations, analytical and differential geometry, topology, number theory, astronomy, and mechanics. A flourishing branch of eighteenth century mathematics to which Euler made many contributions, and of special interest to us here, was that of differential equations. He investigated the existence of singular solutions of first-order equations, and stated the conditions for such equations to be exact. He also developed the technique of making a change of variable for solving second-order equations. Euler's work on problems of elasticity theory later led him to consider the general solution of a differential equation, of whatever order, with constant coefficients. He gave a complete treatment of this problem, first for homogeneous, and then for non-homogeneous equations. Euler also investigated systems of linked differential equations, with their obvious application to dynamical astronomy.

The study of partial differential equations really began, almost as a by-product, as part of the sustained eighteenth century attack on the problem of the vibrating string. Euler's most important paper on the subject, *On the Vibration of Strings*, appeared in 1749. He extended his earlier concept of a function to include piecewise continuous curves.

In laying the analytical foundations of hydrodynamics Euler overcame a fundamental contradiction between the concepts of mathematics and mechanics. For example, a point is usually defined as an element of geometry which has position but no extension; a line is defined as a path traced out by a point in motion; and motion is defined as a change of position in space. But motion and matter cannot be divorced. A point that has no extension lacks

volume and, consequently mass, and can have no momentum. Instead he introduced his historic *fluid particle* concept and thus gave fluid mechanics a powerful instrument of physical and mathematical analysis. A fluid particle is imagined as an infinitesimal body, small enough to be treated mathematically as a point, but large enough to possess such physical properties as volume, mass, density, inertia, etc. A fluid particle to Euler was not a mathematical construct, but a physical point possessing volume V, weight, mass m, and density ρ.

Its mass is $dm = \rho\ dV$, whose integration

$$m = \int\int\int_V \rho\ dxdydz \tag{1}$$

represents, in fact, the law of conservation of mass in fluid flows. Moreover, he recognized that pressure was a point property that varied throughout a flow, and that differences in the pressure at two different points provided a mechanism to accelerate a fluid particle. He treated incompressible flow in a paper in 1752; three years later his equations embraced compressible flow. His approach was to consider the forces acting on a volume-element of the fluid of density ρ, subject to a pressure p and to external forces with components (X, Y, Z) per unit mass. He put these ideas in terms of an equation expressed, in the usual notation of the material derivatives, which he derived for the momentum balance during his residence in St. Petersburg in 1748. He also generalized d'Alembert's equation of continuity to include compressible flow. Euler went further to explain that the force on an object moving in a fluid is due to the pressure distribution over the objects surface. But the derivation of the energy equation did not come about until the development of thermodynamics in the 19th century, beginning with B. de Saint-Venant who used a one-dimensional form of the energy equation to derive an expression for the exit velocity from a nozzle in terms of the pressure ratio across the nozzle.

These non-linear differential equations that result are very difficult to handle. As Euler put it in his 1755 paper:

> *If it is not permitted to us to penetrate to a complete knowledge concerning the motion of fluids, it is not to mechanics, or to the insufficiency of the known principles of motion, that we must attribute the cause. It is analysis itself which abandons us here, since all the theory of the motion of fluids has just been reduced to the solution of analytical formulae*, [4].

Even so, Euler continued to work on the subject and was indeed engaged in writing a treatise on hydromechanics at the time of his death [3].

4 The 19th Century: Mathematical Fluid Mechanics

Louis de Lagrange (1736-1813) also came to the conclusion that Euler's equations could be solved only for irrotational flows. For such flows he derived a general integral of Euler's equations, most usually, but mistakenly, ascribed to Daniel Bernoulli. The reduction of Euler's equations of motion to a single Laplace equation made it possible to carry out extremely complex mathematical operations. It became a cornerstone in the mathematical theory of fluid mechanics. But as this theory grew more refined from Newton to Euler and Lagrange, mathematicians began to recognize its shortcoming in the prediction of the drag of bodies. The first man to develop what we may call a rational theory of air resistance was d'Alembert, a great mathematician and one of the Encyclopaedists of France. He published his findings in a book called *Essai d'une Nouvelle Theorie de la Resistance des Fluides*. In spite of his important contributions to the mathematical theory of fluids, he got a negative result. He ends with the following conclusions:

> *I do not see then, I admit, how one can explain the resistance of fluids by the theory in a satisfactory manner. It seems to me on the contrary that this theory, dealt with and studied with profound attention, gives, at least in most cases, resistance absolutely zero; a singular paradox which I leave to geometricians to explain.*

This statement is what we call the paradox of d'Alembert. It means that purely mathematical theory leads to the conclusion that if we move a body through the air and neglect friction, the body does not encounter resistance. Evidently this was a result which could not be of much help to practical designers, and is far from what we experience in reality.

4.1 Vortex Discontinuities and Resistance

With Hermann Helmholtz (1821-1894) hydrodynamics made the most notable progress since d'Alembert, Euler and Lagrange. Like them he also investigated irrotational motion. However, Helmholtz realized, as Euler had already observed in his paper *Principes Generaux du Mouvements des Fluides* of 1755, that there may be cases in which no velocity potential exists. Helmholtz went on to discover special cases of such motion not satisfying a velocity potential which he named *vortex motions*, and thus opened a new field of research. Before Helmholtz it was generally held that flow without vorticity was a well-founded theoretical assumption. Doubts arose when large discrepancies with reality had been recognized, and even Euler had already pointed out that the assumption of potential flow is not always justified. But it was Helmholtz who openly rejected the potential assumption and, with his paper on vortical motions, opened the door to important new discoveries. This was the beginning of the classical theory of vorticity. His studies of jets in air led to the hypothesis that a surface of discontinuity forms in the velocity field. Up

to this time such discontinuities in velocity had not been considered by the theory. He argued, however, that there is nothing in the theory that forbids two adjacent fluid layers from slipping past one another with a finite velocity, i.e. a tangential discontinuity, or vortex sheet. Helmholtz did retain the idea that viscous forces may be neglected in a fluid with vorticity. These subtle but extremely important differences among the concepts of potential flow, fluid with vorticity, and viscous flow are expressed in precise terms as follows:

> *In potential flow vorticity is zero in the whole fluid (except for singular points), and viscous forces are neglected. In inviscid flow, a mathematical model of real flow, vorticity is present but viscous forces are still neglected (no diffusion of vorticity). No restricting assumptions at all on vorticity and viscous forces apply in real viscous flow.*

The idea of the Helmholtz surface of discontinuity prompted Lord Rayleigh (1842-1919) in 1876 to propose an inviscid wake behind a plate perpendicular to a stream which then experiences drag and thus solves the d'Alembert paradox. That Kelvin's theorem on the constancy of the circulation is not violated by vortex-sheets springing from the boundaries of immersed bodies, has been clearly explained by Prandtl. And so began another line of attack on the problem to understand resistance [5].

The first theoretical deduction of a formula for the drag was provided by the so-called theory of free stream-lines, developed for flow past a flat plate, by Kirchhoff and Rayleigh according to the methods used by Helmholtz for two-dimensional jets, and extended by Levi-Civita and others to the case of curved rigid boundaries. According to this theory there is, in two-dimensional flow past a flat plate perpendicular to the stream, for example, a mass of fluid at rest behind the plate, separated from the stream by two stream-lines springing from the edges of the plate.

The velocity is discontinuous across these stream-lines, which are therefore the traces of vortex-sheets. The velocity just outside the *free* stream-lines is constant, and equal to the velocity u_∞ of the undisturbed stream. The pressure in the stagnant fluid is constant and equal to p_∞, the pressure at infinity. This theory has considerable theoretical, but very little practical importance, its results being largely in disagreement with the results of observation in real fluids of small viscosity. Thus, for two-dimensional motion past a flat plate at right angles to the stream, the theoretical result for the drag coefficient, $\frac{D}{\frac{1}{2}\rho u_\infty^2 b}$, is 0.880, where b is the breadth of the plate: the measured value is nearly 2. The discrepancy arises largely from the fact that there is actually a defect of pressure, or suction, at the rear, the pressure being much less than p_∞. For the plate at right angles to the stream, it is nearly constant and equal to $p_\infty - 0.7\rho u_\infty^2$ right across the rear, and similar features are present in other typical cases. In other important respects the theory is widely at variance with reality, since behind a bluff obstacle in a stream the observed motion either is an irregular, eddying one, or for two-dimensional motion at certain Reynolds numbers has, for some distance behind the obstacle, the appearance

of a double trail of vortices with opposite rotations. Even if a motion like that past a perpendicular plate, or any similar one with vortex-sheets, is allowed to occur in an inviscid fluid, it would not persist, since it would be unstable. The notion that the stream leaves the plate at the edges is, however, valuable and in accordance with reality; and a vortex sheet (more accurately, for real fluids, a thin vortex-layer) does begin to be formed from the edges of the plate. But this vortex-sheet or layer is not fully developed either in a real or an inviscid fluid; it curls round on itself, and something much more in the nature of concentrated vortices is formed.

4.2 The Boundary Layer and Separation

Around 1900, there was a mathematical theory of the mechanics of ideal, i.e. non-viscous, fluids. The first result of this theory was the paradox of d'Alembert, stating that the resistance of a body moving uniformly in a non-viscous fluid is zero if the fluid closes behind the body. If a *separation* of the flow from the body is assumed, as for example by Rayleigh, the theory leads to a value of the force quantitatively at variance with experimental facts [6].

One needs of course to bring viscosity into account in order to predict drag with quantitative accuracy. The use of vortex sheets then is one of modeling. If one has to start with the solution of the Euler equations, because the Navier-Stokes equations are too difficult to solve, one must introduce the discontinuity line artificially, that is, in an axiomatic way. This is certainly true for smooth bluff bodies. If the body has a streamline shape and a salient edge, the vortex-sheet theory comes much closer to reality, as evidenced by the numerical solution of the Euler equations for flow around airfoils with sharp trailing edges, because the sharp edge fixes the point of separation. In three dimensions reasonable predictions are given for flow past delta wings with sharp leading edges, presumably because, unlike the bluff body, the shed vortex-sheet here is stable due to the roll-up process. But outside of these two regimes, one must be rather dubious about the realism of an Euler solution because of the uncertainty in the place of separation.

These considerations bring in the boundary-layer concept. Indeed, the existence of the boundary layer was not known around 1900. In 1904 Ludwig Prandtl published his epoch-making work [7], where he described it as well as its separation from a body surface. The boundary layer – due to the sticking of the fluid to the body surface – is a thin flow sheet adjacent to the latter in which viscosity plays a major role.

This discovery spawned a host of work, new insights and other discoveries, see, e. g., [8]. The connection between lift and drag of a body with skin friction, form drag, separation and induced drag was established. New flow-physics problems with high practical relevance came in, were worked on, and partly are not yet fully mastered like laminar-turbulent transition, turbulent flow and turbulent separation. Boundary-layer theory and boundary-layer

methods were developed which permitted to treat many practical flow problems. Moreover, although the solution of the Navier-Stokes equations – the boundary-layer equations are included in the latter as special case – in general was not possible for the lack of computer recourses, the matter of boundary conditions for these equations at body surfaces, which was open until that time, was settled.

4.3 Shock Waves

The explanation of drag was also sought by investigating other phenomena, namely compressibility. Galileo was the first to point out that the denser the fluid, the greater is its resistance. Christian Huyghens, Rene Descartes (1596-1650) and others developed this fact of nature into the concept that a body moving in a homogeneous fluid can experience different levels of drag. But the conclusion lacked clarity and remained abstract for a long time. Trying to work out the significance of compressibility, Euler and especially Lagrange sought mathematical relationships between density and pressure, but with little progress. Rather it was Helmholtz's ideas of a surface of tangential discontinuity that led others to explore further and generalize the concept of discontinuities. A tangential discontinuity, or vortex sheet, is a stream surface and no fluid passes through it. Once Felix Savart (1791-1841) showed that sound waves propagate in water in the same way as in solids, the way opened to see discontinuities as propagating waves. Pierre Henry Hugoniot (1851-1887) put this together in his concept of an *acceleration wave*. He wrote the equations that hold across such surfaces and proved that there are only two kinds of discontinuities possible in a non-viscous compressible fluid: 1) longitudinal ones which propagate as a wave with finite velocity, and 2) transverse ones which only move with the fluid particles. G.F.B. Riemann (1826-1866), however, was the first who tried to calculate the relations between the states of the gas before and behind the shock wave. He thought that the change across a shock is isentropic, and his results, of course were wrong. They were corrected by W.J.M. Rankine (1820-1872) in a paper *On the Thermodynamic Theory of Waves of Finite Longitudinal Disturbance* in the Philosophical Transactions of the Royal Society, 1870. By assuming that the internal structure of the shock wave was a region of dissipation, and not isentropic, he was able to derive the equations for the change across the shock. Hugoniot independently rediscovered these equations and published them in a paper in 1887 in a form much like those we use today.

Both Rankine and Hugoniot noted that rarefaction as well as compression shocks were possible, but the ambiguity was not resolved until 1910. First Lord Rayleigh (1842-1919) and then G.I. Taylor invoked the second law of thermodynamics to show that a compression shock is the only one physically possible. Thus the fundamental understanding of shock waves had evolved over the course of 40 years.

The phenomenon of shock waves was also being studied experimentally [2]. Ernst Mach (1838-1916), an Austrian physicist and ballistician used the schlieren technique to make shocks visible. Invented by A. Töpler (1836-1912), a German physicist who worked in the field of acoustics, this technique is an optical system that records density changes. In Berlin the ballistician C. Crantz studied experimentally the relationship between the speed of its flight and the drag of a bullet, the behaviour of the air in front of a fast moving body, and the influence of the shape of a body on the buildup of drag. He also conceived the idea of the shock tube. Later J. Schatte further refined the optical method of visualization of waves and flow patterns. His outstanding schlieren and interferometer pictures of supersonic flow and shock waves created by bullets received an enthusiastic reaction from many physicists, aerodynamicists, and military experts. Mach, however, was the first to show that compressibility effects in gas depend not simply on the flow velocity but rather on the ratio of velocity to the speed of sound. In honor of his work J. Ackeret named this ratio the *Mach number*.

While Mach was studying the ballistics of supersonic projectiles, another field of progressing technology in compressible flow was the design of turbines, starting with steam turbines late last century, and extending to gas turbines early this century with the work of A. Stodola in Zurich.

5 The 20th Century: The Computational Era

In 1888 the Swedish engineer, Carl G. P. de Laval, constructed a single stage steam turbine whose blades were driven by a stream of high-pressure steam from a series of novel convergent-divergent nozzles to speeds previously unattainable, over 30,000 revolutions per minute. He was not entirely certain in 1888 that the flow actually reached supersonic speed in his *Laval nozzle*. The possibility of supersonic flow in such nozzles had been established theoretically, but it had not been verified experimentally, and therefore it was a matter of controversy. In 1903 Stodola measured the pressure distribution along the axis of a convergent-divergent nozzle. In his data he found a large increase in pressure near the exit which agreed with the shock equations of Rankine and Hugoniot. This was the first real quantitative verification of the shock-wave theory. The news of this discovery reached Ludwig Prandtl in Göttingen who went on to contribute greatly to the understanding of quasi-one-dimensional supersonic nozzle flow by producing outstanding schlieren photographs of shocks and Mach waves in the flow.

5.1 Early Methods

Some effort was then made to describe the flow pattern mathematically in the minimum cross section of the Laval nozzle and the shape of the plumes in the jet behind such nozzles by seeking solutions to the Euler equations. Quite

independently G.F.B. Riemann in 1860, P. Molenbrock in 1890, and S.A. Chaplygin in 1902 all came upon the idea of introducing new independent variables to transform the Euler equations into equations in the hodograph plane where they were linearized. However, these attempts came before the boundary-layer theory established the practical value of ideal mathematical flow theory, and they did not attract the immediate interest of large groups of scientists and engineers [6].

During the period 1905 to 1908 Prandtl and Theodor Meyer extended normal shock wave theory to two dimensions and laid down the fundamentals of both oblique shock and expansion wave theory for supersonic flow. Meanwhile the growth of the young airplane industry added a practical interest to the advancement of compressible flow theory in the second decade of the century. Although the flight speeds of all airplanes at that time were certainly within the realm of incompressible flow, the tip speeds of the propellers regularly approached the speed of sound and focussed attention on the effects of compressibility on propeller airfoils. The basis for the theoretical approach here rested on the linearization of the governing equations followed by a search for an analytic solution. Prandtl, Jakob Ackeret, H. Glauert among others made major contributions. Mathematicians had been developing the theory of characteristics as a means to solve general systems of partial differential equations of first order. The French mathematician Jacques Salomon Hadamard in 1903 and the Italian Tullio Levi-Civita in 1932 made major contributions. But Prandtl and Adolf Busemann in 1929 were the first to apply this method to supersonic flow problems, and found exact nonlinear solutions (method of characteristics) to the Euler equations for two-dimensional supersonic flow. Busemann went on to use this method to design supersonic nozzles and ultimately the first practical supersonic wind tunnel in the mid-1930s. But in a potential formulation of supersonic flow around a pointed cone G.I. Taylor and J.W. Maccoll solved the resulting ordinary differential equation for conical flow by numerical integration in 1933. It signified the use of numerical methods for compressible flow problems.

For the most part the development of the airplane at that time called for the analysis of low-speed subcritical flow. That meant that viscosity and vorticity were neglected, and the flow model was the Laplace equation. Based on the theory of complex variables, the approach taken was analytical, the superposition of elementary solutions [9]. As the aerodynamic shapes under investigation grew more complex, it matured in later decades into the computational singularity techniques called boundary integral, or more commonly, panel methods [10]. Viscosity was accounted for by solving the boundary-layer equations of Prandtl's theory using finite-difference methods and mechanical calculating machines [11]. Later there were also attempts, in an iterative fashion, to couple together the external potential flow with the boundary-layer solution. The relaxation method was also being applied to solve the Laplace equation by finite differences [12].

Meanwhile the mathematicians like Hadamard, Courant, and Friedrichs, were building the theory of hyperbolic partial differential equations, with the goal of understanding the fundamental issues like the well-posedness of the problem, the propagation of waves, the smoothness of the solution, and its uniqueness. It was in establishing a fundamental result on uniqueness that led Courant, Friedrichs, and Lewy to their famous stability condition, necessary for the analysis of any practical computing method [13].

5.2 Methods to Solve the Euler Equations: 1950-1970

During the 1940s, however, the two groups, the theoreticians and the practitioners, began to draw closer together. The advent of the jet plane, supersonic missiles, and high-energy blast waves brought demands for solutions to problems that went beyond the reach of methods based on the theory of potential and linear hyperbolic equations. The heart of the difficulty was the numerical treatment of the non-linear occurrence of shock waves. This instigated a large effort by von Neumann, Richtmyer, Lax, and others working closely with computing methods to establish a mathematical theory of non-linear hyperbolic conservation laws for the purpose of computing flows with shocks. (The book by Fox [14] reflects how far these efforts progressed during the 1950s.)

But because many of the transonic and hypersonic problems in aerodynamics are steady, the aeronautical community did not immediately embrace the newly emerging hyperbolic methods. Instead, as was commonplace during the earlier decades, special methods were sought to solve the specific non-linear steady problem. The so-called blunt-body problem is a good example [15]. When a blunt obstacle travels through air at a constant supersonic speed, a shock wave appears in the flow, termed a bow shock because it stands detached from and ahead of the body. If the goal is to predict the location of the bow shock and the flow properties between it and the body, then the appropriate model is the steady Euler equations. Except in a small region between the body and the shock, the speed of the flow is always supersonic. This subsonic pocket is what characterizes the problem and makes it difficult because the equations are of mixed type – elliptic within the pocket and hyperbolic outside where the flow is supersonic. No general mathematical theory has been proposed to solve mixed-type equations, but a number of special methods were devised in the late 1950s to solve specifically the blunt-body problem. Among them were Van Dyke's inverse method [16] that first assumed a shape for the bow shock and performed an unstable but controllable numerical march from it inward to determine the corresponding body shape, and then adjusted the shock shape until the desired body was obtained. Another one was Dorodnitsyn's method of integral relations which reduced the problem to a set of coupled ordinary differential equations [17],[18]. All of these specialized blunt-body methods, however, were restricted to flows at substantial supersonic speeds. The other important aerodynamic problem of mixed type, the case of subsonic but supercritical flow past an airfoil where now a

supersonic pocket is embedded in a subsonic field, for example, could not be solved satisfactorily by these methods. The solution of the transonic airfoil problem was first obtained in 1970 by the relaxation procedure of Murman and Cole for the non-linear small-disturbance potential equation and was the initial use of an upwind scheme in aerodynamics. Oswatitsch and Rues [19] present a good survey of the methods being used up to 1975 to solve transonic aerodynamic problems. It is significant to point out that at the Symposium Transsonicum II in 1975 only one paper (by Rizzi) was given on the use of the hyperbolic time marching method to solve the Euler equations for transonic flow. And even at the GAMM-Workshop on Numerical Methods for Transonic Flow in 1979 in Stockholm [20] the majority of the papers still treated the potential equations. It was not until the 1980s that the interest in solving the Euler equations for transonic aerodynamics blossomed out.

5.3 Time-Marching Technology

For truly time-varying flow problems practitioners of computational fluid dynamics (CFD), primarily in fields other than aerodynamics like meteorology, plasma physics, and geophysics, were beginning to apply the theory that the mathematicians had been laying down for hyperbolic evolutionary equations [13],[14]. By now the development of the theory had advanced from linear problems to the understanding of weak solutions to conservation laws. During the 1960s news of the success with the general time-dependent hyperbolic approach in these other fields spread to the aerodynamics community where it was adapted for the solution of steady flows. The idea was to integrate the unsteady hyperbolic full potential and Euler equations forward in time, while maintaining steady boundary conditions so that, as all the transient fluctuations began to disperse, the steady state was reached asymptotically. Although it demands more arithmetic operations, the resulting time-asymptotic method proved to be both more effective and applicable to a wider class of problems than any of the other more specialized methods, e.g. the blunt-body procedures. This conclusion came about in part because of the broad latitude for algorithm modification afforded by the underlying hyperbolic theory. Another factor was the newly developed stability theory for difference approximations of time-dependent partial differential equations by Lax, Kreiss and others (see Ref. [21]). Perhaps an even greater influence on the development came from the increasing computer power which became generally available at that time, making the additional computational work irrelevant. Supercomputer in its day, the Control Data 6600 appeared in 1964 with the power of 1 Mflops, (1 million floating point operations per second) and was followed by the 7600 in 1968 offering 4 Mflops. And if the user was willing to program with special assembly-language techniques, the performance of these two machines could be doubled to 2 and 8 Mflops respectively. Here then is another important and recurring theme of CFD. If there are computing machines readily available that can carry out the calculations in a reasonable period of time, it

can be more feasible to use a more straight-forward method built from a general theory, even though it requires more computational work, than to use a more detailed method based on a narrower theory with limited application. The blunt-body problem with its various methods is a case in point. Rusanov[22],[23] and Moretti [24] were two pioneers of the time-asymptotic approach for the blunt-body problem which now is used almost to the exclusion of all specialized methods in aerodynamics. The need to study the flow patterns around the space shuttle was one of the driving forces in the development of this technique, and led, for example, to the first application of the finite-volume method to the blunt-body problem by Rizzi and Inouye [25].

5.4 Treatment of Viscous Flows

With the methods to solve the Euler equations the basis was established for the solution of the Navier-Stokes equations. Viscous effects so far could only be described by the solution of the boundary-layer equation in two and three dimensions with the help of space-marching finite-difference or integral methods. Needed is the external inviscid flow field which can be found with solutions of the Euler equations or with methods solving the potential equation. Although of great practical value for many design problems, boundary-layer methods can not treat flow with separation or other strong interactions between viscous and inviscid flow domains.

The solution of the Navier-Stokes equations, or, for turbulent flow, the Reynolds-Averaged Navier-Stokes (RANS) equations, was seriously hampered deep into the 1980s by the small available computer power and storage. Only after new computer technologies and architectures (vector and later parallel computers) became available and at the same time algorithm development had large success (e. g., multigrid methods) numerical solutions of the whole flow field past a body, which includes also separation phenomena, became possible. If the flow field is insensitive to the location of laminar-turbulent transition and turbulent separation is treatable, viscous flow past realistic configurations can be computed today exact and reliable, as is shown with many examples in this book.

We abstain here from the a detailed discussion of the problems of discrete numerical solutions of the Navier-Stokes equations. Much about them can be found in the following contributions.

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Golden Age of French CFD in the 1970-80s: Aerodynamics with Finite Elements and the European Multi-Physics HERMES Program

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Summary CFD played a critical role as design tool in the 1970-80s in French laboratories and aeronautical industries with the rapid progress of computing facilities. Three short contributions by senior scientists and technologists describe how CFD developed rapidly in the French scientific and industrial community and was recognized as a mature tool in aerospace engineering for the aerodynamic design of civil and military aircraft and space vehicles like the European HERMES Space plane.

1 Computational Fluid Dynamics

O. Pironneau, LJLL - UPMC Paris 6

From the very early age of computing up to the end of the cold war, Computational Fluid Dynamics (CFD) was given top priority because of its applications to the design of fighter aircraft, and to the simulation of nuclear explosions. The fundamental equations of fluid dynamics, the Navier-Stokes equations, are non-linear partial differential equations (PDEs). They admit a number of simplifications corresponding to potential flow, boundary layer flow, Euler flow, et cetera. For airplanes each is useful in its own regime but ultimately the full compressible Navier-Stokes equations with turbulence modelling are necessary, together with sensitivity analysis, in order to carry out design improvements and optimizations for advanced aircraft.

By 1970 computers could solve fairly accurately large classes of optimization problems and ordinary differential equations. I had myself solved two of these

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in 1969 on a small computer which seemed to be used by no one else in the Electrical Engineering and Computer Science Department at the University of California, Berkeley. Thus I was almost using a personal computer! The program was typed on a paper ribbon or input directly on the console and, of course, a single spelling mistake was heavily punished.

The PDEs of solid mechanics were among the first to be solved numerically using the Finite Element Method and in three dimensions (3D) even in the sixties, but translating the technique to fluid flows had not yet been done. Thus in those early days scientists at NASA, ONERA, the Los Alamos Laboratory and others where using the finite difference method which is an extension of the tools developed for the ordinary differential equations of rocket trajectory calculations. However, the finite difference method is not adapted to the complex shape of airplanes.

At Dassault Aviation in France, P. Perrier was a strong promoter of numerical simulation because he saw it to be the only way to compete with American industries which had much larger resources for wind tunnel testing. However the constraint was to use an arbitrary mesh. Among the first to solve a flow around an entire wing-body configuration in 3D was J. Periaux at Dassault on an IBM 360.

The Fortran IV language was used at that time via punched cards; graphics were displayed with a pen plotter, mostly on Benson tables, and we note that Benson was a French company. At INRIA at the same time, during the period running from 1974 to 1988, the institute's mainframe computer was not connected to the Benson plotting table and a tedious manual data transfer on tape had to be used resulting in endless delay which required much good will on the part of the computer operators. Personal computers, the Apple II in 1978 in my case, were paving the way to a final relief from the arrogant abuse that some of us had to experience on the part of some computer centers.

The situation improved considerably at the end of the 1970s with the advent of remote graphic terminals connected to virtual memory time-sharing systems, the Honeywell-Bull Multix machine in my case, which meant the possibility of using a local Tektronics graphic display which was remotely connected to the time-sharing computer system. At this time computations for an entire aircraft covering compressible potential flow – a world premiere – were conducted at Dassault-Aviation with our collaboration. This was followed soon after by A. Jameson's finite volume solution of Euler's equations around an almost complete aircraft frame.

Later the Apollo workstation made the biggest and final revolution in the laboratory; now the CPU and the graphics were tightly integrated in one machine and consequently greatly increased the number of computer runs that one could accomplish per day. Most importantly, people such as I became the operators of the computing resource and we were then motivated to learn much more about Computer Science itself, rather than just being numerical users of a remote computing resource.

This type of powerful workstation was used in competition, or in addition to, the minicomputers that were already commonly available at that time. Every decent Computational Fluid Dynamics laboratory had to acquire one of these expensive machines: a budget strain that forced us to hunt for industrial contracts, in itself not a bad thing after all, but also a significant strain on the frontier between applied research and commercial services. At that time, the technical stress was on mesh generation and three-dimensional graphic tools, as much as on algorithmic speedup.

Since that time, the working environment has not changed much. We still use powerful computer graphics on desktop machines with the possibility to defer computing to parallel clusters or mainframes supercomputers. However these set-ups are no longer a financial burden to most laboratories, and Computational Fluid Dynamics is available to everyone at the cost of a top-end personal computer.

2 A First Multiphysics Challenge for CFD: the HERMES Program

P. Perrier, French Academy of Technologies, Dassault Aviation retired

The success of Computational Fluid Dynamic in prediction of the main steady phenomena in subsonic, transonic and in supersonic regimes of aircraft was obvious when the European program HERMES was initiated. However the extension of such CFD into the hypersonic re-entry domain was far to have been proven in quality. Would the European Space Agency rely for HERMES on the rules of design used in US for the Shuttle development? In the positive case it would require a large time delay until sufficient know-how and testing facilities were present in Europe, a delay before the building and the certification of a space plane devoted to the transportation of men. How many years were required before mastering experimental validations with large high-enthalpy hypersonic wind tunnels, high temperature convective and radiative heat transfer on true materials of the Thermal Protection System? Neither CFD codes nor experimental facilities were at the level of inclusion of multiphysics involved in the process of design and development for supporting the anticipated needs. However the success of past common effort of research in CFD put in evidence that the first valuable numerical simulation was near: in French, and soon in European science-industry cooperation, the path was open to an advanced and shorter design as well as a certification procedure.

The procedure, that maybe was a shortcoming towards an European successful program, had to rely basically on computational data for the first time in aerospace industry. So the time devoted to the building of these numerical technologies had to be included in the schedule; it implied for the first time to accept critical points from the beginning, where the state of the art in scientific research and in the related code development had to gain validated

levels. The experimental data gained in small facilities present in the laboratories became more important to the success of the program, being related to its feasibility, than data to appear later in industrial facilities. So an industrial management was organized with all the numerical analysis and physics analysis needed of their modelling, including both the data processing of CFD and the experimental outputs. All computations provided a contribution to the evaluation of the required level of quality. It was a tremendous challenge for the European research and industry to apply a methodology where the quality of numerical simulation was the key point for the advancement of the program. In fact it was the challenge of the complexity of the physics to be addressed at the level necessary for the development of technologies allowing the manned access to space in Europe in a feasible project at low cost.

Three main axis were selected for common effort by industry and research teams: the first effort directed towards acquisition of new or better data in the different disciplines of physics and chemistry, the second effort to benefit from better numerical tools addressing all the critical points in the design whatever it comes from mathematical problems or from practical problems of grids, visualization, quality indicators or correlations with experimental data et cetera, and the third effort coming from industrial computations and its engineering outputs in selection of relevant points for evaluation of criticality (for the program feasibility) thanks to good evaluations plus acceptable uncertainties.

A set of workshops was generated, each covering a domain and/or a discipline where the progresses done and to be done were evaluated on test cases; the challenge being to recover data that may be obtained in computation as in laboratories within limited time and low cost. So the convergence of all these efforts resulted in quantified reductions of uncertainties in each critical area and global progress in feasibility of the complete program. The place of man in such transportation system was requiring such an extreme quality in built-in safety along normal or emergency return trajectories ended by safe landing of the crew in the vehicle or by chutes.

Problems of physics and chemistry. The study of physics involved in reentry trajectories put in evidence the problem of dissociation of air and the effect of variations of the equivalent isentropic exponent inducing large variation of the distance from the body to the front shock-wave and so of the maximal heat fluxes particularly in the case of intersection of shock-waves, generating overheating by spurious entropy layers. High temperatures means dissociation and chemistry adjusted to real flight conditions including catalytic effects and low Reynolds number rarefaction effects and in CFD sets of ordinary differential equations added to basic partial differential equations to solve in the loop of convergence, all contributing to non-linear effects as also complementary radiation cooling and heating.

Problems of numerical analysis. The research had shown that the main problems come from a complex accumulation of uncertainties related to the choice of basic algorithms, of the finite difference, finite volume or finite el-

ement implementation, of the non-linear incorporation, and of efficiency of convergence procedures and its sensors. Only workshops appeared able to quantify specific global uncertainties and led to a concurrent approach: a systematic double and triple output by different discrete approaches, different laboratories or research and industrial groups, at a sufficient level of convergence.

They collaborated for furnishing at the end a valuable approach, being always much better than the rough correlations unable to show where are the presumed problems; for example longitudinal Görtler vortices on deflected flaps were identified as sources of eventual overheating experimentally identified, their contribution was quantified and all was checked on flying demonstrators in USSR as in US. All was also compared to the results of much simpler or integral methods for example a direct Navier-Stokes solver compared to Euler solvers coupled with thin boundary-layer solvers near the wall.

Problems of uncertainties of the multi-physics approach. For each discipline and identification of complexity of physics, a tree of derivation was built coming from more simple test cases, disciplinary or with specific coupling of phenomena. For example a branch for continuous flow fields without separation effects, a branch for rarefied flow effects, another for catalytic effects, another for the geometrical scaling or change in shape et cetera. Each of the branches may be validated independently and so the building of the global uncertainties may be attempted with the help of randomization of the test cases.

Concluding remarks. It was too soon at the end of the program, covering by numerical computation all the critical points, to ascertain completely the quality of work done, whereas the go-ahead sign allowing to build a first experimental vehicle (MAIA) was not given. However the capacities of multi-physics in the refined CFD appeared as a key-point for the codes covering real complex physics programs. Access to that level of quality in hypersonics has been a fruitful exercise for the quality of the research teams involved in many environmental simulations and appeared also as a great achievement for collaborative industry in Europe.

3 Computational Mathematics and the Finite Element Method in Aerodynamics

J. Periaux, CIMNE/UPC and Univ. of Jyvaskyla, Dassault Aviation retired

Pierre Perrier has been very instrumental in launching CFD codes at Dassault Aviation for flow fields simulation in the early 1970s. The boundary singularity method did not allow at that time to compute transonic shocked

flows around civil and military aircraft. When I met the Theoretical Aerodynamic Department in 1970 Pierre Perrier was immediately convinced that the finite element method combined with the variational formulation approach introduced by J. L. Lions's school of Applied Mathematics, using Hilbert spaces for the solution of non linear PDEs, should be the right approach for the 3-D simulation of inviscid and viscous compressible flows. This choice was motivated by the following obvious advantages:

i) an easy treatment of complicated geometries and boundary conditions; ii) a robust control of non-linearities by calculus of variations; iii) an anisotropic refinement of the mesh in sharp-gradient regions like boundary layers, shocks, separated regions and wakes, et cetera.

Pierre Perrier was the driver of the famous GB4P team (Glowinski, Bristeau, Periaux, Perrier, Pironneau, Poirier), a close INRIA-Dassault Aviation tandem, to develop, test and finally validate in house the first 3-D full potential finite element code. The most difficult part of the industrial code TRIPHON was the generation of the 3-D unstructured finite element tetrahedral meshes around a complete aircraft obtained by another team of the Theoretical Aerodynamic Department. The capabilities of this approach for solving problems of industrial interest were illustrated in many scientific papers in the early 1980s, namely on the tri-jet engine AMDBA Falcon 50 at Mach = 0.85 and an angle of attack of 1 degree.

The simulated flow was mainly supersonic on the upper part of the wings. The methods have been used to design later the Falcon series like the Falcon 900 and also the Mirage 2000 with complex high-efficiency air intakes.

Another high interest of the Aerodynamic Department at this time was to simulate the unsteady viscous flow around and inside air intakes at high angle of attack for military applications. This challenging problem was solved by the team GBM3P (Glowinski, Bristeau, Mantel, Periaux, Perrier, Pironneau) with the support of the national DRET Defence Organization. The same finite element method was used for the simulation of unsteady flows of incompressible or compressible viscous fluids modelled by the Navier-Stokes equations.

Operator splitting techniques were introduced to decouple the two main difficulties of the problem, namely the incompressibility (the generalized Stokes sub-problem formulation was proposed by R. Glowinski and O. Pironneau) and the non-linearity (the Least Squares-Conjugate Gradient solution method). The resulting TOURNESOL code implemented by the late B. Mantel with Pl elements for the pressure and Pl-iso-P2 for the velocity components was able to simulate the dynamical vortices of a separated flow in a military type air intake. In this approach the existing computing facilities did not allow the fine calculation of 3-D viscous flow around complete aircraft, the critical difficulty being the accurate computation of boundary and shear layers and the control of the mesh quality. But Pierre Perrier did not wait for these computing facilities to start the development of unstructured mesh adaptation techniques in the mid 1980s with several French research teams at University

of Grenoble (J. Fonlup et al.), INRIA Sophia Antipolis (SINUS Project, A. Dervieux et al.), and also at Rocquencourt (MODULEF, M. Bernadou et al.). The necessity of using adapted unstructured meshes was driven by the accuracy needed to control the numerical entropy of compressible Euler flows at supersonic and hypersonic regimes, in particular for the HERMES program described above.

These unstructured mesh techniques were later generalized and used in 3-D EUGENIE (unstructured Euler) and VIRGINIE (unstructured Navier-Stokes) software by other teams of the Aerodynamic Department to simulate highly compressible Euler and Navier-Stokes turbulent and/or aero-thermal flows for the design of the European HERMES Space Plane and aerodynamic interactions of the military Rafale aircraft with store separation integration studies.

To conclude on the above industrial CFD achievements obtained by close R&D cooperations with universities and institutes I would like to add a personal comment: along the ongoing twenty five years spent in the Aerodynamic Department I learned how the combination of fluid mechanics and aerodynamics could ignite the passion of elegant planes designed by very cooperative teams fueled with innovation.

The way of working of these interacting teams announced the future collaborative platforms to be set up at the beginning of the 21st century.

Code Development in the German Aerospace Industry up to the Mid 1990s

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Summary Reviewed are major developments of discrete numerical solution methods of aerodynamics at the German aerospace industry from the 1970s to the mid 1990s. Then the national project MEGAFLOW was initiated. Considered are potential equation codes, with panel and potential equation methods, Euler codes, boundary-layer methods, and Navier-Stokes codes.

1 Introduction

In the NNFM series the first traces of industrial development of discrete numerical aerodynamic codes in (West-) Germany show up already in the proceedings of the first GAMM-Conference on Numerical Methods in Fluid Mechanics, Cologne-Porz, 1975, [1], see also the Appendix, pages 493 to 494. With this contribution we give an overview of major industrial development and application activities from the 1970s to the mid 1990s. Then the national MEGAFLOW project finally combined and streamlined, under the leadership of the German Aerospace Center DLR[1], the so far existing developments in Germany, at least regarding external aircraft aerodynamics. The structured Navier-Stokes solver FLOWer and then the unstructured solver TAU was the outcome of this focussed code development, see Section 6 of this contribution.

[1] The DLR, until 1997 called DFVLR, was formed in 1969, with the headquarters in Cologne-Porz, out of the legacy research establishments AVA (Göttingen), DFL (Braunschweig), DVL (Berlin, after 1945 Aachen and later Cologne-Porz), and others, see, e. g., [2].

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The code development at the aerospace industry, basically Dornier Aircraft[2](Do[3]) (Friedrichshafen), MBB (Munich-Ottobrunn), later Dasa, now EADS, with its divisions Helicopters (Heli), Military Aircraft (Mil), Missiles (Miss), Space Transportation Systems (Space), and Transport Aircraft (Trans) located in Bremen, initially was made partially with the classical problems: no or low acceptance with other staff and management, limited product value due to small computer power and storage. All overarching was the discussion about the value of aerodynamics. Even at AGARD it was deliberated, whether aerodynamics was longer worthwhile to be considered.

However, by as early as 1980, Do had assembled a large group dedicated to what was then called "theoretical aerodynamics". Already during the early 1980s, methods developed and refined in this group were applied to a variety of aerodynamic problems, also in the German automobile industry. Methods employed at Do in the early 1980s spanned the gamut from simple linear vortex-lattice tools, sophisticated panel methods coupled with state-of-the-art boundary layer codes developed in-house, to full potential, Euler and later even some of the first simple Navier-Stokes solvers.

At MBB, in 1984, E. H. Hirschel and C. Weiland initiated, [3], the research and development project "Numerical Aerodynamics at MBB" with the objectives: increase of the effectiveness of the present codes, coordination of developments, parallel code development if large risks exist, fostering of internal and external (universities, DLR) cooperations, internal and also external exchange of codes. The mentioned divisions participated until 1992, [4], all together with up to 10 experts per year plus further staff from projects.

The problem of insufficient computer power lasted longer. However, in 1985 advances in chip technology, Fig. 1 on page 4 of this book, and vector and parallel computer architectures, Fig. 2, improved the situation, while at the same time algorithm development made large strides. Large international (HERMES project) and national (German Hypersonic Technology Programme) ventures helped then to acquire at industry approximately adequate computer power, which, however, at that time still was small and expensive compared to what is available today.

In the following sections short overviews are given of the different major code developments and applications up to the mid 1990s at the German aerospace industry, taking into account, where necessary, also developments at the DLR. Due to the restricted space, the topics grid generation, aerodynamic shape optimization, flow-physics modelling, and multidisciplinary simulation and optimization are left out, and we look only at:

- potential equation codes, with panel and potential equation methods,
- Euler codes,

[2] The core of the Dornier numerical aerodynamics group joined Dasa Military Aircraft in 1995.

[3] We use in the following sections the codes in brackets instead of the full names of the companies and divisions.

- boundary-layer methods,
- Navier-Stokes codes.

Of course we cannot aim for completeness. Many names and contributions will not show up. We apologize in advance to those colleagues, whose work is not mentioned. Anyway, we hope to be able to sketch a picture of the German industrial aerodynamic code developments and applications[4], interesting also for the formerly involved and for the external colleagues.

2 Potential Equation Codes

2.1 Panel Methods

Panel methods solve basically the Laplace equation for inviscid subsonic or supersonic flow. They come as first-order and higher-order surface panel methods, mean-surface (vortex-lattice) panel methods, and field panel methods. A good overview of the work in that field up to 1976, also in Germany, is given in [5], the report on the Euromech Colloquium 75, held in May 1976 in Braunschweig, Germany. We find there for Germany work on and with first-order panel methods by W. Kraus at `Mil`, H. Struck at `Trans` (VFW-Fokker at that time), and S. R. Ahmed (with the Kraus method) and J. Steinheuer at DFVLR. Higher-order methods in Germany are not mentioned, but work on mean-surface panel methods at `Do` by C. W. Lucchi, at DFVLR by H. Körner for wing-fuselage combinations and by D. Hummes for rotor-wing interferences on helicopters. Work on a field panel method was reported by R. Stricker, `Mil`.

In the second half of the 1970s code development at industry shifted towards potential-equation and later Euler methods. Regarding panel methods we mention therefore only the development of the higher-order subsonic and supersonic singularity method HISSS, developed by L. Fornasier at `Mil` at the beginning of the 1980s, [6]. It found application in a wide range. With it also discrepancies, which can show up with first-order panel methods in wing flow-field results as well as wake structures of lifting wings, were investigated, [7], based on the analysis of 3-D wing boundary-layer solutions in [8].

The HISSS code was sold to Aermacchi, Alenia and CASA, used at `Trans` and `Miss`, and, following the tradition established by P. Sacher, was made available free of charge for research to DLR, ONERA, and several universities in Germany and Europe.

[4] Overviews of German work in numerical and experimental fluid mechanics and aerodynamics can be found in the proceedings of the bi-annual AG STAB/DGLR symposia. However, they were published only since 1996 in the NNFM series, beginning with the proceedings of the 10th symposium, Vol. 60. Later following were the Volumes 72, 77, 87, 92, and 96, see the Annex.

2.2 Potential Equation Methods

At Do, starting with a numerical code on the basis of transonic small perturbation (TSP) theory for the solution of two-dimensional problems, R. Vanino, S. Rohlfs and B. Moeken developed a three-dimensional version. On the basis of this software, the so-called SKF (super-critical wing) for the Alpha-Jet was designed (S. Rohlfs, W. Fritz). The TSP method was extended to incorporate the treatment of unsteady flows (W. Fritz) and was applied in the field of aeroelastics, in particular for the prediction of flutter.

Soon the work started on full potential solutions (S. Leicher), initiated by Jameson's first full-potential code. This method and the TSP method were coupled to the boundary layer method developed by H. W. Stock to account for viscous effects. S. Leicher and W. Fritz intensively applied this approach to the development of the IA63 military aircraft. In 1976, missile separation based on the full potential and slender body theory was computed (W. Fritz).

At Mil A. Eberle developed a potential-equation finite-element method for transonic flow past airfoils and wings, including airfoil optimization, [9]. In 1983 the still existing discrepancies between full potential and Euler method results were analyzed by E. H. Hirschel and C. W. Lucchi. It was found, that a shock at the suction side of an airfoil at transonic speed leads to an effective de-cambering due to the total pressure loss, [10]. Because the shock at the curved airfoil surface is orthogonal to it, [11], a simple correction scheme was devised. This resulted in the full potential method for transonic airfoil flow by C. W. Lucchi, [12], at the same time, when G. H. Klopfer and D. Nixon conceived a similar scheme, [13].

A viscous-inviscid interaction method, based on the full potential equation was devised by G. Dargel and P. Thiede at Trans, [14]. It found much applications in wing design. Similar approaches were developed for multi-element airfoils by F. Arnold and F. Thiele, see, e. g., [15].

For the computation of supersonic flow fields past slender wings, C. Weiland, [16], devised a marching solution for the potential equation. Despite the limitation of the potential-equation approach for supersonic problems, the surface-pressure distribution, which is of interest for the engineer, can be found with sufficient accuracy.

3 Euler Codes

With increasing computer power, solutions of the Euler equations became interesting for industry. The inherent limitations of the potential-equation approach thus could be overcome. The reader can find in [17] a very detailed overview by H. Rieger and W. Schmidt of German Euler codes, developed at industry and DFVLR/DLR in the 1980s and the first half of the 1990s.

For supersonic flows past sharp- and blunt-nosed bodies in a large angle-of-attack range, C. Weiland, at that time still with the DFVLR in Cologne-Porz,

later at Mil and finally at Space, developed in the second half of the 1970s time- and space-marching solution methods, initially based on Rusanows "progonka" scheme, [18].

The developments at Do began with Jameson's 2-D Euler method, see, e. g., [19], but rather soon the method IKARUS as Euler/Navier-Stokes code for three-dimensional applications was available, [20]. It is interesting to note that the 2-D-Euler method was applied by H. W. Stock and W. Haase to the layout of the second throat of the European Transonic Wind Tunnel (ETW), [21]. Studies on vortex-flows (including vortex-breakdown) emanating from delta wing configurations were performed by S. Hitzel, [22], [23]. Application to store separation with a code extension for implicit, time-accurate unsteady flows was made by E. Gerteisen, [24]. The 2-D Euler method was forwarded to the DLR and became later on the starting point for the development of the well-known FLOWer code, Section 6. Later the unstructured AIRPLANE code of Jameson, Baker, and Weatherill was taken over, refined, parallelized, [25], and applied to a host of steady and unsteady flow problems.

A. Eberle from Mil presented at the fourth GAMM-Conference on Numerical Methods in Fluid Mechanics (Paris, France, 1982) a study of three time-stepping solution schemes for the Euler equations for airfoils and inlets, [26]. In the following years he developed the Euler solver EUFLEX (Euler solver using characteristic flux extrapolation), [27]. From it the solver for time-accurate unsteady flow solutions was derived by A. Brenneis, see, e. g., [28], and the Navier-Stokes solver NSFLEX by M. Schmatz, see the next section. Much of the developments at Mil, also that of N. C. Bissinger for inlet flow computations, and of R. Deslandes for store separation problems is discussed and referenced in [29].

In 1982, at the fourth GAMM-Conference Eriksson and Rizzi presented Euler solutions of flow past a highly swept delta wing with sharp leading edges, [30]. The results led to speculations and hypotheses regarding the origin of the entropy rise, respectively the appearance of rotational flow in the lee-side vortices. At the symposium "International Vortex-Flow Experiment on Euler-Code Validation" at Stockholm, Sweden, 1986, E. H. Hirschel and A. Rizzi demonstrated, [31], that the effect represents the vortex sheets emanating from trailing edges or swept leading edges. At ordinary lifting wings the vortex sheet leaves the wing only at the trailing edge. For this topic see also [29] and [32].

At Trans, at the beginning of the 1990s, a close cooperation with DFVLR Braunschweig, N. Kroll, R. Radespiel, and C.-C. Rossow, was initiated. The Euler code MELINA, [33], [34], was developed from the codes CATS and CEVCATS of DLR, see Section 6. The Euler code ROTFLEX, was derived from EULFLEX by H. Stahl-Cucinelli, Heli, for helicopter blades, [35], at Miss EUFLEX was adapted to the special needs of missile aerodynamics.

The Euler codes at Do, Mil, and Trans were, in one or the other form, combined with boundary-layer codes, in order to take into account viscous effects. Boundary-layer displacement was either modelled by thickening of the geometry or by applying the equivalent inviscid source concept, see, e. g., [36].

From the mid 1980s on the HERMES project (the European winged reentry vehicle), the German Hypersonic Technology Programme with the $M = 6.8$ airbreathing lower stage SÄNGER as reference concept and the upper stage HORUS, posed large challenges for the computation of hypersonic flow fields with mild and strong high-temperature real-gas effects, see, e. g., [37]. Involved were `Do`, `Mil`, and `Space`, where C. Weiland, since 1984 head of the aerothermodynamics department, developed with G. Hartmann, S. Menne, and M. Pfitzner the aerothermodynamic Euler codes DAINV-Space, [38], and DAINV-Split, [39]. The Euler methods at the different companies were applied to external flow fields, see, e. g., [40], [41], inlet flow, e. g., [42], flows in rocket-engine nozzles (ARIANE), [43], upper stage separation (SÄNGER), e. g., [44], and thermal loads determination, for HERMES with a coupled Euler/second-order boundary-layer method, e. g., [45].

4 Boundary-Layer Methods

Numerical solution methods for the two-dimensional and three-dimensional – we concentrate our review on the latter – boundary-layer equations are, despite of the progress of Navier-Stokes methods, still of interest for research as well as industrial problems. They permit to find with little computational effort wall-shear stress, thermal loads and integral properties (boundary layer thickness, displacement thicknesses et cetera) of attached viscous flow, if needed with very high accuracy.

First work on finite-difference methods for the solution of the three-dimensional equations was made at the DFVLR in Cologne-Porz by E. Krause, E. H. Hirschel and Th. Bothmann at the end of the 1960s and in Göttingen by W. Geissler at the begin of the 1970s. In the 1970s in Cologne-Porz work, especially on wing boundary-layers, was performed, with the investigation of laminar-turbulent stability and transition criteria in the background. For this surface-oriented coordinates are needed, and consequently general formulations of the geometrical and mathematical aspects of first- and higher-order boundary layers were worked on, see, e. g., [36], [46].

In the second half of the 1970s H. W. Stock developed at `Do` a three-dimensional integral boundary-layer method, [47], [48]. Integral methods work with main-flow and cross-flow profile families in surface-normal direction, hence only a two-dimensional surface-tangential difference solution is performed. Such methods are even faster than pure finite-difference methods and, in addition, they yield directly the boundary layer thickness, displacement thicknesses and so on, see, e. g., [49]. The code was later coupled in a two-dimensional version to an Euler method for infinite swept geometries. The resulting DOFOIL code was used for airfoil optimization.

E. H. Hirschel, since 1980 at `Mil` employed in the first half of the 1980s the integral method of J. Cousteix from ONERA, [50], to a host of fuselage and wing configurations, see, e. g. [51], [52]. F. Monnoyer, since the mid 1980s at

Mil, developed his second-order boundary-layer finite-difference method, [53], into the SOBOL code. It found application especially in the HERMES project for the determination of thermal loads at the radiation-cooled windward side of the vehicle, see, e. g., [45], [54]. With the extension to high-temperature real-gas effects by Ch. Mundt, and coupled to the Euler method of M. Pfitzner, [39], it was a very effective tool, superior at that time to the evolving Navier-Stokes solutions. SOBOL was also an important element of the zonal solutions of the Navier-Stokes equations, which were pursued in the second half of 1980s at Mil, see the next section. Like the panel method HISSS, it was made available free of charge for external scientific users. The user group of SOBOL encompassed DLR, FFA, ABB, SAAB, and several universities in Germany and Europe.

At Trans P. Thiede and E. Elsholz took over the finite-difference method of D. Schwamborn, [55], which he had developed at the DFVLR Cologne-Porz. It was used for boundary-layer calculations around wing leading edges, which became important in the 1980s/1990s in view of the boundary-layer control work[5] at Trans. In this context also linear stability codes were developed. G. Schrauf, Trans, devised in 1988 a solver for three-dimensional compressible boundary layers, [58], which was followed by semi-empirical (e^N-method) schemes, see, e. g., [59], and also the work at Do by H. W. Stock and E. Degenhart, [60].

It is very deplorable, that the work of the group of U. Dallmann at DLR Göttingen on non-empirical transition prediction (NOLOT method), see, e. g., [61], was more or less stopped, one year before his untimely death in 2001. The solution of non-linear, non-local parabolized stability equations (PSE) probably is the most promising approach in view of transition prediction and control for practical design problems, once the receptivity problem has been solved.

5 Navier-Stokes Codes

The Navier-Stokes equations for the computation of both steady and unsteady flows represent the highest simulation level in the continuum flow domain. For turbulent flow simulations with statistical turbulence models they are called Reynolds-Averaged Navier-Stokes (RANS) equations. Because of their large computation power and storage needs, their broad application in aerospace industry became possible only in the 1990s, see Part III and also [62].

However, the work on solutions in Germany was beginning much earlier. E. H. Hirschel at DFVLR in Cologne-Porz developed around 1970 a finite-difference method for the solution of the truly parabolized Navier-Stokes equations. He investigated with it the two-dimensional hypersonic attached viscous flow past a flat plate with thermo-chemical non-equilibrium of a binary gas,

[5] For that topic see also [56] and [57].

[63]. E. Elsholz and W. Haase at the Technical University Berlin developed a three-dimensional Navier-Stokes finite-difference solver in terms of the incompressible vorticity-transport equations and presented 1975 the first results of laminar flow past an inclined ellipsoid, [64].

W. Haase, since 1980 at Do, extended at the beginning of 1980s the Jameson's 2-D Euler method to a full Navier-Stokes code, [65], for airfoil design and later, optimization purposes. The 2-D Navier-Stokes method, in an axisymmetric version, was applied to internal flows with moving meshes in Diesel engines by K. Misegades. Moreover, the 2-D Navier-Stokes method was the first test bed for advanced turbulence models, e. g., the $k - \tau$ model implemented by F. Magagnato, [66], and much effort was placed on a validation of flow-physics models in general. Later H. W. Stock and W. Haase successfully coupled the semi-empirical e^N transition prediction method with a Navier-Stokes method, [67]. The 2-D Navier-Stokes method also served as a tool for other applications, e. g. the hydrofoil developments by H. Echtle. As the aforementioned Navier-Stokes method was restricted to single-block computations, W. Fritz developed an additional 2-D Navier-Stokes method for multi-block configurations, probably the first of this kind. H. Rieger developed a thin-layer (parabolized) Navier-Stokes code, and applied it to supersonic and hypersonic flow problems. Eventually the multi-block and multi-grid Euler/Navier-Stokes code IKARUS, developed by S. Leicher, see above, became the "work horse" at Do. Later the unstructured AIRPLANE code of Jameson, Baker, and Weatherill was used also Navier-Stokes code. The Navier-Stokes codes at Do were made available to the aerospace research establishment NLR, to ESTEC, to car industry and to several universities.

At Mil M. A. Schmatz developed in the second half of the 1980s the NSFLEX code, [68], based on the EUFLEX code by A. Eberle. Beginning in 1987 NSFLEX found many applications, since 1988 especially in the hypersonic projects and programmes at that time, [69]. It was also made available for research work at universities, and also ESTEC.

In order to overcome the, in the 1980s still serious, limitations due to the weak computer resources, a zonal solution scheme (Euler and boundary-layer codes in the attached-flow domain, Navier-Stokes solution in the separation/wake domain) was developed by M. A. Schmatz (2-D) and K. Wanie (3-D) at the Technical University München. Later at Mil they combined their scheme with EUFLEX/NSFLEX and the SOBOL boundary-layer code of F. Monnoyer and were able to show, that zonal solutions are viable approaches in aerodynamics, [70], [71]. However, if the search of the zonal boundaries is done automatically, too much computer time is needed and the scheme is no longer advantageous.

At Trans a Navier-Stokes version was derived from the Euler code MELINA, before development activities were given up in favor of the FLOWer developments, Section 6.

At the beginning of the 1990s W. Schröder and G. Hartmann developed at Space the Navier-Stokes code DAVIS-VOL, [72], initially for the simulation

of upper-stage separation problems in the SÄNGER programme, [44]. It later became the "work horse" at Space, with several models to describe high-temperature real-gas effects, turbulent flows and radiation-cooling effects, with applications in a wide range, including even rocket-engine nozzle problems.

6 Towards the Common German MEGAFLOW System

At the beginning of the 1980s H. Körner initiated at the DLR Braunschweig the development of structured Euler and Navier-Stokes codes. N. Kroll, a former student of U. Trottenberg, started in 1981 investigating and scrutinizing the 2-D Euler method which was forwarded to DLR by Do. Together with R. Radespiel and C.-C. Rossow, who joined him in 1981 and 1982, he developed the multi-block structured cell-centered Euler code CATS, see, e. g., [73] and the vertex centered Euler code CEVCATS, see, e. g. [74]. These codes became operational in the second half of the 1980s and at the beginning of the 1990s they were available as three-dimensional Navier-Stokes codes, see, e. g., [75].

In 1993 D. Schwamborn and W. Kordulla at DLR Göttingen decided to develop an unstructured code for the solution of the Euler/Navier-Stokes equations. The work was started by Th. Sonar and in the mid 1990s the TAU (τ, Triangular Adaptive Upwind) code became operational, [76], [77].

The concentration process towards MEGAFLOW started in 1993. The project POPINDA, funded by the German Federal Ministry for Education, Science, Research and Technology (BMBF), was initiated by the DLR, the German National Research Center for Information Technology (GMD) and Trans. Led by A. Schüller, GMD, it was an effort of industry and the research centers to parallelize the structured codes developed and in use at DLR (CEVCATS), Do (IKARUS), Trans (MELINA), and Mil (NSFLEX), [78].

In 1995 at the DLR responsibilities were split: structured codes responsibility (especially FLOWer, in a sense the parallelized extension of CEVCATS) at DLR Braunschweig, unstructured code responsibility (TAU) at DLR Göttingen. These code developments, which finally absorbed the developments at industry, partly also at German universities, resulted in the national project MEGAFLOW, [79], [80]. Emphasis was on the improvement and enhancement in its first phase of FLOWer (1996-1998) and in the second phase of TAU (1999-2002).

The MEGAFLOW software system, resulting from these activities, now is the common German aerodynamic simulation system, meeting the requirements of the German aircraft industry. Coordinated by the German Aerospace Center DLR, it provides with FLOWer and TAU parallel flow prediction and shape optimization capabilities. The interested reader can find details in the contribution by C.-C. Rossow and L. Cambier in Part III of this book.

Note: In the following list of references the volumes of the series are cited without their sub-titles, which give additional information about the contents.

The interested reader can find the complete bibliographical information of each volume in the list of the volumes, Part VI, pp. 494 to 503.

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Discontinuities in Compressible Flows: Italian Contributions

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Summary Valuable results have been achieved over a wide variety of CFD fields by the Italian community during the last decades. Here attention is focused on a specific field: the numerical treatment of discontinuities, especially shock waves, in hyperbolic gasdynamic problems. Italian contributions to the explicit fitting and to the numerical capturing of discontinuities are reviewed in the following.

1 Introduction

Computational Fluid Dynamics (CFD) appeared at the beginning of the 60's. In a short time, it developed on several areas: industrial, environmental, astrophysical, meteorological, biological and others. The American SST project (SuperSonic Transport) started at the end of 1966 and the European Concorde first flew in 1969. Space exploration had already witnessed the first atmospheric reentries: the Soviet Yuri Gagarin from an orbital flight in April 1961 and the American Alan Shephard, one month later, from a suborbital flight. Space Shuttle design was in progress; the first flight took place later, in April 1981. In such a colourful picture of aerospace initiatives, aerodynamic science has very much been focused on high speed regimes, from the transonic to the supersonic and then up to hypersonics, with high temperature effects. Compressibility plays a fundamental role in external and internal flow applications, with the generation of shock waves and contact or shear surfaces.

A classical problem is the supersonic flow past a blunt body (Harvey Allen, 1957), investigated with wind tunnel experiments and analytical studies, but also through first numerical predictions. The steady flow field between the bow shock and the body is characterized by the mixed nature of the governing equations, elliptic in the subsonic pocket about the stagnation point

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and hyperbolic in the downstream neighboring region. The difficulty in dealing numerically with a mixed problem can be successfully overcome with the approach known as the "time dependent" technique [1]. The unsteady flow equations are taken into account to describe a transient. Starting from arbitrary initial conditions, a steady configuration is reached. The governing equations are respected all over the field, as well as the conditions imposed at the boundaries. The mixed nature of the steady flow field, elliptic and hyperbolic in space, is overcome by the hyperbolic nature in time of the unsteady flow equations.

The "time dependent" technique was applied, at the beginning of the 60's, to inviscid compressible flow. It was then extended to more complex physical models, laminar or turbulent flows, reacting flows, multiphasic flows and flows with high temperature effects. Not only steady configurations are searched for and predicted, but also unsteady phenomena are investigated.

In the "time dependent" technique, the time integration is carried out for a system of quasi linear partial differential equations (PDEs), or alternatively, for a system of laws of conservation (LCs). The integration in time of PDEs only allows the correct prediction of flows with discontinuities through their explicit treatment, with the full respect of the related jump conditions. Since the shock wave is the dominant discontinuity, the procedure is called "shock fitting". Obviously, the explicit treatment also has to be extended to contact surfaces or shear flow discontinuities. Alternatively, the integration of the LCs allows the correct prediction of discontinuous flows, without any explicit treatment. The related numerical methods follow the "shock capturing" procedure.

A hot debate characterized the CFD in the 60-70's on which was the more convenient procedure between the "shock fitting" and the "shock capturing". This contribution to Vol.100 of the NNFM series reports on the participation, in this debate, of the most active Italian research groups in this field, in particular those of the Politecnico di Torino, the University "la Sapienza" in Rome and the Politecnico di Bari. This participation refers to a very specific field, among the several and remarkable research activities carried out in Italy over the last forty years. Excellent contributions, spread over the most different CFD fields, have been and are actually being developed within academia, research centers and industry. It is not possible to report them all here, but looking at the more prestigious international journals, one can soon identify the related, large and valuable, scientific production in the worldwide scenario. It is a pleasure to recall here that a CFD group from the Politecnico di Torino participated, on February 1977, at the University of Stuttgart, in the GAMM-Workshop entitled "Boundary Algoritms for Multidimensional Inviscid Hyperbolic Flows" on the numerical test case of the Ringleb flow [2]. The contributions to that Workshop are collected in Vol.1 of the NNFM series, published in 1978 with Professor Karl Förster as editor, see the second contribution to Part I.

2 Shock Fitting

The "shock fitting" procedure is based on the finite difference integration of the differential equations (PDEs) over smooth flow regions. Great care is paid to the prediction of possible generations of shocks. This preliminary operation, "shock detection", is necessary when a shock is not prescribed initially as a finite discontinuity but tends to be formed by the coalescence of "compression" waves at either unknown locations or times: a shock imbedded in a flow field. Shock detection has absorbed much attention but a fully satisfactory answer, in terms of reliability and robustness of the code, has not appeared over the years.

Once a shock is detected or prescribed, it is considered as a line that separates two neighbouring smooth regions. A discretization process, based on two distinct grids which collimate on the shock, follows. Alternatively, the shock can be represented by a line of fluid dynamic discontinuity that moves over a unique grid distributed continuously over the two sides of the discontinuity.

The two lines of investigation, "shock as a boundary between two neighboring grids" and "shock floating over a continuous unique grid", have been widely studied and experimented. The former appears more robust, but requires the capability of the two grids, which merge on the shock, to follow the shock itself with their deformation during its movement, with possible topological difficulties. The second one can be delicate because of the one-sided finite differences on the two sides of the shock evaluated on a continuously variable stencil during the displacement of the shock through the grid.

The scientific guide of Gino Moretti, who has acted in first person or in close collaboration with young American and European scientists, has been fundamental for the development of both lines of investigations. The latter group of scientists are mostly Italian, from Turin, Rome and Bari who visited him in the USA. He has worked hard on "shock fitting", with great ingenuity and passion. Rightfully, he is considered the founding father of this procedure.

It is convenient to recall Moretti's pioneering work which was presented in 1966 [1], where it has proved how "shock fitting" provides excellent results in predicting the supersonic flow past a blunt body. The shock is here considered as the boundary between the upstream uniform supersonic prescribed region, where obviously nothing is computed, and the following downstream region bounded by the body and the shock itself. During the transient of the "time dependent" technique, the shock moves and the grid in the shock layer is continuously deformed up to the steady final configuration, The results reported in [1] are really surprising for what was considered a non simple problem at that time: a ridiculously small grid (4x10) and very good comparisons with experimental data. The CPU time was modest, even for the primitive computers available in the 60's.

Such numerical success has to be ascribed to the explicit treatment of the bow shock, in spite of the rough grid used in the smooth shock layer. Most

of the merit comes from the compatibility equations. Once matched to the Rankine-Hugoniot (R-H) conditions, they allow the shock to move extensively and to reach a stable steady configuration, in agreement with the physics and the hyperbolic mathematical character of the governing equations. This was one of the first suggestions on the transfer of the "upwind" idea from the well known method of characteristics to a finite difference algorithm.

As mentioned later on, S.K. Godunov [3] had suggested a similar idea, a short time before, but developing a "shock capturing" procedure for the LCs. The quality of the results, obtained by integrating the PDEs with the support of the compatibility equations at the fitted shock, prompted further studies. Among them, the "lambda scheme" [4] where the use of the compatibility equations is extended all over the smooth flow field.

Gino Moretti founded a school of thought and numerical practice in the "shock fitting" procedure. Many young Italian researchers have followed him in this adventure, as proved by the rich scientific production on this matter.

3 Shock Capturing

The "shock capturing" procedure represents an alternative to "shock fitting". The detection of the shock is not required here, nor is the explicit tracking of a discontinuity. The shock shows up in the middle of the flow field as a sharp variation of the fluid dynamic properties computed numerically over a few points of the grid. The grid itself can be at rest or be deformed independently from the shock movement.

The integration obviously has to be performed on the LCs and the algorithm has to fulfill the conservativity requirement. The finite volume appears as the more natural and suitable approximation for space discretization.

At the beginning, in the 70's, the fluxes on the interfaces between neighbouring volumes were obtained with centred evaluations. However, severe oscillations arose about the resulting captured shocks. The violation of domains of dependence, which in turn are respected by the compatibility equations in the shock fitting procedure, is responsible for this problem.

In order to keep these oscillations under control, an artificial numerical viscosity is introduced and the oscillations disappear. In the transonic regime the results are very good: satisfactory accuracy and high computational efficiency in terms of CPU time. However, moving up to higher speeds, the amount of artificial viscosity needed to control the oscillations becomes rather large. The captured shocks are spread more and more over the grid and the sharpness of the capturing is lost. In the hypersonic regime, the quality of the solutions becomes unacceptable and the code robustness decreases.

New families of schemes for integrating the LCs were then proposed, at the beginning of the 80's. These are known as "upwind" schemes. In order to understand the meaning of this denomination, within the context of "shock capturing", it is convenient to quote [5]: "To approximate a hyperbolic system

of conservation laws with so-called upwind differences, we must first establish which way the wind blows. More precisely, we must determine in which direction each of a variety of signals moves through the computational grid. For this purpose, a physical model of the interaction between computational cells is needed: at present two such models are in use". They are specified a few lines afterwards, "flux-difference splitting (FDS)" and "flux-vector splitting (FVS)". Several other schemes or families of schemes followed: HLL, HLLE, HLLC, AUSM and others derived from the previous ones in some hybridized form. The reader can refer to classical CFD books on this matter and also to [6] for a critical and comparative analysis of them.

The integration of the LCs with "upwind" methods respects "the two basic aspects of fluid dynamics, conservation and nonlinear wave propagation, both of them properly accounted for" [7]. The propagation of waves, which does not appear directly on the LCs, becomes explicit by introducing PDEs into the evaluation of the fluxes at the interfaces. The former centred algorithms are replaced by biased evaluations in order to respect the domains of dependence. The Riemann problem (RP) is introduced and its solution is also obtained on the basis of the PDEs. It is worthwhile noting that the "upwind" idea, borrowed from the old method of characteristics, was revitalized almost at the same time by two arrays of scientists: the first dedicated to "shock fitting", with the proposal of the "lambda" scheme for the PDEs [4], and the other focused on "shock capturing", with the development of "upwind" schemes for the LCs [7] [8] [9].

As mentioned above, Godunov had in fact already introduced the "upwind" idea for the LCs some years before, but with limited success at that time. Two decades were to pass before Godunov's suggestion in "upwind" schemes for the LCs was rediscovered. Contributions have also been proposed in "shock capturing" studies by the Italian CFD community.

4 Not Only Time Dependency, Compressibility or Shocks

The numerical treatment of discontinuities is a fundamental issue in "time dependent" methods for compressible flows. However, the same issue also appears, in a specular form, in "space marching" methods for supersonic steady flows. Both the "fitting" and the "capturing" are candidate procedures for predicting shocks in these supersonic steady flows, for the inviscid ones governed by the Euler model and for the viscous ones described by the parabolized form of the Navier-Stokes equations. It should also be recalled that any contribution to flows with shocks in compressible flows can easily be transferred to the corresponding "shallow waters" problems. Attention is then paid to "bores" or "hydraulic jumps". Finally, even though shocks represent a discontinuity of great interest, shear flow discontinuities were also deeply investigated in

the frame of an original approach to solve the "inverse problem" for the design of aerodynamic components. Italian researchers have been engaged in investigations of these problems.

5 Contributions from the Italian CFD Community

It is not easy to organize an overview of the contributions made by the Italian CFD community over the last decades. Even by confining the analysis to the narrow field of the numerical treatment of discontinuities in compressible flows, the related scientific production, developed since the middle of the 70's, is large and diversified. Here attention is only focused on the scientific activities published in international journals, while the several and important contributions presented at conferences and workshops are skipped over.

The above community is closely connected to the cultural roots and scientific directions received from Gino Moretti. However, the same hot debate present at an international level on the treatment of discontinuities can also be found in this community which is split into two opposite arrays, one working on "shock fitting" and the other on "upwind" schemes for "shock capturing". In this case, the debate is not in fact so hot, but softer and warmer, because both procedures are based on the propagation of waves. Their contributions are reviewed in the following, starting with the "fitting" array and continuing with the "capturing" one.

5.1 "Fitting" Contributions

The array working on fitting has been active, since the 70's, in the three Italian academic institutions mentioned above. As for the two lines that consider the computational grid, namely (1) two distinct grids adapted on the discontinuity which separates them as an intermediate boundary or (2) the discontinuity which floats on a wholly independent grid, the first one is only used in the case of contact-shear surfaces or shocks with a uniform upstream prescribed field while the second one prevails in most shock applications.

At the beginning, one-dimensional hyperbolic problems were considered, such as 1D unsteady flows (1D-UN) or two dimensional steady supersonic flows (2D-SS). Among the different studies, a low dissipation and dispersion method, suited for possible 1D-UN investigations on non linear axial mode instabilities applied to combustion problems for rocket engines, was proposed in [10] and [11]. Studies have also been performed for 2D-SS flows either with ideal gas [12] and with non equilibrium high temperature effects which move the centre of pressure along a hypersonic flying body [13]. The above one-dimensional studies (1D-UN and 2D-SS) are important to suggest new numerical methods, but extension to multi-dimensional applications must follow, as reported in the conclusions of the previously cited works.

Investigations were then carried out on two-dimensional hyperbolic problems, in particular 2D-UN, in transonic and supersonic regimes. Original contributions have been dedicated to external and internal transonic flows, [14] to [17]. The non conservative "lambda" formulation is here ingenuously modified by introducing the proper jump conditions. Hypersonic flows in non-equilibrium about blunt bodies were investigated in the European "Hermes" project which involved a cooperation among academia, research centres and industry. The Italian contribution is worthy of mention, [18] to [20]. Here the bow shock is treated explicitly, in a classical fashion. The common base of the above 2D-UN activities is the "lambda" scheme which is also formulated in a formal manner for boundaries, in particular for the bow shock [21].

The 2D-UN shocks considered up to now show simple topological structures. On the contrary, the 2D and axisymmetric structures of shocks investigated in propulsion nozzles are much more complex, [22] to [26]. The results refer also to unsteady phenomena with complicated shock interactions and are very interesting. On the basis of these investigations, shock fitting appears to be a well developed, mature and robust procedure. As anticipated, attention has also been dedicated to the treatment of discontinuities in shallow water applications, where the Froude number replaces the Mach number and the bore, i. e. the hydraulic jump, is treated just like the gas-dynamic shock. Extensions from gasdynamics to shallow waters have been proposed for 1D-UN, 2D-SS and 2D-UN flows [27]. Particular mention should be made of the explicit treatment of shear surfaces. Besides the examples already seen in propulsion, with the jet discharged from a nozzle, an original solution was proposed for inverse design problems, in order to determine particular geometries through the unsteady motion of impermeable surfaces [28] [29].

5.2 "Capturing" Contributions

These contributions have been developed more recently, in the 80's, essentially in Turin. The first studies were focused on one-dimensional hyperbolic problems (1D-UN and 2D-SS). The capturing of discontinuities is obtained by integrating the LCs with a "flux-difference splitting" (FDS) scheme. An approximate solver is used to solve the RP defined on the interfaces that contour a finite volume [30]. According to the suggestions of Osher [8], the shocks involved in the solution of the RP are considered isentropic, but the path of the waves is opposite, as in the original proposal by Godunov [3] and in the subsequent one by Roe [9]. This approximated solution for 1D-UN flows was followed by a similar approximate solver for 2D-SS flows [31].

More recently, the 1D-UN studies have been extended to the coupling of fluid dynamic equations (Euler or N-S) with Maxwell equations, for a weakly ionized gas in a magnetic field. The propagation of waves is much more complex than in the classical fluid dynamics. Studies on this matter have been developed in a joint collaboration with ESA-ESTEC [32].

On the basis of the above one-dimensional hyperbolic problems, extensions to multi-dimensional cases have been carried out for 2D-UN and 3D-SS problems. In 2D-UN problems, attention is first dedicated to the inviscid transonic flow about a circular cylinder, with the generation of the vortical wake due to unsteady shocks at the cylinder wall. The wake is unsteady and periodic, similar to the Von Karman one. A preliminary study [33] was followed by a more complete and exhaustive analysis performed at the ETH in Zürich [34].

Interest in 2D-UN flows has also been directed towards non-equilibrium hypersonic flows, at the time of the corresponding "fitting" contributions, in the frame of the "Hermes" project. In a joint research carried out with the Space Group Department of Deutsche Aerospace in Münich, comparisons were made of the results obtained for classical 2D and axially symmetric configurations for reentry vehicles. In the German contribution, the bow shock is "fitted", in the Italian one it is "captured" [35]. The comparisons have proved to be very satisfactory, considering that the two contributions follow opposite procedures at the shocks and totally different numerical schemes elsewhere. Always in the wake of the "Hermes" project and in the frame of AGARD and RTO activities, several studies have been performed on complex interactions of shocks and contact-shear surfaces in hypersonic non equilibrium laminar flows. Numerical predictions have been compared with experimental results obtained at ONERA and CALSPAN [36].

A disturbing numerical instability, the "carbuncle", has emerged with FDS methods on the bow shock about a blunt body, and also on a shock propagating in a gas at rest, as well as in other simple problems. The "carbuncle" has been experimented worldwide by several researchers. It has been deeply investigated in order to understand the reason for its appearance and to prescribe a cure to avoid it [6]. Note that the "carbuncle" arises in the shock "capturing" region whereas the "fitting" of the bow shock does not suffer of any numerical problem [6]: a positive score for "fitting" over "capturing"!

Studies on 3D-SS flows have been carried out alongside those on 2D-UN flows. On the basis of the Euler governing equations, supersonic flows about pointed cones have been investigated, where conical configurations are achieved through a "space marching technique" along the axis of the body. The lift-off of the Ferri entropy singularity from the leeward side towards the shock layer is predicted, with recirculating supersonic cross flow bubbles and the generation of conical vortical structures [37]. Here the bow shock, which assumes an asymptotic conical shape, is fitted and treated explicitly, but cross-flow shocks, which are responsible for the vortical conical structures in the shock layer, are captured numerically with an FDS method.

Always in the domain of 3D-SS flows, great attention has been dedicated to "corner flows". In the case of the Euler model, complex conical structures of shocks and contact-shear surfaces have been predicted. For the 90° corner, symmetric and nonsymmetric structures were predicted at different ramp angles and upstream Mach number [38]. Later, laminar flows were considered

in the parabolized form of the N-S equations, and numerical predictions were compared with experimental data obtained by Hummel at DLR [39].

The above activities have been conducted in the Italian academic environment. However, applications have also been developed outside academia. Intense work on hypersonic vehicles has been carried out, since the 80's, at CIRA (Italian Center for Aerospace Research), as well as at the actual Thales Alenia Space Italy, through continuous interactions with the Politecnico di Torino for over more then two decades. Complex interactions of strong shocks are expected to occur and play a dominant role. Capturing methods founded on the FDS approach are widely used within these activities. These close cooperations have generated joint activities in the European "Hermes" scientific adventure and in the frame of the activities prompted by AGARD and RTO.

More recently, the CAST (Innovative Aerothermodynamic Configurations for Space Transportation Systems) project, founded by ASI (the Italian Space Agency), has actually been promoting a renewed and stimulating involvement among the same actors for the numerical predictions of hypersonic flows.

6 Conclusions

Intense and passionate studies have been undertaken over the last forty years on the numerical treatment of discontinuities in compressible flows. The subject has been widely investigated and seems to have now reached a well established position.

"Fitting" represents a very accurate procedure in problems with relative simple shock interactions and topological structures. For instance, in classical blunt body flow, "fitting" provides excellent results, with minimal coding effort, as in the case where FDS "capturing" seems more vulnerable because of carbuncle instabilities. However, in the complicated problems found in high speed transportation, "fitting" requires coding efforts which may result to be very heavy. On the other hand, the more and more powerful computational resources need to cope with other aspects of the flow, such as for instance, turbulence phenomena. They also allow the use of grids fine enough to sharply and neatly capture any discontinuities. Perhaps "fitting" appears now less appealing in practical applications than it certainly did two decades ago.

On the contrary, "capturing" has received a widespread acceptance, certainly in "commercial codes", but also in "home-made codes" specifically created for basic and applied research. The flexibility in dealing with any unexpected complicated shock structure, the relatively low effort required to write the codes and the resulting high robustness have led to widespread exploitation of the "capturing" procedure.

It is not easy to say a final word on this debate, which has been so thoroughly investigated and with such passion!

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Flashback: 30 Years Numerical Fluid Mechanics and Aerodynamics in Japan, other Asian Countries and the Western Pacific Rim

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Dedication

Three authors were originally assigned to write this article. Prof. Kunio Kuwahara was one of them. Unfortunately, Prof. Kunio Kuwahara died September 13, 2008, during the period when this manuscript was prepared. The other two authors dedicate this article to Prof. Kunio Kuwahara. His effort in the field of CFD was remarkable. A lot of well-recognized researchers finished their ph. D. under his supervision. A lot of his friends in the world were influenced by and received benefits of Prof. Kuwahara's remarkable talent. May he rest in peace.

Summary We glance back at the history of CFD in Asia, especially in Japan. It is quite clear that contributions from Asian countries have increased tremendously in the last 20 to 30 years of CFD research. Advanced supercomputers have been timely developed by Japanese industries and a good environment of CFD research using High Performance Computers has been supplied to the researchers especially in Japan. A number of CFD researchers either learned CFD in U. S. or in Japan and came back to their own countries in Asia. Such incidence obviously supports the CFD development in Asia. This paper describes the fact sheet to support the development and some features of the history of CFD development in Asia, especially in Japan.

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1 Asian Contribution from a Statistical View Point

Computational Fluid Dynamics (CFD) has made remarkable progress in the past 30 to 40 years especially with commercial supercomputers that were first born in late 1970s. As can be found in automobiles and aircraft, CFD became a part of the development process in many engineering fields.

There are now a lot of international symposiums associated with CFD. Among them, the most traditional one, which disappeared by the merger of two existing conferences, was the so called ICNMFD. The exact name was International Conference of Numerical Methods in Fluid Dynamics and it was held every other year. The first conference was held in Novosibirsk, USSR in 1969. Since then, the conferences were held either in Europe or America until the 9th conference held in Saclay, France. The 10th Conference was the first one held in the Asian countries, namely in Beijing, China in 1986. The 14th conference again came to Asia, to Bangalore, India in 1994. The very unique feature of the ICNMFD was that the conference was operated in a single session manner, where all the audience listens to the talks. Therefore, tough selection always existed for the presentations. There was a numerical algorithm that is now well known and widely spread, which was sometimes rejected for the presentation due to improper reviews that misunderstood the importance of the contribution.

Prof. Koichi Oshima at the Institute of Space and Astronautical Science, Japan established a new conference series called ISCFD (International Symposium on Computational Fluid Dynamics) in 1985. This series of symposiums adopted parallel sessions, and larger number of presentations more in the area of applications were presented. These two conferences: ICNMFD and ISCFD were held every other year until 1999, but people decided to merge these two conferences. They established a new series of conferences named ICCFD (International Conference on Computational Fluid Dynamics). The memorable first conference was held in Kyoto with Prof. Nobuyuki Satofuka as the chairperson. The 5th conference was recently held in Seoul, Korea in July 2008. Now the international scientific committee operates a series of the conferences. Noteworthy is that the first ICCFD meeting was held in Asia, and three more conferences of this series were held in Asia and the Pacific Rim (2nd ICCFD in Sidney with Prof. Srinivas as chairperson and 5th ICCFD in Seoul with Prof. Yoo as chairperson). Asian countries contribute much more now than they did in 1970s and 1980s.

The reality of the contribution of Asian countries can be recognized from the number of presentations in these conferences. There were 69 presentations at the 7th ICNMFD conference held at NASA Ames R. C. and Stanford University, USA, in 1980. Among them, presentations from Asian countries were 8: Japan 4 and China 4, no contributions from India, Korea, Taiwan and other Asian countries. There were 144 presentations at the 3rd ICCFD conference held in Toronto, Canada in 2004. Among them, presentations from Asian countries were 35: Japan 20, China 5, Taiwan 3, Korea 4, India 3.

Asian contributions changed from less than 10 percent in early 1980 to about 25 percent in early 2000. The rate would obviously be much higher for the conferences when being held in Asian countries such as the one held in Seoul, Korea 2008.

From these statistics, it is obvious that contributions from Asian countries increased remarkably in the last 20 to 30 yeas since a number of researchers in Asian countries started to join the CFD research field. This is due to the strong effort by some professors and researchers in Asia.

Talking about the Japanese effort for CFD research, there were a few important incidences that pushed CFD in Japan forward. One is the CFD research group established for the research fund in 1987. The title of the research activity was just "Computational Fluid Dynamics". Principal researcher were Prof. Michiru Yasuhara, Nagoya University and Prof. Hisaaki Daiguji, Tohoku University. The group consists of many CFD researchers in wide variety of research fields. Also, domestic CFD symposium was established in 1987 as a place for the presentation of the result of this research group. More about the research group and the symposium established in 1987 will be given in the next section. As will be discussed later, CFD societies were established in Asian countries, and a number of conferences were held, with some of them still in progress.

2 CFD History in Asia, Mainly in Japan

Some observations mainly from the CFD history in Japan are presented, since it is almost impossible to cover the entire important development that has happened in Asia and the Pacific Rim.

2.1 Early 1980s

Supercomputers became available very early in the 1980s for the CFD community in aerospace. The introduction of supercomputers drastically changed the types of flow simulations, but CFD in Japan has a long history much before that. Prof. Mitsutoshi Kawaguchi simulated the two-dimensional flow over a cylinder and the computed result was published in 1955, [1]. In much later years, he told us that it took more than one year with a few students working in parallel using not computers but mechanical calculators. It was surely the first parallel computation. In 1983, Dr. Tetsuya Kawamura and Prof. Kunio Kuwahara simulated the same flow field using a supercomputer, [2]. They also showed that surface roughness drastically reduces the drag of the cylinder. Even though the surface geometry was modified, it showed that CFD can capture the drag crisis with the help of supercomputers. The numerical integration scheme for incompressible flows was called "Kawamura-Kuwahara (K-K) scheme" and later became used by many engineering fields like automobile design. Kuwahara's noteworthy contribution were demonstrations of

possible simulations of flow at relatively high-Reynolds numbers without using turbulence models. Theory says that such simulations require very fine grid resolution of Kolmogorov's scale, but they showed that the main structure of large-scale turbulent flows may be captured with much less grid resolution under certain conditions.

In the area of numerical algorithms for compressible flows, Prof. Nobuyuki Satofuka and his group at the Kyoto Institute of Technology was very active. They tried to extend explicit time integration methods and proposed extensions of Runge Kutta method like, Rational Runge Kutta (RRK). Later, they introduced a "method of lines" which separates time integration schemes and space discretization schemes not only for compressible flows but also for incompressible flows. They also studied parallel computations of such schemes, [3].

CFD especially in Japan made remarkable progress with the performance increase of Japanese supercomputers developed by three Japanese vendors, Hitachi, Fujitsu and NEC. It is obvious that the progress of CFD in Japan is supported by such supercomputers. The first author entered CFD research just before commercial supercomputers became available and is one of the few people that felt the strong effect of such computers. In fact, the three-dimensional compressible Navier-Stokes solver named LANS3D, which was developed by the first author and Prof. Shigeru Obayashi (graduate student of University of Tokyo at that time), now at Tohoku University, showed that computations became 55 times faster on a Fujitsu VP400 than the fastest scalar machine M380 at that time, with very little modifications of the program, [4]. The computation was associated with the national project: collaboration between Japanese heavy industries and Boeing Company supported by MITI (Ministry of International Trade and Industry). The project was called 7J7 at Boeing and YXX in Japan, and the new airplane was to replace the 737 aircraft. Unfortunately, the project was not realized due to market request changes. However, the research was a practical use of advanced CFD technology and made impact to let industries know the effect of CFD.

2.2 Mid 1980s – Early 1990s

CFD made favorable and smooth progress from the middle of the 1980s to the middle of 1990s in Asia as well as in the world. In Japan, CFD research was approved to be one of the important research topics under the Grants-in-Aid for Scientific Research as mentioned in the first section. CFD researchers in all the research fields such as aerospace, mechanical engineering, civil engineering, nuclear engineering, and even astrophysics, joined the group. This research opportunity promoted discussions of researchers among different disciplines and that accelerated CFD research remarkably in Japan. This activity continued three years and ended in 1989. One noteworthy effect in addition was, that the first domestic CFD symposium was held in 1987, the first year of the research activity. There were about 100 presentations as well as 7 invited

talks. Now, this annual symposium has come to the 22nd one in 2008 and the symposium has been keeping more than 200 presentations and 400 to 500 participants, regularly. When looking back to the number of presentations at this symposium, we can tell the trend of CFD in Japan.

The other noteworthy fact were two symposiums (1St ISCFD1985 Tokyo in 1986 and 10th ICNMFD Beijing in 1986) held in Asia as mentioned earlier. These international symposiums obviously prompted Asian CFD activities.

About the research topics, simulations using Navier-Stokes equations were well established both for compressible and incompressible flows. A lot of practical applications appeared. So-called zonal methods appeared in the simulations using structured grids and unstructured grids, both for handling more complicated body geometries. This world trend is true also in Asian CFD activities. When looking back at the number of presentations in Japanese domestic symposia, we notice an increase of simulations using finite element methods. We also notice that practical applications became more than doubled compared to the number of presentations in the late 1980s. There were a lot of proposals about numerical algorithms not only in Europe and U.S. but also in Asia in the late 1980s to the early 1990s. One reason was the trend of developing experimental vehicles for future hypersonic and reusable launch vehicles. Hypersonic flow simulations required analysis of chemical reacting flows (mainly gas dissociations) that prohibits overshoots of heating and pressure increases at shock waves. TVD schemes appeared based on that request.

2.3 Mid 1990s – Early 2000s

Based on the activities under the Grants-in-Aid for Scientific Research, the Japanese CFD society (JSCFD) was established in 1992. Also, a CFD Journal was founded as a part of the activities of the society. Note that JSCFD joined The Japan Society of Fluid Mechanics (JSFM) in 2002 and continues its activity under JSFM.

From the late 1980s, Japan-Russia joint symposia on CFD were held every other year. The Asian CFD society was established in 1993 with the chairpersons Prof. Koichi Oshima in Japan and Prof. F. G. Zhuang in China. The first Asian CFD symposium was held in Hong Kong in 1995 with Prof. W. H. Hui as chairperson. Such activities continued for a while, but disappeared probably because CFD became well established both in academia and industry in each country and hence the role of such activities was finished.

In 1995, the Korean Society of Computational Fluids Engineering was established and promoted CFD in Korea.

Among the research topics a clear feature, again observed from the statistics of Japanese domestic CFD symposia, was turbulence research. LES simulations became feasible, although limited to flow simulations at low Reynolds numbers, such simulations started to show future possibility of LES simulations of practical problems. Japanese automobile companies moved to Kuwa-

hara's method that did not use any turbulence model. There were discussions about unresolved direct simulations using less number of grid points than required for theoretically approved direct simulations, but the results were much better than many of the results using turbulence models.

2.4 Early 2000s – Present

There are two issues about CFD in Asia in recent years. First, CFD simulations, although mostly relying on commercial software, began to be widely used in academic studies in developing countries in Asia. Numbers of young students visited countries like Japan, Korea or the USA and learned much about CFD, came back to their own countries and promoted CFD research. Second, gradual changes of CFD simulations occurred in the last few years in Asia as well as in Western countries. The change is from the use of Reynolds-averaged Navier-Stokes equations (RANS) to Large Eddy Simulations (including RANS/LES hybrid methods) for practical problems. RANS have been mainly be used as basic equations to be solved since early to middle of 1980s when supercomputers became available. However, RANS use turbulence models, which contaminates even global flow structures. We all know that there exist "scale effects" and that was why big wind tunnels were constructed all over the world. Given the parameter of Reynolds number, CFD, theoretically, was considered to solve this problem. However, the use of turbulence models, which were necessary for practical simulations, made it difficult to meet this important goal. Recent progress seems to move CFD such that this problem can be tackled, [5].

The fact is obviously supported by computer progress. In November 2008, supercomputer (SC) '08 was held in Austin, Texas. Top10 of the supercomputer speeds, which is always announced in the SC conference, is now more than 180 TFLOPS and Top1 is over 1 PFLOP (Roadrunner at Los Alamos National Laboratory by IBM). In 1985, Top1 was about 1GFLOPS, top supercomputer achieved 106 faster speeds in 23 years. Note that the Chinese Shuguang 4000A, so-called "Magic Cube" supercomputer located in Shanghai became 10th of them and is to be used in many engineering areas.

Japanese government has a big project to develop a 10PFLOPS supercomputer in 2011. It is true that a good computer environment always supports good research, but leading-edge research could be done even under limited computer resources with innovative ideas.

3 Final Remarks

From the historical overview of CFD in Asian countries especially in Japan, it becomes quite clear that contributions from Asian countries have increased tremendously in the last 20 to 30 years. Advanced supercomputers that have been timely developed were a key-accelerating factor. Academic efforts such

as conferences and workshops organized in Asian countries were another important factor. The authors would like the reader to remember that current successful CFD research in Asian countries relies on the dedicated efforts by our predecessors in the CFD research area in Asia.

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Computational Fluid Mechanics in Russia

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Summary The paper presents the review of the development of Computational Fluid Dynamics and Aerodynamics in the time frame 1960-2007 in the USSR and, later, in Russia. The organization of scientific investigations in the given fields is shown. Reviewed are the theory of difference schemes, splitting methods, irregular grids, and the particle-in-cell method. Finally, notes on software packages and computing systems are presented.

1 Organization of Scientific Research in Computational Hydromechanics and Aerodynamics

The rapid development of aero- and hydrodynamics in USSR in the second half of the last century can largely be attributed to some federal-scale measures taken at that time. Let us consider the most significant of those.

In 1953, the Institute of Applied Mathematics of the USSR Academy of Sciences (now the Institute of Applied Mathematics of the Russian Academy of Sciences (RAS)) was established in Moscow. It was organized and headed (in 1953–1978) by M. V. Keldysh, an eminent scientist and the president of the USSR Academy of Sciences. The establishment of the institute and the recruitment of the leading researchers of the country were largely due to the state program of space investigations, which has stimulated significantly the development of computational fluid dynamics (CFD). The Institute succeeded in the calculations of the challenging problems on explosion gas dynamics and supersonic flow around aircraft, unique in scale and complexity. In early 1960s, before similar calculations in USA, the numerical experiments on computer systems were done, leading to the epoch-making discovery of the T-layer effect[1] [27, 36]. This outstanding scientific event symbolized the establishment of a new field in the applied mathematics, i.e. numerical modeling, which

[1] Magnetohydrodynamic effect used for the non-intrusive influence of flow properties.

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had before been considered only as an auxiliary process in studying physical phenomena.

The team of the Institute included the researchers associated with the most important achievements of Russian science in computational fluid mechanics and aerodynamics: V. Ya. Arsenin, K. I. Babenko, G.P. Voskresenskii, S. K. Godunov, V. F. Dyatchenko, A. I. Zhukov, A. V. Zabrodin, N. N. Kalitkin, O. V. Lokutsyevskii, Yu.P. Popov, G. P. Prokopov, V. V. Rusanov, V. S. Ryabenkii, A. A. Samarskii, K. A. Semendyaev, A. N. Tikhonov, R. P. Fedorenko, N. N. Yanenko and others.

The Institute of Applied Mathematics of the USSR Academy of Sciences became a parent research institution, out of which several other research institutes separated at different times, which further became the leading ones in the considered scientific field, such as the Computing Center and the Institute of Mathematical Modeling.

The Computing Center of the USSR Academy of Sciences was established in 1955. One of the most important research directions since the moment of its establishment has been the development of numerical methods for mathematical physics and their application to applied problems, primarily in the field of aerospace investigations. In 1960, the laboratory of gas dynamics and the laboratory of general mechanics and hydrodynamics were organized. Applied directions varied for different periods but their basic purpose, consisting in the development of the fundamentals of computational mathematics, has been preserved. From 1955 to 1989 the Computing Center of the USSR Academy of Sciences was headed by Academician A. A. Dorodnitsyn — an eminent Soviet scientist, who made a fundamental contribution to various fields of science including gas dynamics, aerodynamics of wing, boundary layer theory, hydrodynamics, computational mathematics, information science. One of his most important scientific achievements was his comprehensive study of supersonic gas flows and development of numerical methods for their computation. Among A.A. Dorodnitsin's disciples are Academician O.M. Belotserkovskii, Doctor of Physics and Mathematics P.I. Chushkin, Professor Yu.D. Shmyglevskii and other researchers who contributed significantly to the development of computational fluid dynamics.

O.M. Belotserkovskii was the rector of the Moscow Institute of Physics and Technology since 1962 to 1987. In 1967 he set up and headed a chair of computational mathematics in this institute. The staff of this chair included such well-known researchers in the field of hydro- and gasdynamics as V.S. Ryabenkii (theory of difference schemes stability, method of potentials), R.P. Fedorenko (multigrid method and hybrid difference schemes), K. M. Magomedov (grid characteristic method in cooperation with O. M. Belotserkovskii), L. A. Chudov (smoothing operators), Dz. V. Lokutsyevskii (sweep method), V. V. Schennikov (viscous fluid dynamics), Yu. M. Davydov (particle-in-cell method in collaboration with O. M. Belotserkovskii), A. I. Tolstykh (compact schemes and adaptive computational grids), V. A. Guschin (hybrid difference scheme of the second order of accuracy) and many others.

In 1957 the Siberian Branch (SB) of the USSR Academy of Sciences was established with formidable tasks on Siberia development. In 1964 under the guidance of G.I. Marchuk (who later became the President of the USSR Academy of Sciences), the Computing Center of the SB of the USSR Academy of Sciences was organized, which took an active part in the development of various directions of computational mathematics. G.I. Marchuk organized research in mathematical modeling of hydrothermodynamics of atmosphere and ocean. N.N. Yanenko began to set up a department at the Computing Center, which was to develop numerical methods for solving various problems of continuum mechanics. The new methods for solving problems of gas dynamics (Yu.I. Shokin, V.M. Kovenya, Yu.A. Berezin and others) and hydrodynamics (B. G. Kuznetsov) started to develop especially actively.

Academician Nikolai Nikolaevitch Yanenko made a great contribution to the development of mathematics, mechanics and new scientific directions connected with the computer techniques and its applications. Moreover, he was an outstanding organizer of science and his research teams in the Urals and in Siberia formed the famous Yanenko school. In 1976 – 1984 N.N. Yanenko headed the Institute of Theoretical and Applied Mechanics of the Siberian Branch of the USSR Academy of Sciences.

N.N. Yanenko's student Academician Yu. I. Shokin became Yanenko's successor in the field of computational mathematics, organized and heads today the Institute of Computational Technologies SB RAS. Y.I. Shokin is the editor-in-chief of the Journal of Computational Technologies, also created by him. The first issue of the journal was published in 1996 (its predecessor was the collected papers of the same title published in 1992–1995). The journal publishes reviews and original papers in computational and applied mathematics, mathematical modeling, interval analysis, and computer technologies.

The other another Russian journal, similar in the subject, Mathematical Modelling, was set up in 1989 and headed by Academician A.A. Samarskii. Since 1953 to 1991, A.A. Samarskii headed a department at the M.V. Keldysh Institute of Applied Mathematics. In 1991 he founded the RAS Institute of Mathematical Modeling and headed it up to 1998. It is impossible to overestimate A.A. Samarskii's contribution to the development of computational mathematics and mathematical modeling. He is the author of over 30 monographs on the theory of difference schemes and mathematical modeling.

The great success achieved by Russian scientists in computational hydromechanics in 1960s – 1970s can mostly be attributed to the organization of research, making it possible to combine a very high mathematical culture of developing computational methods with their simultaneous application to the solution of complex practically significant problems of gas dynamics and hydrodynamics. This development resulted in successful bringing fundamental methods of numerical analysis up to technologies in the country's leading scientific centers and further implementation of these methods in many research and design centers.

2 Problems and Methods of Computational Hydromechanics and Aerodynamics

In the 1960s – 1980s a new direction of human activity emerged, combining both fundamental scientific problems and topical technical issues due to the rapid development of computational power. Computational mathematics and information science became a practical instrument of cognition in all industrial and social spheres. Perhaps in the first place it concerned the urgent problems of aerodynamics, which began to be solved by the first computers in order to increase efficiency.

The establishment of computational hydro- and gas dynamics as a separate scientific discipline was completed by the end of 1980s by working out the "formula" of the computational experiment, its computer resources support accompanied by the development of methodology and technology of mathematical modeling. The credit for the formation of this discipline should largely be given to N.N. Yanenko who in collaboration with A.N. Konovalov, V.I. Karnachuk, and others introduced and developed some fundamental concepts and postulates [17, 43]. In 1972–1973 N.N. Yanenko formulated his famous technological chain of modern computational mathematics: *real phenomenon — physical model — mathematical model — numerical algorithm — computer program — computer calculations — analysis of results — formulation of new knowledge about the subject of research.*

This formula was often discussed and debated. N.N. Yanenko organized the all-Union Seminar on application program packages for the problems of mathematical physics. Eight meetings held over 1971–83 in Novosibirsk and other Soviet cities, recruited hundreds of the country's leading specialists including Academicians A.A. Samarskii and O.M. Belotserkovskii and played a great role in the development of the national computational informatics. During those discussions the problem of systematization and optimization of methods, which are applied to every interconnected step of the technological chain, was formulated as well as of the determination of certain relations between the elements of those structures and global optimization of the entire computation chain. When some link of the technological chain proved insufficient in the course of the computational experiment for obtaining the required knowledge about some phenomenon, it initiated new research in one or another sphere, sometimes a purely theoretical sphere. Historically, the problems of hydroaerodynamics, which have a great variety in statements, the correctness of a mathematical model, the availability of suitable (in accuracy, economic efficiency etc.) numerical methods and the algorithms of their implementation were at different development stages especially in 1950s – 1960s. In 1960s, the attention was focused on the construction and investigation of computational algorithms.

3 Developments in the Theory of Difference Schemes for Hydroaerodynamics

The theory of difference schemes was of a great importance in the development of computational hydromechanics, especially of gas dynamics. At the first attempts of solving really difficult nonlinear problems of aerohydrodynamics, including shock waves, contact discontinuities, multiscale time and space characteristics, complex geometry of computation domain, it was found out that computational methods, in addition to approximation and stability required for convergence of numerical solution, must retain a set of special properties. Those are primarily fundamental properties inherent in the initial differential equations (conservatism, invariance, preservation of balance between various energy types, monotonicity etc.). All this raised new problems in the theory of difference schemes, the foundations of which had been already laid by 1960s [12].

The Godunov difference scheme [11, 13, 14] for the calculation of discontinuous solutions of gas dynamic equations by the "shock-capturing" method became world-famous. Unlike the schemes for hyperbolic equations, well known in 1950s, this scheme was characterized by the adequate "smearing" of shock waves. The scheme was based on the idea of preserving the solution monotonicity over the transition to the next time computation time layer and the implementation of difference analogues of the conservation laws in every computation cell. The scheme was realized in terms of calculating the disintegration of gas-dynamic discontinuities at boundaries between cells. The basic idea proved so fruitful that the first publication was followed by numerous modifications of Godunov's scheme, and in 1997, the international symposium Godunov's Method in Gas Dynamics was held in the USA.

The importance of using conservative difference schemes was emphasized in the early 1950s by A.N. Tikhonov and A.A. Samarskii [35]. They suggested the integro-interpolation method for constructing conservative difference schemes and developed the example of a neoconservative difference scheme, which provides the second order of accuracy in the class of smooth coefficients and diverges in the class of discontinuous coefficients. Later, many Russian researchers studied the issues of conservatism, full conservatism and balance preservation for individual energy types as applied to the problems of computational hydroaerodynamics where a difference scheme is understood as the approximation of integral conservation laws in the class of discontinuous solutions. Fully conservative difference schemes for the equations of gas dynamics in Lagrangian coordinates, in which the "difference conservation laws" are fulfilled for various types of energy, were first suggested in the works of A.A. Samarskii and Yu.P. Popov [25, 27]. The further development of this direction for a multidimensional case were the variational schemes and method of supporting operators [9, 29]. Yu.I. Shokin and Z.I. Fedotova developed fully conservative difference schemes for the equations of gas dynamics using the method of differential approximation (see [31, 32] and references therein).

Noting that shock-capturing methods were the most universal ones, N.N. Yanenko identified two problems here: the problem of interpreting numerical solutions, containing a shock wave "smeared" over several grid cells, and the problem of increasing the accuracy of numerical solutions in the vicinity of discontinuities. The interpretation problem includes the localization of various singularities in gas flows and their classification. Original results (the development of the so-called differential analyzer) and a review of publications devoted to this topic can be found in the monograph [39]. As about the second problem on increasing the accuracy of numerical solutions in the vicinity of discontinuities (conservation of contact discontinuity, removing the "entropy trace" and other non-physical fluctuations), it has been studied by many authors (see the survey in [26]). Of special interest are the publications by V.F. Kuropatenko, who abandoned the uniform difference methods and worked out a class of schemes [20], which singles out any quantity of strong, weak, and contact discontinuities. This method makes it possible to calculate complex gas-dynamic flows with phase transfers.

It should be noted that the method of differential approximation, developed in the works by N.N. Yanenko, Yu.I. Shokin, and their disciples (the first publications date back to 1968), appeared to be extremely fruitful for computational hydromechanics since it can be used to construct, study, and classify various classes of grid methods retaining properties of the approximated systems of differential equations with the required order. In particular, in 1970 a work was published, where for the first time a problem of constructing invariant difference schemes was formulated and solved retaining the same group of transformations in the first approximation as the approximated system of the gas-dynamic equations (see publications [31, 32] for extensive presentation of the theory and numerous examples). In recent years, the direction associated with the application of invariant-group analysis to the difference equations has been actively developed by V.A. Dorodnitsin [8].

4 Development of Splitting Methods for Difference Schemes of Hydroaerodynamics

The development of the splitting method began due to the necessity of solving multidimensional problems of hydroaerodynamics. Many researchers dealing with the application of grid methods to the problems of hydromechanics contributed to addressing this issue, i.e. developed specific methods for reducing a complex problem to a set of simpler ones, and at the first stage of the research – for the replacement of a multidimensional differential problem by a sequence of one-dimensional problems [40, 18, 21, 19].

The first monograph, which was translated into English, presents a bibliography of first publications on the splitting methods. We shall only note that the first splitting scheme suggested by Russian mathematicians was in the

publication by K.A. Bagrinovskii and S.K. Godunov in 1957. This difference scheme explicitly approximates a hyperbolic system of equations.

The implicit scheme of splitting with respect to independent spatial variables for the thermal conductivity equation was published by N.N. Yanenko two years later. It was the first economically efficient and absolutely stable difference scheme, approximating the multidimensional equation on an integer step, and requiring scalar three-point sweeps for the implementation. In N.N. Yanenko's monograph [40], which was published in 1967 and later translated into three languages, is the comprehensive bibliography of the works over that period.

The splitting method appeared to be especially fruitful in aerohydrodynamics. The monograph [18] is devoted to the construction and investigation of implicit difference schemes for the Navier-Stokes equations of compressible heat-conducting gas. It was based on the original works of the authors and their disciples. The investigations in this direction are continued by expanding the range of the problems being solved. For the solution of the most complicated problems of hydrogasdynamics, V.M. Kovenya and his students use, improve and develop the most modern methods and technologies in the field of finite-difference schemes. The monograph [19] in addition to the original material presents the description of the entire technological chain of a computational experiment in the considered class of aerohydrodynamic problems, and also gives the description of the software package ZAMER.

5 Development of High-Order Difference Methods

A large group of scientists was engaged in developing schemes of high-order approximation for enhancing the calculation accuracy in the problems of gas and hydrodynamics. One of the first schemes of the third order was the well-known scheme of Rusanov (1968), and schemes developed by Balakin (1970), Yeremin, and Lipnitskii (1971).

A.I. Tolstykh [37] and V.I. Pinchukov [24] were also very successful (their monographs present the comprehensive reviews of studies by other authors). In his recent works, A.I. Tolstykh considers the schemes, using linear combinations of basis operators, which are rational functions of three-point operators and parameter-dependent. It was shown that assigning N various parameter values makes it possible to obtain the values of coefficients of those linear combinations in such a way that those provide orders of approximation proportional to N. In addition the action of multioperators on the specified grid functions can be calculated in parallel and simultaneously, using N processors, which enables the user to increase the scheme orders without additional computer-time consumption.

6 Irregular Grids (Curvilinear, Moving)

An alternative to the schemes, which smear shock waves, are the methods based on identification of discontinuities both strong and weak. These methods impose special requirements on the computation grid, which has to be adjusted to the position of the discontinuities and move along with them. This involves a number of problems of grid generation, especially in two-dimensional problems. Many Russian scientists studied the problems of grid construction in connection with the solution of hydroaerodynamic problems (S.K. Godunov, N.N. Yanenko, A.F. Sidorov and others). Among the first to consider this problem were S.K. Godunov and G.P. Prokopov in 1967. They employed the methods of complex variable theory and conformal mappings. Their multi-author monograph [14] gives a detailed description of both the theoretical basis of the method and the results of numerical modeling by applying this method to a wide range of problems of multidimensional stationary and nonstationary gas dynamics. Later this direction was successfully developed by A.F. Sidorov and his school [34] in the Institute of Mathematics and Mechanics of the Ural Branch of RAS, and also in the RAS Institute of Applied Mathematics.

The demand for the solution of essentially nonlinear problems, characterized by medium deformation, presence of interface zones and unstable modes, lead to the construction of solution-adaptive grids. In the mid-1970s, N.N. Yanenko suggested the variational principle of controlling a moving grid, under which the following limitations were imposed on a grid: grid refinement in the area of large gradients, proximity to Langrangian grids and minimum grid distortion. This direction brought many remarkable results, and the research is continued.

The main trends in the development of the methods for constructing difference grids are based on the application of elliptical nonlinear equations including control functions for controlling the required properties of difference grids. In addition the results obtained by the Riemannian differential geometry are applied, which allows giving a uniform representation of difference grid generation for all arbitrary physical geometries (curves, surfaces, domains) as a well-posed mathematical problem and to provide a comprehensive and reliable control of difference grid characteristics [42].

In recent years, the grid generation methods, as an object of intensive research, are forming a special field of computational mathematics. One may say that achievements in this area are ahead of the practical applications of grids.

Examples of numerical methods, where the method potential is in good agreement with the application of arbitrary moving Langrangian grids in the case of strong deformations, are the variational difference schemes and the method of supporting operators. For those the methods for automatic construction of irregular adaptive grids for solving problems in complex-geometry domains have been successfully developed [33]. These grids are characterized

by moving nodes, which minimize the error of the difference scheme approximation, and provide essential accuracy enhancement for dynamic problems and uniform convergence in boundary layers.

In recent years, the use of unstructured grids in hydrodynamics is expanding. These grids were first implemented in the finite element method. The idea of this method was formulated in the USSR as early as in 1935, but insufficient computation capacity had retarded their development in our country. At present, triangular grids are efficiently used in the method of supporting operators [30] as well as in the integro-interpolation difference schemes, or the balance method (recently the term *finite-volume method* is more often used). In the work [28] the monotonous difference schemes were constructed on the basis of the balance method for convection-diffusion problem; the conclusion was made that this construction could be done easily and simply, and the finite element method had no advantages over it.

7 The Particle-in-Cell (PIC) Method

By the early 1980s the situation in computational hydrodynamics was characterized by N.N. Yanenko in the following way: there are theoretical foundations laid for modeling steady flows and algorithms have been constructed, which predetermine their further development (this concerns both finite difference methods and finite element methods). At the same time N.N. Yanenko noted that the concept of stable solution depends on the choice of a mathematical model and stability criteria (e.g., models of averaged turbulent flow are mathematically stable although they describe an unstable process). Therefore, N.N. Yanenko posed the problem of modeling *transition processes* – the arising and development of instability [41]. This problem is far from being solved yet, although it could be assumed that particle-in-cell method and other methods relating to it could be efficient in modeling such problems.

In its early variants, the particle-in-cell method provided a satisfactory description of unstable and significantly distorted boundaries due to the splitting of the entire process into two stages: at first only inertial forces are taken into account, and then the free-molecule flow is described (with an alternation taking place at every time interval of the method). Updating of the density, momentum, and energy is attained by averaging over particles in every elementary cell and then thermodynamic parameters and velocities are obtained. The method can be interpreted as the splitting into physical processes, when every stage is described using various approaches (grid and Liouville). Later the particle-in-cell method was further developed, the proportion of Liouville and grid stages determined the variety in modifications (method of markers, method of flows, etc.). In particular, O.M. Belotserkovskii and Yu.M. Davydov developed "large-particle" method, the advantage of which is the use of resource-sparing efficient difference schemes, and the construction of

approximational viscosity allows stabilizing unsteady flow. This method was successfully applied to the solution of aerodynamics problems [4].

On considering the perspectives of computational hydrodynamics, N.N. Yanenko noted the lack of continual physico-mathematical models describing unsteady and turbulent flows. He repeatedly argued for the discrete models resulting from the phenomenological approach. Of interest is also his opinion about the difference scheme emerging not as a result of an approximation of some differential equation but as a self-sufficient mathematical model claiming to describe a physical phenomenon. For the solution of free-boundary problems, the idea of the direct discrete modeling was implemented by N. Yanenko's disciple A.M. Frank, who developed and explained a number of discrete models of incompressible fluid resulting directly from the variational principles of classical mechanics [10].

A large contribution to numerical modeling of hydrodynamic instabilities and turbulence was made by O.M. Belotserkovskii. He suggested a discrete dissipative model reflecting the contribution of small-scale subgrid pulsations for various resolution scales based on the concept of structural turbulence for mathematical modeling of ordered motion and large-scale "coherent" vortices [5].

8 Solution Methods for Navier–Stokes Equations

Since the late 1960s the attention of the scientific community was focused on the numerical solution of viscous fluid flow described by the full Navier-Stokes equations. The numerical integration of boundary-value problems for the Navier-Stokes equations is rather difficult for several reasons. One of these reasons is a higher order of the system in comparison with the system of Euler equations. In the case of nonviscous fluid, while using the velocity-pressure variables, the specific difficulties are connected with the continuity equation. A.A. Dorodnitsin deserves the credit for creating such an important direction in computational hydrodynamics as the development of iterative methods with splitting of the boundary conditions (BC) of the solution for boundary-value problems for the Navier-Stokes equations. Actually, in spite of the possibility of formal splitting of the Navier-Stokes system into sequential scalar equations of second order, the boundary conditions, which are practically interesting, however "bind" the system and do not allow the splitting into simpler separate boundary-value problems (a frequent problem for the splitting methods). In the case of two-dimensional flows A.A. Dorodnitsin suggested to substitute the no-slip condition on the wall for a more general condition containing a small iterative parameter [6]. In the later works a similar approach was applied to three-dimensional flows [2].

A large group of researchers participated in the development, theoretical and numerical studies of the iterative methods with BC splitting includes: B.V. Paltsev, V.Yu. Belash, A.S. Lozinskii, N.A. Meller, I.I. Chechel, E.G.

Khlyupina, and others. At first the iterative methods with splitting of boundary conditions were employed, and then the algorithms of the multigrid methods were developed. A large cycle of works was done in the numerical finite element implementation of those methods. It turned out that both velocities and pressure can be approximated similarly by bilinear finite elements, neglecting the fulfillment of matching conditions such as Ladyzhenskaya–Babuska–Brezzi conditions required for the finite element approximation of the entire problem.

The calculations were also done for nonstationary problems with time discretization of Crank-Nicholson type. For a singularly perturbed system of the Stokes type with a large parameter, for a nonsingular Stokes system, for a stationary Navier-Stokes system, as well as for a nonstationary Stokes system, the methods were developed, which were characterized by unquestionable advantages, because they provided the simplicity of algorithms and high rates of convergence; high accuracy, equal for both velocities and pressure; good transition to domains of a more general form and the possibility to perform calculations on the grids with high resolution. By means of the developed methods, in particular high-accuracy numerical solutions of the problem of stationary viscous incompressible fluid flows between rotating spheres under small Reynolds numbers were obtained [2, 22].

N.N. Yanenko's school paid great attention to the comprehensive study of the Navier-Stokes equations [42]. Among the achievements within the frame of the fractional step method, obtained by then, the discovery of the artificial compressibility method should be specially noted, consisting in the introduction of a time derivative of the pressure with a small parameter into the Navier-Stokes equations for viscous incompressible fluids. This procedure makes it possible to change over to the Cauchy – Kovalevskaya type equations with a small parameter. Further in the works of N.N. Yanenko and Yu.Ya. Belov the respective theorems were proved about the convergence of the solution of the approximating system to the solution of the initial system.

For the solution of the approximating system of equations, N.N. Yanenko suggested the implicit splitting schemes, which appeared to be an efficient method for solving hydrodynamic problems within the frame of the Navier-Stokes equations. A significant contribution to the development and justification of numerical methods for the Navier-Stokes equations as well as in development of software was made by the members of N.N. Yanenko's scientific team (first at the Computing Center of the Siberian Branch of the USSR Academy of Sciences and then at the Institute of Theoretical and Applied Mechanics) including B.G. Kuznetsov, B.P. Kolobov, V.N. Shepelenko, Sh.S. Smagulov, G.G. Chernykh and others. Sh.S. Smagulov, a full member of the Engineering Academy of the Republic of Kazakhstan, who largely determined the organization of research in fluid dynamics in the Republic of Kazakhstan, first proved the well-posedness of the initial boundary value problem for the nonlinear degenerate equations of magnetic hydrodynamics. He also suggested a new numerical method for solving the equations of viscous incompressible

fluid in stream function – vorticity formulation, and obtained the fundamental results in justification and application of the fictitious domain method.

B.G. Kuznetsov's disciple Professor G.G. Chernykh and his colleagues studied viscous flows within the frame of the hierarchy of modern semi-empirical models of turbulence and the method of splitting into spatial variables. The evolution of the turbulent wake behind a self-propelling body in a linearly stratified fluid was investigated. In particular it was shown that a process of anisotropic degeneration of turbulence can be adequately described with the help of the models containing the refined approximations of triple correlations of the velocity field, allowing taking into account in more detail the gravity effect, and the modified equation of dissipation velocity transfer (see, for instance, [38]).

One of the chapters of [23] is devoted to the numerical modeling of heat and mass exchange based on the Navier-Stokes equations. The finite difference method is considered, the prototype of which is the T.V. Kuskova's scheme. Later after modifications, connected with the calculations of transient turbulent modes of convection, this scheme was known as the Polezhayev's scheme. The monograph presents a review of works devoted to the methods for the solution of the Navier-Stokes equations for incompressible fluids.

N.N. Yanenko considered the multidimensional Navier-Stokes equations of compressible heat-conducting gas as the most comprehensive model of hydrodynamics. Analyzing the variety of problems and methods for their solution within the framework of these equations, he formalized the concept of the splitting methods by subdividing them into analytic, physical, and geometrical splitting. It allowed providing the uniform position for describing difference schemes. The problem of the development of economically efficient and reliable schemes is closely connected with technological problems of developing software packages and systems. These questions are described in detail in the monograph by N.N. Yanenko and V.M. Kovenya [18]. The investigations in this direction are continued by expanding the range of the problems being solved [3].

9 Software Packages, Computer Systems

On the basis of the modular analysis of problems and algorithms of mathematical physics, the technological paradigms were created as well as specific developments of application program packages including refined system and functional content. N.N. Yanenko's colleagues (V.M. Kovenya, A.P. Lymarev, A.D. Rychkov and others) implemented large-scale software systems ARFA, ISTOK, ZAMER and SPRUT for scientific research in the field of aerodynamics and hydrodynamics based on then-advanced principles of architectures and operation organization [16]. The software package SAFRA [15] (developed by M.M. Gorbunov-Posadov, V.L. Karpov, D.A. Koryagin and others) was intended for the solution of a large range of gas-dynamic problems taking into

account various physical processes. The software package GAMMA (hydromechanic modules and algorithms) was also developed [1].

In 1980s first commercial general-purpose CFD-codes emerged abroad, and 1990s witnessed the rapid development of the CFD-code industry due to the fast growth of computer performance. Unfortunately, Russia and CIS countries lost many of their leading positions due to the lack of funding resulting from reconstruction of the country economy.

In recent years the research activity in Russia has been intensified. On the basis of original methods of numerical modeling of flows in flow passages of turbomachines, which allow calculating three-dimensional flow fields for various problem formulations, using stationary and nonstationary Euler and Reynolds equations of incompressible fluid, the system of computer-aided multipurpose optimization of a water wheel shape was created. This system enables one to simultaneously enhance several criteria of the water wheel including its performance characteristics for several operating modes. The optimization method was realized as a program tool CADRUN-opt. A parallel version of the program was developed for the calculation on multiprocessor computing systems [3].

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CFD Developments in the Northern European Countries

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Summary This chapter briefly surveys the CFD developments in the Nordic countries. The focus chosen is on the major current tools in use with just sketchy indication of the origins of these tools and how they evolved from earlier legacy codes. The developments in Sweden surveyed here are selected from four domains: fundamental studies of turbulence and transition, ship hydrodynamics, aeronautical CFD and numerical weather prediction. The developments in Norway begin with a historical survey of the formulation of models and then lead into present-day contributors of computational methods and codes. The developments in Denmark focus mainly on wind turbine aerodynamics and how the Danes have successfully developed the EllipSys3D code and became leaders in the wind energy business. In Finland at Helsinki University of Technology researchers have produced the FINFLO code and applied it to computational aerodynamics, ship flows and to the development of new turbulence models. Work at the Finnish Meteorological Institute is also mentioned.

1 Developments in Sweden

The developments in Sweden surveyed here are selected from four domains: 1) fundamental studies of turbulence and transition, 2) ship hydrodynamics, 3) aeronautical CFD and 4) numerical weather prediction.

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1.1 DNS Code for Studying Wall-Bounded Turbulent Boundary Layers

The Mechanics Department at KTH has developed a DNS code for fundamental studies of turbulent wall-bounded boundary layers. One aspect of this research shows that according to linear theory non-modal growth mainly associated with streaky structures in the streamwise direction can cause large transient amplification. Non-linear calculations have shown that when the optimal disturbances from linear theory are used as initial conditions, the threshold amplitudes required for transition to turbulence is lower than for general disturbances. Recent calculations have also shown that these results carry over into the spatial development of disturbances in boundary layers.

Another part of the research involves direct numerical simulations (DNS) of transition to turbulence where these transient growth mechanisms play a major role. This bypass of the traditional Tollmien-Schlichting instability waves is involved in many shear flow transition scenarios. Previously transition associated with localized disturbances has been investigated, and at present the transition in boundary layers starting with a pair of oblique waves is investigated. These waves generate elongated streaks in the streamwise velocity which rapidly grow due to the non-modal mechanism. The secondary instability of these streaks has also been studied, both using DNS and secondary instability theory. A new direction in the research is to simulate transition in a boundary layer subjected to free-stream turbulence, where the turbulence is initiated close to the leading edge by a random distribution of continuous spectrum modes. See URLwww.mech.kth.se/mech/ for more details.

1.2 CFD for Ship Flows

The main research area within the Shipping and Marine Technology Department of Chalmers University of Technology (CUT) over the past 20 years has been computational fluid dynamics (CFD) applied to ship flows. Three main branches of the research may be distinguished: potential flow panel methods with a free surface, Navier Stokes methods with or without a free surface and automatic shape optimisation. See URLwww.chalmers.se/smt/EN for more details.

Lead times are being shortened more and more in ship design, particularly at the initial phase. Many alternatives have to be evaluated in a short period of time. Time can be saved by using the efficient potential flow panel methods, which predict important quantities like waves and wave resistance rapidly, yet with enough accuracy for hull ranking, e.g. to enable wave wash predictions at large distances from a ship. To accomplish this, the original Rankine source method is extended to also include Kelvin sources.

Viscous effects are also important. The viscous resistance is often the largest component and the inflow to the propeller is critical. Therefore a good

viscous solver such as a Reynolds-Averaged Navier-Stokes solver is also necessary. The Navier-Stokes solver, named CHAPMAN, uses an overlapping composite grid. CHAPMAN was mainly developed and reported within the European project CALYPSO, and the main development work was made in a spin-off company: FLOWTECH International AB and the code is SHIPFLOW, commercialised and marketed by FLOWTECH International AB. Turbulence modeling for stern flows includes bilge vortices. Eight models ranging from the standard k-ϵ model to a Reynolds stress model have been investigated both for a ship hull and for other more generic cases including longitudinal vortices. Another important aspect of hydrodynamic RANS methods is the treatment of the free surface. LES modeling is also available in SHIPFLOW.

Automatic shape optimisation is incorporated in SHIPFLOW by the Method of Moving Asymptotes (MMA) and with the adjoint equation technique, allowing a simple hull shape and a bulb to be optimised from a total resistance point of view. Other work involves optimising a fast mono-hull and a catamaran from a wave wash point of view. This work is part of the large scale European project FANTASTIC.

Over the past ten years the software SHIPFLOW has developed into the world standard for ship hydrodynamics CFD. Developed by naval architects, physicists and numerical analysts, SHIPFLOW is optimized for ship hydrodynamics design. Specialization means efficiency and user-friendliness. No general purpose code can compete with SHIPFLOW in hull design: grids are automatically generated, resistance and propulsion data are presented using conventions from naval architecture, and the solvers are adapted for hull geometries. See URLwww.flowtech.se for more details.

1.3 Aerospace CFD Applications

Early-Legacy Euler & Navier-Stokes Solvers

Starting in the 1980s practical applications of 3D Euler solvers began to appear worldwide in the solution of aerodynamic problems related to atmospheric flight, and researchers at FFA in Stockholm (later re-organized into FOI The Swedish Defence Research Agency) were among these early developers. For example, already in 1981 Rizzi and Eriksson had developed the WINGAS code, a single-block structured-grid Euler solver, and presented Euler solutions of transonic flow past the ONERA M6 wing [1]. Later that same year they further refined the method into the DELTA code using an O-O grid topology specialized for vortex flow over delta wings. They applied this code to obtain the first Euler solution for vortex flow shed from the leading-edge of a sharp delta wing [2].

Navier-Stokes solvers for practical 3D problems began to appear at the end of the 1980s. Researchers at FFA were again among the frontline developers with the structured single-block NSWING code, and presented a viscous solution of transonic flow past the ONERA M6 wing [3]. These early Euler and

NS solvers later became the legacy to an international project that produced the structured multi-block NS solver EURANUS [4].

National Aerospace Code - Edge

By the end of the 1990s FFA-FOI decided to develop a NS solver using unstructured grids. Using EURANUS as a base, a project was set up to construct Edge, a NS solver developed at FOI (sv.: Totalforsvarets forskningsinstitut) since 1997 for unstructured grids of arbitrary elements[1]. It solves the three-dimensional, compressible Reynolds-Averaged Navier-Stokes (RANS) equations on hybrid grids and features several turbulence models from algebraic to state-of-the-art two-equation models. The code also includes LES and DES models and the ability to run in 'Euler´ and laminar mode. Time-accurate and aero-elastic simulations are also possible. Edge is an industrial-strength code designed for realistic, large scale, parallel computations. The unstructured formulation allows Edge to be used for problems of arbitrarily complex geometry. However, Edge can be run on any Unix/Linux platform including small PC computers. The Edge flow solver is based on a node-centered finite volume scheme. For steady flows, the equations are integrated towards steady state with an explicit multi-stage Runge-Kutta scheme. To accelerate convergence, residual smoothing and a multi-grid technique can be employed. Low Mach-number preconditioning is also available. Time-accurate computations are implemented using dual time-stepping: implicit time marching with explicit sub-iterations. For more details, please refer to the Documentation pages and articles in the Publications section on the homepage www.edge.foi.se/. The copyright holder is FOI, and an individual user-based written agreement with FOI is required to get access to the code.

1.4 Numerical Weather Prediction

Meteorological Analysis and Prediction is the research unit of the Swedish Meteorological Office (SMHI) and works primarily with development of Numerical Weather Prediction (NWP) models. The forecast models utilize numerical methods in order to simulate the flow of the atmosphere. This research unit actively works within the following fields all in order to reach a common goal - better weather forecasts: 1) Data Assimilation. 2) Ensemble Prediction System, 3) Physical Parameterisation, 4) Studies of Processes and Phenomena, 5) Long Range Forecasting and 6) Observational Systems.

The aim of this research is to improve meteorological predictions at different forecast ranges, and to get a more in-depth understanding of the atmosphere. To achieve these goals research and development is carried out

[1] See also the contribution by C.-C. Rossow and L. Cambier in Part III of this book.

in the field of numerical modeling and statistical processing. A close contact with all parts of SMHI is crucial for understanding the needs for further developments and ensuring constructive feedback on the products. See URL-www.smhi.se/cmp/jsp/polopoly.jsp?d=5222&l=en and URLwww.smhi.se/cmp/jsp/polopoly.jsp?d=6026&l=en for more details.

Numerical Modelling and Data Assimilation For Short Range Forecasting (1-2 days)

The first of two main forecasting tools at the research department of SMHI are the HIgh Resolution Limited Area Modeling system (HIRLAM), developed within the nordic HIRLAM project where both Sweden and Finland participated, funded by the Nordic council. The second is the ALADIN system. The hydrostatic HIRLAM forecasting system is applied over different Northern Europe areas at an horizontal resolution of approximately 5 to 30 km, using 40-60 vertical levels. It contains an advanced data assimilation system based on variational techniques to obtain the best possible initial model state by blending information from various observation types with a short range forecast. Presently the emphasis is on improved utilisation of various remote sensing data as well as further refinements and experimentation with 4-dimensional variational data assimilation. The ALADIN forecasting system is applied in hydrostatic as well as non-hydrostatic mode over different areas and at a horizontal resolution of 3 to 10 km, using 60 vertical levels. The forecast models predicts future atmospheric states by integrating forward in time utilizing the governing equations of the atmosphere. SMHI has expertise on physical parameterisations of physical processes that cannot be resolved by the model as well as land-surface processes. For prediction at very short-ranges (0-6 hours approximately), where it is important to use the most recent observations and have forecasting products almost immediately available, a 'nowcasting' system is applied.

2 Developments in Norway

As a starter for describing the developments of fluid mechanics in Norway one is tempted to mention the historical names of the mathematician Niels Henrik Abel (1802-1829), the propeller theoretician Theodore Theodorsen (1897-1978), Ragnar Fjørtoft (1913-1998) and Arnt Eliassen (1915-2000) of whom both the latter two persons contributed to numerical weather forecasting. Enok Johannes Palm (born 1924) from the University of Oslo made further meteorological studies, in particular on convection and interfacial waves in fluids.

Since Norway does not have an aeronautical industry, it is well worth to point out that the Royal Norwegian Air Force activated a program in the beginning of 1960s to develop and build two prototypes of a rescue helicopter.

However, the program ended in a non-fatal flight crash. Since the project involved several student works from e.g. the Norwegian Institute of Technology (NTH), it was a good start to stimulate to further aerodynamic studies. This was accomplished by sending five dedicated students a year to the Royal Institute of Technology (KTH) in Stockholm. The program has now terminated for financial reason.

In 1973 the Department of Aero- and Gas Dynamics was established at NTH and Torstein Fanneløp and Helge Nørstrud were to take the initial Chairs. Nørstrud had previously (1965-1968) studied for his Doctorate at the Technical University of Vienna (under Professor Klaus Oswatitsch) and continued his work on numerical solutions for transonic flow over wings and wing profiles. See references [5], [6], [7].

The computer program OLGA was initially developed in 1979/80 at the Institute for Energy Technology (IFE) at Kjeller outside Oslo. The code has later been improved in order to simulate the transport of oil, gas and water in pipelines

In the latter part of 1985 and in 1987 Lars-Erik Eriksson came as a Visiting Professor to NTH to participate in a project on numerical flow modeling of gas turbine compressors. His valuable experience on numerical flow analysis led in 1988 to the forming of the company CFD norway together with Erland Ørbekk and Helge Nørstrud. This company has since participated in numerous projects nationally and internationally. Key area of research topics were connected to atmospheric flow over topography, building aerodynamics, aerodynamics and aerothermodynamics of airplanes and aerospace vehicles, propulsion systems and lately to marine application of Computational Fluid Dynamics (CFD).

Norway is a member of the North Atlantic Treaty Organization (NATO) and as such it have had delegates to the former Advisory Group for Aerospace Research & Development (AGARD), including in the Fluid Dynamics Panel. This has been most valuable access to other NATO countries developments within fluid mechanics and a stimulating forum for exchange of ideas and research results. Furthermore, the von Karman Institute for Fluid Dynamics (VKI) in Rhode-St-Genèse, Belgium has fostered many Norwegian graduates from their departments. Several faculty members at the Norwegian University of Science and Engineering (NTNU) have earned their Diploma or Doctorate from that school. Bernhard Müller also attended VKI and is since 2007 appointed as Professor of Computational Fluid Dynamics at NTNU (formerly NTH)

Numerical fluid dynamics demand high computer power and the advances of performance in Norway have followed the internationally trend from small workstations to supercomputers including software. The University of Bergen (Centre of Computational Sciences) announced in June 2007 to acquire the new 51 Teraflops Cray XT4 supercomputer (trillion floating point operation per second) for Norwegian research in fields including large-scale simulation of ocean processes, computational physics and applied mathematics. Two hun-

dred and twenty-four Sun Fire x2200 nodes will soon expand the computer cluster Titan at the University of Oslo. Since Norway is a nation of rich oil and gas offshore resources, this will promote further fluid dynamic computations such as reservoir flow prediction, multiphase flow computations and meteorological simulations. In this context it is appropriate to mention the work of Helge Ingolf Andersson of NTNU in direct Navier-Stokes flow simulation (DNS) which requires extensively computer performance.

3 Developments in Denmark - Wind Turbine Aerodynamics

At the Department of Wind Energy at the Risø National laboratory there has been ongoing research in wind turbine aerodynamics for the last 25 years. The problem of rotor aerodynamics and related phenomena have been investigated at Risø National Laboratory using a wide variety of the available techniques, wind tunnel experiments, full scale experiments in the atmosphere, engineering aerodynamic models as the Blade Element Momentum (BEM) method, and computational fluid dynamics methods as the actuator disc model and full Reynolds Averaged Navier-Stokes computations. See URLwww.risoe.dk/Risoe_dk/Home/About_risoe/research_departments/VEA/AED.aspx for more details.

For the last 10 years there has been an ongoing development of the ElipSys3D Reynolds Averaged Navier-Stokes code, in a close co-operation between the Department of Mechanical Engineering, DTU and the Department of Wind Energy, Risø. See URLwww.risoe.dk and URLwww.fluid.dtu.dk/ English.aspx for more details. The code has been designed to take advantages of modern distributed memory and shared memory machines, and a large effort has been invested making it efficient, both in single and multiprocessor mode. There is an ongoing development of both numerical algorithms and physical models in the code. The EllipSys3D Navier-Stokes code has matured to a level where important issues about the aerodynamics of wind turbines can be investigated. Many of these computations are time true computations. Due to the large range of time and spatial scales, large domains and long integration times are needed to resolve the geometry and obtain time periodic responses or sufficient statistical information. The need for massive computer capacity are therefore paramount for these types of computations, and the efficient parallelized EllipSys3D code has proven well suited to these types of investigations. Simulations have a significant impact on technical applications such as micro-siting of wind turbines, prediction of dynamic loads on engineering structures and atmospheric transport of pollution.

3.1 EllipSys3D Code

The in-house flow solver EllipSys3D is developed in co-operation between the Department of Mechanical Engineering at DTU and The Department of Wind Energy at Risø National Laboratory, see [8], [9] and [10]. The EllipSys3D code is a multi-block finite volume discretization of the incompressible Reynolds Averaged Navier-Stokes (RANS) equations in general curvilinear coordinates. As the code solves the incompressible flow equations, no equation of state exists for the pressure, and the SIMPLE algorithm of is used to enforce the pressure/velocity coupling. The EllipSys3D code is parallelized with the Message Pass Interface (MPI) library for executions on distributed memory machines, using a non-overlapping domain decomposition technique. The solution is advanced in time using a 2nd order iterative time-stepping (or dual time-stepping) method, and is 2nd order accurate in space. Several turbulence models for aerodynamic applications are available in the code.

4 Developments in Finland

At Helsinki University of Technology (TKK) fluid mechanics is connected to several disciplines, including chemistry, physics, mechanical and civil engineering. In mechanical engineering the research has had a concrete target, the simulation of flying vehicles. This research produced a computer code called FINFLO, which has been applied to computational aerodynamics and ship flows. The in-house computer code has been the basis of theoretical work, mainly the development of new turbulence models, and also the foundation for education in this field at TKK.

Classical experimental and theoretical methods have been elementary parts of education in aerodynamics and ship hydrodynamics. When the new campus for the university was being built in Otaniemi during the 1950s and 1960s, the large laboratory buildings, i.e. wind tunnels and towing tanks, became landmarks in the area. Lacking proper resources, these facilities have never been utilized effectively, but they were considered to be necessary for research in fluid mechanics. Approximate integral equations, potential theory and boundary-layer methods were the computational methods applied.

The first effort to develop more sophisticated in-house computer codes and to study appropriate numerical methods was made in the early 1970s. The fact that Navier-Stokes equations can be solved numerically and that there are computers efficient enough to do the job was the subject of informal discussions among the researchers. As the Finnish universities got access to a very efficient computer, the Univac 1108, Navier-Stokes methods were used independently by Professor Göran Öhman at Abo Academi University and by Professor Seppo Laine at TKK. For a short period of time the Univac was the most efficient computer in Europe. At first it was easy to get a lot of CPU time, since the computer, although shared by all the universities in the

country, was more than enough for the tiny demand. The demand situation changed rapidly, but in 1972 Professor Laine was among the heaviest users of the machine. This use resulted in his doctoral thesis concerning the flow over a backward-facing step. The aim was to study the stability of a boundary-layer flow and a possible transition. Hence, an accurate time-dependent scheme was employed. Later, the method was modified by others for a general coordinate system and was applied for a bulge on a flat plate.

The methods used in the 1970s were based on vorticity and stream function, and were thus limited. Later, novel developments in CFD gradually faded them away, as did the increase in computing power. During the next decade the foundations of modern CFD were completed and, while new supercomputers were being used elsewhere, in Finland people were arguing that the era of large computer centres would soon be over. Finally in 1987 the computational sciences received a boost when the first vector processor was bought. The funding of this acquisition was abnormal, but since then the needs of the computational sciences have been better served by the Ministry of Education. The late 1980s were economically good for the Finnish universities and in addition to budget funding, project work increased rapidly. In CFD this ushered in a new period.

4.1 FINFLO Code

As project work started to flourish at the Finnish universities it was easy to start new areas of research as long as there was funding available. In CFD, industrial applications involving incompressible flows were funded mainly by the power companies, whereas research on compressible flows was funded solely by the Finnish Air Force in the beginning. This cooperation has lasted for over 20 years and has resulted in the computer code FINFLO, Furthermore, the CFD group at Helsinki University of Technology owes its very existence to the Air Force-driven projects. See URLwww.cfdthermo.tkk.fi/finflo.html and URLwww.finflo.fi for more details.

As funding and the vector processor were available, adequate personnel were needed to do the job. Elsewhere at the same time a couple of guys had been looking for new challenges. Computational methods were already being used in many areas of technology, including nuclear reactor thermal hydraulics. At the Technical Research Centre of Finland (VTT) one-dimensional computer codes had been developed for a two-phase flow and Timo Siikonen, later a professor at HUT, was among the young, brave, but inexperienced staff at VTT. Professor Laine belonged to a steering group of a technology program run by VTT. A natural consequence of these circumstances was the start of a new CFD project at TKK from the beginning of 1987.

Soon it became evident that the upwind first-order methods applied in thermal hydraulics as well as the vorticity-stream function formulation belonged to an entirely different world than a compressible flow with shocks. On the IBM 3090 machine the solutions literally blew up on the display of

the computer terminal. A lot of tests with the existing methods were made and new lessons were learned. The then-popular MacCormack method was selected on the basis of one-dimensional test cases. Maybe the reason was the intrinsic dissipation of the method, and as a consequence Jameson-type methods never became popular in Finland.

It was satisfying to start from scratch. The programs could be designed so that all the internal DO-loops were vectorized. After the clumsy beginning with the compressible flow, everything seemed to work for a while. However, a nightmare started as implicit two-dimensional results were obtained. The steady solution of the MacCormack method is dependent on the time-step size. With a large time-step the solution is oscillatory and a two-dimensional plot resembles a mineral called 'rapakivi'. This funny name was introduced by the Air Force people monitoring the project.

However, the research went on and a cure for the rapakivi symptom was found from Van Leer's excellent papers. Upwinding again, a bit more complex than that for the incompressible flow, but the behaviour of the scheme was familiar. Later, mainly Roe's scheme and other approaches based on the upwind principle have been applied. The resulting code was named FINFLO in 1990 [11]. Subsequent development was based on roughly the same roadmap as elsewhere: multi-grid, multi-block, parallelization, and development of turbulence closures. Very early on, the code was also applied for various practical cases. Today FINFLO can be called 'over-matured', but it is still a useful tool in research and is applied in aerodynamical simulations. As a side product incompressible solution methods have been developed. The Ship Laboratory of TKK and VTT developed models to cover free-surface flows. At Lappeenranta University of Technology the code has been used to study radial compressors. A new generation of research scientists has been able to develop improved turbulence models [12],[13].

Recently, in addition to FINFLO new software has been written at TKK and also theoretical work has been made in LES and DNS [14],[15]. Especially the most demanding computations are performed on the supercomputers offered by the Finnish IT centre for science (CSC). CSC has also made advances in numerical methods: their multiphysics software ELMER can be applied for CFD and they provide commercial software for the Finnish universities. In Finland the use of commercial codes started at Tampere University of Technology and at VTT in the early 1980s in a close cooperation with industry. Today commercial CFD codes are applied in many different areas in Finnish enterprises.

Finnish Meteorological Institute (FMI) has made considerable developments in numerical weather prediction since 1980s. The model development takes place within the framework of the international HIRLAM program. FMI's main contribution to the project include the development of data assimilation system, use of remote sensing data, and the development of physical parametrizations of the model. Since 2003, FMI has also acted as the Lead Center for the RCR (Regular Cycle with the Reference) runs, within which

capacity it has the special duty of running the official reference version of the HIRLAM as its operational weather forecast model. The HIRLAM model has been used operationally since 1990. At present, four 48 hour regional forecasts and four 48 hour mesoscale forecasts for the Northern Europe are produced daily, respectively. In addition, pre-operational test runs with a very high resolution model being developed in co-operation between HIRLAM and Meteo France are being performed.

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Some Developments in Computational Aerodynamics in the UK

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Summary The UK has been responsible for many seminal contributions to the general field of computational fluid mechanics and heat and mass transfer. Attempting to review all of them would be an impossible task within the space constraints imposed on us. Instead, we restrict ourselves to two particularly prominent areas, in which we can claim to have specialist knowledge, namely methods for simulating problems involving complex geometries and methods for the modelling of turbulence within the framework of the Reynolds–averaged Navier Stokes equations.

1 Introduction

Computational Fluid Dynamics (CFD) is a large, complex and highly interactive collection of mathematical, numerical and IT tools and models of physical processes, all targeting the computational solution of the differential equations that describe, in a supposedly exact manner, the conservation of mass, momentum, species concentration and energy within any fluid flow within ducted

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systems and around solid bodies. The complexity and multi–facetted nature of the subject precludes a discussion of any but some of its key ingredients. Moreover, in an article that aims to summarise the contribution to the subject by any one nation or geographical entity, a further restriction arises from the global nature of CFD, not merely in respect of its current widespread exploitation in the academic and industrial research communities, but also in respect of its emergence and evolution from its very beginning.

Among the numerous subjects that would justify being included in the present article, the authors are of the view that two key areas in which the UK community may claim to have made seminal contributions are

1. numerical solution methods for complex geometries;
2. modelling turbulence within the framework of the Reynolds–averaged Navier Stokes equations.

In what follows, the focus in the former is on the development of block–structured, body–fitted–grid and unstructured–grid methods, especially for external aerodynamic applications, both being prerequisites to the application of CFD to practically relevant complex configurations. The latter is concerned, principally, with the highly challenging task of devising statistical closure models that represent realistically the response of the Reynolds stresses in the RANS equations to the strain field over a broad range of flow conditions.

2 Contributions to Methods for Dealing with Complex Aerodynamic Configurations

Early computational simulations involving realistic aerodynamic geometries were based upon the use of panel methods. These boundary element methods only involved highly simplified flow physics, but they could readily deal with complicated geometries. This lack of realistic physics restricted the ability to predict key flow field features and, in particular, the aerodynamic properties. Work in the 1970s, on the solution of the full potential equation, brought greater realism to the simulations. However, these domain based methods required the discretisation of the computational volume surrounding the aerodynamic configuration of interest. Since techniques for constructing such discretisations for domains of complex shape were not available at that time, the application of full potential methods was restricted to relatively simple wing and wing–body configurations [33].

In early 1980s, the pioneering work on the solution of the Euler equations [36] was accompanied by an increasing industrial requirement for the use of CFD in the aerodynamic design process. This resulted in major efforts by the international community to develop robust methods for the generation of computational grids for complicated and realistic aerodynamic shapes. The two most successful approaches, classified as structured multi–block methods and unstructured methods, were both pursued in the UK.

2.1 The Multi–Block Method

The fundamental problem in generating structured grids around complicated geometries is the inherent issue of the mapping between the real physical domain, that includes the geometry of interest, and an idealised computational domain, that is topologically a single cuboid. The form of the mapping defines the topology of the mesh, where the generic mesh topologies are termed $\mathcal{C}$, $\mathcal{O}$ (polar) and $\mathcal{H}$ (Cartesian). For complicated geometries, such as a complete aircraft configuration, it proves to be extremely difficult to construct a mapping that results in a mesh suitable for accurate computations. Indeed, the construction of such a mapping may not be possible for certain mesh topologies. Central to the multi–block approach for overcoming this problem is the idea that the complete computational domain, between the aerodynamic configuration and some outer boundary, is conceptually broken down into a set of blocks. The union of the blocks fills the flow field, without holes or overlaps. Each block is chosen to be topologically equivalent to a cuboid, in that it has six faces and eight corners. Then, in principle, each block can be mapped into a unit cube in computational space, without change in topological structure. Cartesian grids in the unit cube in computational space map back to curvilinear grids in the physical space. Any appropriate technique may be used to perform the mapping, but the most popular approach has been to use the elliptic grid generation method of Thompson [78].

The major development of the multi–block approach to grid generation in the UK was funded by the Royal Aircraft Establishment, Farnborough and conducted by researchers at the Aircraft Research Association, Bedford. A series of papers describe the developments in the method, from the early ideas [87] through to applications on realistic configurations [77]. Similar techniques were being applied by groups in other countries, notably in the US [75, 76] and in The Netherlands [5]. The multi–block approach benefitted from the fact that the major advances that were being achieved in flow solvers, particularly for the Euler equations [36], could be easily incorporated within the framework.

In principle, the multi–block approach provides a means of generating grids for geometrical shapes and domains of arbitrary complexity. The method, combined with Euler solvers, enabled some of the early flow simulations involving realistic aircraft configurations. However, for general use, the key problem was how to sub–divide the domain automatically into a set of blocks, with the constraint that the block decomposition resulted in an appropriate grid topology. One of the earliest approaches was that of Roberts [64], who employed a series of embedded polar or $\mathcal{O}$ meshes around a geometry. Another approach was to represent a geometry as a simple cartoon [70]. Some efforts were dedicated to utilising the rapidly emerging graphics workstation hardware and software to allow the user to interactively construct the blocks [1]. However, although some of these methods proved useful for a limited set of geometries, no generally applicable method was devised and this remains an

area for research activity even today. With these limitations, the multi–block method has still been widely used within industry and applied extensively in the design of modern aircraft.

2.2 Unstructured Grid Methods

Work on the development of truly unstructured grid methods for external aerodynamics at Swansea University started in the early 1980s. Although the main attraction was the promise of an ability to readily handle complex geometries, there was also the hope that an unstructured grid environment would enable practical mesh adaptivity to be successfully accomplished. At that time, the wider CFD community was concerned about the viability, computational efficiency and accuracy of the unstructured grid approach.

Viability was addressed in initial 2D work, with the compressible Euler equations and with simple artificial viscosity models [46], and included a practical demonstration of the use of mesh adaptivity for both steady flows [48] and transient flows involving significant boundary movement [17]. Mesh generation was achieved using an advancing front method [59]. The full power of the approach was immediately apparent with the 3D extension [60] and the rapid level of capability that was achieved was demonstrated in 1988, when a valid tetrahedral grid for a computational domain surrounding a complete F18 configuration was presented at a NASA Langley Peer Review Meeting on Grid Generation. A view of the surface triangulation for this grid is shown in Fig. 1.

Computational efficiency was enhanced through a series of algorithmic and programming developments. The original element based algorithms [53] were replaced by edge based procedures, while a multigrid process, employing a sequence of unnested unstructured grids, was added to accelerate the convergence to steady state [61]. This formed the basis of the original versions of the FELISA and FLITE3D computer systems for the simulation of 3D Euler flows, jointly developed at Swansea and at Imperial College London. Simulation work, undertaken in collaboration with Rolls Royce [57], provided an initial demonstration of the capabilities of the FLITE3D system for the analysis of flow about installed nacelles. The efficiency of the method on the early vector computers was improved by the use of colouring techniques, designed to reduce the penalties associated with indirect addressing [47, 18], while implementations on parallel platforms with distributed memory were achieved for both steady flows [54] and unsteady flow simulations on adaptive moving meshes [79]. The efficiency of the volume mesh generation process was improved by replacing the advancing front method with an approach based upon the Delaunay/Voronoi dual geometrical construction [85, 35]. The Delaunay triangulation of a set of points is central to the procedure but, for efficient mesh generation, automatic point creation [88, 50] and boundary recovery [86] are critically important. The technique was used to generate large meshes, of up to a billion cells, in parallel [89]. For effective Navier Stokes

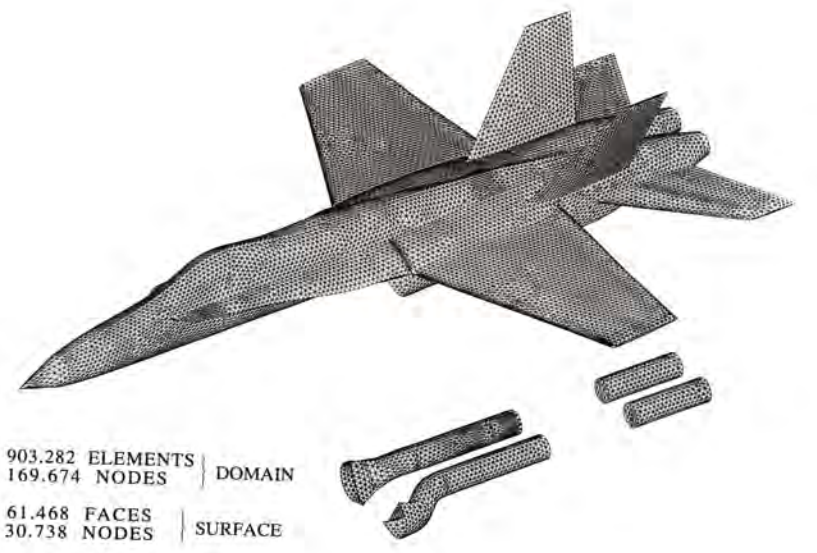

Fig. 1. View of the discretised surface for an unstructured volume grid, produced in 1988, for an F18 configuration (Reprinted from Computer Methods in Applied Mechanics and Engineering, Vol 87, K. Morgan, J. Peraire and J. Peiró, The computation of 3D flows using unstructured grids, pages 335–352, Copyright (1991), with permission from Elsevier).

simulations, anisotropic meshes were constructed using an advancing layers method [32].

The accuracy of the computations was improved by implementing high resolution extensions, using both flux corrected transport [49] and upwind methods [81], and by constructing better artificial viscosity models [11, 52].

At the University of Oxford, a distributed memory parallel computing framework for unstructured grids [10] was developed and this formed an essential ingredient in the development of the Rolls Royce corporate CFD code HYDRA. Using an energy analysis linked to algebraic stability theory, the stability of a Navier Stokes discretisation [23] and a preconditioned Euler discretisation [25] on unstructured grids were analysed. The adjoint approach to aerodynamic design was extended to enable the modelling of problems involving complex geometries and unstructured grids [26] and the adjoint iterative process and the handling of strong boundary conditions was also explained [24].

At the Rolls Royce Vibration UTC at Imperial College London, the AU3D code was developed to enable the simulation of the unsteady flow and fluid/structure interaction problems that characterise large scale turbomachinery problems [68]. This work led to a capability for the analysis of flutter

mechanisms [82], bird strike prediction [34] and the modelling of rotating stall and surge [80].

Turbomachinery flows were also successfully simulated using the adaptive NEWT code at the CFD Laboratory, University of Cambridge [13]. The applications included unsteady rotor/stator interactions [14] and the influence of casing treatment on fan performance [3]. The capabilities of the NEWT code were extended to enable the modelling of explosions [6].

The unstructured mesh approach has impacted upon industrial practice in the UK. For example, the British Aerospace Sowerby Research Centre Newsletter reported in 1997 that its implementation had led to spectacular time savings for flow solutions in large scale analyses, with overnight turnaround now being achieved for simulations which previously could have taken up to six months [20].

3 Contributions to CFD Based on the Navier Stokes Equations

The addition of the fluid viscosity and associated strain–rate tensor into the Euler equations yields the set of Navier–Stokes (NS) equations. At low speed – or rather low Reynolds number and strain rate – this addition has benign consequences, in most circumstances, in so far as the flow described by the equations is laminar and its computation relatively easy. Indeed, viscosity tends to promote numerical stability, by damping oscillations, although much depends upon whether the solution algorithm is explicit or implicit. Any physical unsteadiness that is (appropriately) not damped – for example, that associated with vortex shedding behind bluff bodies – is periodic and has a single time scale or is accompanied very few sub–harmonics. In such circumstances, the NS equations pose no noteworthy computational challenges over and above those encountered when solving the Euler equations, perhaps with the exception of the need for high resolution of thin shear layers. However, as the Reynolds number increases, physical instabilities provoked by the non–linear inertia terms amplify, and flow becomes transitional and eventually turbulent. It is in these circumstances that viscosity has a profound impact on the flow the NS equations describe and the challenges associated with the solution of the equation.

A fully–established turbulent flow contains a vast number of mutually interacting eddies having a wide range of length and time scales. Order–of–magnitude considerations show that the ratio of largest eddies, of length scale, L, and smallest eddies, of length scale η, the so called Kolmogorov scale, increases with Reynolds number in accord with $L/\eta \sim Re^{3/4}$, where Re is formed with appropriate mean–flow length and velocity scales. Thus, as turbulence is three–dimensional and temporally evolving, the computa-

tional resource requirements tend to rise in accord with[1] $cpu \sim Re^3$. This makes the direct solution of the NS equations a formidable task at any but very modest Reynolds numbers. For example, a fully–developed channel flow at bulk–flow Reynolds number of 40,000 requires, for full resolution, a grid of around 0.5×10^9 nodes and of order 10^6 cpu hours on a parallel cluster of 3GHz Xeon or Opteron processors, generating several Terabytes of data that need to be processed in order to determine the statistical properties of the flow. In complex strain (e.g. separation) and geometry, the resource requirement can be substantially higher than the above, rather conservative, estimate.

In the 1960s, the emergence of mainframe computers in the USA, such as the IBM 7090 and CDC 6400, began to offer the level of resource, in terms of both cpu power and memory, necessary to embark on simulations that would resolve the three–dimensional, spatial structure and temporal evolution of turbulent flows in detail. Related developments in this area will be outlined later. The flows that could be addressed at that time were very simple, however, and could only be computed with very coarse grids. For example, early (large eddy) simulations by Deardorf [15] at Oregon State University for a fully–developed channel flow were performed with a grid of only $24 \times 20 \times 14$ nodes. The realisation that simulation would not be a tenable route to predicting practical fluid–flow and heat–transfer problems for many years to come, thus provided a powerful impetus for the development of Reynolds–averaged Navier–Stokes (RANS) methods and associated statistical turbulence models, an area in which the UK exercised undisputed global leadership over many years, starting around 1968.

The reference to Reynolds–averaged NS equations, reflects the fact that Osborne Reynolds (1842–1912) is the father of statistical turbulence modelling, for which the RANS equations form the foundation. In a landmark paper, presented in 1885 to the Royal Society of Great Britain, Reynolds [63] derived the ensemble–averaged NS equations and introduced important statistical ideas and supplementary equations, including the equation for the turbulence energy. The RANS equations arise upon the insertion of the velocity and pressure decompositions $\tilde{U}_i = \bar{U}_i + u_i$ $(i = 1, 2, 3)$, $\tilde{P} = \bar{P} + p$, into the NS equations, followed by time– or ensemble–averaging of the equations. Here, the tilde denotes the time–dependent (turbulent) value, the overbar the corresponding time–averaged value and the lower case letters identify turbulent fluctuations. A profound consequence of the time–averaging process is the appearance of the correlations $\overline{u_i u_j}$, referred to as the (kinematic) Reynolds stresses. The essential benefit derived, in principle, from time averaging is that the RANS equations, if solvable, circumvent the need to resolve the time evolution of turbulence. Moreover, in the case of flows which are statistically homogeneous in one direction, the RANS equations apply in their two–dimensional form, allowing a wide range of planar and axisymmetric flows to be computed, in principle, with very economical two–dimensional grids. However, the RANS

[1] $cpu \equiv$ central processing unit time.

equations can only be solved if the Reynolds stresses are modelled in terms of known or determinable quantities. The formulation of general turbulence models and their successful incorporation into computational prediction schemes formed a major body of research and development in the 1970s and 1980s, leading to the extensive and widespread commercial exploitation of CFD.

Although early research on statistical turbulence modelling was pursued in a number of countries, notably by Prandlt [62], Rotta [66] and von Karman [83] in Germany, Chou [7] in China and Kolmogorov [41] and Davidov [12] in Russia, it was not until the late 1960s that practically useful, general–purpose turbulence models emerged. These developments were initiated and directed at Imperial College London, by Brian Spalding, and involved many outstanding colleagues, including Brian Launder, Kemal Hanjalic, William Jones, Wolfgang Rodi, Micha Wolfshtein, Michael Gibson, Aki Runchal, Suhar Patankar, Stephen Pope and David Gosman.

A *golden period* of around 10 years saw the emergence of the $k - l$ model (Wolfshtein [90]), alternative forms of the $k-\epsilon$ model (Jones and Launder [38]), Launder and Spalding [43]), the Reynolds–stress–transport model (Launder et al [42], Hanjalic and Launder [31], Gibson and Launder [22]) and the algebraic form of the latter (Rodi [65]). Simultaneously, a range of numerical codes for computing turbulent flows were developed, again mainly at Imperial College London, into which the new models were incorporated and which were then applied to a wide variety of flows and transport phenomena, including heat and mass transfer and combustion.

The code GENMIX (Spalding [72]) for thin–shear flows, and several other codes, including TEACH, for more general flows developed by Spalding, Gosman and their colleagues (Gosman et al [29], Patankar and Spalding [56], Gosman and Pun [28], Gosman and Ideriah [30], Gosman et al [27]) dominated the turbulent flow CFD scene. This work laid the foundation for the development of the more sophisticated commercial codes PHOENIX and STAR within the companies CHAM and Computational Dynamics, respectively. Outside Imperial College London, the code FLUENT was developed at the University of Sheffield by Boysan et al [4], to form the foundation of the company FLUENT.

All these codes incorporated variants of the k–ϵ eddy–viscosity models, and later, also Gibson and Launder's version of the Reynolds–stress–transport model for high–Reynolds–number flows. In the 1980s, the centre of gravity of turbulence–modelling research in the UK moved to UMIST in Manchester, where, for some 20 years, under the direction of Brian Launder and Michael Leschziner, the emphasis was on the development and exploitation of advanced Reynolds–stress–transport and non–linear eddy viscosity models for physically and geometrically complex two– and three–dimensional incompressible and compressible flows (e.g. Fu et al [19], El–Baz and Launder [16], Craft and Launder [8], Craft et al [9], Lien and Leschziner [45], Apsley and Leschziner [2], Leschziner et al [44]) in aero–mechanical engineering, including heat transfer.

Towards the end of the 1990s, research on turbulence modelling, worldwide, saw a marked decline, although the overwhelming majority of commercial and industrial CFD codes continue to rely on such models. One reason for this decline was the increased availability of high–performance computers, allowing LES to be performed for an ever wider range of conditions, especially if the primary motivation is to gain insight into fundamental turbulence mechanisms in laboratory flows. However, an arguably more important reason was a degree of disappointment that the enormous efforts put into turbulence modelling over some 30 years had not yielded models that were sufficiently general to enable accurate predictions to be derived for complex three–dimensional flows, especially when involving separation from curved surfaces. Specifically, an inability to break the barrier posed by the use of a single surrogate length–scale equation (be it for the dissipation, ϵ, the specific dissipation, ϵ/k, or the time scale, k/ϵ), and the lack of insight on how to progress beyond the status reached by around 1995, are regarded to be major obstacles to a significant broadening of the range of applicability of conventional statistical models. Much effort is now underway to bring LES and hybrid RANS–LES methods into CFD practice, but there are still many obstacles to overcome, some associated with the high computational cost and others with accuracy, resolution, subgrid–scale modelling, sensitivity to meshing and difficulties with specifying unsteady boundary conditions at inlets.

The science that provided impetus for pioneering work on simulating turbulence was meteorology, an area in which the use of the Reynolds averaged Navier Stokes equations was regarded as neither effective nor appropriate. Interestingly, this early work, in the late 1960s did not attempt to resolve the entire spectrum of turbulence, but applied the concept of large eddy simulation, as suggested by Smagorinsky [71] who also formulated the first subgrid–scale model that accounted, in a statistical form, for the dissipative effect of the small–scale part of the turbulence spectrum that could not be resolved by the relatively coarse grids that were used for LES.

As noted earlier, Deardorf [15] was the first to compute a turbulent channel flow, using a very coarse grid of $24 \times 20 \times 14$ nodes. Soon after, Schumann [69] published landmark simulations for channel and annular flows, and LES was then pursued with great vigour for studying engineering flows at Stanford University by Moin and his many co–workers (e.g. Moin and Kim [51]). First full–spectrum simulations — referred to as Direct Numerical Simulations or DNS — were performed by Orszag [55] at MIT, with an emphasis on studying the physics of isotropic, homogeneous turbulence — an area that is still an important subject of study, now pursued mostly in Japan by Kaneda et al [40] on the Earth Simulator in Yokohama, with grids of up to 10^{10} nodes. As with LES, the Stanford University group around Moin eventually emerged as a leading proponent of DNS, performing many landmark simulations for fundamentally important turbulent flows (Kim et al [39]).

The seat of early research in the UK on simulation was Queen Mary College, University of London. This research was led by Lesley and Voke (e.g.

Gavrilakis et al [21], Voke et al [84]) and focused mainly on channel flow and developing turbulent boundary layers, computed with spectral codes. Much of the subsequent work in the UK on LES and DNS in the 1990s and beyond can be traced to this early leadership by Lesley, with Peter Voke at Surrey University and John Williams at Queen Mary College, being two well–known collaborators.

At present, primary centres of simulation research in the UK are Southampton University (N. Sandham, DNS), Manchester University (D. Laurence, LES), Imperial College London (M. Leschziner, W. Jones, LES) and Loughborough University (J.J. McGuirk, LES) and Queen Mary University of London (J. Williams, LES, E. Avital, DNS and LES). Most of the LES work is directed towards complex flows and geometries having an increasingly industrial relevance. Although the emphasis is often on laboratory flows, offering insight into fundamental issues, research into hybrid RANS–LES schemes, especially at Imperial College London (Temmerman et al [73], Tessicini et al [74]) and at Manchester University (Jarrin et al [37]), targets industrial applications at high Reynolds numbers. This work involves, in most cases, the application of finite–volume codes, while research in DNS (Sandham et al [67]) aims at fundamental issues and is being pursued with spectral or high–order finite–difference codes.

The cursory historical review provided above justifies the claim that the UK has made an outstanding contribution to the area of turbulent–flow CFD. In particular, it has unquestionably exercised global leadership, especially in the 1960s and 1970s, in the area of turbulence modelling and the development of computational codes for the prediction of turbulent flows. This work spawned much of the commercial software that is applied globally today by companies such as CD and ANSYS (FLUENT) to the solution of industrial problems. Starting in the early 1990s, the emphasis in the area of turbulent–flow research has shifted gradually away from RANS towards LES, DNS and, more recently, hybrid LES–RANS methods. These approaches rely especially heavily on massive computing power and therefore major investment by the state and universities in large facilities. The lack of investment in the UK, relative to several other countries, including the USA, Japan and Germany, has put the UK in a less favourable position than it was in earlier decades. While the UK continues to be a strong player in all areas of turbulent–flow simulation, the community engaged in this area is now broad and global, with the USA being the leader and Japan, France, Italy, Germany, Sweden and the Netherlands being major contributors.

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The Development of Numerical Fluid Mechanics and Aerodynamics since the 1960s: US and Canada

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Summary CFD in North America greatly increased its utility in the 1970's with the development, locally and abroad, of high-resolution finite-volume methods. These methods permeated aerodynamics in the 1980's, when Euler and Navier-Stokes models became the standard of industry; since then, aerospace engineering has remained at the forefront of CFD development. During the 1990's, research emphasis shifted from fundamental discretizations to practical matters such as generating and using unstructured/adaptive grids, and high-performance computing. At the start of the 21st century, increasingly complex applications are driving a quest for compact higher-order algorithms; these borrow greatly from finite-element methodology.

1 The Dawn of Modern CFD

1.1 The Starting Position, 40 Years Ago

Let us consider the state of affairs in numerical fluid mechanics in the USA in the late 1960's. Gone were the days of initial exploration of first-order methods by the national laboratories, reported in detail in Academic Press's book series "Methods in Computational Physics" [3].

But second-order methods, that is, the method of Lax and Wendroff [79] for hyperbolic conservation laws and its predictor-corrector variants [22], were not living up to their promise of greater accuracy. Numerical oscillations and nonlinear instabilities would plague the solutions as soon as shock waves would appear.

On the positive side, Academic Press and Livermore editors Bernie Alder, John Killeen and Sydney Fernbach demonstrated a keen vision in having the

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book series succeeded by the new *Journal of Computational Physics*. It was in this journal that the breakthroughs were reported that transformed numerical fluid mechanics – eventually renamed Computational Fluid Dynamics (CFD) – into the powerful tool we know it to be today.

Volume 3 (1968) of *J. Comp. Phys.* contains an article by IBM scientist Jacob Fromm [44] presenting a second-order upwind-biased advection scheme that later became the basis of the standard of industry in compressible CFD, the MUSCL code of Van Leer [141] and Woodward; see Section 2. The journal also served to publish (Vol. 5, 1970) the contributions to the First International Conference on Numerical Methods in Fluid Mechanics, held in Novosibirsk, USSR, July 1969. In this issue we see a paper on *third-order* Euler methods by V. V. Rusanov [124], which inspired a later paper by Burstein and Mirin [21]. Without the problems affecting second-order methods solved, these higher-order extensions were futile.

Meanwhile, coping with second-order methods continued, within and outside of *J. Comp. Phys.*. Burstein [22] used a 2-D predictor-corrector form of the Lax-Wendroff scheme to march in time toward a steady Euler solution of flow over a blunt body (a step). Noteworthy are the sophisticated, solution-gradient-based third-order smoothing terms added to fight nonlinear instabilities and shock-induced oscillations; these are the Euler extension of terms included in [79] for the 1-D Lagrangean equations.

In a much-quoted AIAA paper, R. W. MacCormack [90] developed nonlinear 1-D and 2-D variants of the Lax-Wendroff scheme aimed at reducing the operation count; these dominated numerical aerodynamics for many years to come. This scheme contains a simplified third-order smoothing term with its coefficient proportional to the pressure gradient.

1.2 The Birth of High-Resolution Schemes

To appreciate the difficulty of designing a second-order method for the compressible Euler equations that produces oscillation-free shock structures it is useful to first consider modeling the linear advection of a step function. Here we immediately run into a "barrier" theorem included in Godunov's [46] famous 1959 paper: *if an advection scheme preserves the monotonicity of the solution it is at most first-order accurate.* This result could discourage anyone attempting to improve advection schemes; fortunately, there is a way to circumvent it. In the proof of this theorem it is tacitly assumed that the linear advection equation is approximated by a linear discretization; once *nonlinear* discretizations are admitted the theorem no longer stands.

The realization that Godunov's theorem could be circumvented came at the start of the 1970s, when, within the span of one year, three independent approaches were launched for the construction of oscillation-free higher-order advection schemes. The authors: astrophysicists Jay P. Boris (USA) [14], Bram van Leer (Netherlands) [139], and aeronautical engineer Vladimir P. Kolgan (USSR) [76]. In this chapter I shall discuss in detail only the work of Boris and

collaborators [15, 16, 17, 158]; Van Leer's work of the 1970s was largely carried out in the Netherlands and is referenced here only for the purpose of comparison. Kolgan's [76] approach is the same as Van Leer's but remained less developed and little known, not in the least because Kolgan died at an early age in 1978. It is not even mentioned in the contribution on Computational Fluid Mechanics in Russia.

Boris (then and now at the Naval Research Laboratory) presented the first non-oscillatory second-order advection scheme SHASTA - Sharp and Smooth Transport Algorithm — at a seminar course in Trieste, Italy, in August 1971 [14]. His was a predictor-corrector approach: a non-oscillatory first-order scheme is followed by a corrector step that removes the leading, dissipative term of the truncation error ("anti-diffusion"). The corrector fluxes, however, are *limited* where necessary in order to prevent new extrema to arise. The family of methods generated by this procedure was named "Flux-Corrected Transport" or FCT.

FCT methods are particularly suited and widely used for unsteady high-energy flows such as arise in weapons research; they have not found much ground in aerospace engineering, which is more focused on steady flows. One additional reason is that in FCT schemes the limiting is strongly coupled to the update step, causing the limiter to erratically switch on and off, which in turn may lead to undesirable staircase-like solution contours.

Van Leer's approach to numerical advection is essentially a Discontinuous Galerkin technique in which the solution is represented by polynomial sub-cell distributions, with limiting applied to the values of the derivatives of these distributions. In the finite-volume version of this technique the sub-cell distributions are obtained by interpolating cell-averaged values; thus, the problem of avoiding numerical oscillations becomes a matter of non-oscillatory initial-value interpolation, irrespective of the update equation. This point of view has proved particularly fruitful; in the USA it has led to the development of Essentially Non-Oscillatory (ENO) interpolation (see Sub-Section 3.1) and even made its mark on the field of image restoration, in particular, edge sharpening [80].

Characteristic of the above approach is that at each cell interface a discontinuity arises in all flow variables. Already in the 1950s Godunov [46] had observed that unique fluxes can be obtained by interpreting the situation at an interface at the beginning of a time step as Riemann's initial-value problem (a generalization of what is known in gas dynamics as the "shock-tube problem"), of which the unique solution is known. These interface fluxes automatically lend upwind bias to the finite volume scheme that incorporates them. Algorithms that produce fluxes from exact or approximate[1] solutions of

[1] The justification of using only an approximation is that conservative schemes suppress most of the information in Riemann solutions anyway, by averaging over them in the final update.

Riemann's problem were soon called exact or approximate "Riemann solver" see further Sub-Section 3.1.

The first 2-D Euler code based on Van Leer's [140] advection schemes with piecewise linear subcell distributions, written and tested in 1975-77 by Van Leer's collaborator, astrophysicist Paul Woodward, was named MUSCL, for "Monotone Upstream Scheme for Conservation Laws" this acronym became generic for codes of this type. Woodward took the code to the Lawrence Livermore National Laboratory, where he further advanced and popularized the MUSCL approach and its sequel PPM (Piecewise Parabolic Method) in collaboration with numerical analyst Phil Colella [33, 34]. A landmark paper is their 1984 JCP review [156], an elaborate comparative study in which Godunov-type schemes, FCT and more traditional methods are pitted against one another.

The MUSCL scheme was greatly simplified when a predictor-corrector formulation by Steve Hancock (a former student of Maurice Holt at UC Berkeley) came along [136, 144]; this is an extension to hyperbolic systems of Van Leer's finite-volume version ([140], Scheme I) of Fromm's [44] advection scheme.

2 Computational Aerodynamics in the 1970s

While high-resolution methods were developed by researchers dedicated to a fully compressible flow model, the aerodynamics community was still served by simpler flow models, in particular, forms of the potential flow equations for homentropic, irrotational flow. Incompressible potential flow was treated by panel methods such as found in Boeing's PanAir code; Mach-number effects for subsonic and supersonic flows were included in the small-disturbance equations, still linear. For transonic flow, however, the equations are inherently nonlinear.

The first successful numerical technique for steady transonic flow was based on the transonic small-disturbance equation and due to applied mathematician Julian Cole and his student Earll Murman [100, 99]; here the centered stencil used in the subsonic flow region automatically switches to an upwind stencil in the supersonic region, and to a special stencil at sonic points. An intriguing flaw of this scheme was that the transonic switch did not distinguish between an admissible compression shock and an inadmissible expansion shock, and thus could lead to the appearance of the latter in smooth flow[2]. This problem was later removed by Antony Jameson (economist by education) [66] through upstream biasing of density values appearing in the scheme, creating the artificial diffusion needed to break down expansion shocks. He also

[2] A decade later, expansion shocks turned up in Euler solutions obtained with Roe's numerical flux (see Sub-Section 3.1). The issue of "entropy-satisfying" fluxes became a topic of interest to applied mathematicians (Harten, Lax, Osher, Tadmor, Goodman, LeVeque); the standard of industry is an "entropy fix" based on the work of Harten, Goodman and LeVeque [145].

introduced differencing in a frame normal to the shock ("rotated differences"), for greater robustness and precision. Jameson's techniques became part of the FLO22 code (developed with David Caughey), and of Boeing's influential TranAir code [72], formulated on a non-conforming Cartesian grid, with embedded solid-body boundary conditions. This workhorse code is still used extensively for airplane analysis and design.

Jameson's influence on aeronautical CFD can hardly be overestimated. Starting in the late 60s he contributed a sequence of aerodynamics codes for increasingly complete flow models, from small-disturbance to full Navier-Stokes. Most influential were his efficient 2-D Euler code FLO57 and its multi-grid version FLO87, which definitively sold the aerospace community on the full Euler flow model.

Another strong force in the development of CFD in the aeronautical community was Flow Research Corp., a company that counted among its employees such influential scientists as Joe Steger, Earll Murman, Mohammed Hafez, Woodrow Whitlow and Wen-huei Jou, who all eventually ended up at high positions in academia, national labs and industry. Hafez and Whitlow are known for co-authoring the first transonic-flow code based on the full potential equation [53]. Hafez remained dedicated to the full potential equation after it had been superseded by the Euler equations, developing a non-isentropic correction [154] to the transonic shock position.

Yet the broadest effort in developing CFD algorithms and codes for aerodynamics in the 1970s was located at NASA's Ames Research Center. While Terry Holst and collaborators were refining POTFLOW [60], a full-potential flow code, Dick Beam and Bob Warming pioneered an implicit, compressible Navier-Stokes scheme, implemented with aid of a kind of dimensional splitting, "approximate factorization," due to Briley and McDonald, also at ARC [93]. This scheme formed the basis of the ARC2D/3D codes developed by Tom Pulliam, Joe Steger and others [112].

In retrospect the development of this Navier-Stokes solver must be regarded as premature. At this time knowledge of limiting had not yet reached aeronautics, so the Euler discretization embedded in the Beam-Warming scheme, based on central differencing, was oscillatory in the presence of shocks, and not a good basis for a Navier-Stokes scheme.

Subsequent work by Steger and Warming on forward/backward splitting of the Euler fluxes [128], a crude approximate Riemann solver[3], was a step in a more promising direction, although the splitting was mainly intended for approximate LU factorization of implicit operators. Furthermore, a new interaction of Peter Goorjian (ARC) with Björn Engquist and Stan Osher (both at

[3] A better term is "approximate Boltzmann solver", [56] since it can be interpreted as being based on the concept of molecular transport rather than wave propagation. The Steger-Warming flux is a special case of the flux used in the "Beam Scheme" of astrophysicist Kevin Prendergast [126], which is based on a crude quasi-molecular velocity-distribution function.

UCLA) in 1979 gave birth to the entropy-satisfying upwind Engquist-Osher flux [42] (also based on flux splitting) for the small-disturbance transonic potential equation; it eventually morphed into a much-used approximate Riemann solver for the full Euler equations. This leads us right into the 1980s.

3 The Heyday of CFD: 1980-1998

3.1 Impact of High-Resolution Schemes

The emergence of higher-order Godunov-type methods created several strong research trends in the 1980s; much of the research activity was concentrated at and emanated from the Institute for Computer Applications in Science and Engineering (ICASE) at NASA's Langley Research Center, established in 1972 by the Universities Space Research Administration (USRA). After a modest start in 1972, ICASE came to play a crucial role in the further development of CFD, for aeronautics or for general use, in the US as well as worldwide; its period of high impact stretched from 1980 through 1998[4].

ICASE was set up to bring together Langley engineers and scientists from all over the country and the world, and it handled this task extremely well. One of its earliest successes was the result of introducing to LaRC of multigrid analyst Achi Brandt (Weizmann Institute, Rehovot, Israel). His collaboration with Jerry South, Jr., chief of the Theoretical Aerodynamics Branch (ThAB), on solving the full potential equation marks the first application of multigrid relaxation to an aeronautical flow problem [73]. Another mathematician from Israel, David Gottlieb (now at Brown University) introduced spectral methods [50] to ICASE and LaRC. Spectral methods became a prominent tool for research of turbulence and the transition to turbulence; at ICASE a sizable group dedicated to such studies included M. Y. Husseini, T. A. Zang, C. Canuto and A. Quarteroni [24].

Even more significant was the arrival of Van Leer at ICASE in 1979; this marks the introduction of Godunov-type high-resolution schemes to LaRC and, subsequently, to the general aeronautics community. Soon ICASE became a center of knowledge exchange and collaboration among applied mathematicians, physicists and aerospace engineers on the subjects of limiters and non-oscillatory interpolation, as well as upwind fluxes based on approximate Riemann solvers; research in these topics proliferated. An anthology of ICASE-based papers on these topics, with historical and technical notes, can be found in the book *"Upwind and High-Resolution Schemes"* [61].

[4] With the de-emphasis of algorithm development by funding agencies in the late 90s ICASE's focus had to shift, and shortly after its 30th anniversary it closed. Its successor became the National Institute of Aerospace (NIA), run by Virginia Tech, Georgia Tech and other schools; this institute still has to find a formula for success.

The use of upwind fluxes, which promote diagonal dominance in implicit schemes, further created a revival of classical relaxation methods, and a new perspective on convergence acceleration; see below in this section.

Among the regular visitors of ICASE, one of the most productive and influential was Ami Harten (Tel Aviv University), because he also was a regular at ARC and UCLA. At ICASE he collaborated with his former advisor Peter Lax (NYU) and Van Leer on a review of upwind differencing [56], which features an approximate Riemann solver that is in wide use for large, complex hyperbolic systems[5]. At ICASE he also developed local sufficient conditions to make a scheme Total-Variation-Diminishing (TVD) [54]. The total variation of a discrete solution (sum of absolute differences) will increase with the birth of a new extremum; thus, a TVD scheme guarantees a non-oscillatory solution when applied to a single *nonlinear* conservation law.

Harten's motivation for this work was to put the theory of limiting on a mathematical footing broad enough to allow extension to multiple space dimensions. Unfortunately it was shown by mathematicians Jonathan Goodman and Randy LeVeque [49] that the total variation is too crude a functional to be of use in constraining multi-dimensional discrete functions: a multi-dimensional TVD advection scheme can be no better than first-order accurate. Around 1985 Harten re-examined non-oscillatory interpolation theory while at UCLA and, together with Osher, Engquist, Sukumar Chakravarthy (Rockwell), and Chi-Wang Shu, developed the concept of ENO [58, 57, 55, 127], which does generalize to multi-dimensional solutions [1]. ENO is a systematic procedure that selects the discrete stencil whose data will give the smoothest interpolant, i. e. the function with the lowest values of its derivatives. ENO schemes are only Total-Variation-Bounded (TVB). ENO was succeeded by Weighted ENO (WENO) [71], which includes a higher-order target scheme and switches stencil only when really needed to prevent oscillations.

Another researcher whose career in CFD took off at ICASE was Philip Roe (Royal Aircraft Establishment, UK). His approximate Riemann solver [119], presented first in 1980 at the 7th International Conference on Numerical Methods in Fluid Dynamics (Stanford/ARC), became the most popular one among all such solvers. Though not developed in the USA, it is useful to describe it here, if only for the sake of comparison. It is based on a local linearization of the conservation laws, valid in the vicinity of the interface between two cells; the linearization is with respect to a smart average of the neighboring states ("Roe average"). While new for the Euler equations, it turns out that a similar linearization of the Lagrangean equations goes back to an early paper by Godunov [47].

[5] There is much confusion about this paper in the literature. There are actually two Riemann solvers in the paper; the first one, a two-wave model and very diffusive, is just an exercise in developing the second one, which includes three waves. Most people, though, when referring to the Harten-Lax-Van Leer (HLL) flux, mean the first solver.

The Riemann solver of Osher [107] treats any acoustic wave as a simple wave, whether it actually is an expansion wave, or a shock. Both Osher and Roe solvers can be used to split flux differences across a mesh into parts attributable to either forward- or backward-moving waves; this technique is called "fluctuation splitting" after Roe, or "flux-difference splitting". Less accurate are the solvers based on the Boltzmann approach [56], in which the distribution functions of adjacent cells are merged; this leads to formulas commonly known as "flux-vector splitting" or simply "flux splitting." The best-known representatives are the Steger-Warming splitting discussed earlier, and Van Leer's flux splitting [143], developed at ICASE.

Van Leer and Wim Mulder [97, 148] demonstrated that classical relaxation methods for elliptic equations (from point-Jacobi to line-Gauss/Seidel) are effective when applied to upwind second-order discretizations of the Euler equations in two dimensions [NB: this work was not done in the USA]. Independently, Osher and Chakravarthy [106] soon came to the same conclusions. Mulder also experimented with multigrid relaxation for the Euler equations and in 1989, while at UCLA, developed a semi-coarsening strategy [98] that overcomes the lack of convergence caused by alignment of the grid with the flow.

Meanwhile, vector computing was becoming a standard capability of computer architecture, and this significantly upset the order of preference held by relaxation methods on the basis of their performance on scalar computers. Sequential methods such as Gauss-Seidel, where one result follows from another, can not make use of vector processing in one dimension; in multidimensional calculations, though, it is possible to process a stack of 1-D or 2-D Gauss-Seidel relaxations with vector operations. The same holds for line relaxation, which by itself does not vectorize well. In view of these complications, the "checkerboard" variant of Jacobi relaxation (update every other point) and the "zebra" variant of line relaxation (update every other line), which vectorize well, became popular for a while. Note that most of these relaxation methods are inspired on structured hexahedral grids; it is cumbersome to extend them to unstructured tetrahedral grids [52].

The collective knowledge of limiters, Riemann solvers and relaxation methods was put to use in a collaboration between Van Leer and Jim Thomas and Kyle Anderson, both at NASA Langley's Analytical Methods Branch, and Bob Walters of Virginia Tech, in the development of the CFL2D/3D code [122], which is still in use. During this development it became clear that non-differentiable components in the residual calculations, notably, nonsmooth limiters and flux functions, could slow down or even halt convergence to a steady state. When using an implicit time-marching scheme it is now customary to use only differentiable limiters such as Van Leer's harmonic limiter [140], Van Albada's [136], Koren's [77], or the one developed especially by V. Venkatakrishnan [152] with easy convergence in mind.

A different approach to discretization of the Euler equations was launched in 1981 by Jameson, Wolfgang Schmidt († 2008) and Eli Turkel (Tel Aviv

University) [69]. Their numerical flux is never upwind; it is the sum of an algebraic flux average and a third-order stabilizing artificial-diffusion term with a scalar coefficient; limiting is accomplished by trading this term for a first-order term with a coefficient proportional to the second difference of the pressure. While this approach is not automatically non-oscillatory when applied to a linear advection equation, it does give non-oscillatory shock profiles in the class of steady-flow problems for which it was intended. The time-marching method combined with this spatial discretization was a four-stage Runge-Kutta method, after Rizzi [118], who had pioneered the use of Runge-Kutta methods for Euler schemes. In addition the scheme included several explicit convergence-acceleration devices, in particular, residual smoothing (averaging of the local residual with neighboring values) and enthalpy damping. Later, Jameson added multigrid relaxation [67] and used up to five stages, with or without residual smoothing, in order to get strong high-frequency damping, as required in a multigrid strategy.

Jameson's design of multistage methods suited for multigrid relaxation was done by trial and error. The procedure was made automatic and in some sense optimized by Van Leer and students [150, 89].

Multigrid relaxation is only one of many convergence-acceleration techniques used in aerodynamics. Any type of vector-sequence acceleration, such as GMRES [125], Bi-Conjugate-Gradients [137] or other Krylov methods [23], can be used to solve the large systems of nonlinear equations arising in CFD, or as a preconditioner for a final solver. Preconditioning can be a powerful tool for clustering eigenvalues of a system to be solved; in Sub-Section 3.2 local preconditioning of the Euler and Navier-Stokes equations figures prominently.

The Euler era in aeronautical CFD lasted only 5 years; by 1986, when a Euler solution of flow over a full fighter aircraft[6] adorned the cover of Aviation Week [9], Navier-Stokes solvers based on high-resolution Euler schemes had already been presented at the 7th AIAA CFD Conference in 1985, [134]. Inclusion in a Navier-Stokes discretization does put a constraint on the approximate Riemann solver used for computing the inviscid fluxes: its implied artificial dissipation should not interfere with the structure of attached boundary layers [151]. This rules out the use of flux-vector splitting, which causes artificial diffusion of tangential momentum across the boundary layer [30], thus visually thickening the layer except on excessively fine grids. For the same reason Jameson's Euler flux, which contains a scalar dissipation coefficient, is not tenable in a Navier-Stokes code, as demonstrated by Allmaras [4]. Turkel and Swanson [133] avoided the unwanted diffusion by replacing the scalar coefficient by a matrix; this makes Jameson's flux mimic an upwind flux, with the effect of limiting included; see Van Leer [142].

Liou and Steffen [85] succeeded in modifying Van Leer's Eulerian flux splitting by taking out the advection terms and treating these by flux-difference

[6] The calculation was actually done by A. Eberle (MBB Military Aircraft), using yet another Riemann solver, see [41].

splitting; only terms containing the pressure remain traditionally flux-split. The resulting numerical flux function, named Advection-Upwind/Splitting Method (AUSM), is still very simple and compatible with the Navier-Stokes equations; a number of variations exist [84].

Meanwhile, at the national laboratories (LANL, Sandia, LLNL), where CFD was intensively used in weapons and energy research (including radiative hydrodynamics), the impact of high-resolution schemes was felt in phases. The labs were quick to embrace the concept of limiting second-order terms, including it in the re-map step of their Eulerian-Lagrangean codes, which until then had been first-order accurate by necessity. This gave such an improvement in overall accuracy that no immediate need was felt to also include the other obvious component of Godunov-type schemes, the Riemann solver. It was owing to the considerable efforts of Woodward, Phil Colella [156, 34] and others, that the full numerical technology of higher-order Godunov methods slowly became accepted at the national laboratories. In this regard it is interesting to note that the concept of Discontinuous Galerkin (DG) methods for fluid dynamics, which can be regarded as the ultimate way of generating Godunov-type methods, was actually invented at LANL by Reed and Hill [117], and has now become the focus of CFD method development in aeronautics; see Section 4.

Toward the end of the 1980s most developers and users of high-resolution codes for gas dynamics and aerodynamics were rather satisfied with the performance of their codes in a wide range of flow problems. Yet I must conclude this subsection with a discussion of one notable exception: the hypersonic flow regime. By 1988 it was clear that highly successful finite-volume codes like CFL2D produced bizarre solutions of steady flow around a blunt body on perfectly smooth grids, if the Mach number rose above 5. Typically, the bow-shock would exhibit a tumor-like growth or "carbuncle;" the correct steady solution, obtainable for symmetric flow problems by only solving for half of the flow field, no longer was an attractor.

Since then, insight into the carbuncle instability has greatly improved. There is a complete analysis of 1-D shock-position instability by Barth [11]; the instabilities become more complex when a 1-D normal shock, grid-aligned, is studied with a 2-D code [114] – this is called the 1.5-D case. Still greater complexity arises in genuinely 2-D and 3-D flow problems. Phil Roe and students have studied the carbuncle in great detail and come up with a variety of flux modifications combating the carbuncle [65], but to date no numerical flux function has been found that is carbuncle-proof in all dimensions [74].[7]

The carbuncle problem is exacerbated on unstructured grids. To this date it is recommended that hypersonics calculations be carried on multiblock structured grids composed of hexahedrals [105].

[7] The best candidate right now is a multi-dimensional flux function, due to Hiroaki Nishikawa, which has been implemented in the code FUN3D [103].

This greatest unresolved problem of classical finite-volume schemes has been deemed worthy of the only illustration of this chapter, Figure 1 (from Kitamura et al. [74]).

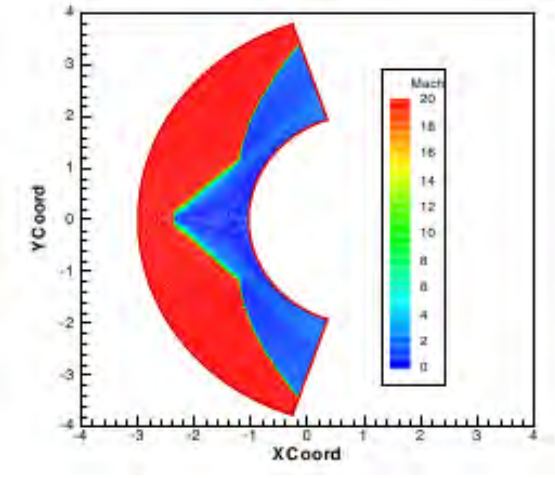

Fig. 1. The dreaded Carbuncle. Bow shock for Mach 6 flow about a cylinder. First-order Roe scheme. Contours of Pressure Coefficient.

3.2 Emphasis on Grids, Parallel Computing, and More

In spite of the carbuncle, toward 1990 research gradually shifted away from developing basic Euler and Navier-Stokes discretizations, with one exception: the study of genuinely multi-dimensional Euler methods, to be discussed further below. Otherwise, CFD research turned to adaptive and unstructured grids, and formulating schemes for such grids. Convergence acceleration remained a research focus; furthermore, there was a growing research activity in more complex fluid problems, such as multi-fluid dynamics and multi-scale flow. Funding agencies were shifting moneys from focused fundamental research to high-performance (= massively parallel) computing and communication (HPCC) and grand-challenge applications; support for basic research never fully recovered.

Cartesian grids with cut cells at solid boundaries and tree-structured adaptive refinement (quadtree, octree) were developed for pure Euler calculations and scored great successes in practical applications. A landmark is the study of Berger and Aftosmis [2] of the flow around a C-150 transport plane, in particular, the current in which exiting paratroopers would be immersed. The authors arrive at a recommendation of increasing the plane's angle of attack

when unloading troopers. Worth mentioning is also the space-weather prediction software BATS-R-US, which tracks a solar coronal emission all the way till it arrives at the earth, using adaptive meshes to represent a range of scales from tens of kilometers near the earth to the 1 AU distance from Sun to Earth (see the contribution by K. G. Powell in Part IV).

Fully unstructured grids for aeronautical problems, first with triangular, later with tetrahedral cells, were developed at the same time as the cut-Cartesian grids. Tim Baker († 2006) and Jameson [68] were the first to produce 3-D inviscid flow solutions for a simplified airplane on a tetrahedral grid. When formulating the Euler conservation laws on such a grid, one has the choice between a cell-based approach, where the cells are the volumes over which conservation is guaranteed, and a node-based approached, where conservation is guaranteed on the cells of a dual grid centered around the nodal points. Either approach has produced efficient computational codes. Node-based codes include Jameson-Baker [68], LaRC's FUN3D [5], Mavriplis's NSU3D [92], and OVERFLOW [70]. AVUS [59] is and example of a cell-based code. In addition, the so-called residual-distribution schemes, to be discussed below, are all node-based.

Pure cut-Cartesian grids proved to be unsuited for viscous flows [32]; they have to be blended with prismatic boundary-layer grid. The same is true if the main space-filling grid is tetrahedral. In some approaches developed later, e.g., those by M. S. Liou (DRAGON) [159] and Z.-J. Wang [155], the tetrahedral and prismatic grids are merged into in one framework without any distinction. The opposite is true in the CHIMERA [13] approach of Steger(† 1992) and Peter Buning, which is particularly effective in multi-body flow calculations. Here, each body gets its own grid wrapped around it, resulting in overset grids betweeen which interpolation routines are defined for data transfer. The approach is useful for fixed bodies as well as bodies moving with respect to each other, as with store separation or the launching of an escape vehicle. A landmark result was the flow around the Space Shuttle with booster rockets attached, computed as early as 1989 [20].

A key result on moving grids was the calculation in 1987 by Man Mohan Rai [116] of flow over a 2-D stationary blade row followed by a moving blade row, discretized on two grids sliding along one another.

In the area of convergence acceleration, some researchers concentrated on the key problem of reducing the complexity of computing steady solutions to the theoretical minimum. Specifically, solving a discrete problem with N unknowns should not require more than KN operations (the "complexity"), where K is a bounded number independent of N. It was clear that multigrid relaxation should be part of the solution strategy. Multigrid expert Achi Brandt [18] used a slightly different terminology: to him "textbook multigrid convergence" means bringing down the residual to the level of the truncation error within a few (say, 5) multigrid cycles. This goal includes not just achieving $O(N)$ complexity, but also bringing down the coefficient K to the lowest achievable value.

$O(N)$ complexity of steady Euler solutions was first achieved at the end of a long line of research started by Van Leer and collaborators [150, 89, 88] and finished by David Darmofal and K. Siu [37] in 1998. Key ingredients in this approach are optimal local preconditioning (to make the Euler equations behave as a scalar equation insofar as this is possible), optimally smoothing time-marching schemes (to efficiently damp high-frequency modes at each grid level), and multigrid relaxation with semi-coarsening (to overcome the flow-alignment problem; see Sub-Section 3.1). Darmofal and Siu showed that with regular full coarsening the complexity for an Euler calculation of lifting flow increases to about $O(N^{1.5})$, and without local preconditioning convergence stalls.

In contrast, $O(N)$ complexity of steady Navier-Stokes solutions has not been achieved; the computational work typically scales with N^2 or worse. One reason is that no optimal multi-D local preconditioner has been developed to date[8].

Local preconditioning itself has a long lineage; it descends from A. Chorin's [27] artificial compressibility technique, which allows to compute incompressible flow by marching in time with a hyperbolic system. This in turn was generalized by Turkel and optimized for subsonic flow [135], to speed up steady-flow calculations in the nearly incompressible regime. Many applications of this basic preconditioning are due to C. Merkle and collaborators [153, 26, 43]. In 1991 Van Leer et al. [146] proved that the lowest condition number achievable among the characteristic speeds by local preconditioning of the Euler equations is $|1 - M^2|^{-\frac{1}{2}}$, where M is the Mach number. This preconditioning separates the residual component due to acoustic waves from the residual components due to advection; this allows separate scaling of the different processes, which in turn can be used to reduce the spread in wave speeds (equivalent to reducing the system's condition number), thus speeding up explicit marching toward a steady state at any Mach number. Another benefit of the residual splitting is its use in residual-distribution schemes, discussed toward the end of this section.

A general theory of optimal local preconditioning for 2-D hyperbolic systems was developed by Roe [121]. It was applied successfully to the 2-D MHD equations [104], but obtaining the optimal preconditioner for MHD is sufficiently expensive to make its widespread application doubtful.

Two-fluid dynamics became greatly simplified with the appearance of the "level-set method" of Mulder, Osher and Sethian [96], related to older Volume-of-Fluid methods [45], but particularly easy to implement. In this method a scalar function measures the distance to the fluid interface; the zero level (con-

[8] Chris Depcik and Van Leer [40] demonstrated that optimal local preconditioning for the Navier-Stokes equations, while feasible, leads to an unphysical growing (antidiffusive) mode for certain combinations of Mach and Reynolds numbers. A scheme including such preconditioning must have a mechanism to damp such modes, for instance, through time-impliciteness.

tour) of the function indicates the interface itself. An advection equation or conservation law for this function is added to and integrated along with the Euler equations. Under the rule of this equation, the scalar function loses its property of distance function, so renormalization is needed at regular time intervals. The method can be used for compressible [113] as well as incompressible flow [130].

This chapter would not be complete without touching on the subject of genuinely multidimensional methods for the Euler equations. These started out as techniques of switching automatically to a shock-attached coordinate frame [38, 82, 35] in order to achieve a grid-insensitive shock representation, in particular, to avoid smearing of oblique steady shocks. A more fundamental technique, proposed independently by Roe [123] and Ijaz Parpia [109], sought to enrich the rotated Riemann solver with a shear wave running normal to the other waves. This model is suited for steady-flow calculations; it efficiently removes pressure oscillations across a detached boundary layer and, unexpectedly, leading-edge entropy errors.

In 1986, though, Roe [120] already published an even more ambitious concept based on an unstructured nodal-point scheme, in which the Riemann solver, previously used to decompose the flux imbalance at a cell interface, was interpreted in multiple dimensions as a multidimensional wave model that would explain the flux integral along the entire cell boundary, i.e., the residual [95]. Contributions due to the waves would be distributed in some suitable fashion over downwind nodes; the sum of all contributions at one node would serve to update the state at the node. This scatter-gather approach had an Achilles heel: the wave model. The model was not unique and there were always more plane waves than state quantities, making the steady state a matter of cancelling rather than vanishing waves - not a road to high accuracy.

It took until 1994 before it was realized that the discrete acoustic waves had to be taken out of the model and treated collectively as the acoustic part of the residual. The tool by which this was achieved was a splitting of the Euler residual into a hyperbolic (advection) and an elliptic (acoustic) part, previously derived for the sake of locally preconditioning the Euler equations (see above).

This class of multi-D schemes, nowadays called "residual-distribution schemes," matured during the 1990s owing chiefly to the efforts of Roe et al. at the University of Michigan in Ann Arbor and Herman Deconinck et al. at the Von Kármán Institute near Brussels. Milestones were the doctoral theses of Lisa Mesaros (1995, UMich [94]) and Henri Paillère (1995, VKI [108]).

The approach has become popular only in Europe, where it is actually used for solving industrial flow problems. A comprehensive report describing the European effort up to 1996 is the BRITE/EURAM project book edited by Deconinck and Koren (1997 [39]).

The state of the art is still represented reliably by the theses of Dutchman Erwin van der Weide (1998, TU Delft, Netherlands [138]) and Roumanian

Doru Caraeni (2000, TI Lund, Sweden [25]). Van der Weide solves complex steady viscous rocket-base-flow problems. His findings are that the method does fulfil its promise of uniform resolution regardless of direction, but that convergence to a steady solution suffers, probably because of the compact, highly nonlinear limiters. Caraeni develops a third-order-accurate scheme for Large-Eddy Simulation (LES). Temporal accuracy is achieved by using the scheme only in an inner iterative (pseudo-time) loop, which solves an outer, implicit update scheme.

It remains a challenge to include Navier-Stokes terms in a residual-distribution strategy, although theoretically this should be feasible. Some progress in this direction has recently been made by Nishikawa [102].

4 Latest Developments

During the past decade, CFD in the USA has become more powerful than ever, owing to the circumstance that massively parallel computing has come within reach of every research group. There is a great diversity in challenging applications; the trend seems to be toward handling increasingly complex physics in the presence of an increasingly complex geometry. It is not my intention to present an inventory of such applications; I will restrict myself to illuminating some accompanying developments in CFD methodology.

The first building block to be recast when describing a more complex physical system is the inviscid part of the numerical flux function or, equivalently, the approximate Riemann solver. When the equation systems get larger and their eigenvector/value structure more intricate, detailed Riemann solvers with separate contributions from all waves are increasingly difficult and costly to obtain. For the 8 equations of magnetohydrodynamics[9] (MHD) a Roe-type solver is known [111], but in computational practice, specifically, in space-weather prediction (see Part IV of this book), one routinely resorts to a three-wave solver of the Harten-Lax-Van Leer type, due to Linde (HLLL) [83]. And the even larger systems of equations (≥ 10) obtainable for low-density flow by taking multiple moments of the Boltzmann equation [51, 81, 19] are now exclusively treated with the HLLL solver [132].

A completely different way of simplifying the inviscid numerical fluxes is to avoid the need for a Riemann solver by discretizing the equations on a staggered grid, in the spirit of the Lax-Friedrichs scheme [78]. Schemes of this type have the property that the solution changes even for a zero time-step, due to its projection onto the staggered grid; this projection gives an averaging or diffusion error. In consequence, the truncation error of such a

[9] The standard conservation form of these equations, used to derive jump relations, is not suited for CFD discretizations because of one Galilein-noninvariant eigenvalue. Powell [110] added nonconservative source terms $\sim \nabla \cdot B$, which formally vanish, to regularize the eigenstructure, thus rediscovering a form of the equations derived earlier by Godunov [48].

scheme always has a term inversely proportional to Δt in its truncation error, and the time-step must not be made arbitrarily small on a fixed grid. These schemes therefore are not suited for defining the spatial operator in a Method-of-Lines (Runge-Kutta, multistage) time-marching approach. In spite of their inherent crudeness, a staggered scheme is a practical choice when the equation system is large or unexplored and a Riemann solver may be costly or not even available.

While the Lax-Friedrichs scheme is only first-order accurate, the Tadmor-Nessyahu [101] scheme, formed on a more elaborate stencil, has second-order accuracy and is adequate for fluid dynamics. Particularly advanced are the formulations and applications of this method by the Canadian mathematician Paul Arminjon and students [6], who has used it as the basis of an efficient MHD code [7].

Much flow complexity in today's challenging applications derives from geometrical complexity. The use of unstructured, adaptively refined grids can solve the problems of discretizing space in the presence of complex boundaries, and making sure that the solution has the detail where needed. But on such grids conventional finite-volume methods lose or compromise at least one desirable property out of the following three: accuracy (one order is easily lost), monotonicity (oscillations arise in advection, or the maximum principle is violated in elliptic steady solutions), conservation (sometimes sacrificed for the sake of accuracy or monotonicity [31]). The higher the targeted accuracy of the method, the closer to impossible becomes the preservation of desirable properties. Thus, the use of the highest-order finite-volume schemes available, viz., WENO schemes, is restricted to fundamental flow research on uniform rectangular grids such as the study of turbulence (Direct Navier-Stokes or DNS simulations) or transition to turbulence [157].

The direction in which CFD methodology is currently evolving in the USA borrows generously from finite-element methods. Specifically, when expanding the subcell solution in terms of a set of basis functions, it is becoming commonplace to treat the coefficients of the expansion as independent quantities, each with its own update equation, rather than to compute these by interpolating the solution in the cell's neighborhood. This potentially allows one to maintain an arbitrarily high order of accuracy, which in turn may be used to counter the effects of poor grid quality. By trading the mesh size (h) for the order of accuracy (p) where the solution is smooth, and vice versa where intricate spatial detail asks to be resolved, one arrives at a so-called $h - p$ refinement strategy, also regarded as essential to modern CFD.

Examples of methods in this class are the vintage Discontinuous Galerkin (DG) method [117] and Spectral Element (SE) method [91], and the much more recent Spectral Volume (SV) and Spectral Difference (SD) methods, both developed by Zhi-Jian Wang [129, 87]. DG typically uses a polynomial basis per cell, whereas SE obviously uses harmonic basis functions. SV and SD define the subcell solution by discrete solution values, but there is a polynomial basis in the background. There is increasing evidence that DG, SV

and SD may be implementations of the same method by different quadrature-related formulas [63]; we may expect blending of the boundaries between these methods in the future.

DG is the oldest, most researched and most applied of the above methods, so it is worth being discussed here in more detail. Originally developed at LANL for neutron transport by Reed and Hill [117], it is a finite-element interpretation and implementation of the class of upwind advection schemes. It was developed independently in Europe by Van Leer ([140], Schemes III and VI), who extended it to a coupled space-time method, but at the time was unable to generalize this idea for a nonlinear hyperbolic system [141]. After that, the decelopment of DG for hyperbolic systems stalled for more than a decade.

Later applications to hyperbolic systems by Shu and Bernardo Cockburn [28], understandably, used the spatial DG operator in a semi-discretization, combined with multi-stage marching in time. It was not until 2004 that Hung Huynh [62] succeeded in formulating an explicit space-time scheme for the Euler equations that reduces to Van Leer's 1977 Scheme III for linear advection; it is more efficient than DG/Runge-Kutta [131].

DG schemes for hyperbolic systems, just as finite-volume schemes, include Riemann solvers to compute inviscid fluxes, and limiters to make the solution non-oscillatory. A bottle-neck in the development of high-order DG methods is the absence of limiters suited for DG; current limiters are borrowed from finite-volume methods [29] and are too crude to preserve the subtleties of the DG discretization, resulting in loss of accuracy. For piecewise linear 1-D solutions Huynh [62] has developed a satisfactory DG limiter, but it is not clear how to extend it to multiple dimensions. In fact, one of the great unsolved problems remaining in CFD, whether one regards traditional finite-volume methods or DG methods, is to develop a multidimensional limiter for piecewise linear solutions, usable on unstructured grids.

Fortunately it is *not* necessary to develop such limiters for piecewise polynomial solutions of a higher degree, owing to the development of *hierarchical reconstruction* by Yingjie Liu [86] and others. Here one takes derivatives of the solution to the point that the distribution becomes piecewise linear; after limiting this derivative the linear part of the next lower derivative is limited, and so on, all the way back to the original solution.

While DG for advection was inspired by upwind finite-volume schemes and benefited from the available Riemann solvers and limiters, applying the DG concept to diffusion terms — as needed when solving advection-diffusion or Navier-Stokes problems — is not natural and had to be developed without a leading example. As a result the methodology got mired in finite-element tricks. To define a unique diffusive flux at a point where neither the solution nor its derivative are defined, penalty terms were evoked, with little physical motivation. Going back as far as 1978, the first DG schemes for diffusion were inconsistent or marginally stable, until G.A. Baker [10] and Arnold [8] introduced a stabilizing interface penalty term. It took until 1998 before Shu

and Cockburn came up with the now popular Local DG (LDG) method [29], inspired by rewriting the diffusion equation as a first-order system of two equations. This procedure, though, squares the condition number of the operator's eigenvalues, and therefore causes an overly restrictive stability condition on the time step.

Not suffering from this drawback are the methods of Bassi and Rebay [12]; Darmofal and his DG group at MIT [36] combined LDG with the compactness of Bassi-Rebay, and named the resulting scheme Central DG (CDG). Finally, the DG-for-diffusion scene was swept clean by Van Leer and coworkers [149, 147, 115] through the development of the Recovery-based DG method (RDG). In this technique one recovers from the piecewise polynomial solution on a pair of neighboring cells a single higher-order polynomial that is indistinguishable from the former in the weak sense. Great economy results from applying this recovery procedure to the piecewise continuous basis functions on the pair of cells; in this way a smooth *recovery basis* is obtained that can be used throughout any fixed-grid calculation. The solution is expanded in terms of the recovery basis when computing the diffusive fluxes, and in terms of the discontinuous basis when computing the advective fluxes; the sets of expansion coefficients are *identical*. Huynh [64] has shown that CDG and Bassi-Rebay can be interpreted as lower-order approximations to RDG.

In recent years it has been recognized that multistage time-marching, though convenient and versatile, does not bring out the best of the DG discretization. Space-time DG appears to be the way to go, but so far has been used only for linearized equation systems, such as encountered in aeroelasticity [75]. Relevant is that Suzuki [131] has shown an order-of-magnitude increase in efficiency when combining the spatial DG operator with Hancock's time-marching method as formulated by Huynh [62]. The latter becomes a true space-time DG method when applied to a linear hyperbolic system, and may be regarded as a first iteration step toward space-time DG for a nonlinear system.

At the start of the 21st century there clearly is no lack of challenging research topics in CFD-method development.

5 CFD in Canada

Most developments in CFD described above took place in the US, many with contributions from new immigrants attracted to the US by growth in the CFD field. It bears mentioning, however, that Canada also has an active CFD community, including the CFD Society of Canada, which holds an annual conference. Fred Habashi, of McGill University in Montreal, serves as Editor-in-Chief of The International Journal of Computational Fluid Dynamics, one of the most respected journals in CFD. Other prolific Canadian CFD researchers include Paul Arminjon of the University of Montreal, David Zingg and Clinton Groth of the University of Toronto, Carl Ollivier-Gooch of the

University of British Columbia, Konstantin Kabin of the University of Alberta, and Jean-Yves Trepanier of Lécole Polytechnique Montréal.

6 Concluding Remarks

Within the scope of this contribution I have tried to narrate the story of four decades of CFD in the USA and Canada with emphasis on method development, and following the longer arches of research, rather than reviewing several hundred individual research papers. The perception of these lines of research, often intertwining and branching, and the perspective they offer, are mine, formed by my participation in CFD research during the entire period described.

Many names and contributions fell by the wayside – I apologize in advance to those authors, and to the readers who will not find their favorite references among those cited. I have had to skip entire subjects that were on my original ambitious list, having neither the space for these nor the time to complete the extra writing.

I hope that the chapter will offer some new historical insights to those working in CFD development and/or applications, and will raise the interest in CFD of those who only have a limited familiarity with the subject.

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European Numerical Aerodynamics Simulation Systems

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Summary This contribution gives an overview of methods used for flow simulation in the European aeronautical industry, where they are now widely accepted as analysis and design tools. However, in contrast to other industries, they are usually not provided by commercial software vendors but are developed, supplied, and maintained by national European Research Establishments. The status of the codes developed by the European aeronautical research centers ARA, CIRA, DLR, FOI, NLR, ONERA, and a code developed by Dassault is outlined, and some results of their application are highlighted.

1 Introduction

Numerical flow simulation has matured to a point where it is widely accepted as analysis and design tool in the European aeronautical industry. In contrast to other industries, the simulation methods used for aerodynamic analysis and design in Europe's aeronautical industry are usually not provided by commercial software vendors but are developed, supplied, and maintained by national European Research Establishments. One reason for this is that aerodynamic analysis and design requires very high levels of reliability and accuracy, which result from long time expertise and active research in numerics, modelling and validation. Also, a few aeronautical companies still use in-house software. In the following, we will give an overview of the major aerodynamics simulation systems currently in routine use. As a consequence, systems mainly developed and applied in an academic environment will not be considered. Furthermore, the focus will be on methods used in aerodynamic airframe design, whereas applications in the aerospace engine industry and general applications in e.g. the

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automotive or energy industry will not be taken into account. This overview does not claim to be exhaustive, and to avoid any bias the different systems will be presented in alphabetical order of the European nations of their origin. Large parts of this overview are based on the excellent review of Ref. [1].

2 France

The major CFD system developed in France is the multi-application *elsA* software system, which is developed by the French aerospace research center Onera in co-operation with Cerfacs and some other selected research partners, and which is used by several major aerospace companies, such as Airbus, Safran group, Eurocopter, MBDA, and others. The *elsA* software system [2] to [4] deals with complex external and internal flow simulations and multi-disciplinary applications like aeroelasticity, aeroacoustics, and aerothermics. The aim of the development of *elsA*, which started at Onera in 1997, was to group a very broad range of CFD capabilities available in legacy software in a new generation interoperable and evolving software package. Object-Oriented techniques were selected for designing a tool able to tackle industrial problems and to welcome further innovative CFD developments. Today, the large variety of CFD capabilities available in *elsA* is the result of the capitalization of research results during the last ten years.

The *elsA* multi-application CFD simulation platform solves the perfect gas compressible 3-D Navier-Stokes equations for arbitrary moving, possibly deforming, bodies, from the low subsonic to the high supersonic flow regime. A large variety of turbulence models from eddy viscosity to full Differential Reynolds Stress models (DRSM) is available in *elsA*. The range of turbulence models includes classical one-equation and two-equation transport models, more advanced two-equation models, multiscale four-equation models, one-layer or two-layer Explicit Algebraic Reynolds Stress models. Transition prediction capability is based on application of criteria that either were previously developed at Onera for use in boundary layer codes, or are issued from classical criteria from literature. These criteria allow the description of Tollmien-Schlichting instabilities (including laminar separation bubble predictions), cross-flow instabilities, bypass for high external turbulence rate, attachment line contamination, wall roughness [5]. In order to deal with flows exhibiting strong unsteadiness and large separated regions, the user can perform Detached Eddy Simulations (DES), Zonal Detached Eddy Simulations (ZDES), Delayed Detached Eddy Simulations (DDES), Monotone-integrated Large Eddy Simulations (MILES) and Large Eddy Simulations (LES) with subgrid models.

High flexibility advanced techniques of multiblock structured meshes are available in *elsA*. In addition to totally or partially coincident matching techniques, these advanced techniques include totally non-coincident (TNC) quasi-conservative matchings, "Hierarchical Mesh Refinement" technique, and

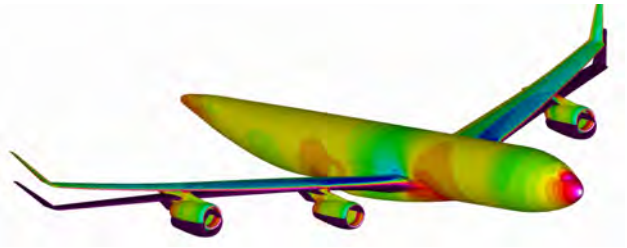
Chimera technique for overlapping meshes [6]. Besides these techniques, Onera is also pursuing the development of hybrid multiblock capabilities (including unstructured blocks) and of Cartesian solver capabilities.

The flow equations are solved by a cell centred finite-volume method. Space discretization schemes include second order upwind or centred schemes, and a third order Residual Based Compact scheme. The semi-discrete equations are integrated, either by multistage Runge-Kutta schemes with implicit residual smoothing, or by backward Euler integration with implicit schemes solved by robust LU relaxation methods [7]. An efficient multigrid technique can be selected in order to accelerate convergence. For time accurate computations, the implicit dual time stepping method or the second-order backward difference Gear integration scheme are employed. Preconditioning is used for low speed flow simulations.

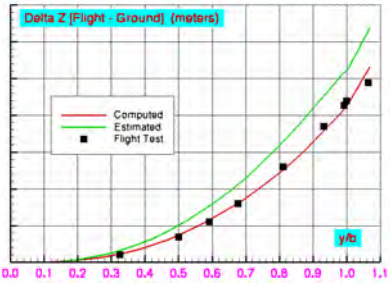
elsA also includes a module dealing with aeroelasticity [8]. This module allows harmonic forced motion simulations, static coupling simulations (using either a reduced flexibility matrix or a modal approach) and dynamic coupling simulations (using a modal approach). Linearized unsteady aerodynamic functionalities for structural harmonic motion are also available in *elsA*. A module dealing with calculation of sensitivities by linearized equation or by adjoint solver techniques is useful for optimization and control [9].

Today, *elsA* is a routinely used design tool in the process chains of aeronautical industry partners. Airbus has chosen *elsA* as multiblock structured CFD software at all European Airbus sites. In turbomachinery industry, *elsA* is used in the design teams of Snecma, Turbomeca and Techspace Aero. Figure 1 shows an example of an application for a static fluid/structure coupling simulation around a civil wing/body/pylons/nacelles aircraft configuration.

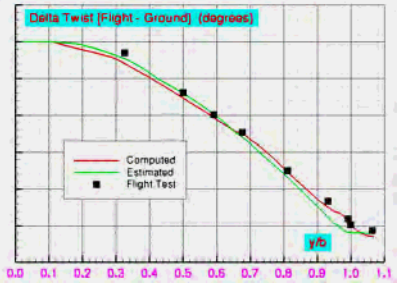
The French aircraft company Dassault Aviation develops and uses the in-house CFD software system Aether (for AEro-THERmodynamics). Aether is one of the very few finite element codes used in the European Aeronautical industry. It assembles elementary technologies from diverse partner research centers and universities. The Aether software [10] uses unstructured grids with an adaptive grid local refinement capability. It is based on a SUPG (Streamline-Upwind Petrov-Galerkin) formulation, with the Galerkin/least-squares formulation being a full space-time finite element approach. For steady calculations, time integration is carried out by a fully implicit iterative time marching technique using the GMRES (Generalized Minimal RESidual) algorithm. For unsteady calculations, time marching is carried out either by an implicit iterative algorithm, or by explicit Runge-Kutta techniques. In particular, the second-order-in-time implicit Gear scheme is available in the Aether software. The Dual Time Stepping method allows a steady solution of each sub-state resulting from an unsteady marching; this steady solution also relies on the GMRES-based implicit solver used for steady calculations. Aether is highly parallelized, and excellent scalability has been recently verified using up to a thousand processors.



a) Difference between computed flight shape and ground shape, and computed wall pressure field



Spanwise evolutions of bending deformation



Spanwise evolutions of twist deformation

b) Comparison between initial estimation, numerical simulation results and flight test data

Fig. 1. Transport aircraft: Fluid/structure static coupling simulation with *elsA*.

The Aether software deals with the Navier-Stokes equations completed by RANS or URANS turbulence models: one- or two-equation models relying on the Boussinesq hypothesis, EARSM and DRSM models, and semi-deterministic models. Among these models, the two-layer (k,ε) model with SST non-equilibrium correction is frequently used in Aether calculations. As one of the major research partners of Dassault Aviation, Onera contributes to transition and turbulence modeling in Aether. Recent developments in Aether [11] on LES and DES approaches have been performed to deal with aerodynamic design problems involving flows with strong non-equilibrium and high anisotropy. Novel subgrid scale models based on a variational multiscale approach have been implemented in Aether for LES calculations. Two versions of the DES approach (one based on the Spalart-Allmaras model, and the second on the (k, ε) model with SST correction) are currently in use. Aether provides capabilities for multiphysics simulations, such as fluid/structure interaction and optimum shape design [12].

This Aether software system is used for the aerodynamic design of business jets, military aircraft or space projects [13]. Aether includes several thermochemical models that are used for both space applications and the detailed thermal analysis of jets for Infrared Signature analysis. It was first applied to the design of the Hermes space plane. Recent applications include the aero-

dynamic design of the long range Falcon 7X, see Figure 2, or the Neuron UCAV.

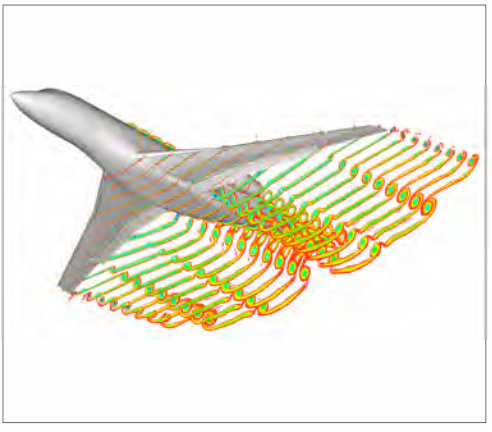


Fig. 2. Wake calculation of the Falcon 7X high-lift configuration with Aether.

As described in [14] for the Falcon 7X business jet, solution of the RANS equations is today routinely used for both design and identification phases of aircraft development at Dassault Aviation. More than 500 full aircraft RANS calculations were performed for the design of the Falcon 7X, relying on very efficient processes combining 3-D unstructured mesh generation, RANS solver and post-processing of the data.

3 Germany

In Germany, the aerodynamics simulation capability is represented by the MEGAFLOW software system, which is a result of several national German CFD projects initiated to meet the requirements of the German aircraft industry. Coordinated by the German Aerospace Center DLR, a network of aircraft industry, DLR, and several universities has been created with the goal to focus and direct development activities for numerical flow simulation towards a common aerodynamic simulation system providing both a block-structured (FLOWer code) and a hybrid (TAU code) parallel flow prediction and shape optimization capability, see Refs. [15] to [17].

With respect to mesh generation, DLR developed the block-structured mesh generator MegaCads as a tool for research applications. MegaCads features parametric construction of multi-block grids with arbitrary grid topology, generation of high-quality grids through advanced elliptic and parabolic grid generation techniques, construction of overlapping grids, and batch functionality for efficient integration into an automatic optimization loop for aero-

dynamic shape design [18]; however MegaCads does not provide automatic definition of block topologies. MegaCads was extended towards the generation of mixed, i.e. structured and unstructured meshes, where block-structured meshes with highly stretched cells are employed for boundary layer resolution and the outer field is discretized using tetrahedral elements [19]. For generating unstructured meshes, DLR uses the commercially available unstructured hybrid grid generation package Centaur, where DLR established a strategic cooperation with the Centaur provider CentaurSoft [20].

The major research effort at DLR is devoted to methods solving the Reynolds Averaged Navier-Stokes (RANS) equations, and DLR followes both the structured and the unstructured approach. The structured multi-block code FLOWer employs a second order finite-volume formulation on block-structured meshes using either the cell vertex or the cell-centered approach. For spatial discretization a central scheme combined with scalar or matrix artificial viscosity and several upwind discretization schemes are available. Integration in time is performed using explicit multistage time-stepping schemes. For steady calculations convergence is accelerated by implicit residual smoothing, local time stepping and multigrid. Preconditioning is used for low speed flows. For time accurate calculations an implicit time integration according to the dual time stepping approach is employed.

The influence of turbulence is modeled by a variety of turbulence models with major effort spent on Differential Reynolds Stress Models (DRSM), and Large Eddy Simulation capabilities were introduced. Transition prediction is enabled by a module consisting of a laminar boundary layer code and an e^N-database method based on linear stability theory [21]. FLOWer allows coupling to structural mechanics to compute configurations in aeroelastic equilibrium, where both high-fidelity models (ANSYS, NASTRAN) or simplified models (beam model and discrete structure solvers) can be considered. To enhance flexibility within the structured approach, the Chimera-technique of overlapping grids was implemented. For aerodynamic design, FLOWer includes an inverse design option based on prescribed pressure distributions, and for optimization the adjoint equations can be solved.

The unstructured, edge-based TAU code [22] uses unstructured hybrid grids, where the mesh may consist of a combination of prismatic, pyramidal, tetrahedral and hexahedral cells. To fully exploit the advantages of hybrid grids, a grid adaptation algorithm based on local grid refinement/derefinement and wall-normal mesh movement in semi-structured near-wall layers was implemented. Spatial discretization is based on either the primary or dual grid with implementation of a central scheme with artificial dissipation and several upwind methods. The hybrid TAU-code uses either explicit Runge-Kutta multistage schemes in combination with an explicit residual smoothing or a Lower-Upper Symmetric Gauss-Seidel (LU-SGS) scheme, and to accelerate convergence a multigrid procedure was developed based on the agglomeration of control volumes. Computation of unsteady flows is achieved by em-

ploying the dual time stepping approach, and for the calculation of low-speed flows the compressible flow equations are appropriately preconditioned.

The TAU code features a similar suite of turbulence models as the FLOWer code, and options are available to perform Detached Eddy Simulation (DES), eXtra-Large Eddy Simulation (X-LES), or Delayed Detached Eddy Simulation (DDES). Analogously to the FLOWer code, TAU enables transition prediction, provides coupling interfaces to structural mechanics for aeroelastic equilibrium with efficient mesh deformation techniques, and allows the use of the Chimera technique. The TAU code also features options for aerodynamic design such as an inverse design module, and allows for solution of the adjoint equations. The solution of the adjoint equations was also used to allow goal-oriented mesh adaptation and to provide reliable error estimation [23]. To further enhance efficiency, the TAU code is currently being extended to locally apply structured solution algorithms. The TAU-Code has been established at all European Airbus sites as the standard hybrid flow solver for complex applications.

To explore the potential of numerical methods beyond the state-of-the-art second order accurate TAU code, DLR pursues research on higher order methods based on the finite element Discontinuous Galerkin approach, with employing techniques for goal oriented mesh adaptation [24].

The MEGAFLOW software is intensively used at DLR and the German aircraft industry for many aerodynamic problems of fixed-wing aircraft and helicopters. Fixed wing applications range from cruise and high-lift transport aircraft configurations to maneuvering military aircraft. Figure 3 shows a TAU solution for the computation of vortices generated at the nacelle strakes of a large civil transport aircraft with deployed high-lift system [25], where the TAU mesh adaptation was extensively used for vortex resolution.

Due to the high efficiency for unsteady flows the FLOWer code was used to compute the flow around the NH 90 helicopter with trimmed and elastic main rotor [26]. The corresponding computational grid and the computed unsteady surface pressure distribution on the complete helicopter is shown in Figure 4. Since modeling of real gas effects is incorporated into the TAU code, it is also used for a variety of spacecraft applications, especially with respect to the complex aerothermodynamic phenomena of re-entry problems.

4 Italy

The Italian Aerospace Research Center CIRA has developed for more than 15 years the flow solver ZEN (Zonal Euler/Navier-Stokes) [27] which is integrated in the ZENFLOW computational system. The system is composed of a domain modeller ZENDOMO, a grid generator ZENGRID, and the ZEN code. Besides ZENGRID and other in-house methods, at CIRA the grid generation capability is also based on commercial codes. The commercial grid

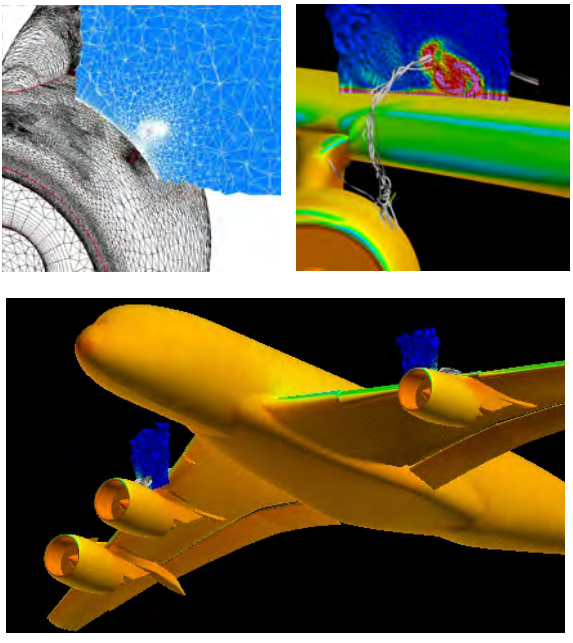


Fig. 3. Computation of nacelle strake vortices on a transport aircraft configuration.

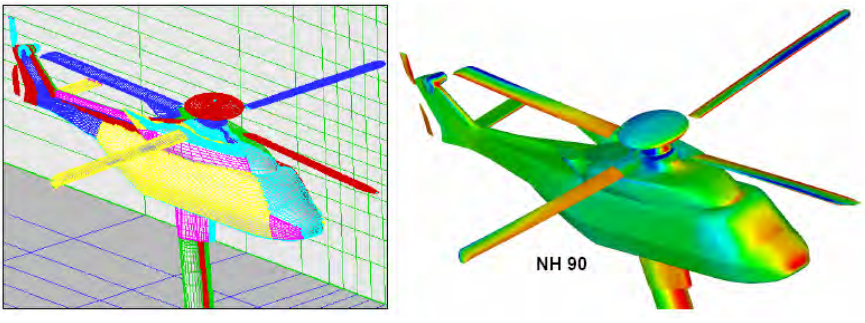


Fig. 4. Computational mesh and surface pressure distribution for the NH 90 helicopter.

generator ICEM-CFD is in use for multi-block structured grids and it has been interfaced with the flow solver ZEN.

The ZEN solver is based on multi-block structured grids and allows the aerodynamic analysis of three-dimensional configurations for subsonic, transonic and supersonic regimes. The flow modeling is based on the multi-zone approach, in which different equations can be solved in different regions. Three models are available: Euler, thin-layer Navier-Stokes and Reynolds-averaged

Navier-Stokes equations. Spatial discretization is performed by a second-order accurate, cell-centered, finite-volume method using central differences with an adaptive artificial dissipation model using a TVD switch. The discretized time-dependent system of equations is integrated towards steady state using an explicit Runge-Kutta scheme, accelerated by local time stepping, implicit residual averaging, and multigrid.

Substantial effort has been dedicated to the development of turbulence models and to validate their applicability to a wide range of flow problems [28]. The turbulence models most frequently used are: algebraic Baldwin-Lomax model, Spalart-Allmaras model, Myong-Kasagi (k, ε) model, Wilcox, TNT and Menter SST (k, ω) models. One of the implemented models is based on the adoption of a non-linear constitutive relation for the Reynolds stress tensor.

A new version (U-ZEN) [29] based on the U-RANS equations has been developed. The flow solver in U-ZEN uses the Dual Time Stepping method [30], where for the sub-iterations in pseudo-time the same techniques as in the steady version (ZEN) are employed. In addition, CIRA is completing the development of a U-RANS Chimera capability mainly dedicated to rotorcraft applications. The development of a method based on the use of Cartesian grids and specifically on the "Immersed Boundaries" approach is also launched at CIRA [32]. The flow solver has already been validated for the solution of inviscid flow, see Figure 5 and Figure 6, and laminar flows; at the moment the flow solver is being validated for the RANS equations with a wall turbulence modelling.

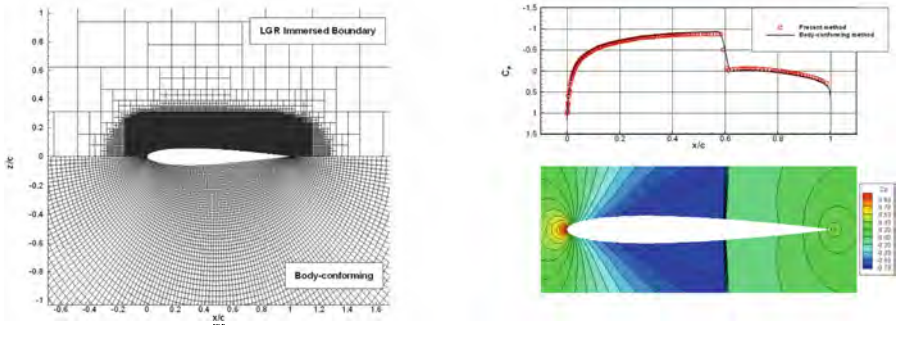


Fig. 5. Immersed versus body conforming grid and Euler solution around the NACA0012 airfoil.

The ZEN solver is heavily used at CIRA within the framework of national and European projects, and for activities contracted by Italian aeronautical industries. The ZENFLOW aerodynamic analysis system has been used in several applications; i.e. flows around launchers [33], high lift flow modelling [28], analysis of icing performance degradation [34]. For flow control applications, a CIRA synthetic jet model was shown to be able to reproduce, with

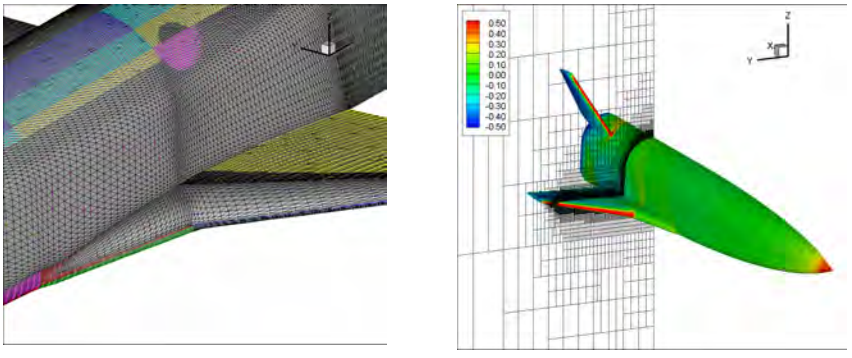


Fig. 6. Surface geometry, immersed boundary grid and Euler solution for the CIRA-USV.

satisfactory accuracy, the main steady and unsteady characteristics of a turbulent flow separation when controlled by synthetic jets [31]. ZENFLOW is also part of a software system for three-dimensional aerodynamic optimisation and has been used in the European projects AEROSHAPE and VELA. This versatile system is based on hybrid-type optimizers [35]. The flow solver codes are also included in a commercial MDO environment.

5 The Netherlands

The National Aerospace Laboratory NLR of the Netherlands developed ENFLOW, a complete system for the accurate simulation of 3D flows around civil and military aircraft and spacecraft, see Ref. [36]. The ENFLOW system is based on multi-block structured grids and allows the computation of both steady state and time-dependent flows. The ENFLOW CFD system consists of the ENDOMO domain modeller and the ENGRID structured grid generator as pre-processor, the ENSOLV flow solver, and the ENADAP grid adaptation tool [37].

The multiblock mesh generation is performed in a semi-automatic manner. Starting point of the process is the airtight representation of the geometries to be represented. In the multiblock approach the flow domain has to be discretized into curvilinear mesh blocks which have to be mapped to a computational domain. In the NLR structured grid generation process, first a Cartesian abstraction of the geometry description is created, and field blocks are generated in Cartesian space. The corresponding simple cubical blocks in the Cartesian space are then automatically mapped into physical space by a grid deformation technique. Grid quality is then enhanced by an elliptic smoothing algorithm.

Figure 7 gives an impression of the grid blocks in Cartesian space and the

corresponding grid in the physical domain. Details of the mesh generation process may be found in Refs. [38], [39].

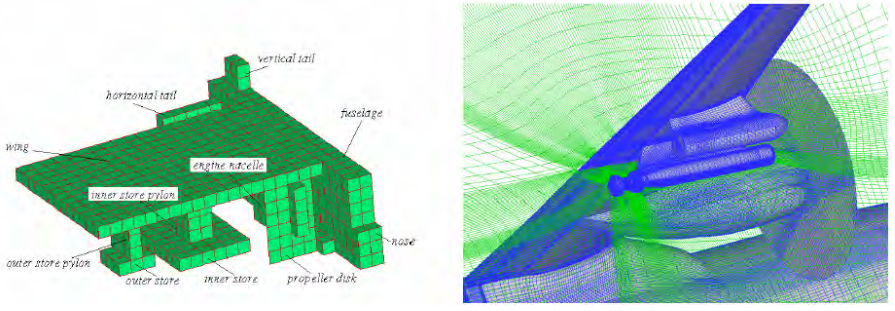


Fig. 7. Cartesian mapping technique and grid for a propeller aircraft carrying a torpedo.

The flow solver ENFLOW is capable of solving the Euler and Reynolds-averaged Navier-Stokes equations in multi-block grids for arbitrary configurations. The configurations under investigation can either be fixed or moving relative to an inertial reference frame, and can be either rigid of flexible. The flow equations are solved in full conservation form and are discretized in space by a second-order accurate, cell-centered, finite-volume method using central differences with scalar or matrix-based articificial dissipation. For steady flow simulations, the discretized time-dependent system of equations is integrated towards steady state using a five-stage explicit Runge-Kutta scheme, accelerated by local time stepping, implicit residual averaging, and multigrid. In case of time-accurate simulations, the flow solver uses the dual time stepping technique, where for the sub-iterations in pseudo-time the same techniques as for steady flow simulation are employed. The flow solver features a variety of turbulence models, including the Turbulent-Non-Turbulent (TNT) k-omega model [40], the EARSM model [41], and a hybrid RANS-LES model for eXtra-Large Eddy Simulation (X-LES) [42].

Applications of the ENFLOW system cover complex geometries as well as complex physics. In Ref. [37], dynamic aeroelastic simulations are performed to compute flutter and Limit Cycle Oscillations (LCO). Besides validation studies including flutter of the AGARD 445.6 wing, flutter and inviscid LCO of the NACA-64A010 airfoil, and LCO of the NLR-7301 airfoil, LCO are computed for the F-16 aircraft in a heavy store loading configuration. A detailed study of the complex flow physics was performed in [38] for the full-scale F-16XL aircraft, where emphasis was on capturing the complex vortex interactions at several flight conditions, see Figure 8. The capability of the ENFLOW system for multi-body simulations is demonstrated Ref. [39], where separation and trajectory of a torpedo released from a twin-engine propeller aircraft were analyzed.

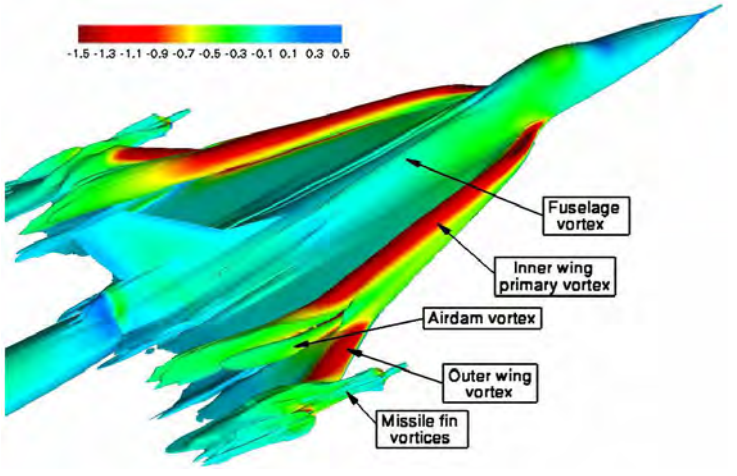


Fig. 8. Iso-surfaces of computed vorticity on a F-16 aircraft.

Besides following the structured grid approach, NLR is also pursuing the hybrid grid approach. In the European projects FASTLO I (1996-1998) and FASTFLO II (1998-2000), both coordinated by NLR, the objective was to develop a fully automated CFD system [43]. In this context, NLR developed a mesh generator suitable to provide inviscid and viscous hybrid grids. In combination with the DLR-TAU code, NLR used the FASTFLO mesh generator for the simulation of aeroelastic phenomena [44] and high-lift flows [45].

Another topic of current CFD research work at NLR is the development of a higher order code on the basis of the finite element Discontinuous Galerkin approach, where particular emphasis is laid on wake resolution of flows for helicopter applications [46].

6 Sweden

At the Swedish Defense Research Agency FOI, the CFD flow solver EDGE is being developed [47]. The code is developed and maintained by a team based at FOI and in collaboration with selected research partners. EDGE is the main CFD tool for Saab Aerosystems, where it is used in the JAS 39 Gripen program and other aerospace projects. The EDGE code was originally created in 1997 at FFA, the Swedish Aeronautical Research Institute, which in 2001 was merged into FOI. The development of EDGE has largely been motivated by Saab's need for a scalable, high-quality flow solver capable of handling realistic aircraft geometries. However, EDGE is also the foundation of a wide range of research activities both within FOI and elsewhere. The

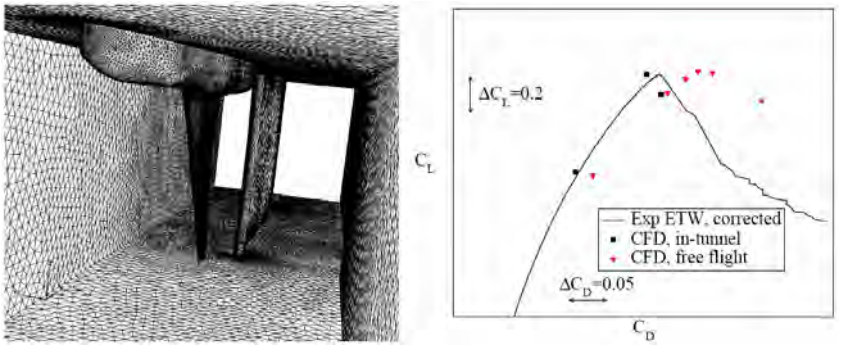


Fig. 9. Wind tunnel installation effects on a 3-element high lift configuration.

current EDGE system comprises the solver, pre-processor, and a large suite of supporting programs, see Ref. [48].

The EDGE flow solver employs an edge-based, finite-volume formulation, where the flow is represented by the compressible Navier-Stokes equations. The control volumes are defined on the dual mesh with each control volume containing a node of the primary mesh where the unknowns are stored. The dual mesh structure is generated by the EDGE pre-processor, which also performs agglomeration of control volumes for the multigrid, and mesh partioning for parallel applications. Discretization of the convective terms can either be performed by employing a central differences plus artificial dissipation scheme, or by using a second order upwind scheme. The viscous terms are split into normal and tangential operators, where for the thin-layer part a compact discretization following Ref. [49] is used. The discretized flow equations are integrated in time explicitly using a multi-stage Runge-Kutta scheme. Time-accurate solutions are obtained using an implicit dual time-stepping technique with explicit subiterations. A wide range of RANS turbulence models are available in the EDGE code, from the one-equation Spalart-Allmaras model, Explicit Algebraic Reynolds Stress Models (EARSM) [49], to full Differential Reynolds Stress Models (DRSM). Lately, also transition prediction models are being integrated and evaluated. Additionally, hybrid RANS/LES and full LES models have been implemented, [51]. Furthermore, the EDGE solver can also solve the adjoint equations, thus providing the basis for efficient shape optimization [52].

The EDGE code is applied within research and industrial projects. EDGE has been validated for drag prediction in the 2nd and 3rd Drag Prediction Workshops and is among the best codes for unstructured grids [53]. FOI is active in high lift applications of European projects like EUROLIFT II, and an example is given in Figure 9, where wind tunnel installation effects were investigated for a three-element high-lift take-off configuration [54].

Within Saab, the EDGE code was e.g. applied for aerodynamic analysis of the fighter JAS 39 Gripen, Figure 10, the aircraft Saab 2000, the UCAV demonstrator Neuron, and the helicopter Skeldar V150.

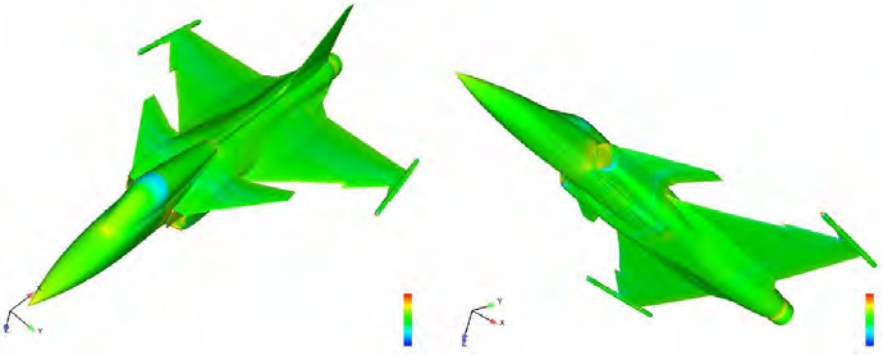


Fig. 10. Pressure distribution over the Gripen 39A fighter aircraft.

7 United Kingdom

The major CFD system developed and applied in the UK is the SOLAR CFD system. The evolution of SOLAR started in the 1990s, when the external aerodynamics community in the UK aerospace industry recognized that their existing systems were limited in meeting their needs. This resulted in a collaborative effort of research groups of Airbus, BAE Systems, the Aircraft Research Association (ARA), and QinetiQ (then Defence Evaluation Research Agency, DERA) to enable accurate, rapid-response viscous/turbulent flow predictions [55], [56]. Each team had experience of contemporary CFD systems including the BAE multiblock system RANSMB [57], SAUNA [58], FAME [59], and FLITE3D [60].

The SOLAR CFD system generates meshes well suited for turbulent flow prediction, since it has many qualities of a structured multiblock grid in the near wall region. The meshes that are formed by the SOLAR mesh modules MERCURY and VENUS predominantly contain hexahedra with less than 10% of other cell types. SOLAR meshes are created in two phases. First, a real space advancing front quadrilateral surface mesh is generated using MERCURY. The volume mesh is then generated in two separate phases using the VENUS module. First a partial volume mesh is generated by advancing layers of cells from the surface mesh to form the near wall mesh. Finally, in the original formulation, the far-field mesh is completed using an octree Cartesian algorithm mapped onto the grown layer using cut cell techniques. The background Cartesian mesh is refined using a background spacing file to

create a mesh with sensible sizes related to the geometry and other spacing requirements. Thus the SOLAR mesh predominantly consists of hexahedral cells with prisms and tetrahedra created as required to maintain mesh quality. The mesh contains 'hanging faces' where there is no longer a one-to-one mapping between neighbouring cells across a single cell face.

An alternative far-field mesh formulation has been created more recently, based on a tetrahedral mesh which is interfaced to the near-field mesh using a buffer layer composed of pyramids and tetrahedra. This approach gives conforming mesh element faces without hanging faces or nodes.

The flow solver JUPITER of the SOLAR CFD system solves the compressible three dimensional Reynolds Averaged Navier-Stokes (RANS) equations in strong conservation form. The flow solver algorithm is explicit with convergence acceleration by a multi-stage Runge-Kutta time stepping scheme with artificial dissipation and local time stepping. Convergence is further enhanced by the use of a suitable multigrid technique based on automatically generated agglomerated cells. The hybrid mesh is treated as an unstructured system, where the discretization uses the hybrid scheme described in [55] and data storage at cell centers. For the discretization of the inviscid fluxes, the CUSP scheme of Jameson is employed with careful construction of the required gradients for second order accuracy [56]. For modelling the influence of turbulence, the k-g model of Kalitzin, Gould, and Benton is implemented [61].

Both SOLAR far-field mesh formulations are acceptable to JUPITER. The tetrahedral far-field variant was specifically developed for compatibility with the TAU code.

The SOLAR system was applied to a variety of complex configurations, such as generic military wing body and civil transport aircraft, where the accuracy of the hybrid approach was verified by direct comparison with results from methods using purely structured meshes [56]. The capability of the SOLAR system for efficient automatic generation of high-quality hybrid meshes for viscous flow calculations was demonstrated in Ref. [62] for different application fields including power plant installation and store carriage and release, and Figure 11 gives a view of the SOLAR mesh generated around the Tornado military aircraft configuration using anisotropic sources.

In Ref. [63], the SOLAR mesh generation system was successfully applied to the semi-automatic generation of viscous meshes around two- and threedimensional high-lift systems. Although fully unstructured, the method proved to capture strongly directional flow features such as boundary layers and shock waves by employing highly anisotropic quad- and hex-dominated surface and near field volume meshes. In Figure 12 a view of the surface grid of the TC-217 high-lift configuration investigated within the European EUROLIFT program is given.

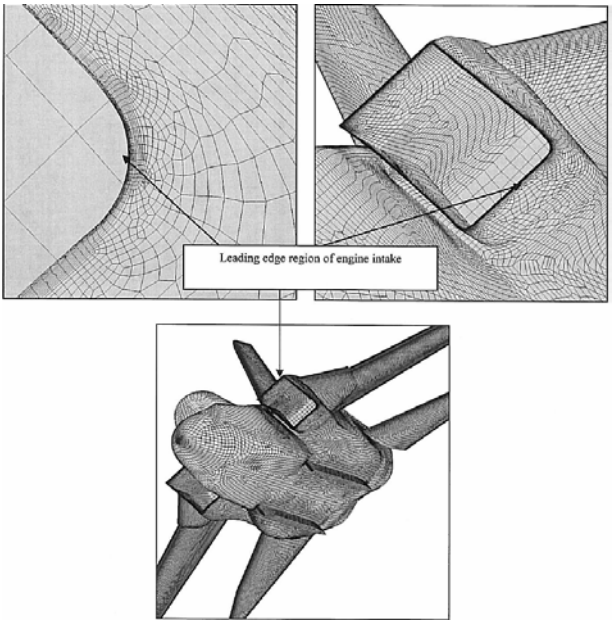


Fig. 11. Global and close-up views of surface grid for Tornado aircraft.

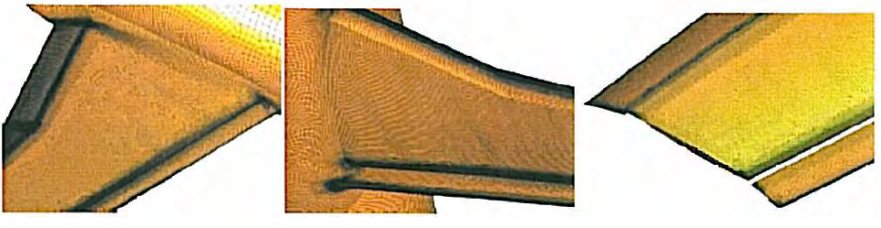


Fig. 12. Anisotropic quadrilateral surface grid on TC-217 high lift configuration.

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Numerical Aerodynamics in Transport Aircraft Design

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Summary Computational Fluid Dynamics (CFD) has become a vital tool for Aerodynamic Development. It has enabled sophisticated design optimization and comprehensive aerodynamic analysis of aircraft, and thus provides an effective means to cope with complex product requirements. Major applications demonstrate the essence and value of high fidelity CFD in a wide field. The outlook to future needs shows a high potential of CFD to lead to a complete change of paradigm of the work of the Aerodynamic Engineer which is strongly supported by upcoming development projects on simulation technology.

1 Introduction

More than 15 years ago massive use of 3D CFD started to find its breakthrough in aeronautical industry [1]. Step by step routine use extended from the simplified up to the most complex configurations and geometrical shapes. Furthermore, flow modeling improved from inviscid flow simulation to the standard use of Reynolds Averaged Navier-Stokes (RANS) equations with 2-equation or full RSM (Reynolds Stress Model) turbulence models. Now, flow modeling is on its way to DES (Detached Eddy Simulation) and LES (Large Eddy Simulation), although not ready yet for routine use in the industrial frame.

In the past CFD valued itself mainly through extensive use for aerodynamic cruise design. Wing and other components' shape design was mainly supported by all kind of approximative methods up to full Navier-Stokes simulations. But in recent years due to effective improvement [2] a tremendous increase has occurred in the use of CFD for many types of aerodynamic work (Fig. 1).

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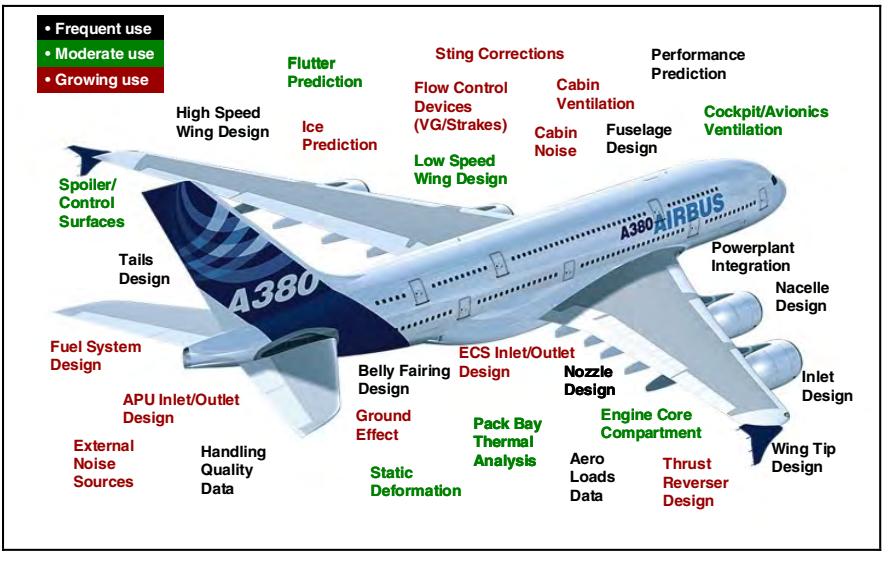

Fig. 1. Use of CFD in aircraft development at Airbus (from [3]).

The ability to tackle most complex configurations in acceptable time and with reasonable computational costs has also allowed high-lift design efforts to take considerable advantage of the capability. The next two areas that will be heavily influenced by CFD are the generation of aerodynamic data for loads and for handling qualities. Use of high-fidelity CFD in these areas is significantly growing.

In the distant future, it is plausible that numerical simulations will be performed for the whole flying aircraft, including all relevant disciplines. Sustained improvement of physical models, algorithms and hardware give rise to an optimistic view for the next 15 years [3].

2 The Design Task

Aircraft design makes – as is commonly observed for complex products – more and more use of numerical simulation. This capability essentially helps to find solutions which provide an optimum for the desired range of application in an economical as well as an ecological sense.

Overall aircraft configuration design is usually developed through an optimization process which has to rely on aerodynamic performance prediction based on theoretical/simplified aerodynamic models. This is due to the fact that the detailed shapes are developed later within the design process – based on a selected configuration.

CFD methods only come into play during the detailed design process. A typical application there is the assessment of the aircraft performance and to perform certain sensitivity studies around the major cruise design point. Mach flexibility, for example, is a typical topic for investigation (Fig. 2).

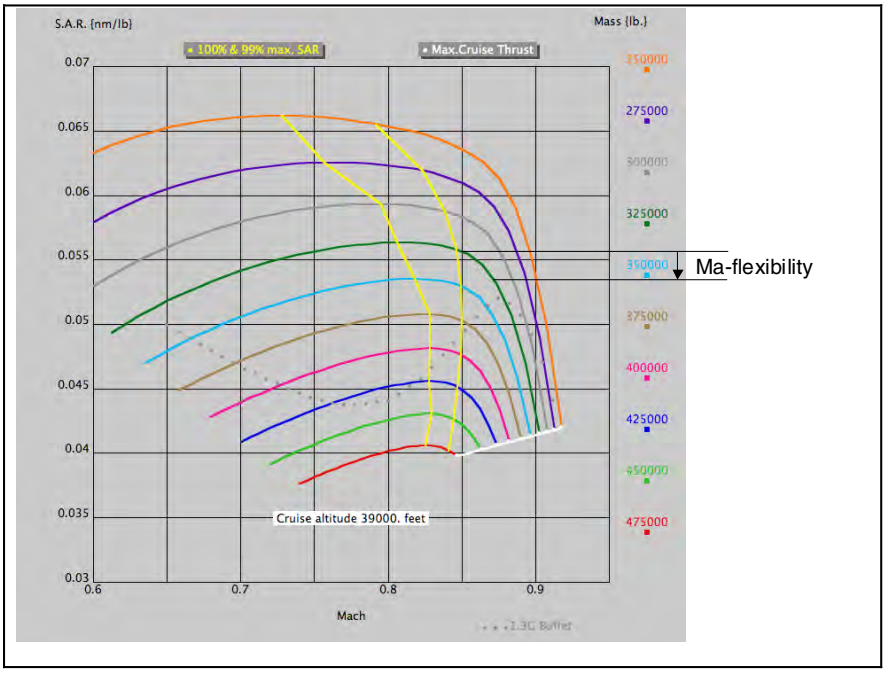

Fig. 2. Mach flexibility investigation.

The role of the wind tunnel is currently changing. It is moving from being a design tool to becoming a tool that validates the designs obtained through the use of CFD. Fig. 3 shows a typical example of the comparison of global lift and moment coefficients versus angle of attack. Overall excellent agreement over a range of Reynolds numbers convinces the aerodynamic engineer of the quality of his numerical tools.

CFD is also used for flight performance prediction which formerly was mainly based on wind tunnel data to provide incremental results relative to a baseline aircraft with known flight performance characteristics. Recent exercises have revealed that CFD based scaling seems to be as accurate as, or better than, wind tunnel based scaling (Fig. 4).

Figure 5 illustrates an example of routine use of CFD for the design and analysis of a typical aircraft in cruise [5].

This configuration consists of a wing, fuselage, pylon, engine group, empennage, and flap-support fairings. The engine group includes fan and core

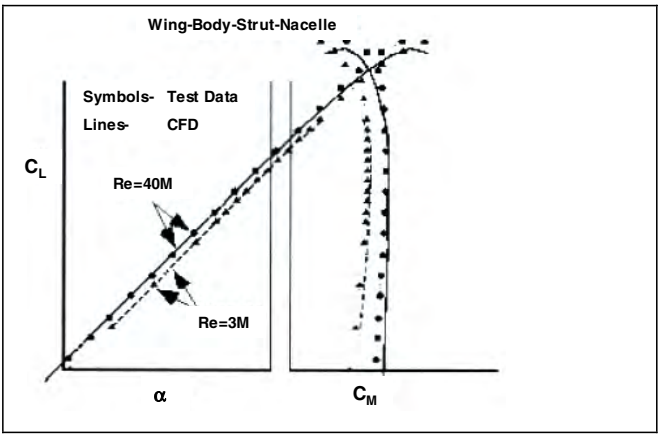

Fig. 3. Aircraft longitudinal characteristics – CFD data compared to wind tunnel data (from [4]).

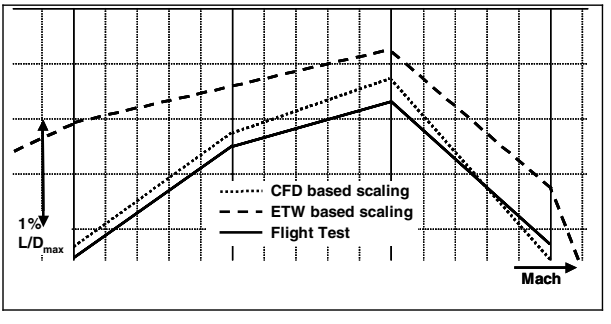

Fig. 4. Flight Performance estimates – CFD and wind tunnel prediction vs. flight test results (from [3]).

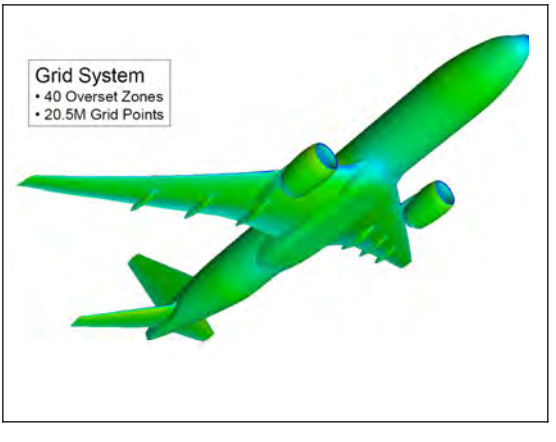

Fig. 5. Complete transport aircraft at cruise condition in static trim.

cowls with bifurcated flows; the power effects are represented with specified mass-flux and thrust related boundary conditions. The empennage consists of a vertical tail with rudder, and a horizontal tail with elevator. The CFD calculations are performed at a specified lifting condition with the aircraft trimmed to its center-of-gravity location. Hence, the angle-of-attack and the incidence of the horizontal tail (and corresponding geometry changes) are part of the solution process. The results of the numerical predictions of the absolute drag are within 1% of flight test data, which is comparable to the uncertainty of the flight data itself. This class of CFD applications is also being coupled with simultaneous computation of aero-elastic deformations.

CFD allows the designer to go into even more detail namely to analyze flows with respect to the physical properties and behaviors related to the aircraft. Surface pressure distribution information is important specifically for the analysis of component interference and proper integration design. Such information is sometimes not easy to obtain from wind tunnel tests, and CFD through its three-dimensional volumetric results can significantly help to understand the flow physics at very detailed levels (Fig. 6).

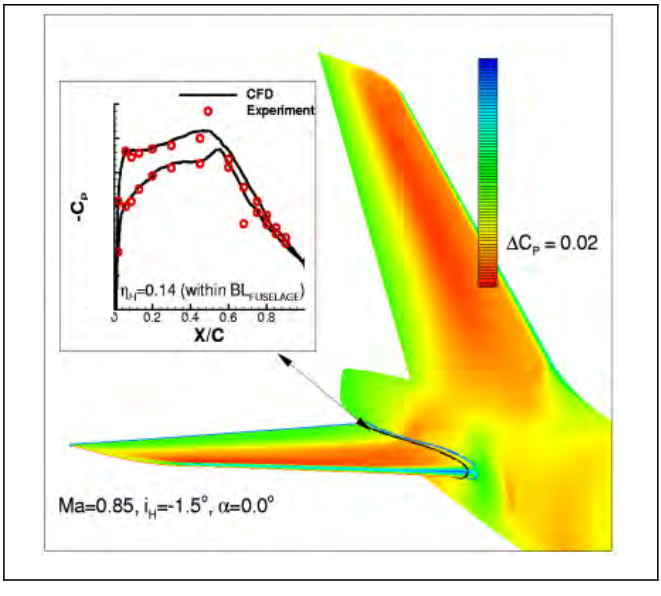

Fig. 6. Flow simulation for the rear end configuration – pressure levels – comparison of inboard section computed pressure with experimental values.

The numerical process is not confined to simulation but can also serve optimization loops. Various methodologies are appropriate for use in the aircraft industry to help finding best solutions for aerodynamic or even multi-disciplinary design optimization problems. The adjoint methodology provided

by Jameson et al. [6] to [9] is suitable to find optimum wing shapes, for example, (Fig. 7).

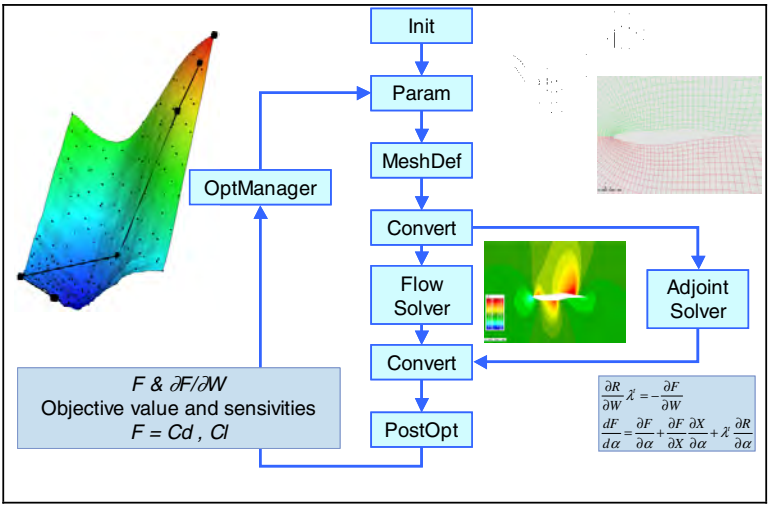

Fig. 7. Shape design process based on numerical optimization using adjoint technology.

For gradient-based search algorithms this technique delivers gradient information with a numerical effort that is independent of the number of parameters. On top of this, information is available on the sensitivity of the optimum towards variations of the single parameters.

Low speed design is a quite more challenging task. It normally deals with both, shape and configuration design. 'Shape' in this case means fixed wing or flap leading edges, whereas 'configuration' deals with slat/flap settings, mainly. Interesting areas are engine integration, multi-functional use of high lift components, simplification of high lift systems, et cetera.

A still challenging problem is maximum lift prediction (Fig. 8). From the physical point of view, separation onset as well as massive separation still poses severe difficulties for physical modeling and subsequently CFD.

Although geometry modeling has achieved a very high degree of complexity, there are still deficiencies between what we get from the wind tunnel and what CFD is telling us. A major rule to be followed has been evolving over the last years: The numerical model has to be as much as possible in line with the physical test arrangement. All single entries like tunnel walls and model support, exposed test equipment, wind tunnel conditions, CFD geometry, turbulence and transition as well as model deformations have to be taken into account. Otherwise detrimental effects will hinder a proper comparison and leave open space for speculations. Several investigations showed considerable improvement for the simulation of single effects (e.g.: half model effect [10],

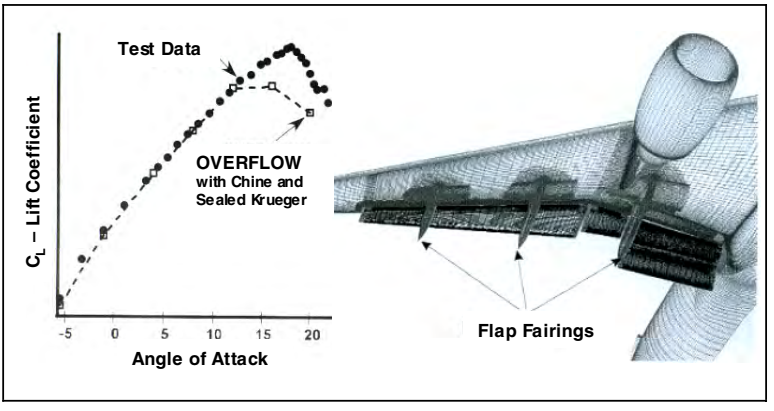

Fig. 8. Maximum lift prediction is still difficult (from [4]).

impact of measurement equipment [11]), however, we finally need all available information.

Integration of laminar-turbulent transition in the flow simulation seems to provide an essential improvement of the flow model. For high lift configurations, it must be recommended to neglect transition tripping in favor of the prediction method (see Fig. 9). However, proper calibration of the transition prediction method is a prerequisite for an accurate physical model.

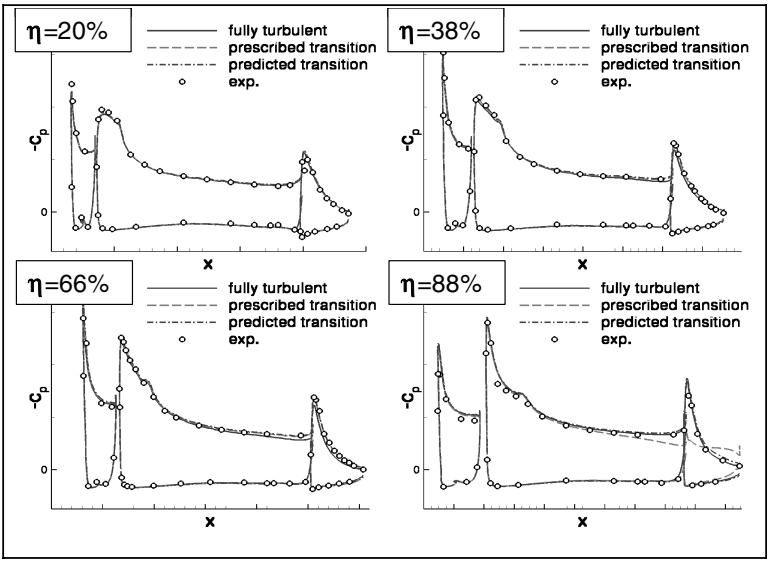

Fig. 9. Impact of integrated transition prediction on high lift wing flow simulation.

3 Aerodynamic Analysis of Flight

While in the past massive aerodynamic data production - for the full flight envelope and beyond - was in principal done by means of the wind tunnel, nowadays, numerical simulation enters this area for the development of an aerodynamic model of the aircraft. By nature, this model has to be complete and precise, as it enters the flight simulator, flight control and structural sizing. A typical analysis is concerned with the effect of airbrakes. Pressure coefficients are used to determine aerodynamic loads on these components and the whole wing. As can be seen in Fig. 10, the CFD based pressure prediction delivers results which fit very well with experimental values.

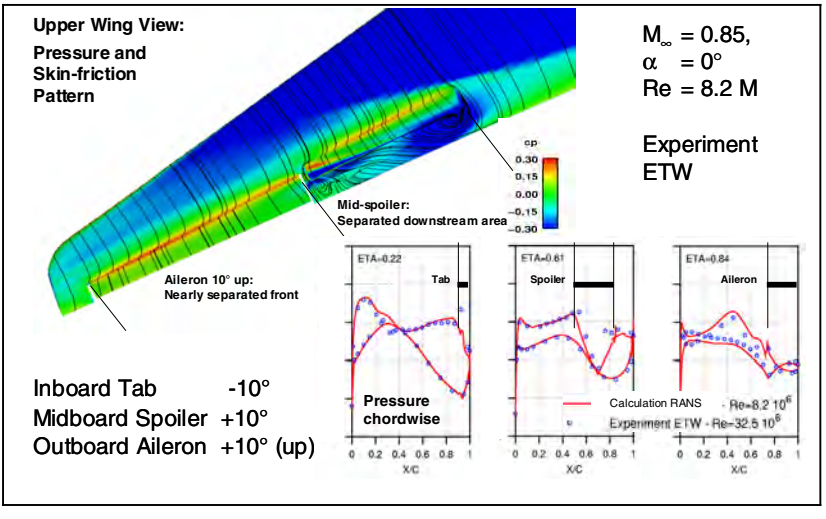

Fig. 10. Flow simulation for spoiler-out case – comparison of chord-wise pressure distributions with experimental values.

Aerodynamic coefficients for single components or the whole aircraft are of major interest for flight simulation. Specifically for tail planes these values determine the efficiency of such elements of the aircraft. As computations show (Fig. 11) it is possible to derive such values from numerical simulation. The results compare very well with experimental data and thus may be used with trust to even explore the parameter range beyond the situations investigated in the wind tunnel.

Massive computations have proven to be appropriate for validation and enhancing the prediction of the ground effect on aerodynamic data. It is quite obvious that wind tunnel measurements in this area are limited to some distance to the ground. They are also very complex because there is a moving ground necessary and the test is required with running engines (Fig. 12).

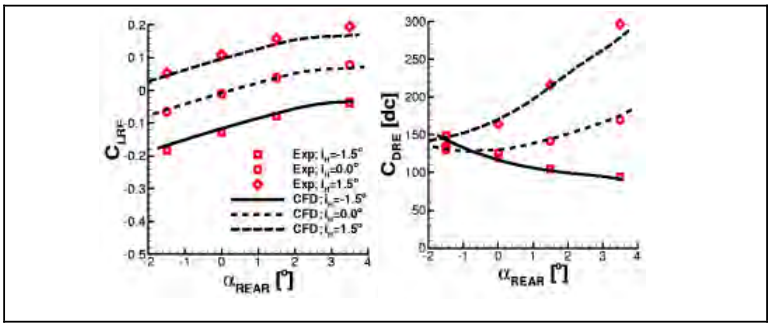

Fig. 11. Flow simulation for tail flows – lift and drag coefficients compared to experimental values along the angle of attack for three different incidences of the horizontal tail plane.

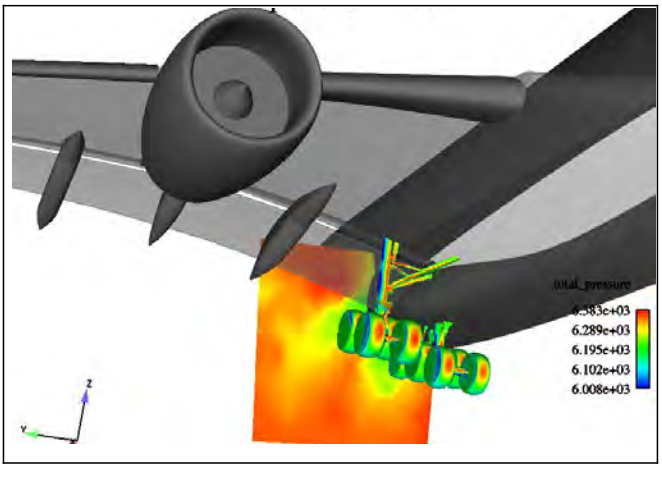

Fig. 12. Ground effect computations using hybrid Navier-Stokes CFD (full high lift configuration including undercarriage).

CFD it now helps to better understand certain aerodynamic effects. CFD based ground effect investigations therefore became an increasing application within the aircraft development process.

4 Problem Diagnosis

CFD is increasingly used to analyze complex flow situations. Fig. 13 shows a typical example: At what speed and directions does the airflow run through the interior of a military transport airplane in case of open paratroop doors and cargo ramp? How will persons inside be affected by the flow? Some CFD calculations simulating the case can yield an answer to those questions. Strong

vortical flow at moderate speed was detected with implications even to the far interior of the open cargo room. This result helped to understand the situation and adapt the design according to needs of the aircraft's customers.

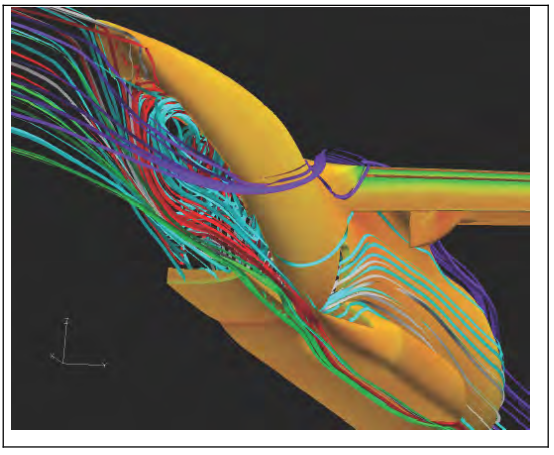

Fig. 13. Airflow through military transport aircraft at open parachutists door and cargo ramp.

Experimental investigation of this case wouldn't have made sense because an extra model with very specific 3D flow measurement equipment would have been necessary, not to speak of time and cost. Thus CFD appeared as a good alternative providing a lot of detailed information.

CFD could also help to investigate in areas where there is only restricted or even no access by measurement equipment. A typical example is the sting correction for wind tunnel models. By what amount has the drag coefficient measured at the respective gauge to be corrected due to inflow effects into the sting support chamber in the model. Fig. 14 shows a model with rear sting support. The sting does not fully close the hole in the model so that some flow can creep into the chamber. This flow will have an effect on the measured drag value because some forces apply to internal walls in main flow direction.

This analysis helped to find out the dependency of these forces on angle of attack and other parameters of the flow. Thus complete specific corrections could be developed.

5 Conclusion

Since some years, advanced CFD (RANS) made its way into routine use for aircraft aerodynamic design and data production. A steep gradient can be observed for the use of related methods and tools, including high performance

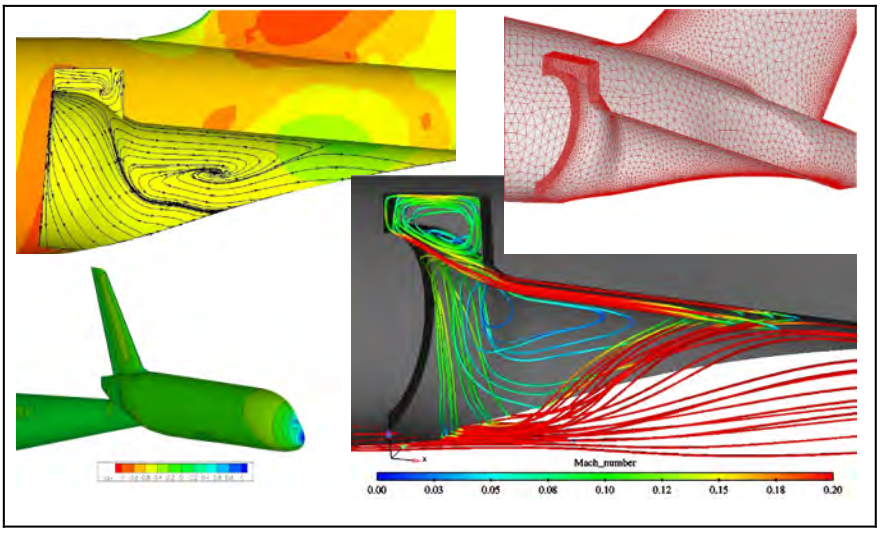

Fig. 14. Sting support impact analysis by CFD.

computers. The future could be imagined as providing full aircraft multidisciplinary simulation. Although a tremendous effort is still necessary, the past progress is fascinating. Industry – which is always a step behind academic research – has started to take full advantage of highly sophisticated models, methods and tools, in a comprehensive manner. And activities have been initiated to increase the power of numerical simulation by orders of magnitude within the next decade.

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Numerical Aerothermodynamic Design in the European Space Industry

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Summary In the mid 1980s France launched an industrial programme for the development of a winged space vehicle called HERMES. Approximately three years later HERMES became an European Program under the supervision of the European Space Agency ESA. This was the focal point for the begin of activities in the frame of numerical aerothermodynamics in particular in space industry. The companies Dassault Aviation, Aerospatiale, Saab, Dornier and MBB were partners in this project and have pushed forward in a special research program the physical modelling and the numerical methods for solving the governing equations of aerothermodynamics. After the run-down of the HERMES project somewhere in 1993 several smaller international and national activities were undertaken in order to further extend and harmonize the level of competence in this aerothermodynamics. Some of the projects and programs were the Crew Return Vehicle (CRV), the Manned Space Transportation Programme (MSTP), the X-38 project, the Technology for Future Space Transportation Systems (TETRA) and the PHOENIX demonstrator. This report addresses some details of the work in the above mentioned projects.

1 Introduction

In the last two and a half decades we have seen in Europe some demanding technology programs and development projects to broaden the design competence for evolving space vehicles. In the frame of the aerothermodynamic discipline these activities have moved forward:

- the physical modelling of high temperature real gas flow,
- the numerical methods in particular for hypersonic flow applications,
- the description of wall boundary conditions including wall catalycity,
- the generation of grids for complex vehicle configurations with deflected flaps, elevons and rudders,

E.H. Hirschel et al. (Eds.): 100 Vol. of 'Notes on Num. Fluid Mech.', NNFM 100, pp. 221–230.
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- the design of non-winged and winged vehicle shapes, for which aerothermodynamic data bases were established.

The focal point of these activities was the HERMES programme which was started in 1984 originally as a pure French project. In November 1987 this became an European programme under the supervision of the European Space Agency ESA. HERMES was a winged re-entry vehicle (RV-W).

Approximately at the same time in Germany and France studies were started with the goal to develop two stage to orbit transportation systems (TSTO). The lower stages of these systems are hypersonic winged airbreathing vehicles, also characterized as cruise and acceleration vehicles (CAV), [1]. Germany called this system SÄNGER [2], and France STAR-H [3].

After cancellation of these projects sometime in the years 1993-1994 Europe has taken part in the development of a Crew Return Vehicle (CRV) for the International Space Station (ISS) directed by NASA [4]. For this mission a lifting body was chosen, whose shape was based on the former NASA vehicle X-24A, and was named X-38. Such lifting bodies glide un-powered from an orbit along a given trajectory down to a specified altitude and conduct the final descent and landing by a steerable parafoil system. The parafoil system is a must, because the aerodynamic performance of a lifting body in the subsonic flight regime is too low for an aero-assisted terminal approach and landing, see, e. g., [5].

During the time between the end of the HERMES programme and the beginning of the X-38 project, in Europe a solution of the transportation problem to and from the ISS was considered on the basis of a non-winged re-entry vehicle (RV-NW), [6] to [9]. Such a vehicle could be either a classical capsule or a bicone.

European aerospace industry[1] was strongly involved in all these projects, in particular in the HERMES programme.

Most of the vehicles mentioned above were never built and flown with the exception that

- NASA conducted drop tests with some versions of the X-38 vehicle in order to test the subsonic aerodynamics and parafoil landing system [10],
- in Europe an Aerodynamic Re-entry Demonstrator (ARD) was developed and manufactured with which a suborbital flight was successfully performed [11],
- in Germany a winged demonstrator PHOENIX was built, which carried out a drop test to investigate subsonic flight and landing capabilities [12].

[1] Messerschmitt-Bölkow-Blohm (later Dasa and EADS-ST) and Dornier in Germany, Aerospatiale (later EADS-LV) and Dassault Aviation in France, and Saab in Sweden.

2 Particular Requirements on Physical Modelling

In the beginning of the 1980s the numerical methods for solving the various partial differential equations of fluid motion were not in such an advanced state, that three-dimensional solutions around complex configurations including high temperature real gas effects could be achieved[2]. The sets of equations mainly considered at that time are:

- the Euler equations,
- the boundary layer equations,
- the Navier-Stokes equations.

A great challenge was the mathematical formulation of physical models for the description of real gas flow in chemical and thermal non-equilibrium as well as in equilibrium, and to incorporate that in the corresponding numerical solution methods. In the frame of the research and development program, which had accompanied the HERMES project, intensive activities were conducted for improving the theoretical and numerical capabilities in this regard.

The results of this work are documented in the three volumes of the proceedings of the two Antibes workshops in 1990 and 1991 [13].

Another challenge was a proper mathematical description of turbulence for engineering purposes by models which are able to numerically simulate at least the main effects of the corresponding flow fields. The goal was to predict more precisely the pressure and the shear stress distribution along the whole surface of the vehicle in order to improve the accuracy for the determination of the aerodynamic coefficients. The same was true for the prediction of the heat flux from the gas to the wall and the wall temperature distribution, the so called thermal loads, which are decisive for the design of the thermal protection system (TPS).

Intensive work was done in this regard on European level in the frame of the Manned Space Transportation Programme (MSTP) in the mid of the 1990s [14], and the X-38 project in the second half of the 1990s, as well as on national level in Germany's Technology for Future Space Transportation Systems (TETRA) program in the years 1999-2001 [15], [16].

Today, one can summarize that indeed these activities have advanced the capabilities for the prediction of turbulent flows past space vehicles and as long as the flow is attached the numerically determined data have agreed often rather well with experiments [17]. But of course in regions with flow separation, e.g., on the leeward side and in the base area of space vehicles, the progress was somewhat lower in particular with respect to the flow topology. The prediction of laminar-turbulent transition remains as major problem.

[2] We address here, due to space restrictions, only two of the major physical problems, namely real gas effects and turbulence modelling. Of course there are a lot of others, for example the view factor approach of hot radiation cooled non-convex surfaces, laminar-turbulent transition, catalytic surface effects, jet/airflow interaction, et cetera.

3 Particular Requirements on Numerical Methods

As already mentioned in the last subsection, 25 years ago, the numerical methods for solving the governing equations of fluid dynamics were not able to treat properly hypersonic flows past complex space vehicles. To have a successful simulation procedure in this regard for industrial applications the numerical method must show at least the following features:

- conservation of mass, momentum and energy (enthalpy) in the flow field,
- proper treatment of discontinuities like bow and embedded shocks, shear layers, et cetera,
- full three dimensionality including gap, step and base area resolutions,
- resolution of regions of interactions between shocks, boundary layers, entropy layers and vortices,
- suitable formulations of boundary conditions for pressure, temperature (or heat flux) and wall catalysis including surface radiation for cooling purposes.

In the sequel of the development of advanced numerical methods these items were covered. For industrial purposes three methods were intensively applied to the aforesaid projects and programs[3]. These are ONERA's FLU3M/ NEQ code used by EADS-LV (former Aerospatiale) [11], the CEVCATS-N code of the DLR [18], [19], and the DAVIS-VOL code of EADS-ST (former Dasa) [15], [20], [21]. These codes have in common that they are based on the finite-volume approach and that they have used structured grids[4].

4 Presentation of Selected Results

The purpose of space vehicles consists in transporting payloads into the space, e.g. in several Earth orbits or beyond, and returning from it. In doing so the vehicles have to fly along ascent and descent trajectories, which are mainly characterized by strong variations of Mach number, angle of attack, flight path angle and atmospheric density. This has the consequence that the states of the flow fields along such trajectories differ substantially. Solutions of numerical simulations supporting the assemblage of the aerodynamic and the aerothermal data bases must have the capacity to do so in this wide parameter range.

In fact there exists a large number of numerical investigations and flow field solutions past several non-winged and winged space vehicles on various trajectory points. It is now the intention to present here some of them.

[3] Of course there are other codes from research institutes and universities but at that time they were not so significant in industrial design work.

[4] In the nearer past codes were developed using unstructured grids for improving the flexibility in the application to complex shapes like the *elsa* code in France and the τ code in Germany.

4.1 Non-Winged Space Vehicles

At first we will start with presenting numerical investigations of the flow fields past capsules, where our interest is focused on three items. Firstly, the influence of high temperature real gas effects on the aerodynamic coefficients of the ARD capsule, secondly the flow topology on the aft part of the VIKING capsule including the radiation adiabatic wall temperature distribution, and thirdly the heat flux in the stagnation point of the OREX probe. Fig. 1 shows the shapes of the three vehicles.

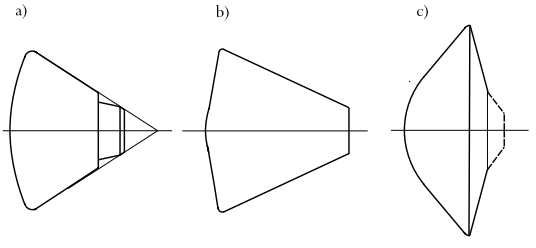

Fig. 1. a) ARD shape, b) VIKING shape, c) OREX shape.

Since real gas effects are so important for reliable entry flight from space, in the European Manned Space Transportation Programme (MSTP) strong efforts were undertaken to reveal this problem. More than 120 complete three-dimensional Euler and Navier-Stokes computations past the ARD capsule with perfect, equilibrium and non-equilibrium thermochemical state of the air were performed and compared with flight data [11], [22]. All computations were carried out for an angle of attack $\alpha = -20°$, Fig. 2.

The axial force C_x is best represented by the equilibrium assumption (upper left) and the normal force coefficient C_z by the non-equilibrium one (upper right). The aerodynamic performance L/D is not much affected, but the non-equilibrium state seems to be the appropriate on (lower left). Finally the trim angle α_{trim} in particular for high Mach numbers agrees fairly well with the non-equilibrium data (lower right). Indeed, for high Mach numbers the difference of α_{trim} between perfect gas prediction and flight data are more than 2°, which is in agreement with the observation during the APOLLO flights.

From a Navier-Stokes solution around the VIKING shape with $M_\infty = 3$, $H = 35\ km$, $\alpha = -25°$ the skin friction lines and the radiation adiabatic wall temperatures on the lower aft part of the body are shown in Fig. 3. The pattern of the skin friction lines is very complex. One can identify attachment and separation lines (left), which coincide well with regions of higher (attachments) and lower wall temperatures (separations) (right).

The authors of [23] report about numerical simulations with different physical modelling, which were conducted for flows past the OREX probe. In

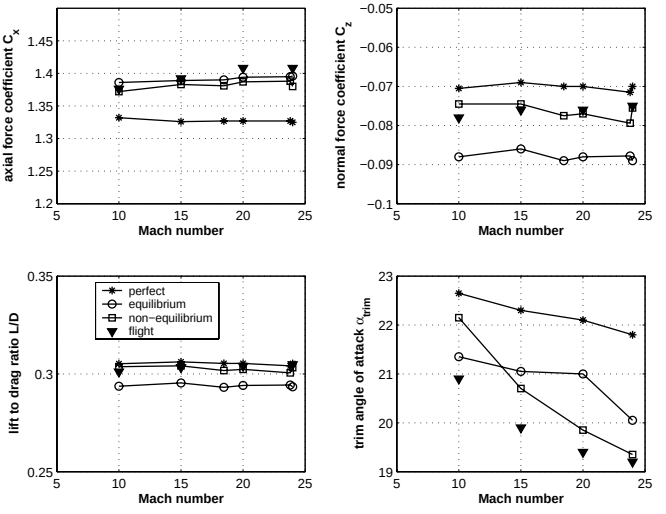

Fig. 2. Influence of high temperature real gas effects on the aerodynamics of the ARD capsule, angle of attack $\alpha = -20°$, [11], [22].

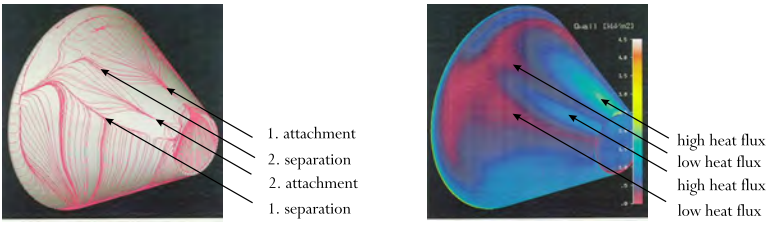

Fig. 3. Pattern of skin friction lines on the surface of the VIKING shape (left), radiation adiabatic wall temperature distribution (right), view from rear, $M_\infty = 3$, $H = 35\ km$, $\alpha = -25°$, [8].

particular it was investigated in what regime of the re-entry trajectory catalytic surface effects, slip conditions and thermal non-equilibrium gas states are important. The outcome was that for $105.0\ km \gtrapprox H \gtrapprox 84.0\ km$ slip flow and thermal non-equilibrium gas effects must be taken into account. The wall catalycity does not play any particular role, since the recombination probability is very low there. For lower altitudes the influence of thermal non-equilibrium and slip flow decreases and the wall catalycity becomes more important. The comparison of the predicted data at the stagnation point with data from OREX free-flight confirms unambiguously this trend, Fig. 4.

4.2 Winged Space Vehicles.

With Fig. 5 we demonstrate the advancements the numerical methods have undergone during the period of the HERMES project. At that time (1991-

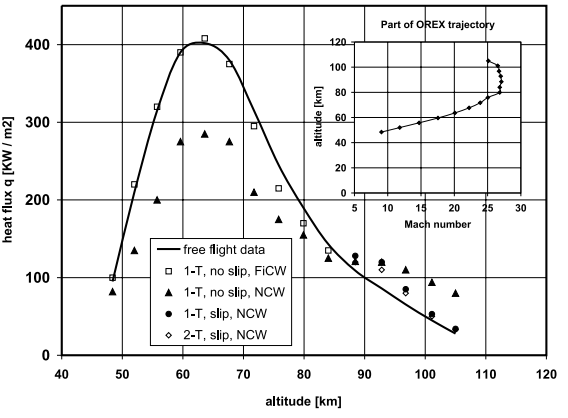

Fig. 4. Heat flux in the gas at the wall at the stagnation point of the OREX probe. Free-flight data and CFD analysis. FiCW; finite rate catalytic wall, NCW: non-catalytic wall, 1-T: one temperature model, 2-T: two-temperature model, [23].

1994), the industrial companies Dassault Aviation, Aerospatiale, Dornier, Dasa (former MBB) and Saab were able to produce fully three-dimensional solutions past the HERMES configuration with various physical modellings[5].

The plots a) and b) of Fig. 5 exhibit the evaluation of two Navier-Stokes solutions produced with the FLU3M code, [24], one with equilibrium real gas for $M_\infty = 25$, $\alpha = 30°$, $Re = 3.58 \cdot 10^5\,(\alpha)$, and the other one with perfect gas for $M_\infty = 10$, $\alpha = 30°, Re = 2.1 \cdot 10^6\,(\beta)$. The body flap and the elevons are deflected but without gaps between them. In a) the pressure distributions on the windward side are shown, whereas b) presents the skin-friction lines on the leeward side which give a first insight into the flow topology with separation in the wing area and attachment on top of the fuselage.

The effectiveness of the aerodynamic controls, body flaps, elevons and rudders, can only be determined accurately if the gaps between these devices are numerically modelled. Fig. 5 c) shows an equilibrium real gas Euler solution, where the flows in the base and the wake as well as between the gaps are simulated. Displayed is the Mach number distribution at the wall, [4]. Further Fig. 5 d) presents the probably first complete Euler solution (1990), with a non-equilibrium real gas approach around the HERMES shape.

Surely, the dynamics of advancement in the development of numerical methods for aerothermodynamics was reduced after the run-down of the HERMES project in the beginning of the 1990s. But nevertheless at the end of the last century a stabilization of the quality of numerical methods could be observed,

[5] Of course some of them did it with the support of the National Research Establishments ONERA, France and DLR, Germany.

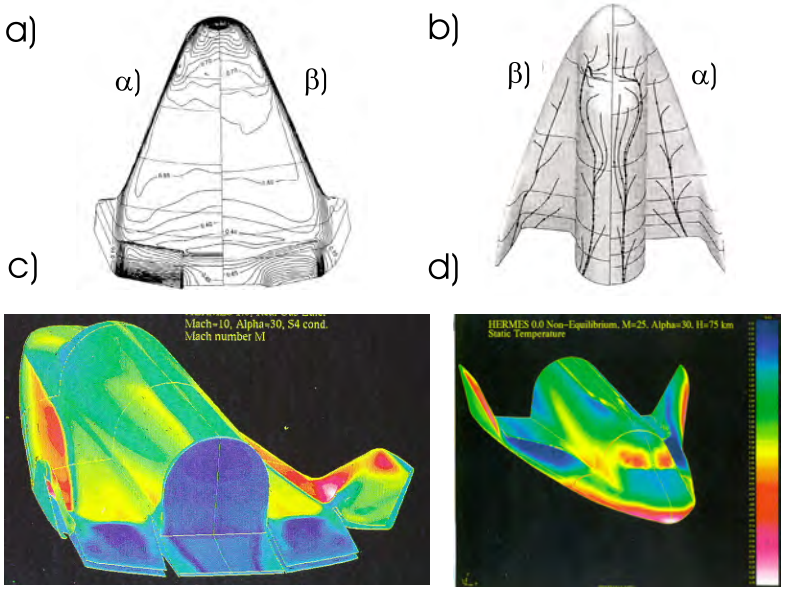

Fig. 5. HERMES flow field computations: Navier Stokes solutions using the FLU3M code, [24], a) pressure distribution on windward side, b) skin friction lines on leeward side; α) equilibrium real gas, $M_\infty = 25,\ \alpha = 30°,\ Re = 3.58 \cdot 10^5,\ \beta$) perfect gas $M_\infty = 10,\ \alpha = 30°, Re = 2.1 \cdot 10^6$; Euler solutions using the Dasa code, [4], c) Mach number distribution on surface, equilibrium real gas, $M_\infty = 10,\ \alpha = 30°$, d) wall temperature, non-equilibrium real gas $M_\infty = 25,\ \alpha = 30°,\ H = 75\ km$.

so that they are also used in the process of data base generation, [10], [22], [25]. Further the application of suitable turbulence models for engineering purposes has yielded first reliable results. We state this with Fig. 6.

A comparison of laminar and turbulent Navier Stokes solutions, achieved by the CEVCATS code, past the X-38 shape for $M_\infty = 6, \alpha = 40°, Re = 3.25{\cdot}10^6$, with a transition model being used, is shown in Fig. 6 a), [26]. The turbulent regime was computed by the one equation Spalart-Allmaras model.

A two equation $k - \omega$ based turbulence model (SST) was employed for the Navier Stokes computation with the DAVIS-VOL code for the same flow situation as above, [17], where a rapid transition was prescribed at the position where the flow was tripped in the LaRC experiment performed by NASA, [15]. Fig. 6 b) shows the comparison of the heat fluxes between the experiment and the numerical simulation, firstly as an isoline plot on the windward side and secondly as a x-y diagram along the marked line.

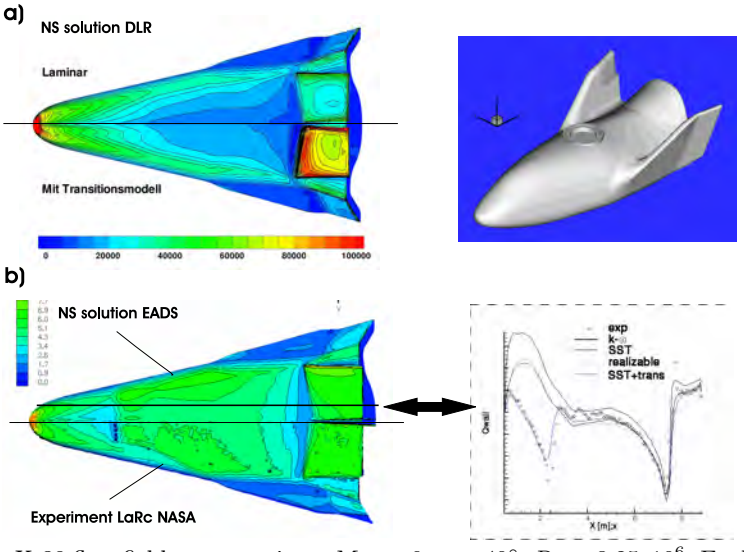

Fig. 6. X-38 flow field computations, $M_\infty = 6$, $\alpha = 40°$, $Re = 3.25 \cdot 10^6$. Evaluation of heat flux distributions on windward side: a) Navier Stokes solution using the CEVCATS code, [26], b) Navier Stokes solution using the DAVIS-VOL code, [15].

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The Second International Vortex Flow Experiment (VFE-2): Status 2007

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Summary In order to understand the vortical flow around delta wings especially with rounded leading edges and to collect new flow field data for comparison with numerical results, the Second International Vortex Flow Experiment (VFE-2) has been carried out in 2003 to 2008 within the framework of an RTO Task Group. The tested configuration was a flat plate 65° swept delta wing with interchangeable sharp and rounded leading edges. Five different models were tested in various wind tunnels worldwide. The program of work and some of the main experimental and numerical results are presented in this paper, and an outlook concerning future investigations on this configuration is given.

1 Introduction

The First International Vortex Flow Experiment (VFE-1) [1], [2] has been carried out in 1984 - 1986 on a cropped 65° delta wing-fuselage combination in order to validate the various Euler codes. It turned out that these were not well suited for the calculation of the pressure distribution on slender sharp edged wings, since the secondary separation is not modelled.

In the last fifteen years considerable progress has been achieved in the numerical calculation of vortical flows by taking into account viscous effects through solutions of the RANS equations. This means that Reynolds number effects are now included and secondary vortices turn out. However, the pressure distribution on the upper surface of the wing is very sensitive to the formation of the viscous regions of the flow field, especially the boundary layers and the secondary vortices [3]. For turbulent flows in solutions of the RANS equations a turbulence model is necessary, which has to cover both the attached boundary layers and the secondary vortex area properly. In order to validate the results of Navier-Stokes calculations new and more detailed

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experimental data are necessary, and therefore a Second International Vortex Flow Experiment (VFE-2) has been proposed in [4]. Since up to now most investigations of this kind were carried out for sharp edged wings, VFE-2 has been designed to concentrate mainly on wings with rounded leading edges.

2 Test Configuration

The configuration for VFE-2 has been chosen in such a way that all flow regimes (i. e. attached flow, separated vortical flow without and with vortex breakdown and separated deadwater-type flow) are covered properly, and this lead to a delta wing with a leading edge sweep of 65°. Concerning the thickness distribution a flat plate inner portion in combination with interchangeable leading edges was desired, and these requirements were fulfilled by the NASA configuration [5], which is shown in Fig. 1. Sets of one sharp and three rounded leading edges were available. The geometry of the wing as well as the shape of the sting is given by analytical expressions described in all details in [5]. New wind tunnel models could be built quite easily and overall aerodynamic coefficients and pressure distributions in certain cross sections were already available for a large variety of Reynolds numbers and Mach numbers [5], [6].

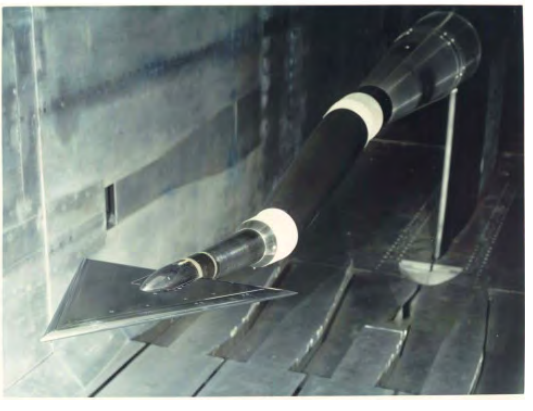

Fig. 1. 65° delta wing (A = 1.85) at cryogenic tests in the National Transonic Facility (NTF), NASA Langley Research Center [5] (By courtesy of J. M. Luckring).

3 Program of Work

The VFE-2 has been carried out within the framework of the RTO Task Group AVT-113 "Understanding and Modelling Vortical Flows to Improve the Technology Readiness Level for Military Aircraft". New experimental investigations were performed on various wind tunnel models:

- **Model 1** was on loan from NASA, USA, (Aerodynamic coefficients and PSI provided). It has been tested at DLR Goettingen, Germany, (PSP and PIV) and at ONERA Lille, France, (Forces and moments, PIV).
- **Model 2** has been built at TU Munich, Germany, (PIV and hot-wire investigations of the flow field). It has been tested also at DLR Cologne, Germany, under cryogenic conditions (PIV and IR/TSP for laminar/turbulent transition).
- **Model 3** has been built at Glasgow University, UK, (Unsteady force and pressure measurements at high angles of attack).
- **Models 4 and 5** (Sharp and rounded LE) have been built at ONERA Lille, France, (Forces and moments, pressure distributions, flow visualization, PIV). They were also tested at TUBITAK-SAGE Ankara, Turkey, (Forces and moments, laminar/turbulent transition).

The experimental investigations were accompanied by numerical calculations of the flow on structured and unstructured grids by the partners. All experimental results as well as the related numerical results according to the various computer codes were distributed among the participants by means of a Virtual Laboratory [7], [8].

4 Results

Results of the PSP investigations on model 1 obtained by the PSP team (R. Engler, Ch. Klein, R. Konrath) of DLR Goettingen, Germany, according to [3] are shown in Fig. 2 (M is the free-stream Mach number, R_{mac} the Reynolds number related to the mean aerodynamic chord (mac)). For the configuration

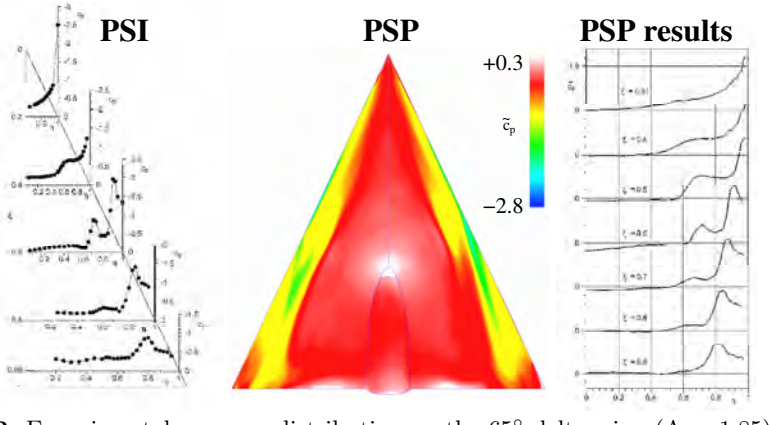

Fig. 2. Experimental pressure distribution on the 65° delta wing (A = 1.85) with rounded leading edges (medium radius) for M = 0.4, $R_{mac} = 3 \cdot 10^6$, $\alpha = 13°$. PSI and PSP results from DLR Goettingen ($\tilde{c}_p$ pressure coefficients without offset correction).

with rounded leading edges at $\alpha = 13°$ the flow is attached in the front part whereas in the rear part a vortical flow is established. It consists of two vortices on each side: A strong outer vortex and a weaker inner vortex both associated with corresponding suction regions on the wing surface.

Numerical calculations have been carried out at EADS Munich (W. Fritz), Germany, for the same case using the code FLOWER and the k-ω turbulence model. Some results are shown in Fig. 3.

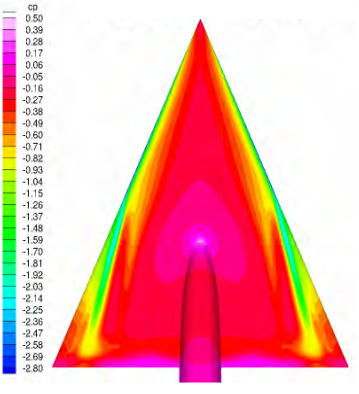

Fig. 3. Numerical pressure distribution on the 65° delta wing (A = 1.85) with rounded leading edges (medium radius) for M = 0.4, $R_{mac} = 3 \cdot 10^6$, $\alpha = 13°$. Results from EADS Munich, FLOWER code and k-ω turbulence model.

In spite of some differences regarding the position of the onset of vortical flow, the two-vortex configuration turns out very well. Surprisingly the inner vortex is as large as the outer one as shown in Fig. 4.

The outer vortex is fed by vorticity up to the trailing edge, whereas the inner vortex decays downstream more and more. The numerical results came up just after the PSP measurements at DLR Goettingen and they have been used as a guideline for the optical setup for the subsequent investigations of the PIV team (A. Schroeder, J. Kompenhans, R. Konrath) of DLR Goettingen, Germany. The results according to Fig. 5 show excellent agreement with the numerical findings.

The vortical flow field with a well developed single primary vortex on each side of the configuration has been investigated by means of PIV and HWA at $\alpha = 18°$ (no vortex breakdown) and at $\alpha = 23°$ (with vortex breakdown over the wing). Results for the time-averaged flow field and the velocity fluctuations are shown in Fig. 6 for the sharp leading edge case at $\alpha = 18°$ and in Fig. 7 for the rounded leading edge case at $\alpha = 23°$. In both cases the details of the unsteady flow field will be compared with numerical results in order to check the validity of the various turbulence models and of the prediction of vortex breakdown.

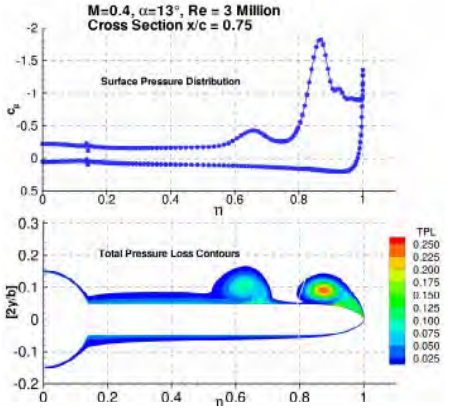

Fig. 4. Numerical pressure distribution and vortex pattern, described by total pressure loss contours, in the cross section at x/c = 0.75 for the the 65° delta wing (A = 1.85) with rounded leading edges (medium radius) for M = 0.4, $R_{mac} = 3 \cdot 10^6$, $\alpha = 13°$. Results from EADS Munich, FLOWER code and k-ω turbulence model.

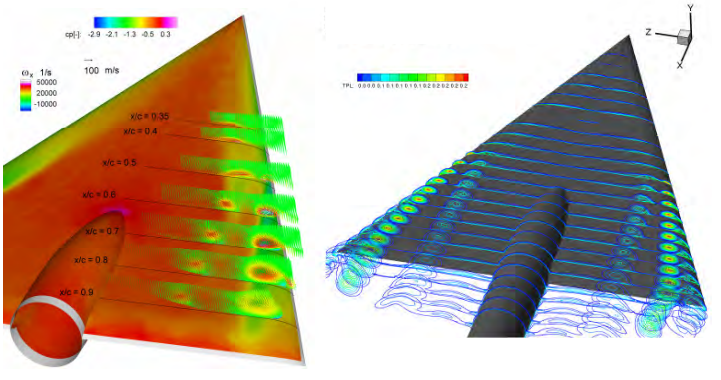

Fig. 5. Pressure (surface color), velocity (vectors), and vorticity (vector color) distributions above the 65° delta wing (A=1.85) with rounded leading edges (medium radius) for M = 0.4, $R_{mac} = 3 \cdot 10^6$, $\alpha = 13°$. Comparison of the PSP and PIV measurements at DLR Goettingen with the numerical solution of EADS Munich.

Towards the end of the working period of the RTO Task Group, many numerical results became available for the now existing experimental data.

For the calculation of the flow around a delta wing the fully developed vortical flow without vortex breakdown is the simplest case. For this reason $\alpha = 18°$ has been chosen for the VFE-2 configuration to be the standard case for sharp and medium radius rounded leading edges. All numerical codes applied on structured and unstructured grids were able to calculate this flow, and various turbulence models have been applied in these calculations.

At very large angles of attack the spiral mode of vortex breakdown takes place within the vortices over the wing. Studies of this phenomenon have been

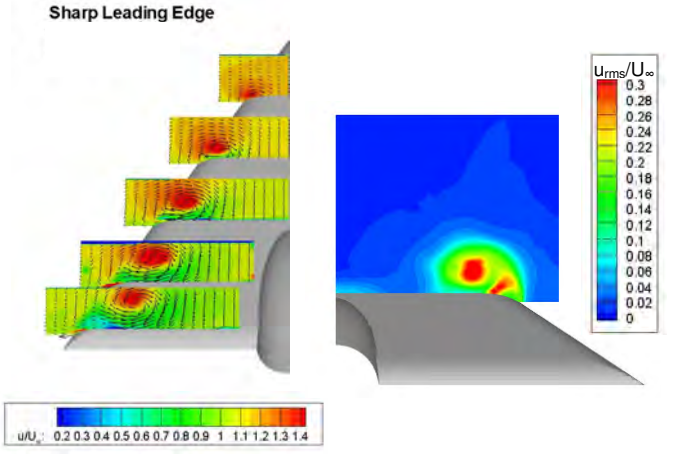

Fig. 6. Flow field around the VFE-2 configuration with sharp leading edges at M $\approx$ 0.1, $R_{mac} = 1 \cdot 10^6$, $\alpha = 18°$. PIV results for the time-averaged flow field (left) and HWA results for the velocity fluctuations at x/c = 0.6 (right) according to measurements by TU Munich.

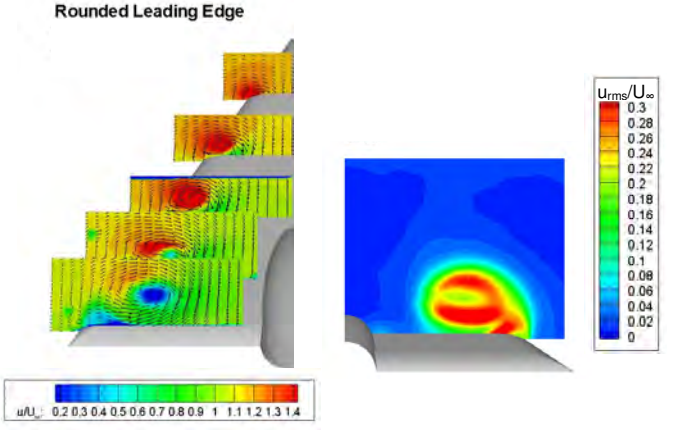

Fig. 7. Flow field around the VFE-2 configuration with rounded leading edges (medium radius) at M $\approx$ 0.1, $R_{mac} = 1 \cdot 10^6$, $\alpha = 23°$. PIV results for the time-averaged flow field (left) and HWA results for the velocity fluctuations at x/c = 0.8 (right) according to measurements by TU Munich.

carried out for $\alpha = 23°$ Due to the unsteadiness of the flow field time-accurate CFD codes have to be applied. In transonic flow in the vicinity of the sting mount of the VFE-2 configuration terminating shocks occur in the flow field, which lead to a considerable upstream shift of the vortex breakdown onset. From the very beginning of VFE-2 this phenomenon has been studied numerically, in the first place on structured grids, but later other members of the VFE-2 team joined with solutions on unstructured grids. The experimentally

detected effects of the shock waves on the vortex breakdown location in the flow field could be predicted nicely by various numerical methods.

The numerical simulation for the partly developed vortical flow on the VFE-2 configuration at $\alpha = 13°$ with two co-rotating vortices turned out to be the most difficult case. The first successful treatment of this problem within VFE-2 on a structured grid has been shown in Figs. 3 to 5. In the meantime also results for co-rotating vortices on unstructured grids are available. In this kind of solutions serious convergence problems have to be overcome, especially for low Reynolds numbers and low Mach numbers, and therefore further improvements on this subject are necessary. Due to the lack of experimental information about the onset of the inner primary vortex and the interference between the two vortices in the onset region of the outer primary vortex, reliable numerical results will play an important role in the understanding of the flow physics.

Fig. 8 shows latest (autumn 2007) calculated results on a structured grid by EADS Munich (left) and on an unstructured grid by DLR Braunschweig (right). It is expected that the detailed analysis of this kind of numerical solutions will lead a proper understanding of the flow structure.

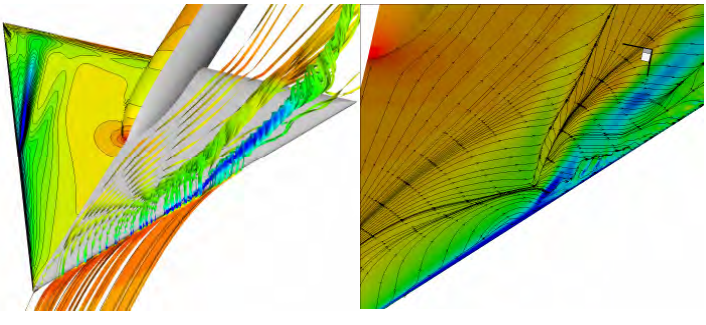

Fig. 8. Numerical solutions for the flow around the VFE-2 configuration with medium radius rounded leading edges at M = 0.4, $R_{mac} = 3 \cdot 10^6$, $\alpha = 13.3°$. EADS solution on a structured grid with pressure distribution and streamlines in the flow field (left) and DLR solution on an unstructured grid with pressure distribution and upper surface friction lines (right).

Up to now the Second International Vortex Flow Experiment (VFE-2) has been carried out within the framework of an RTO Task Group, in which specialists in CFD and in experimental techniques worked closely together. The Task Group of the RTO Applied Vehicles Technology Panel AVT-113 acted 2003 to 2008, and many results of the VFE-2 have been published so far, [9] to [32]. At the end of the RTO phase of VFE-2, main results of this cooperation have been presented in two sessions at the 46th AIAA Aerospace Sciences Meeting 2008, [33] to [47], and all results will be included in a Final Scientific Report to be published by RTO in 2008.

5 Outlook

The Second International Vortex Flow Experiment (VFE-2) will now enter a new, open phase: Many existing experimental and numerical results will be improved in the future, some inadequately treated problems should be considered anew, and even new tasks can be dealt with. In order to encourage future investigations the Final Scientific Report will provide some material: The VFE-2 configuration is very simple and described in analytical form. Therefore new wind tunnel models can be built quite easily. The Final Scientific Report will contain some experimental data for use in comparisons with future calculations, and in addition a structured and an unstructured starting grid will be included in order to promote new calculations.

The scientific community is invited to join this program for future work.

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Large-Eddy Simulations of Flow Problems of Aeronautical Industry

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Summary Stimulated by the developments in computer technology, numerical algorithms, and physical modeling large-eddy simulations have become more and more mature over the last couple of years such that they can be used to analyze even highly complex flow fields. In the following, a number of industrially related flow problems ranging from open channel flows to combustion chamber flows will be briefly discussed on the one hand, to underline the maturity of the large-eddy simulation approach and on the other hand, to get more and more engineers and scientists interested in the concept of large-eddy simulation.

1 Introduction

Due to the fantastic progress in micro-electronics, in the development of efficient numerical algorithms, and in grid generation methods it is nowadays possible to approximately solve the conservation equations of viscous laminar flows on a PC. This statement is completely different when turbulent flows are considered. The direct numerical simulation (DNS) of turbulent flows can even on today's fastest and most up-to-date machines using the most efficient algorithms only be performed at small Reynolds numbers in the order of $Re : \mathcal{O}(10^4)$. The reason for the drastically rising computational time, when turbulent instead of laminar flows are considered, is the pronounced extension of the temporal and spatial scales at increasing Reynolds numbers.

Since turbulence is always a three-dimensional phenomenon a spatial resolution, i.e., the number of grid points in three dimensions is proportional to $Re^{9/4}$ [1]. In turbulent flow the temporal scale also does decrease at increasing Reynolds number such that the computational effort is enlarged to $Re^{11/4}$. Keeping in mind that most of the technically relevant applications possess a Reynolds number in the range of $Re \approx 10^8$ an extremely powerful computer at 10^{23} $flop/s$ would be required to determine the turbulent flow field. Since

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such a machine will not be available in the near future, DNS will be restricted to fundamental turbulence research.

However, in many technically problems the engineer is only interested in mean distributions or integral solutions such as drag, lift, and heat transfer. That is, a statistical analysis like that based on the Reynolds averaged Navier-Stokes (RANS) equations suffices in numerous industrial flow problems. However, since a perfect and general turbulence model for the Reynolds stress tensor is still lacking, this is more or less implicitly proven by the vast number of varying RANS models [2] to [9], especially flows characterized by intricate phenomena such as unsteady separation and reattachment, complex vortical structures, swirl or rotation, streamline curvature, and transition cannot be computed at sufficient accuracy. Moreover, when finer and finer meshes are used it is the modeling that defines the quality of the final result. That is, if a certain accuracy is required a modeling level less limiting to the accuracy and at less computational effort than a DNS is a must.

The method of large-eddy simulation (LES) is such an alternative. Unlike in DNS only the large scales and their spatio-temporal development are resolved and the physics of the remaining small scales is modelled. The decomposition into large and small scales is often based on the existence of an inertial subrange in the energy spectrum. The smallest resolved scales are to be part of the inertial subrange and as such this condition defines the mesh resolution. The non-resolved vortices, which contain only a small amount of the total energy of the turbulent flow field, have to be modelled. This defines the advantage of the LES approach against the RANS ansatz. The physics of the small vortices can be considered more homogeneous and as such the models to describe the impact of these subgrid scale (SGS) structures can be much simpler than the RANS models. The numerous SGS models range, e.g., from the Smagorinsky model [10] via the structure function models [11], scale similarity models [12], dynamic models [13], approximate deconvolution models [14] to implicit subgrid scale models such as the MILES (monotone integrated large-eddy simulation) approach [15], [16]. General trends and novel developments of significant components of LES methods such as discretizations, SGS models, filter functions, boundary conditions etc. are discussed in various papers and books [11], [17] to [21]. These analyses not only show the susceptibility of the LES method to the overall numerical formulation but also the breadth of the LES applications. It is evident that LES is particularly well-suited for turbulent flows which possess a large scale unsteady character. That is, flow fields which cannot be computed sufficiently accurate by the RANS approach. In other words, transitional flows, vortex detachment, unsteady separation and reattachment and so forth are well-defined problems for LES.

2 LES Solutions

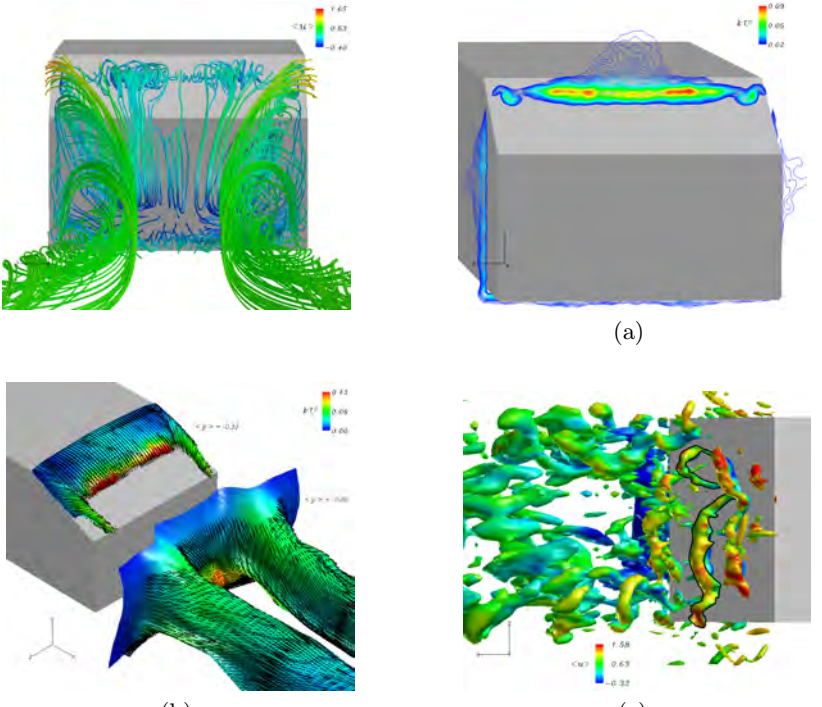
This statement will be substantiated by the following applications which show highly challenging fluid problems such as flows over car models, film cooling flows, coaxial jet flows, reacting flows in a combustion chamber, and the ignition process in a combustion chamber. The intriguing results the details of which are discussed in the literature [22], [23], [24], [25], [26] have been determined by large-eddy simulations. It goes without saying that the following findings represent only an excerpt of many fantastic LES solutions which have been published over the last couple of years. It is beyond the scope of this article to completely list and discuss these results.

2.1 Ahmed Body Car Model

Aerodynamic features of road vehicles are strongly characterized by intricate interactions between flow separations and pronounced trailing vortices in the wake. Therefore, a thorough knowledge of the physical mechanisms to generate such detachments and their interactions with wake vortices is a must to successfully design future cars at low fuel consumption. To analyze the aforementioned flow structures the Ahmed body [27] is often used as reference car model. Flows over this bluff body possess the fundamental aerodynamic features of cars. Its simplified shape enables a detailed comparison of experimental and numerical studies [28].

Recently, Minguez et al. [22] analyzed the flow field over the Ahmed body by a large-eddy simulation based on a multidomain Chebyshev-Fourier approximation. In the streamwise direction, the computational domain is decomposed into eight non-overlapping subdomains of different lengths depending on the flow region. The continuity of the solution at the subdomain interfaces is ensured by an influence matrix technique. In the vertical and streamwise directions a collocation Chebyshev method is applied and a Fourier Galerkin method is used in the spanwise direction. Three subdomains are wrapped around the Ahmed body. In each subdomain the space discretization consists of $41 \times 191 \times 340$ points in the streamwise, vertical, and spanwise direction. Consequently, the simulations are performed using approximately 21 million points. The temporal discretization is based on a fractional step method. It is globally second-order accurate and consists of an explicit transport step, an implicit diffusion step, and a projection step. The large-eddy simulation capability of the spectral solver makes use of the spectral vanishing viscosity stabilization technique [29].

The flow field at $\mathrm{Re} = 768000$ evidences complex time-dependent and highly three-dimensional flow features around the Ahmed body. It is shown in Fig. 1 that the flow separates at the edge of the slant surface and tends to reattach on the slant back. The recirculation zone possesses a nonconstant thickness in the spanwise direction at a weaker intensity and smaller size around the streamwise symmetry plane.



(a) (b) (c)

Fig. 1. Visualization of the vortical structures in the wake of the Ahmed body at a Reynolds number $Re = 768\,000$: (a) Mean three-dimensional streamlines in the wake colored by the mean streamwise velocity $\langle u \rangle$; (b) contour of the turbulent kinetic energy k on the slant; (c) contours $\langle p \rangle = 0.25$ and $\langle p \rangle = -0.07$ of the mean pressure colored by the dimensionless turbulent kinetic energy k, the velocity fields on the slant and in the wake are shown; (d) contours of the pressure fluctuations colored by the mean streamwise velocity $\langle u \rangle$ on the slant and in the wake. Contours of structures reminiscent of horseshoe vortices are highlighted by solid lines. (Courtesy of M. Minguez et al. [22]).

The contours of the turbulent kinetic energy indicate the recirculation to be divided into two bubbles. At the edge of the slant two confined regions are observed where the turbulent kinetic energy peaks. At the edges between the slant and the lateral surfaces of the Ahmed body two large counterrotating cone-like trailing vortices develop. These trailing vortices coincide with the lowest pressure regions in the flow field. They interact with vortical structures over the slant. The Kelvin-Helmholtz instability occurring in the shear layer downstream of the edge of the slant generates vortices the axes of which are almost parallel to the separation line. These vortices propagate downstream. The spanwise variance of the slant recirculation slightly lifts these structures approximately midway down the slant. The contours of the instantaneous pressure fluctuations evidence their shape to be similar to classical horseshoe

vortices. The interaction of the large trailing vortices with the smaller horseshoe vortices generates helical structures rolling up around the trailing wake vortices.

2.2 Film Cooling

To ensure a high thermal efficiency and an extended life cycle for the next generation of gas turbines advanced cooling techniques have to be used which protect the surfaces of the gas turbine components from the hot fluid. The most commonly used technique is the so-called film or effusion cooling where the cooling film is generally created by bleeding of low temperature fluid through discrete holes or rows of evenly spaced holes. From a fundamental point of view the flow physics equals the jet-in-a-crossflow problem, where a fluid exiting a round or rectangular orifice interacts with a transverse outer flow. The resulting highly intricate flow field is characterized by jet shear layer vortices, horseshoe-like cortices, kidney vortices, wake vortices, and other time dependent structures such that the detailed analysis of the mixing process of the coolant and the outer flow is an ideal challenge for a large-eddy simulation.

In a sequel of papers [30] to [31] full large-eddy simulations were performed to analyze the flow structures at various configurations and flow parameters. That is, not only the flow from the plenum through the cooling pipes but also the incoming boundary-layer are computed by an LES. This approach is pursued to avoid problems such as discontinuous solutions in the wall-shear stress distributions. Therefore, an independent spatially developing boundary layer simulation is performed. Based on a slicing technique, the inflow distribution is prescribed using the velocity profile possessing the boundary-layer parameters necessary at the inflow boundary of the jet-in-a-crossflow problem. The auxiliary flow simulation generates its own turbulent inflow data using the compressible rescaling method. The flow field is extracted from a plane near the domain exit and rescaled by some appropriate laws and reintroduced as a boundary condition at the inlet. This procedure results in a straightforward spatially evolving simulation which generates its own inflow data.

The LES method is second-order accurate in time and space. The discretization of the inviscid terms is based on an upwind-based approximation in conjunction with an advection upstream slitting method. The diffusive terms are approximated by a centered scheme. A five-stage Runge-Kutta method is used for the temporal integration. To achieve a high rate of convergence also at low Mach numbers an implicit dual-time stepping scheme plus preconditioning completes the numerical method.

The simulations are performed on block-structured meshes. The grid consists of 12.3 million cells distributed over 40 blocks. The grid points are clustered near the walls. To obtain the time-averaged statistics the flow field is sampled over eight time periods. The operating conditions are been based on a hot gas Mach number of $Ma = 0.2$ and the flat plate Reynolds number at the first row is $Re = 400000$. The velocity ratio between the jet and the crossflow is $u_j/u_\infty = 0.28$ and the static temperature ratio is $T_j/T_\infty = 0.44$.

Fig. 2 shows contours of the mean streamwise velocity at several cross sections. The deflection of the turbulent boundary layer by the first row of cooling jets is evidenced. The velocity field in the interaction region downstream of the first cooling row is anisotropic at strong velocity gradients in the normal and spanwise direction. The injection of the coolant causes a fast growing boundary layer such that the more downstream cooling jets penetrate deeper into the crossflow.

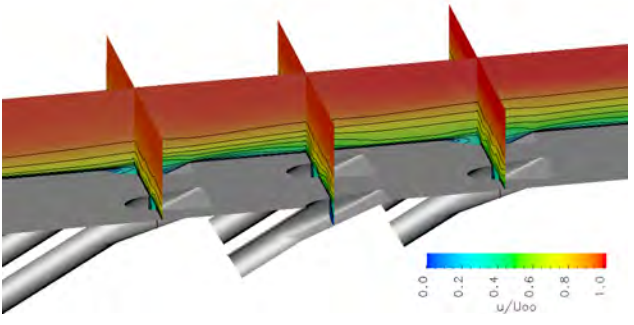


Fig. 2. Mean streamwise velocity at several cross sections.

A snapshot of the instantaneous temperature field at a ratio $T_j/T_\infty = 0.44$ is illustrated in figure 3. The red contours evidence the crossflow temperature level and the blue contours which cover the surface emphasize the lower temperature determined by the coolant. A closer look reveals the weak spanwise effectiveness of the cooling film downstream of the first row and the regeneration of the cooling film through the following jets. Such computations are used to analyze highly intricate temporal and spatial flow structures which can be hardly captured by any measurement.

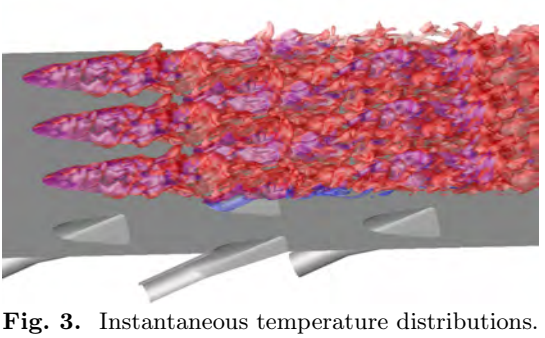


Fig. 3. Instantaneous temperature distributions.

2.3 Coaxial Jet

Due to the increasing air traffic airports all over the world become larger and larger resulting in a continuously growing exposure to air traffic noise in

populated areas. Certification of new aircraft is based on constraints on noise generated by air traffic. At take-off the noise level is primarily determined by the turbulent jets emanating from the engines. These turbulent jets are free shear flows, i.e., mean flow gradients develop in the absence of surfaces. The jet flow is characterized by a main flow direction which possesses a significantly greater velocity than the normal direction. Likewise the gradients in the normal direction are much larger than those in the streamwise direction. High-velocity fluid is permanently ejected through a single or a multi-stream jet. When the fluid exits the nozzle the flow is fully aligned with the nozzle wall and a potential core flow develops. At a single-stream jet a free shear layer is generated between the high-speed fluid and the surrounding fluid downstream of the nozzle lip. The thickness of this shear layer is determined by the boundary layer at the nozzle exit. The entrainment of ambient fluid causes the shear layer to spread in the downstream direction. Simultaneously, the radial extension of the potential core decreases and the flow becomes more and more turbulent. Right downstream of the potential core the jet is fully turbulent.

In the following, the flow field and the acoustics of a transonic coaxial jet with a heated primary stream are studied. The detailed analysis has been presented in [24]. The static temperature in the primary stream is roughly three times higher than the temperature of the secondary stream, i.e., of the bypass flow, the temperature of which equals the ambient temperature. It goes without saying that such a configuration possesses large temperature gradients in the shear layer between the primary and the secondary stream. The jet Mach number of both streams is approximately 0.9. The nozzle geometry and a slice through the computational domain is shown in Figs. 4 and 5.

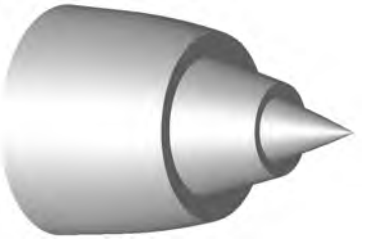


Fig. 4. The nozzle geometry. (Courtesy of N. Andersson et al. [24]).

The Favre-filtered Navier-Stokes equations are solved using a finite-volume method. The solver is based on a third-order low-dissipation upwind scheme for the convective fluxes and a centered difference approach for the diffusive fluxes. The temporal derivatives are approximated using a second-order three-stage Runge-Kutta technique. The computational domain is discretized using a block-structured boundary-filtered mesh with 159 mesh blocks and roughly

20 million nodes. The mesh is generated using a combination of Cartesian and polar mesh blocks to get a homogeneous mesh structure in the radial direction throughout the domain. A block with square cross section is wrapped around the centerline of the primary jet to avoid the centerline singularity, Fig. 5.

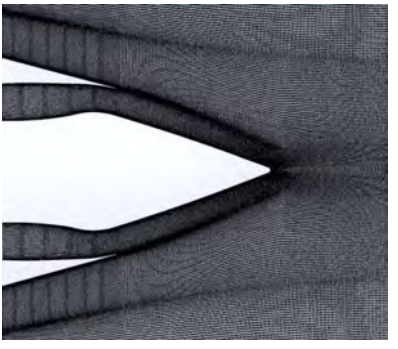
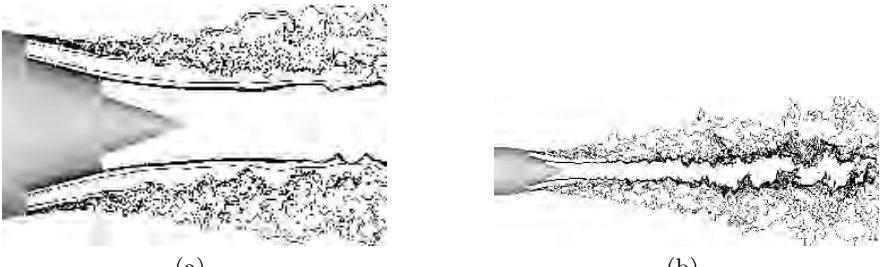


Fig. 5. Mesh in the nozzle exit region. (Courtesy of N. Andersson et al. [24]).

Fig. 6 evidences the development of the inner and outer shear layers by visualizing instantaneous entropy contours close to the nozzle lip and on the entire computational domain. In the outer shear layer small vortical structures are generated right at the nozzle lip. The vortices generated in the initial shear layer break down into smaller structures before they propagate far downstream. The inner shear layer appears to be rather stable. Nevertheless, smaller structures occur in the initial part of this shear layer. This low degree of mixing between the primary and the secondary jet is conjectured to be due to the fact that the velocity and momentum ratios are reversed.



(a) (b)

Fig. 6. Instantaneous entropy contours, (a) near the nozzle exit, (b) on the entire computational domain. (Courtesy of N. Andersson et al. [24]).

To be more precise, the velocity in the primary stream is higher than that in secondary stream whereas the temperature difference leads to a lower momentum flux in the primary stream than in the secondary stream. Furthermore,

initially there is a negative radial velocity component such that the shear layer is concave. This curvature also could have a stabilizing effect. It is evident from Fig. 6(b) that the stability of the inner shear layer causes a rather pronounced extent of the potential core in the streamwise direction. The highly intricate flow structure in the inner and outer shear layers is shown by density contours in Fig. 7.

(a) (b)

Fig. 7. Instantaneous density contours, (a) shear layer between primary and secondary jet, (b) shear layer between secondary jet and surrounding fluid. (Courtesy of N. Andersson et al. [24]).

In the initial part of the inner shear layer, Fig. 7(a), Helmholtz instabilities having ring-like structures occur. In the developing shear layer the vortices deform and axial structures are generated which excite the break up of the inner shear layer. In the outer shear layer the initial mixing process is enhanced (Fig. 7(b)) resulting in small flow structures near the nozzle lip.

The LES data can be used to determine via a hybrid approach [32], [33] the acoustic field generated by the jet flow. The sound pressure levels shown in Fig. 8 are computed using various methods [24], [34], [35]. It is evident from the comparison with the experimental data that it is a must to include in the analysis of the acoustic field not only the shear layer related noise mechanism but also the temperature related sound sources. Otherwise the noise level will be predicted too small.

2.4 Reacting Flow in a Combustion Chamber

In [25] Moin and Apte perform an LES for the turbulent reacting flow in a single sector of a Pratt & Whitney combustor. For the LES, the conservation equations for low Mach number flow with variable density are solved for the gas phase. The numerical method bases on a finite volume, energy conserving scheme for unstructured meshes [36]. A flamelet progress-variable formulation is used for the chemistry. An integration of the chemical state relationships over a presumed probability density function yields the subgrid fluctuations in the mixture fraction, progress variables, and filtered combustion variables. A dynamic Smagorinsky model is used to determine the subgrid terms.

The liquid phase is taken into account in a Lagrangian framework, which requires an efficient particle-tracking method. The particle positions are determined by solving the Basset-Boussinesq-Oseen equations for each individual

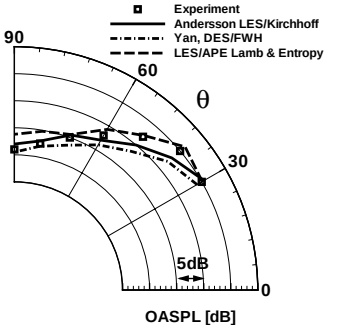


Fig. 8. Directivity at $r/R_s = 60$ generated by the Lamb vector and entropy sources. Comparison with experimental and numerical results (Andersson LES/Kirchhoff [30], Yan DES/FWH [33]). (Courtesy of E. Gröschel et al. [35]).

droplet. Additional correlations, which modify the drag force acting on the particles, are used to account for the deformation of the droplets from the spherical shape. The droplet size is assumed to be smaller than the spatial filter width used in the LES. Effects from subgrid velocity fluctuations on the particle motion are neglected. To reduce the number of particles in the simulation of sprays, parcels which represent a group of droplets, are introduced. These parcels are formed as soon as the local number of droplets within a single control volume exceeds a certain threshold. This method was developed to avoid severe load imbalances due to large variations of the droplet number per subdomain.

To validate the hybrid particle-parcel method the flow through a Pratt & Whitney injector is simulated. The problem exhibits a complex flow structure including vortex breakdown. In the simulation about 3.5 million droplets and 150,000 parcels are tracked. Despite of this hybrid technique still a load-imbalance of the parallel computation is observed, since only one-third of the processors compute the motion of more than 10,000 particles. The comparison of the results of the velocity field and the liquid axial mass flux with experimental data shows a distinctively better agreement than solutions based on the unsteady Reynolds averaged Navier-Stokes equations.

The simulation of the reacting flow in the single sector of the Pratt & Whitney combustor including all models for spray breakup, evaporation, and turbulent combustion, is performed on a mesh with 1.9 million hybrid elements. The mesh inside the inlet and swirler is to a large extent composed of tetraeder, while the combustion chamber is mostly filled with hexaeder, since the latter offer a higher accuracy.

Fig. 9 shows a snapshot of the instantaneous temperature distribution and different cross sections. Good agreement is obtained with experimental data for the time averaged temperature distribution. The results demonstrate that LES is applicable to predict complex turbulent reacting flows in geometries of industrial interest with a higher accuracy than models based on Reynolds

averaged equations. The computing times of 25-30 CPU days are, however, still large such that substantial effort is required for improving the efficiency of the involved algorithms, especially for use of large processor numbers.

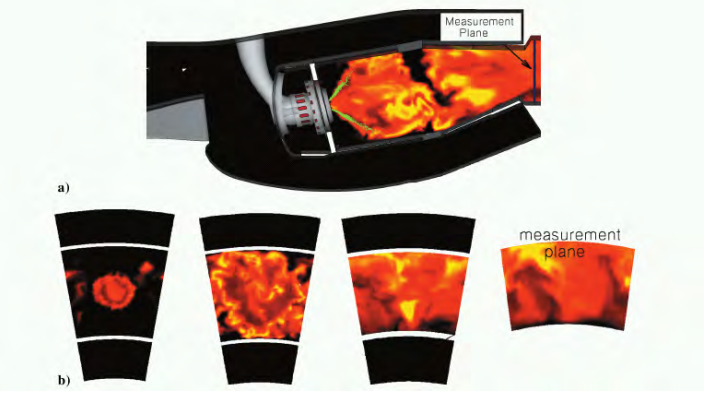


Fig. 9. Instantaneous temperature distribution in a sector of a Pratt & Whitney combustor. Symmetry plane (a) with superimposed droplets and different cross sections (b). (Courtesy of P. Moin and S.V. Apte [25]).

2.5 Ignition Process in a Full Combustion Chamber

The ignition process in a full gas turbine engine is investigated by Boileau et al., [26] using a LES. The 360^o geometry of a combustion chamber demonstrator called VESTA, with 18 individual burners, is resolved by a tetrahedral mesh with 19 million cells and 3.1 million nodes. The numerical method bases on unstructured meshes and solves the Navier-Stokes equations for compressible flows. The time integration is made with an explicit three-stage Runge-Kutta method. A spray model in an Euler-Euler description is used to predict the liquid phase of the fuel. The combustion model involves one-step irreversible chemistry for the fuel JP10. For the flame-turbulence interaction a thickened-flame model is applied, where the flame front is thickened by a certain factor such that it can be resolved on the computational mesh. Since an explicit solution scheme and the Eulerian formulation for the spray model does not require a particle tracking, the whole algorithm can be easily parallelized and a high parallel efficiency can be achieved on 700 processors of a Cray XT3.

The simulation is conducted to demonstrate today's capabilities in the application of numerical methods to predict flame ignition and propagation in a full combustion chamber. Due to the fact that many questions concerning the initial ignition process especially in the presence of liquid fuel are still open, simple and validated models for chemistry, spray, and ignition are used. The results obtained reveal the details of the flame propagation front, starting at the igniters and propagating into the different quadrants of the burner. Fig. 10 shows the flame front 46 ms after ignition. It can be seen that the flame

propagation itself is not symmetrical in each quadrant, which is due to the swirling components of the main air jets. Therefore, the velocity field inside the annular chamber plays an important role for the ignition process. The analysis of the mass flow rates of the reaction products indicates the expansion of the burnt gases to be the major mechanism for the flame propagation.

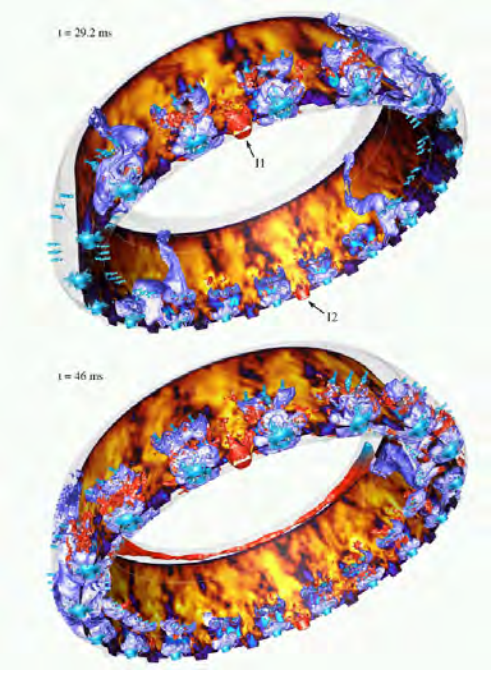


Fig. 10. Two instants of the ignition sequence. A contour in light blue of the progress rate represents the flame front. The two high speed hot jets used for ignition are marked I1 and I2. (Courtesy of M. Boileau et al. [26]).

After the ignition two reaction zones can be distinguished, the first is a partially premixed flame region located close to the main injector which is stabilized by the vortex breakdown of the rotating air jet. The second region, downstream of the premixed flame, has the properties of a diffusion flame, since the oxygen of the primary hole air jets is used to burn the excess fuel from the premixed flame.

This simulation shows that the physics of the ignition process in a full gas turbine combustion chamber can be simulated using the existing methods. The simulation obviously requires the resolution of the full annular geometry, since otherwise the asymmetry of the combustor cannot be captured. Details of the ignition process of an individual flame, in which liquid fuel and detailed kinetics for evaporating sprays in unsteady mixing flows may play an important role, have still to be addressed in more fundamental investigations.

3 Conclusion

The above examples do show that large-eddy simulations can be used to investigate not only fundamental generic problems but also industry related flows. Nevertheless, it has to be emphasized that any large-eddy simulation method is highly susceptible to discretization schemes, filtering, subgrid scale modeling, boundary conditions and their numerical formulation to mention just a few components which determine the final quality of the LES solution. In general, a long-term fundamental expertise in computational fluid dynamics is necessary to perform such computations. Moreover, it goes without saying that extremely powerful computers are required to obtain results in an acceptable computational time. Therefore, although LES is capable of analyzing some selected flows which possess the geometrical and fluid mechanical intricacy of industrial flow problems it has to be kept in mind that the solutions are primarily determined in a research environment. Especially the computing times are still way too high not only for the design process but even the industrial development process.

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Issues of Multidisciplinary Design

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Summary Issues of multidisciplinary design are considered in view of the aerodynamical and structural design of the airframe, i. e. fuselage, wing, and tail unit. Background problems, like Cayley's design paradigm are discussed, as well as ideal-typical airframe definition and development phases, and the industrial challenges which numerical multidisciplinary design and optimization (MDSO) poses. Finally the state of the art of MDSO methods is illustrated.

1 Introduction

In 2002 with Volume 79 the title of the NNFM series was changed to "Notes on Numerical Fluid Mechanics and Multidisciplinary Design". This change was made because volumes were coming up with multidisciplinary topics and the series' title should reflect the widening of its scope. Soon the Volumes 81, 84, 85, 89, and 98, see the pages 494 to 503 of this book, appeared with corresponding content.

Aircraft – as well as in general industrial – design and development, is multidisciplinary by definition. It concerns the work of many disciplines on the whole aircraft, the system, including the sub-systems, like the wing, the fuselage, et cetera. The evolution of discrete numerical simulation and optimization methods of aerodynamics, structure mechanics et cetera has paved the way towards what is called "Multidisciplinary Design Optimization[1] (MDO)". It aims for and effects a higher integration than before of the involved disciplines in the sense of Concurrent Engineering by making use – however not necessarily – of high-performance computation and of information technologies.

[1] The field of classical aeroelasticity can be considered as a special case. It regards problems of flow-structure interaction, for instance flutter, which is treated with linear aerodynamic methods in the frequency domain.

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The potential of MDO for product definition and development in the aerospace sector was early on recognized. In 1991 the AIAA MDO Technical Committee reviewed the current state of the art in the field, [1]. The committee published extended discussions of aspects and problems of MDO in [2]. MDO was – and is – considered as a methodology to exploit the synergism of mutually interacting phenomena occurring in complex technical systems. As can be seen from the following contribution by D. S. Lee et al., this does not necessarily mean problems connected to flow-structure interaction phenomena.

In Germany a group of experts from airframe and from jet propulsion industry, from the German Aerospace Center DLR, and universities published in 1996 a memorandum, [3], pointing out the extreme importance of high-performance computation for aerospace products. A joint project "High-Performance Computation for Cost Reduction and Quality Improvement in Aircraft Engineering" was proposed. The proposed reference problem was the *numerical simulation of the unrestrained flexible and maneuvering air vehicle and its propulsion system in steady and transient movement.* We note only that industry at that time was not yet ready for the project "AMANDA, a Multidisciplinary High Performance Numerical Simulation and Development System for Aircraft", [4], proposed in the frame of the German Aeronautical Research Program.

In the present contribution the topic "multidisciplinary design", respectively MDO, is narrowed to the topic "multidisciplinary simulation and optimization (MDSO)", meaning *high-fidelity multidisciplinary simulation and optimization with discrete numerical methods* of the system aircraft and/or its subsystems.

Industrial design and development work generally is organized according to the second aspect of Cayley's design paradigm: the involved disciplines work in their own departments, weakly coupled in a sequential and iterative way. It is necessary to understand the implications. These are treated in the next section, Section 2, with the two aspects of "Cayley's Design Paradigm" as guiding concepts.

MDSO becomes more and more necessary for several reasons. The first one is, that in general economical and ecological pressures ask for more effective, environment friendly and safe aircraft. The second reason is, that Cayley's design paradigm in terms of its first aspect was substantially weakening in the last decades. This weakening will become even stronger, when aircraft configurations move away from the classical fuselage or tube/wing concept, to maybe blended wing/body concepts. This move happens since long with military aircraft, but in particular with hypersonic flight vehicles. The third reason, closely connected to the first one, is the modelling and simulation of the emerging aircraft during the definition and development phases. This concerns the mathematical model of the aircraft (aerodynamics, structural dynamics,

control devices[2], engines et cetera) which is needed, for instance, by the flight control system (FCS), see, e. g., [6], [7], for avionics integration, systems-simulation, pilot-in-the-loop training and so on. The needed data base(s) for these tasks should be available more exact and earlier than it is now the case.

The background problem is the following: with the present definition and development approach the quantification of the physical properties and the functions of the vehicle's airframe is evolving only slowly. The actual and finally accurate data become available only very late in the development process, after the first - as *perfect-elastic* structure defined and developed - airframe has been assembled. Partly this quantification process extends deep into the flight envelope opening process. This topic is addressed in Sections 3 and 4 of this contribution.

MDSO has many faces. In this contribution the discussion is concentrated on the aerodynamical and structural design and optimization of the airframe. In Section 5 the state of the art of MDSO in view of flow-structure interactions is illustrated.

2 Cayley's Design Paradigm and its Weakening

The definition and development of aircraft basically follows an over decades well proven ideal-typical approach. The background of this approach is given by Cayley's design paradigm. Sir George Cayley (1773 - 1857) was an early British aviation pioneer, who conceived the essentials of the aircraft as we know it today, but who formulated also insights into the design process. A good, albeit short overview of his work can be found in [8].

Cayley's design paradigm (first aspect), [9], see also [10], reads regarding aircraft design (not in his own words):

- Assign functions plainly to corresponding sub-systems, e. g.:
  - wing ⇒ provision of lift,
  - propulsion system ⇒ overcoming of drag,
  - horizontal stabilizer and elevator ⇒ longitudinal trim, stabilization and control,
  - vertical stabilizer and rudder ⇒ lateral (directional) stabilization and control,
  - fuselage ⇒ payload accommodation,
  - et cetera.
- Have the different functions and the corresponding sub-systems only weakly and linearly coupled, then you can treat and optimize each function

[2] The combination of structural dynamics, aeroelastics and flight control is called aeroservoelastics, see, e. g. [5].

and sub-system more or less independently of the others[3], and nevertheless treat and optimize in this way the whole aircraft, which integrates all functions and sub-systems.

This paradigm (first aspect) has been proven to be very effective (ideally it should hold for every technical apparatus). However, the quest for more performance and efficiency, the opening of new flight-speed domains et cetera, has led over the years to higher and higher integrated functions and sub-systems, i. e. a persistent weakening of Cayley's design paradigm[4]. Of course, this is different for different kinds of flight vehicles, and does in each case not necessarily encompass all major functions and sub-systems.

Palpable examples of this weakening are:

- Aeroservoelastics of especially large aircraft, see, e. g., [11].
- Transport aircraft with high/ultra-high by-pass engines, see, e. g., [12].
- High-lift systems.
- Unstable flying aircraft (today fighter aircraft, see, e. g., [13], in future also transport aircraft).
- Airbreathing hypersonic aircraft (very highly coupled lift/propulsion system with pre-compression by an elastic forebody, see, e. g. [14]).

In general it appears, that a strong and non-linear coupling of functions/sub-systems asks also for a strong non-sequential coupling of the in the definition and development involved engineering disciplines like aerodynamics, structural mechanics, et cetera. Two basic cases can be distinguished:

- Cayley's design paradigm is valid for the whole airframe or only negligibly violated: the complete system must not be treated with MDSO, however, it may be necessary to apply MDSO to one or more of the sub-systems, for instance the wing or the tail unit.
- Cayley's design paradigm is invalid for the whole airframe: MDSO must be applied to the complete system.

The treatment of these basic cases in the classical way is partly possible, but it may result in large time and cost increments. Design risks can become

[3] Take the wing as an example. It basically has to be optimized such that it provides everywhere in the flight envelope the needed lift and has, at the same time, adequate static and dynamic structural properties at minimum weight. At cruise it must have optimal aerodynamic quality, i. e. the the product flight Mach number times lift-to-drag ratio ($M_\infty L/D$) must be as large as possible.

[4] The wing of a modern transport aircraft today indeed is a multi-functional sub-system. Its major function is the provision of lift. At the same time it transports the fuel, it carries with the pylons and the nacelles the vehicle's engines, and, moreover, it houses the high-lift system, with very closely coupled flow paths in the case of the latter two functions.

large, and, especially with very strong functions/sub-systems couplings, they can become untenable.

This leads to the second aspect of Cayley' design paradigm: a differentiation similar to that of sub-systems and functions has taken place also of the engineering disciplines, which are involved in the design and development of flight vehicles[5]. This is natural, and was and is indeed also a strong technological driving factor.

The differentiation of the engineering disciplines certainly became necessary early on, and it was instrumental in the evolution of the aircraft as we know it today. However, it had also adverse effects. It led, for instance, to the presently strongly established sequential and iterative design cycles with a weak interaction of the disciplines. It further led in some cases to autonomy drives of disciplines by duplicating skills and tools of other disciplines, which then often did not participate in the sub-sequential developments of the mother disciplines.

3 Ideal-Typical Airframe Definition and Development

Aircraft definition and development involves a host of engineering disciplines which work in different ways together in many so-called design phases. Different denominations are used in different companies and countries, but in general on can distinguish the four product phases shown in Fig. 1. The topic of this contribution concerns the definition and the development phase.

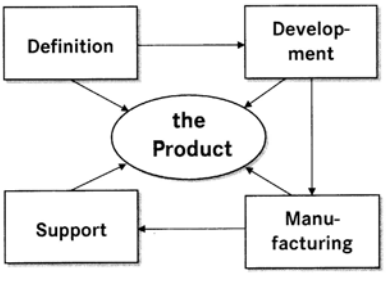

Fig. 1. Schematic of product phases, [9].

A more detailed consideration results in the picture shown in Fig. 2. This is an ideal-typical picture, which also omits that sub-phases are iteratively structured. No time intervals are given, because these can be very different,

[5] This differentiation also holds for university education and for research at universities and research establishments.

depending one the type of aircraft. If a completely new design is made, they will be longer than with a derivative from an existing design.

The product definition phase is considered to consist of the concept phase, the pre-design phase and the design phase, Fig. 2. At the end of the pre-design phase the concept is frozen. No major changes will be made in the following phases, unless major problems show up. Initial data-sets are available, system-simulations have been made, design sensitivities, see, e. g., [10], are established, as well as technology development needs, et cetera.

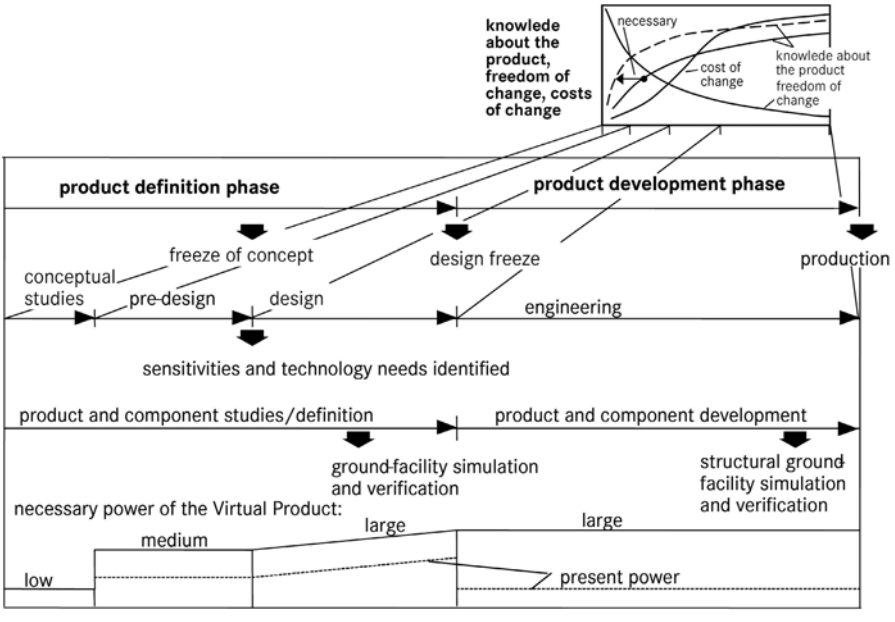

Fig. 2. Ideal-typical schematic of the product definition and development phases and sub-phases, [15]. The figure shows from the left to the right the advancing phases and sub-phases. The abscissa hence can be considered as the time axis, although most of the phases proceed iteratively. In the right upper part corresponding schematics of product knowledge, freedom of change, and cost of change are given. The ordinate there represents a dimensionless scale from zero (below) to one (above).

In the design phase details of the design are worked out. At the end of this phase the design is frozen. The aerodynamic design, besides others, has been verified, see, e. g., Fig. 3 in the introduction to this book, and data sets,

for instance the "aerodynamic model" with a linear elastification[6], have been produced.

If the go-ahead is given, the product development phase is entered. In this phase the detailed engineering work is performed. Finally, maybe after a prototype has been build and tested, the actual manufacture of the aircraft will begin.

In all product phases and sub-phases functions, sub-systems, components et cetera are studied, tested and simulated in ground-simulation facilities, also on the computer. Very important is the fact, that the real static and dynamic aeroelastic properties of the airframe are found very late in the development phase. The structural ground-facility tests of course can only be made, if the airframe has been fully assembled.

In the product definition phase not only the shape, the performance, the flying qualities and so on of the aircraft are settled, but also, which is very important, the final production, operation, and maintenance costs (product life-cycle costs) are implicitly and early fixed to a very large degree. Therefore mistakes in this phase must be avoided as far as possible. In the upper right part of Fig. 2 this is illustrated. The "knowledge" about the product (physical properties and functions of the system and the sub-systems) rises during the phases, but reaches a high level only late in the development process. The final level will only be achieved during system identification with the real, flying aircraft. The "freedom of change" decreases during the phases. The later a major change is made, the higher is the "cost of change", which is obvious.

Changes – actually "repair solutions" – which must be made of the airframe, if the desired properties don't meet the requirements after the late structural ground tests, can be very costly and in any case will increase the structural weight of the vehicle and may lead to other changes, too, [5].

In view of this general problem and in view of the still rising computer power and the numerical simulation capabilities (the second wave of mathematisation of the sciences and engineering) the concept of the "Virtual Product" was put forward in [9], see also [10]:

"The Virtual Product (VP) is a high-fidelity mathematical, respectively numerical representation of the physical properties and the functions of a product".

It effectively should permit to shift the curve of product knowledge to a higher level at an earlier time, in order to avoid and minimize costly changes at later times, Fig. 3. Many other effects are coupled to this major effect, see the detailed discussions, also of the problems of the VP, in [9] and [10].

[6] The aerodynamic data set originally is produced with a rigid model in the wind tunnel. It must be "elastified", because the real airframe is elastic, see e. g. [7]. The real non-linearly elastified aerodynamic model is only available after the structural ground-facility tests have been made, Fig. 2 – with possible repair solutions as a consequence – and finally after the system identification with the real flying aircraft has been performed (flight data measurements).

Numerical multidisciplinary simulation and optimization (MDSO) is one of the major elements of the Virtual Product.

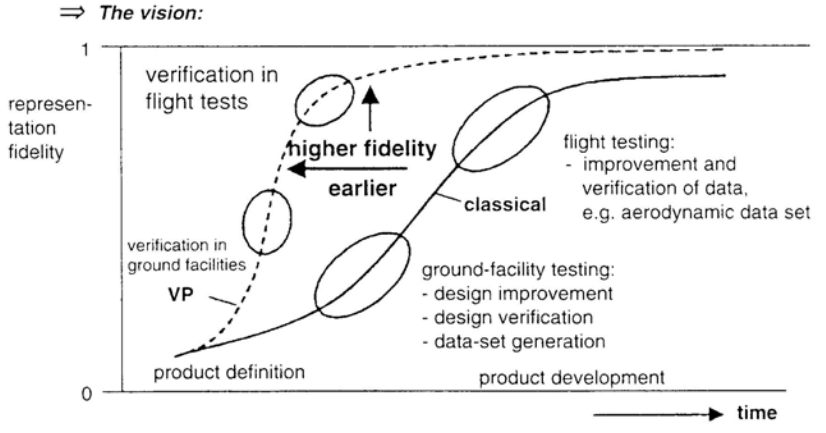

Fig. 3. The desired effect of the Virtual Product in aircraft design: shift of the curve of product knowledge to a higher level at an earlier time, [9].

4 Challenges

The challenges to achieve the desired effect of the Virtual Product are enormous. For general discussions see [9] and [10]. The following discussion concentrates on issues of numerical multidisciplinary simulation and optimization in view of the aerodynamical and structural layout of the airframe.

4.1 Mathematical/Numerical Product Models

Underlying MDSO are mathematical/numerical product models. These have already a long history in the field of aeroelasticity. However, there typically simplified structural and aerodynamic models are used. Nevertheless, the last decade has seen many new developments, mostly due to the advances in nonlinear numerical aerodynamics. Some problems and solutions of time-domain mechanical fluid-structure couplings in MDSO are illustrated in Section 5.

4.2 Flow-Physics and Structure-Physics Models

Flow-physics models for the non-empirical prediction of laminar-turbulent transition, turbulent separation et cetera in steady and unsteady flow are pro-

gressing with respect to predictive accuracy, but are yet not on an adequate level. For a somewhat broader discussion see Section 4 of the introduction to this book.

Here the discussion is concentrated on structure-physics models, in particular on the question *perfect-elastic* versus *real-elastic* properties of the structure, which is one of the open problems in MDSO.

The real airframe is a structure with point-, line-, and plane-wise distributed joints (rivets, screws, gluing and welding zones), which introduce non-linearities, damping, and non-linear deformations (post-buckling belongs to the picture). These govern the real-elastic properties of the structure. Today the determination of the structural properties of the airframe is made in the product definition phase and deep into the development phase with perfect-elastic structures. The real-elastic properties are found only late in the development phase, see Fig. 2, after the structural tests with the assembled airframe have been made. Then especially the dynamic properties of the airframe are determined with frequency-domain approaches.

MDSO, in order to achieve its true potential in view of the desired effects of the Virtual Product, must be able to model to the needed degree the real-elastic properties of the structure. This goal presents enormous challenges. Scale discrepancies as large as in flow with turbulent boundary layers past whole flight-vehicle configurations would have to be mastered. Possible approaches may use statistical models based on parameter identification as in statistical turbulence theory, combined with methods similar to direct numerical or large-eddy simulation. So far the real-elastic airframe properties have not been recognized to the needed degree as an important field of research, neither by the MDSO community nor by the structural mechanics community.

4.3 The Product-Knowledge Problem

In Fig. 2 it is schematically shown how the "knowledge" about the product rises during the phases, first it is rather small, only later it becomes larger. This holds in particular also for the airframe's structure. Indeed, the airframe engineering with the actual design of the structural elements happens during the development phase. MDSO hence has the problem, that especially in the definition phase the structure is not enough defined in order to perform high-fidelity simulations, which in many respects would be desirable already there. This means also that the matter of structure-physics models, as discussed above, is not relevant in the early design phases. The way out are ersatz-models of the structure, like for instance the Timoshenko beam for the load carrying elements of the wing. In industry the "product-knowledge problem" in view of MDSO finally is a matter of systems engineering.

4.4 Implementation and Acceptance at Industry

Implementation and acceptance of MDSO at industry – without or with the Virtual Product approach – need attention and effort as large as the develop-

ment of MDSO itself. Industry is organized and works discipline-oriented, as depicted by the second aspect of Cayley's design paradigm. The problem can also be seen from another perspective. The often discussed and heralded Concurrent Engineering is indeed exactly, as already mentioned, what the Virtual Product approach demands.

The high-fidelity representation of the physical properties and the functions of a product, for which MDSO and the Virtual Product aims, is achieved with new process technologies. That entails changes in systems engineering and processes – indeed, it aims for them – and hence organizational changes. This holds for the whole chain from customer inputs up to aircraft certification. Finally, and this must not be forgotten, it will introduce risks, as any new approach does, and the cost for its implementation must be recovered in due time. The established and proven systems engineering processes can only very carefully be changed and with large costs and at serious risks.

Finally the acceptance problem is addressed. All organization levels, from the management level down to the staff level must accept and approve the new approach. "Cultural" changes are necessary, incentives must be given. MDSO is a tool. Tools are only as good as the people, who wield them. Therefore it is one of the large challenges for industry to build a staff with adequate qualification, [9].

The development of a post-Cayley design paradigm certainly is a topic of research establishments and universities – with strong involvement of aerospace industry. It is to be clarified how and with what capabilities MDSO can and is to be applied in the definition and development phases, what are the consequences for systems engineering and processes, and last but not least for the industrial organization (see also the considerations in [2]).

5 Fluid Structure Interaction as Important Element of MSDO

The work on numerical multidisciplinary design methods in the last decade was motivated by the recognition that simulation procedures combining various disciplines must be developed step by step. There is actually no chance yet to handle during a real design process of a flight vehicle in a coupled manner, for example, the disciplines shape design, aerodynamics, structural mechanics and flight mechanics instantaneously with a MDSO approach.

In the following two examples illustrate the capabilities one has today to combine at least the two disciplines aerodynamics and structures in an interdisciplinary sense. In the literature such methods are summed up by the term "mechanical fluid structure interactions", see, e. g., [14].

The main problem for disciplines analyzing physical states, which interact strongly with each other, is that they have to provide for a fast and precise exchange of data at the corresponding boundaries. Of course, there are various possibilities to do this, but here we concentrate on a procedure, where for the

single disciplines the methods providing the best approximations are used, regardless of consistency with respect to computational grid and integration method. On the other hand this implies a sophisticated interpolation method for the data transfer across the common interface boundary.

A very promising strategy for a suitable treatment of this data transfer is pursued by the authors of [16] to [18]. They introduce besides the meshes for the fluid and structure fields the moving mesh as a third field[7]. The corresponding equations for the three fields are solved simultaneously. The three field approach allows for an employment of a partitioned solution procedure, where best suited numerical simulation methods are applied for the involved disciplines[8].

The time coupling of the joined sets of equations is treated, for example, by a solution strategy based on a staggered scheme of the form shown below, Fig. 4, [16], [20].

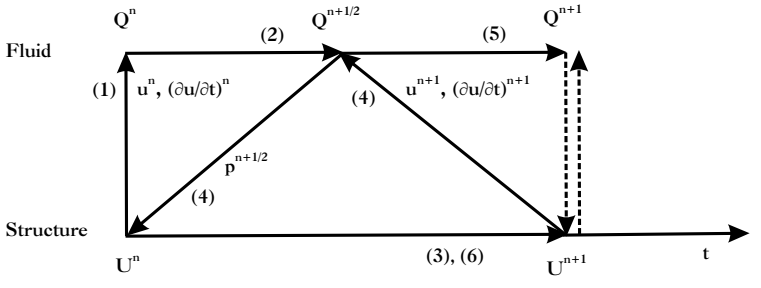

Fig. 4. Staggered scheme with inter-field parallelism for the coupling of the solutions of a three-fields fluid-structure interaction problem, $U = (u, \dot{u})^T$, [20].

This scheme can be described by :

1. Update the fluid mesh coordinates with structural displacements u^n and the velocities $\dot{u}^n$ to conform to the structural boundary at t^n.
2. Advance the flow from t^n to $t^{n+1/2}$.
3. Advance the structure using the pressure and the stress field at t^n from t^n to t^{n+1}.
4. Transfer the pressure and the stress field at $t^{n+1/2}$ to the structural code and transfer the structural displacements u^{n+1} and the velocities $\dot{u}^{n+1}$ to the fluid code.

[7] Note that in the classical way aeroelastic properties as well as aerodynamic loads are determined with, for instance, vortex-lattice methods applied in the skeleton surface of the wing. In this way the true aerodynamic contour of the wing is not taken into account!

[8] In the process chain for fluid-structure coupling of the DLR the coupling is made with the help of an interpolation module, [19].

5. Advance the flow from $t^{n+1/2}$ to t^{n+1}.
6. Re-compute the structure using the pressure and the stress field at $t^{n+1/2}$ from t^n to t^{n+1}.

Fig. 5 shows as first example a static aeroelastic solution for the AMP[9] wing obtained with a method like the one described above, [21]. The solution was performed at ONERA using for the aerodynamics ONERA's inviscid-viscous interaction code VIS25 and for the perfect-elastic structure the NASTRAN code.

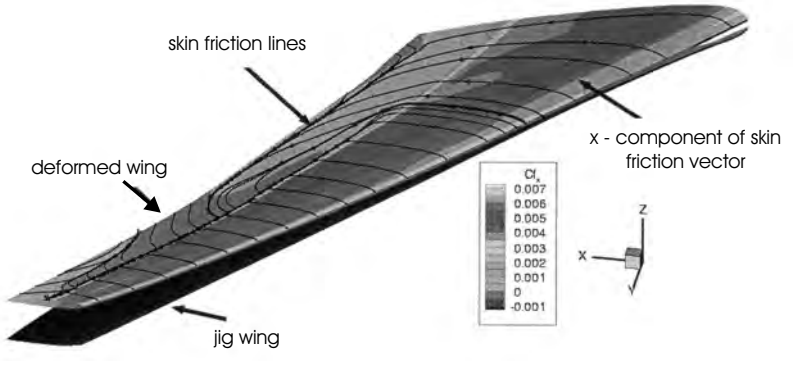

Fig. 5. AMP wing: static aeroelastic solution, [21]. Wing deformations and skin-friction lines for $M_\infty = 0.819$, $\alpha = 3.98°$, $Re = 1.99 \cdot 10^6$, $C_L = 0.58$.

The span-wise deformation and the leading edge deflection for another flow case of the AMP wing is shown in Fig. 6, where experimental data are compared with data from the VIS25 solver and from ONERA's more sophisticated fluid solver CANARI (unsteady Euler equations) again coupled with the NASTRAN code.

The results shown in Fig. 6 are very promising. Compared to the experimental data the leading edge deflection is overpredicted, whereas the twist deformation is better reproduced. Dynamic computations did show that the flutter limits were found – for several dynamic pressures – close to experimental results.

The second example is a result of the application of the DLR process chain, [19], to the wind tunnel model of a full transport aircraft in high-lift configuration with through-flow nacelles. Fig. 7, [22], shows the computed flow field, on the left side for the rigid airframe, on the right side for the elastic airframe. In the latter case both the wing and the high-lift elements were deformable.

[9] AMP $\Longrightarrow$ Aeroelastic Model Program.

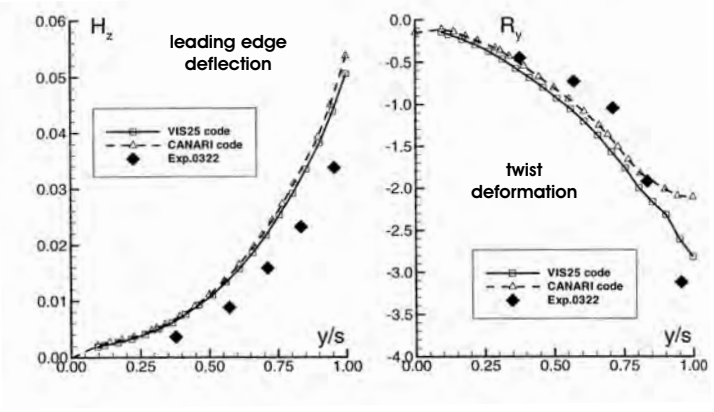

Fig. 6. AMP wing: static aeroelastic solution, [21]. Span-wise leading edge deflection H_z and twist deformation R_y. Flow field found with Euler (CANARI) and viscous-inviscid interaction code (VIS25). Comparison with experimental data of the ONERA S2 wind tunnel, Modane. $M_\infty = 0.862$, $\alpha = 1.6°$, $Re = 3.64 \cdot 10^6$, $C_L = 0.30$.

The differences in the pressure distributions and in the patterns of the skin-friction lines are very small near the wing root, but become larger towards the wing tip, and especially on the extended trailing-edge flap. On the trailing-edge flap the differences are mainly due to changes of the gaps. The changes of the lift and the drag coefficient from the rigid to the elastic airframe are $\Delta C_L = +\,0.5$ per cent, and $\Delta C_D = +\,1.3$ per cent.

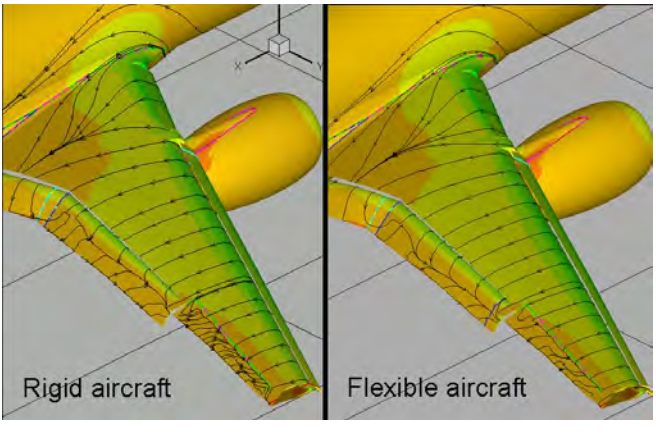

Fig. 7. Wind tunnel model of a transport aircraft in high-lift configuration, $M_\infty = 0.2$, $Re_{mac} = 1.52{\cdot}10^6$, $\alpha = 15.2°$, through-flow nacelles, coupled flow-structure solution. Computed flow field, left rigid airframe, right elastic airframe (wing and high-lift elements), [22].

6 Conclusion

Discrete numerical methods for multidisciplinary simulation and optimization have reached – in view of airframe design tasks – a high level with partly spectacular results. However, this holds so far only for perfect-elastic airframes and structures. A host of problems remains to be solved with MDSO methods as such.

Although the products of aerospace industry need increasingly a more accurate description of their properties and functions, MDSO cannot simply be introduced into the present definition and development processes. The large challenges, which arise in this regard, should be seen in the wider frame of the Virtual Product, which is becoming possible due to the enormous developments in computer power and information technologies in general.

While talking on and promoting MDSO, research and industry have different attitudes – pro (research) and tacitly contra (industry), apart from the aerodynamicists. One can dare to say, that the potential and the chances, but also the implications of high-performance computation – especially that of high-fidelity numerical simulation and optimization (MDSO and the Virtual Product) – for the aerospace industry and their products are, with very few exceptions, neither thematized nor sufficiently understood on higher management levels. As long as this has not changed, the danger is that MDSO will remain in industry, despite its great advances and results, and the indeed existing needs, a mere catchword.

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Evolutionary Optimisation Methods with Uncertainty for Modern Multidisciplinary Design in Aeronautical Engineering

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Summary One of the new challenges in aeronautics is combining and accounting for multiple disciplines while considering *uncertainties* or variability in the design parameters or operating conditions. This paper describes a methodology for robust multidisciplinary design optimisation when there is uncertainty in the operating conditions. The methodology, which is based on canonical evolution algorithms, is enhanced by its coupling with an uncertainty analysis technique. The paper illustrates the use of this methodology on two practical test cases related to Unmanned Aerial Systems (UAS). These are the ideal candidates due to the multi-physics involved and the variability of missions to be performed. Results obtained from the optimisation show that the method is effective to find useful Pareto non-dominated solutions and demonstrate the use of robust design techniques.

1 Introduction

Most of Multi-Objective (MO) and Multidisciplinary Design Optimisation (MDO) problems in aerospace engineering deal with intuitive nature problems [1, 2, 3]. One cannot ignore the fact, that MO and MDO in aerospace engineering frequently deal with situations, where the design input parame-

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ters and flight/flow conditions have some amount of uncertainty. When the optimisation is carried out for fixed values of the design variables and parameters however, converged optimised solution gives good performance at design condition, but poor drag or lift/drag ratio at slightly off-design conditions. The challenge in aeronautics is still to develop a robust design that accounts for uncertainty at design or operating conditions of the engineering system or aircraft. In this work we attempt to remedy this issue and prevent the fluctuation of performance by using a robust design technique [5, 6].

This paper introduces uncertainty-based robust design coupled with evolutionary algorithms and analysis tools for aerodynamics, electro-magnetics to maximise the survivability of Unmanned Aerial Vehicles (UAV/UCAV) at a set of flight conditions and frequencies that affect the Radar Cross Section (RCS). The paper describes the methodology and its numerical implementation for Uncertainty based Multidisciplinary Design Optimisation (U-MDO). The methodology couples a CFD and a RCS analysis software, an advanced evolutionary optimiser (HAPMOEA) [7] and the concept of robust/uncertainty strategy in the design, to produce a set of optimal-stable designs.

The rest of the paper is organised as follows: Section 2 describes the uncertainty based methodology. Analysis and formulation of problems are demonstrated in Section 3. Real-world applications are considered in Section 4 and conclusions are presented in Section 5.

2 Methodology

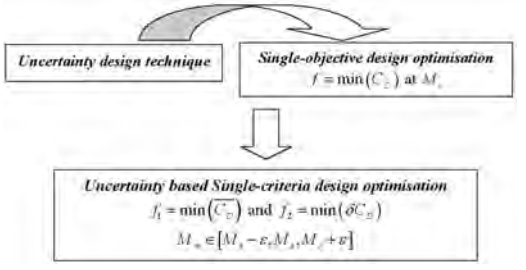
The method couples the Hierarchical Asynchronous Parallel Multi-Objective Evolutionary Algorithms (HAPMOEA software) with several analysis tools. The method is based on Evolution Strategies [8, 9] and incorporates the concepts of Covariance Matrix Adaptation (CMA) [10, 11], Distance Dependent Mutation (DDM) [9], an asynchronous parallel computation [13, 14], multi-fidelity hierarchical topology [12], and Pareto tournament selection. Details of HAPMOEA can be found in reference [7]. The method is enhanced with a robust design technique.

Robust Design Technique (Uncertainty) A robust design technique *Uncertainty* [15] is considered to improve simultaneously both stability and performance of the physical model. The robust design approach can be computed by using two statistical formulas (*mean* and *variance*):

$$\bar{f} = \frac{1}{K}\sum_{j=1}^{k} f_j \ (mean) \ and \ \delta f = \frac{1}{K-1}\left(\sum_{j-1}^{k} |f_j - \bar{f}|\right) (variance).$$

The above equations represent the aerofoil/wing performance and the sensitivity to the variability of input parameters such as geometry, flight condi-

tions, radar frequency, etc. For instance, if *uncertainty* is applied to a single aerodynamic design optimisation, the problem becomes an uncertainty based multi-objective design problems as shown below:



Consequently, the major role of uncertainty technique is to produce not only a low drag coefficient but also low drag sensitivity at uncertain flight conditions by computing mean and variance of the criteria. Full details of uncertainty can be found in the references [5] and [6].

3 Analysis and Formulation of Problem

The type of vehicle considered in this section is a UCAV similar in shape to the Northrop Grumman X-47B [16]. The baseline UCAV is shown in Fig. 1.

Fig. 1. Baseline design in 3D view.

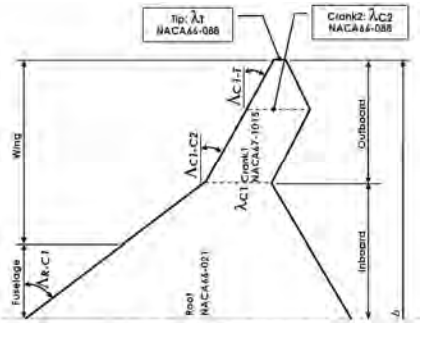


Fig. 2. Baseline UCAV configuration.

The wing planform shape is assumed as an arrow shape with jagged trailing edge. The aircraft maximum gross weight is approximately 46,396 *lb* and empty weight is 37,379 *lb*. The design parameters for the baseline wing configuration are illustrated in Fig. 2. In this test case, the fuselage is assumed from 0 to 25% of the half span. The crank positions are at 46.4% and 75.5% of the half span. Inboard and outboard sweep angles are 55 degrees and 29 degrees. Inboard and outboard taper ratios are 20% and 2% of the root chord.

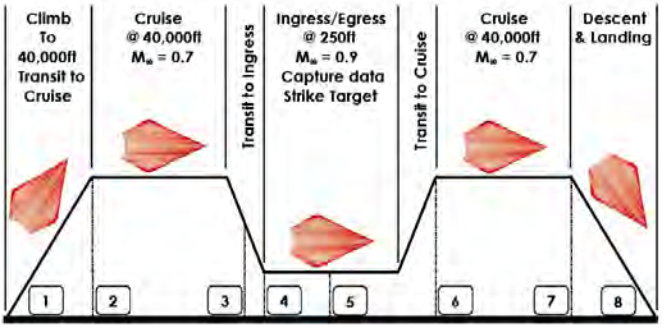


Fig. 3. Mission profile for baseline UCAV.

It is assumed that the baseline design contains three types of aerofoils at root, crank1, crank2 and tip section as illustrated in Fig. 2; NACA 66-021 and NACA 67-1015 are at the inboard sections, while NACA 66-015 and NACA 67-008 are used at the outboard sections. The maximum thickness at the root section is 21% of the root chord; this value is about 3% thicker than that for the X-47B to increase avionics, fuel capacity and missile payloads.

The mission profile for the UCAV considers Reconnaissance, Intelligence, Surveillance and Target Acquisition (RISTA) as illustrated in Fig. 3.

Fig. 4 shows the weight distribution along the mission profile. The weight between *Sector4* and *Sector5* is significantly reduced since 80% of munitions weight is used for target strike. In this paper, flight conditions for *Sector2* to *Sector4* are considered and the minimum lift coefficients (C_{Lmin}) are 0.296 and 0.04 for *Sector2* and *Sector4* as shown in Fig. 5.

The baseline design produces 30% higher lift coefficient at *Sector2* when compared to C_{Lmin}, while only 7% higher at *Sector4*. The aim of optimisation

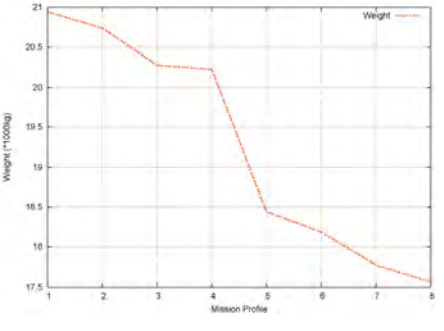


Fig. 4. Weight Distribution.

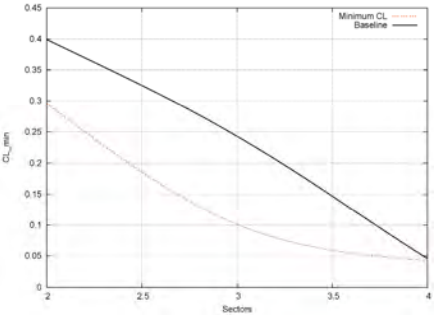


Fig. 5. $C_{L_{Minimum}}$ for Sector2 to Sector4.

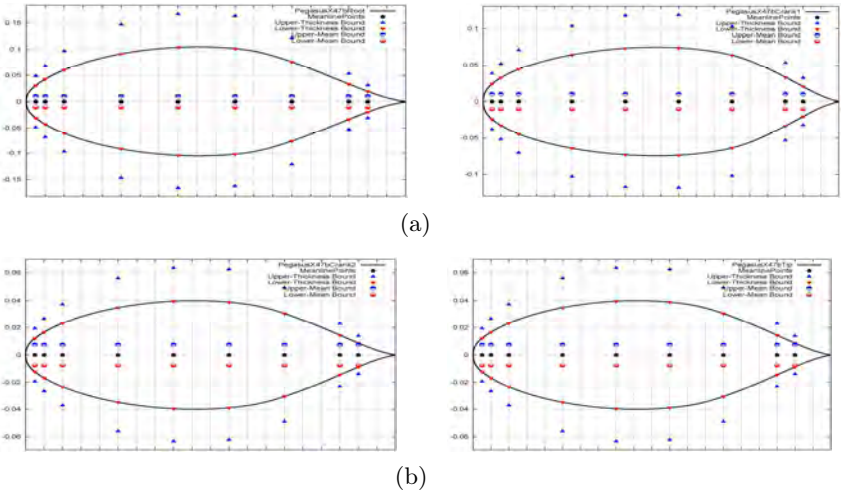


Fig. 6. (a) Root (left) and Crank1 (right) mean and thickness control points. (b) Root (left) and Crank1 (right) mean and thickness control points.

is the improvement of aerodynamic performance at Sector4 while maintaining aerodynamic performance in *Sector2*.

Representation of Design Variables The aerofoil geometry is represented using Bézier curves with a combination of mean line and thickness distribution control points. Example of the upper and lower bounds for mean and thickness control points at root, crank 1, crank 2 and tip sections are illustrated in Figs. 6(a) and 6(b).

The wing planform shape is parameterised by considering the variables described in Table 1 where three wing section areas, three sweep angles and two taper ratios are considered. The taper ratio at crank 2 is not higher than the taper ratio at crank 1, i.e. ($\lambda_{c2} \leq \lambda_{c1}$). Seventy six design variables are considered in total.

Table 1. Wing planform design variables.

Variables	$S_1(m^2)$	$S_2(m^2)$	$S_3(m^2)$	λ_{c1}	λ_{c2}	Λ_{R-c1}	Λ_{c1-c2}	Λ_{c2-r}
Lower	50.46	10.09	5.05	0.15	0.15	49.5^o	25^o	25^o
Upper	63.92	16.82	10.09	0.45	0.45	60.5^o	35^o	35^o

Table 2. Comparison of the objectives.

Description	Baseline	ParetoM1	*ParetoM5*	*ParetoM6*	ParetoM15
$1/\left(\overline{C_L}\right)$	12.232	9.890 (-19%)	*10.056 (-18%)*	*10.096 (-17%)*	10.562 (-14%)
$1/\left(\overline{L/D}\right)$	0.410	0.095 (-77%)	*0.079 (-80%)*	*0.078 (-81%)*	0.068 (-83%)

4 Real World Design Problems

Two real world test cases are selected to illustrate the potential of this methodology with increasing levels of complexity. The first case considers the aerodynamic analysis and optimisation of a J-UCAV (J stands for joint), the second test compares and illustrates the challenge and benefits in industrial environments of introducing a second discipline (electro-magnetics) while accounting for uncertainty in the design parameters and operating conditions.

4.1 Multi-objective Design Optimisation of a J-UCAV

Problem Definition This test case considers the design optimisation of a UCAV wing's aerofoil sections and planform geometry. The objectives are to maximise both mean values of lift coefficient ($\overline{C_L}$) and lift to drag ratio ($\overline{L/D}$) at *Sector2* and *Sector4*. The fitness functions and flight conditions are as follows;

$$f_1 = min\left(1/(\overline{C_L})\right) \ and \ f_2 = min\left(1/(\overline{L/D})\right),$$

$$where \ \overline{C_L} = (C_{L_{Mission2}} + C_{L_{Mission4}})/2 \ and \ \overline{L/D} = (L/D_{Mission2} + L/D_{Mission4})/2.$$

Results The algorithm was allowed to run approximately for 6667 function evaluations and took 200 hours on two 2.4 *GHz* processors. The resulting Pareto set is shown in Fig. 7. The black inverse triangle represents the best solution for the fitness function 1. The blue triangle indicates the best solutions for the fitness function 2. The red squares represent compromised solutions. It can be seen that there is a convex Pareto front between the first and second objective as shown in Section-A.

Table 2 compares the fitness values obtained by the baseline and Pareto members (1, 5, 6 and 15). It can be seen that all non-dominated solutions produce higher $\overline{C_L}$ and $\overline{L/D}$. There was a 17.5% of $\overline{C_L}$ and 80% $\overline{L/D}$ improvement when compared to the baseline design.

The *Sector* sweep is plotted with C_L and C_D in figures 8(a) and 8(b). The range of *Sector* sweep (*Sector2* to *Sector4*) is M_∞ = [0.7:0.9], α = [6.05:0.5] and ATI = [40,000:250].

It can be seen, that all Pareto members (1, 5, 6 and 15) produce a higher C_L when compared to the baseline. Pareto member 1 indicates higher lift

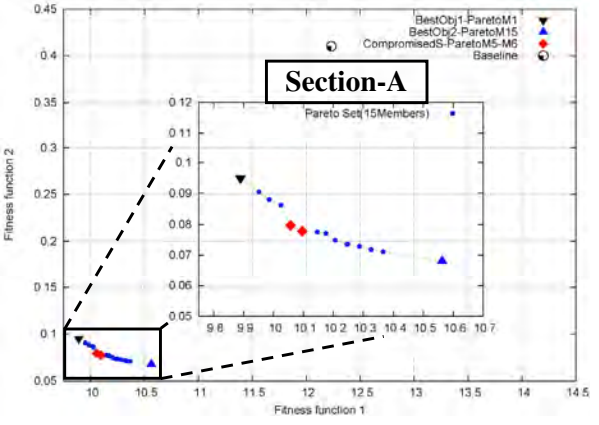


Fig. 7. Pareto optimal front.

coefficient along all sectors when compared to other solutions, while Pareto member 15 has a lower drag coefficient from Sector3. In addition, all Pareto members produce lower C_D without fluctuation compared to the baseline design as shown in Fig. 8(b). Table 3 compares the quality of the drag coefficient obtained from Pareto members and the baseline design. It can be seen that all Pareto members produce lower CD (-60 %) and lower sensitivity at Sector2 to Sector4, when compared to the baseline.

Table 3. Comparison of C_D quality.

Description	Baseline	ParetoM1	*ParetoM5*	*ParetoM6*	ParetoM15
$\overline{C_D}$	0.025	0.011 (-56%)	*0.010 (-60%)*	*0.009 (-64%)*	0.009 (-64%)
δC_D	5.49×10^{-5}	1.49×10^{-5}	*1.54×10^{-5}*	*1.56×10^{-5}*	2.11×10^{-5}

Fig. 8(c) compares the lift to drag ratio obtained by Pareto members (1, 5, 6 and 15) and the baseline design.

It can be seen that all Pareto members produce higher L/D along the Sector sweep, which means an extension of flight range. Even though the MO design method found useful Pareto non-dominated solutions producing aerodynamic improvement at *Sector2* and *Sector4*, there is considerable fluctuation of L/D at $M_\infty \in [0.75{:}0.85]$ (transition point: *Sector2* to *Sector3* and *Sector3* to *Sector4*), where a high dash flight is required. Therefore it is necessary to check the aerodynamic quality along the Sector conditions; $M_\infty \in [0.75{:}0.85]$, $\alpha \in [4.662{:}1.887]$ and $ATI \in [30{,}0062{:}10{,}187]$. This can be done using mean and variance of L/D; the mean value indicates the scalar of objective, while the variance can be interpreted as the stability/sensitivity of the objective.

Table 4 compares the quality of L/D obtained from the Pareto members and the baseline design. The L/D variances of the optimal solutions are higher

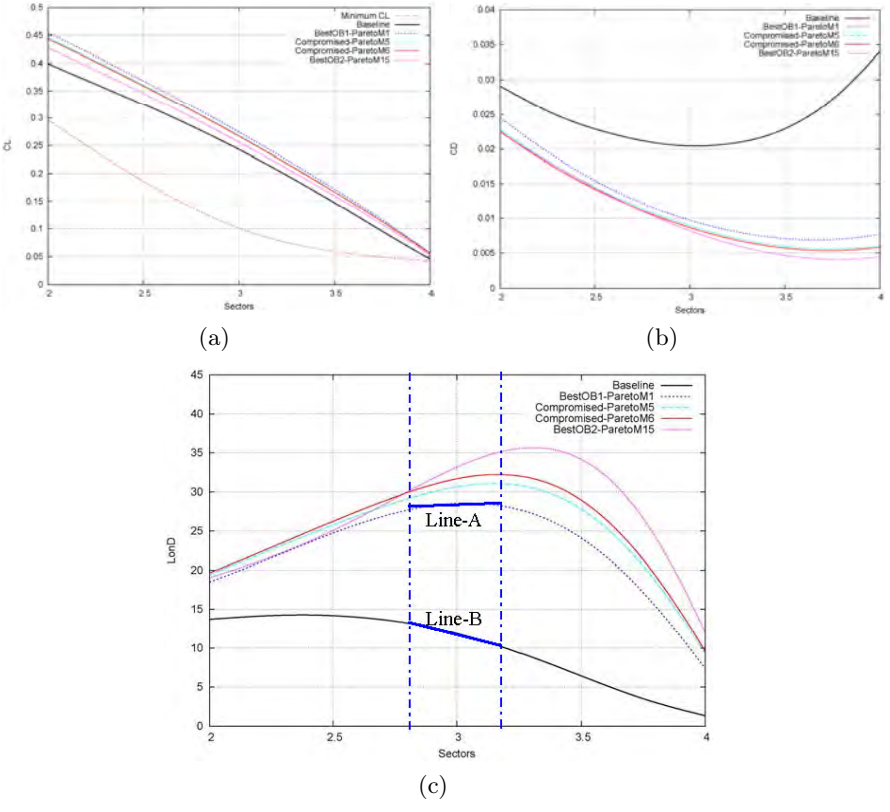


Fig. 8. a) C_L vs. Sector sweep. b) C_D vs. Sector sweep. c) L/D vs. Sector sweep.

than of the baseline design. This means Pareto members are overoptimised solutions to maximise an aerodynamic performance at design conditions.

Table 4. Comparison of the L/D quality.

Description	Baseline	ParetoM1	*ParetoM5*	*ParetoM6*	ParetoM15
$\overline{L/D}$	10.525	27.62	*30.03*	*31.05*	33.222
$\delta L/D$	8.25	23.53	*42.08*	*50.19*	127.10

This fluctuation can lead to structural or control failure at the transition point. This fluctuation can be avoided by using a robust design technique during optimisation. However, particular care is required for deciding variability of flight conditions. For instance, if the variable operating conditions are con-

sidered between blue centre lines in Fig. 8(c), then the variance (Line-B) of the baseline is higher than Pareto member 1 (Line-A), even though the baseline is more stable (low sensitivity) from *Sector2* to *Sector4* conditions. The introduction of uncertainty with effective variability of operating conditions is implemented in the next subsection to produce stable solutions for both the drag coefficient and lift to drag ratio.

4.2 Uncertainty Based MDO of the J-UCAV

Problem Definition The two disciplines aerodynamics and electromagnetics are considered to maximise the survivability of the UCAV when operating on a target strike mission. The first objective is to maximise the mean of L/D in the aircraft Sector3, while minimising the second fitness function variance of L/D to reduce fluctuation (Fig. 8(c)) at variable flight conditions. A third fitness function considers mono (Sector2) and bi-static (Sector4) radar analysis at variable radar frequency to produce a stealth UCAV. The RCS quality (scalar and stability) is expressed as one combined statistical formula in terms of the mean and variance.

The variabilities of design conditions (end of *Sector2* to beginning of *Sector4*) are:

$$M_{\infty i} \in [0.75, 0.775, M_s = 0.80, 0.825, 0.85],$$

$$\alpha_{\infty i} \in [4.662^o, 3.968^o, \alpha_s = 3.275^o, 2.581^o, 1.887^o],$$

$$ATI_{\infty i} \in [30062, 25093, ATI_s = 20125ft, 15156, 10187],$$

$$F_{\infty i} \in [1.0, 1.25, F_s = 1.5GHz, 1.75, 2.0],$$

where M_s, α_s, ATI_s and F_s represent the standard design condition.

The fitness functions for this problem are defined as:

$$fitness(f_1) = min\left(\frac{1}{\overline{L/D}}\right) - (mean),$$

$$fitness(f_2) = min\left(\delta\frac{L}{D}\right) - (variance),$$

$$fitness(f_3) = min(RCS_{Quality}) =$$

$$= \frac{1}{2}\left[(\overline{RCS}_{mono} + \delta RCS_{mono}) + (\overline{RCS}_{bi} + \delta RCS_{bi})\right],$$

where $\frac{\overline{L}}{D} = 1/K\sum_{i=1}^{k}(L/D_i)\frac{M_{\infty i}^2}{M_s^2}$ and $\delta\frac{L}{D} = \frac{1}{(K-1)}\sum_{i=1}^{k}\left(L/D_i\frac{M_{\infty i}^2}{M_s^2} - \overline{L/D}\right)^2$,

and $\theta = [0^o : 3^o : 360^o]$ and $\phi = [0^o : 0^o : 0^o]$ (*Mono-static*),

and $\theta_0 = 135^o, \phi_0 = 90^o at \theta = [0^o : 3^o : 360^o], \phi = [0^o : 0^o : 0^o]$ (*Bi-static*).

Results The algorithm was allowed to run approximately for 539 function evaluations and took 200 hours on two 2.4 *GHz* processors.

The resulting Pareto set is shown in Fig. 9 where the black inverse triangle (Pareto member 1) represents the best solution for fitness function1. The red square (Pareto member 10) represents the best solution for fitness function 2. The blue triangle (Pareto member 10) indicates the best solution for the third fitness. The light blue square (Pareto member 8) indicates the compromised solution. It can be seen all Pareto members produce higher L/D with low sensitivity while their wing planform shapes have low observability.

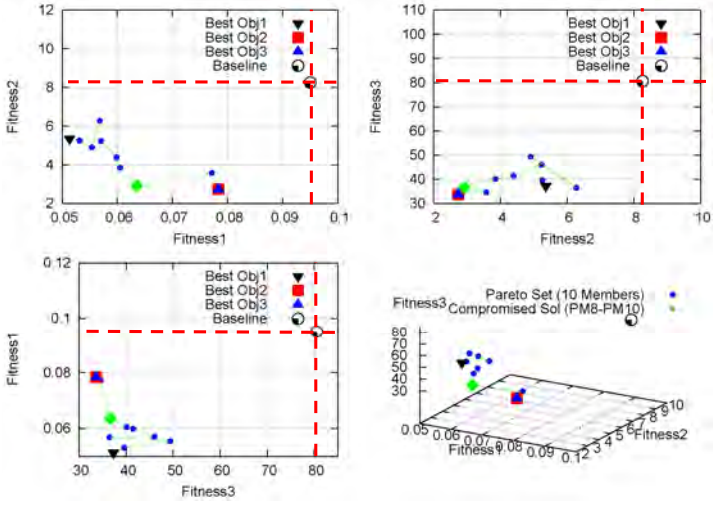


Fig. 9. Pareto optimal front.

Table 5 compares the mean and variance of lift to drag ratio and RCS quality obtained by Pareto members (1, 8, 10) and the baseline design.

Pareto member 1 produces lower inverse mean lift to drag ratio by 46% with 35% reduction of sensitivity, when compared to the baseline design. The sensitivity $\delta(L/D)$ of Pareto member 10 is lower by 67% with 18% improvement in $1/\sqrt{L/D}$. These indicate that all Pareto members produce higher aerodynamic performance with less sensitivity at the start of *Sector3* to the end of *Sector3*, where the fluctuation is shown in Fig. 8(c). In addition all Pareto members have RCS quality improvement (more than 50%) when compared to the baseline design.

Table 5. Comparison of the objectives.

Description	Baseline	ParetoM1	*ParetoM8*	*ParetoM10*
$1/\overline{L/D}$	0.095	0.051 (-46%)	*0.063 (-34%)*	*0.078 (-18%)*
$\delta(L/D)$	8.25	5.35 (-35%)	*2.91 (-65%)*	*2.73 (-67%)*
$RCS_{Quality}$	80.58	37.29 (-53%)	*36.67 (-54%)*	*33.62 (-58%)*

Figs. 10(a) -10(c) compare the Sector sweep vs. C_L, C_D and L/D obtained from current non-dominated solutions (Pareto members 1∼10), Pareto member 5 (denoted as AeroPM5) from the previous test (Section 4.1) and the baseline design.

The range of *Sector* sweep is from *Sector2* to *Sector4*. Fig. 10(a) shows that the current Pareto members (1 and 2) and AeroPM5 produce higher C_L along

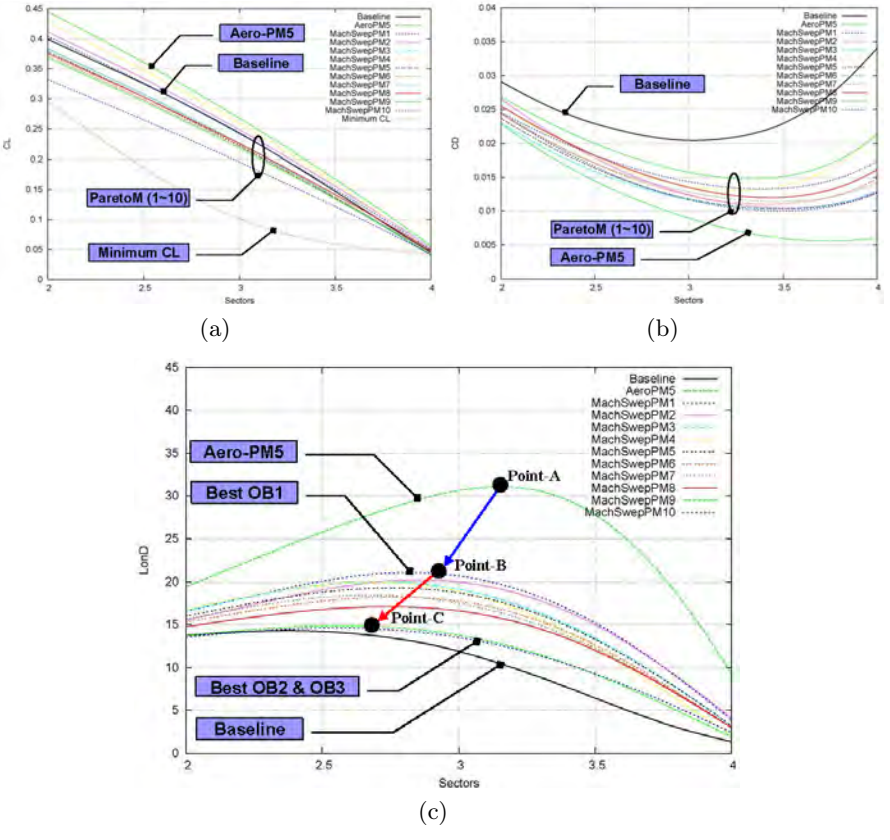


Fig. 10. a) C_L vs. Sector sweep. b) C_D vs. Sector sweep. c) L/D vs. Sector sweep.

Table 6. Comparison of C_D quality.

Description	Baseline	AeroPM5	ParetoM1	*ParetoM8*	*ParetoM10*
$\overline{C_D}$	0.025	0.010 (-60%)	0.012 (-52%)	*0.014 (-44%)*	*0.015 (-40%)*
δC_D	5.49×10^{-5}	1.54×10^{-5}	7.917×10^{-6}	6.48×10^{-6}	3.83×10^{-6}

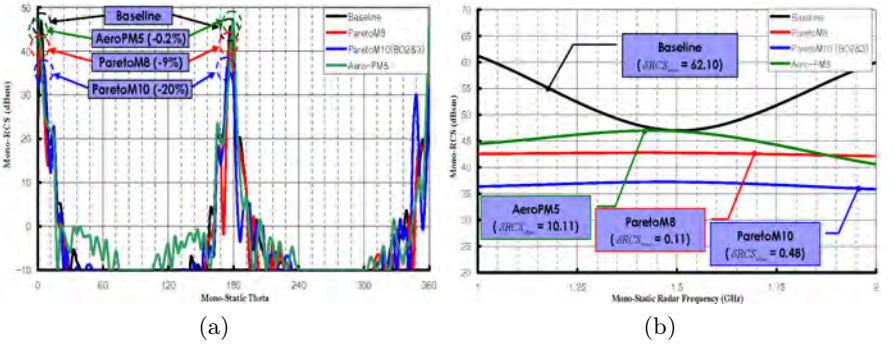
the Sector sweep when compared to the baseline design. Pareto members (3 to 10) have a lower C_L when compared to the baseline design while having a higher C_L value than C_{Lmin}.

Fig. 10(b) and Table 6 compare the mean and sensitive of C_D obtained by Pareto members (1 to 10), AeroPM5 and the baseline design. AeroPM5 produces lower drag when compared to the other Pareto members and the baseline, whereas the current Pareto members have much lower C_D sensitivity along the Sector sweep.

Fig. 10(c) compares the L/D along the Sector sweep obtained by Pareto members (1 to 10), AeroPM5 from the previous test and the baseline design. It can be seen that Pareto member 1 and AeroPM5 produce higher L/D than the baseline design, while Pareto member 10 produces lower sensitivity. It can be seen that one of the benefits of the uncertainty design technique is that the maximum L/D point (Point-A) of AeroPM5 moves to the maximum L/D point (Point-B) of Pareto member 1 and then the designs and solutions move to Point-C of Pareto member 10 which corresponds to and reflects the *variance*.

Fig. 11(a) compares the mono-static RCS analysis obtained by Pareto members (8 and 10), AeroPM5 from Section 4.1 and the baseline design at the standard design frequency (1.5GHz).

It can be seen that Pareto members 8 and 10 produce 9 % and 20 % lower *RCS* when compared to the baseline design while AeroPM5 produces almost

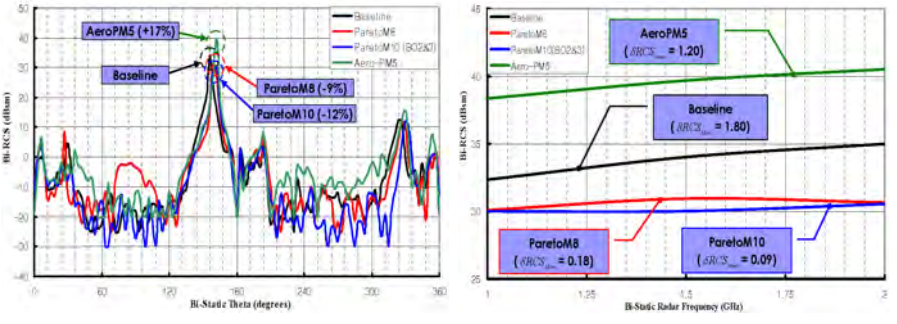


(a) (b)

Fig. 11. a) RCS_{Mono} at standard frequency. b) RCS_{Mono} vs. $F_{Mono-static}$.

the same RCS as the baseline design. Fig. 11(b) illustrates a frequency sweep corresponding to mono-static RCS analysis. The variance value for Pareto member 8 is lower while the baseline design value highly fluctuates at the standard design radar frequency ($1.5\,GHz$).

Fig. 12(a) compares the bi-static RCS analysis obtained by Pareto members (8 and 10), AeroPM5 and the baseline design at the standard design frequency (1.5GHz). Even though AeroPM5 produces higher aerodynamic performance, its bi-static RCS indicates that it has 17 % more chance to be detected, compared to the baseline design. Pareto members 8 and 10 have 9% and 12 % lower observability when compared to the baseline design. Fig. 12(b) compares the bi-static RCS at variable frequencies and shows the lowest RCS variance is achieved by Pareto member 10 ($\delta RCS_{BI} = 0.09$).



(a) (b)

Fig. 12. a) RCS_{Bi} at standard frequency. b) RCS_{Bi} vs. $F_{Bi-static}$.

5 Conclusions

A new methodology for the design and optimisation of UCAV aerofoil sections and wing planform shapes has been proposed and investigated numerically. The methodology couples a robust multidisciplinary evolutionary algorithm, with aerodynamic and RCS analysis software. The results of the method show that by introducing another discipline and a robust design analysis it is possible to compute a set of useful Pareto non-dominated solutions that produces 55 % lower sensitivity and 35 % higher aerodynamic performance with 55 % lower observability at variable flight conditions and radar frequencies when compared to the baseline design. Future work will focus on coupling the method with other game strategies such as Nash and hierarchical game. Results obtained from different games will be compared in terms of efficiency and design quality in a forthcoming paper.

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CFD Application in Automotive Industry

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Summary With the growing interest in environmental issues, the automotive industry is required to implement a range of measures such as increasing fuel efficiency or decreasing pollutants from exhaust gases. It is no doubt that CFD is an encouraging technology to develop an innovative idea by providing valuable data which conventional experimental methods can not measure. Compared with other industries, the automotive industry has been taking the initiative in introducing Computer Aided Engineering (CAE) at various stages of manufacturing. Thus, we can look into the state of the art of engineering CFD by reviewing its applications in automotive engineering.

1 Introduction

The main concern of automotive CFD is the treatment of turbulence. In fact, we have to treat generally higher Reynolds-number turbulence up to $Re \sim O(10^6)$, but it will be impossible to apply Direct Numerical Simulation (DNS) in the foreseeable future. Especially in the development stage of a new model, we have to obtain a reasonable numerical prediction within a couple of days at reasonable costs. Thus, conventional Reynolds-Averaged Navier-Stokes (RANS) simulation has been the most popular method, and commercial softwares are generally utilized to avoid excessive development cost for the CFD code. In addition to the accuracy of the solver, easiness of mesh generation, robustness and parallel efficiency of the solver are considered when we select commercial software among various candidates. Analysis scales are up to some million numerical meshes using computer cluster sys-

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tems, but occasionally, some ten million scale simulations are conducted on a supercomputer at the research stage.

With rapid development of hardware systems, unsteady or transient turbulence simulation now comes within range. The validity of the unsteady simulation is, in addition to its high accuracy compared with RANS, its applicability of predicting unsteady aerodynamic phenomena including aeroacoustics. Two promising methods for the time-dependent simulation are the Large Eddy Simulation (LES) and the Lattice Boltzmann Method (LBM). The LES is based on the spatially filtered Navier-Stokes equations, while the LBM is based on the mesoscopic Boltzmann equation. The validity of the LBM is its handiness of mesh generation and robustness of the numerical scheme, while its problem is that the effect of the numerical model on the macroscopic flow process is unclear. In both cases, the main issue to be solved is the treatment of the solid surface where the very thin turbulent boundary layer appears.

2 Vehicle Aerodynamics

For years, wind tunnels have been the main tool to assess vehicle aerodynamic performance. However, owing to the high cost for measurements, as well as the shorter time period of the vehicle design process, CFD is expected to be an alternative to the experimental measurements. In fact, CFD has been most extensively used in this category in the automotive industry.

The panel method was the only CFD available around thirty years ago, when a powerful computer was not available. In that method, fluid is supposed to be irrotational and velocity-potential is solved via a boundary integral equation transformed from the Laplace equation. The method is used together with the boundary layer method for the viscous treatment. The typical example [1] applied to a vehicle body is shown on the left of Fig. 1. It is impressive that even such an ad hoc method somehow properly capture the pressure distribution on the upper surface, while serious discrepancy is found on the vehicle floor and the rear end region where the flow separates from the body.

In the 80's, remarkable progress of supercomputers and engineering workstations made it possible to conduct 3-D Navier-Stokes simulation. Two major methods for the turbulence treatment at the time were: RANS in which turbulence is expressed as the Reynolds stress in the momentum equations and only the mean quantities are solved, and quasi DNS in which only larger eddies are solved in a time dependent simulation and smaller turbulent eddies are dissipated numerically by the upwind method. Generally the unstructured finite volume (FV) method is adopted for the former method, while the boundary-fitted coordinate (BFC) is employed for the latter case. The total numerical mesh number available was less than one hundred thousands at the time and a simplified car shape without an engine room was treated.

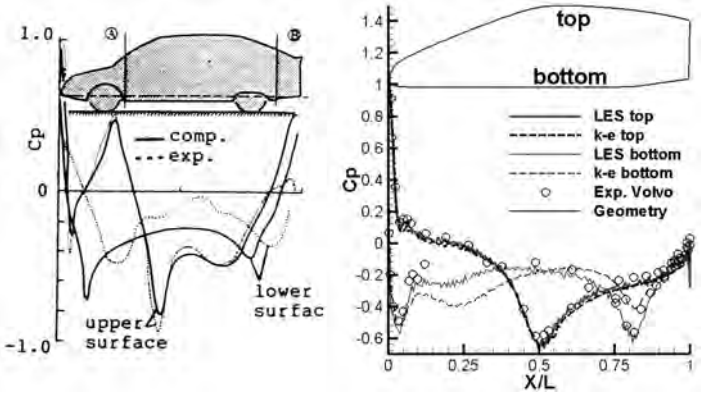

Fig. 1. Surface pressure distributions on the vehicle center line. Left: Panel method (reprinted with permission from SAE Paper 920338 ©1992 SAE International). Right: LES and RANS.

GFlops-class supercomputers were available in the 90's, and full-scale vehicle aerodynamic simulation with some million numerical meshes was going to be possible at the time. A landmark of a time-depending 3-D CFD for a full-scale vehicle was conducted in 1990 [2] using a quasi-DNS method with the upwind K-K scheme. CFD was realized to be a powerful tool for the vehicle aerodynamic assessment. However at the same time, some problems were recognized, such as the strong dependency on the adopted turbulence models, numerical treatments including the boundary conditions, numerical meshes and schemes [3].

In the 2000's, RANS methods were going to be commonly utilized in the automotive industry as a supplementary tools of wind tunnel measurements. The problems of RANS are: one is its strong dependence on turbulence model as mentioned above, and the other is its difficulty of capturing the unsteady flow characteristics. In addition, recently greater attention is paid to unsteady aerodynamic forces generated from sudden steering action, overtaking, or cross wind; all of which are difficult to estimate not only by a RANS method but also by a wind tunnel test, and an alternative method to the conventional manners is strongly desired. LES will be an encouraging solution to the problem, because it can reproduce unsteady turbulence characteristics with high accuracy, but in turn it requires excessively large computational resources. Consequently only few attempts have been made so far to apply LES to the assessment of vehicle aerodynamics. In 2002, the world-fastest massively parallel supercomputer Earth Simulator (ES) was developed in Japan, which consists of 5120 vector processors with the peak performance of 40TFlops. In 2006, high-performance computing LES of the flow around vehicles was conducted on ES to investigate the validity of the large-scale LES on vehicle aerodynamics [4]. They used some ten million numerical meshes and compared the results with the conventional RANS (standard k- model) method.

As shown on the right of Fig. 1, surface pressure distributions of LES and experimental data show excellent correlation on both top and bottom surface of the vehicle, while relatively large discrepancy appears between RANS and experiments on the bottom surface.

In 2007, high-performance computing (HPC)-LES of flows around a full-scale formula car and a motorcycle were conducted on ES using some ten to one hundred million meshes [5] (see Fig. 2).

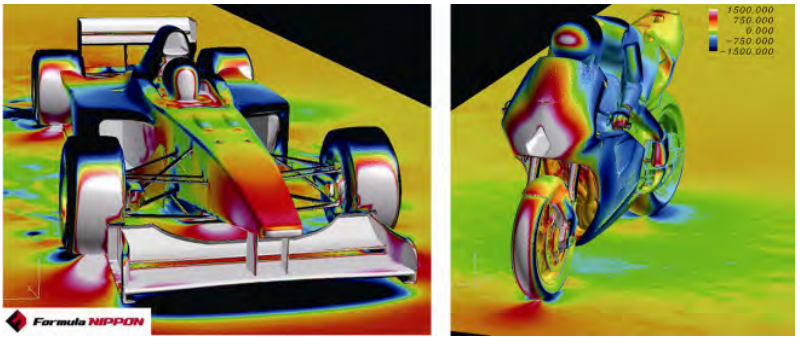

Fig. 2. HPC-LES of unsteady flow around a full-scale formula car and a motorcycle: Snap-shots of the surface pressure.

LES successfully predicted the lift coefficient, which is only about 1% larger than the wind tunnel data. Compared with the results of the panel method and LES in Fig. 1, which describes the progress of CFD for the thirty years, improvement of the underbody profile should be noted. Our next target concerning CFD and vehicle aerodynamics will be the estimation of unsteady aerodynamic forces acting on vehicles in the conditions of such as a sudden cross-wind and a steering action, or overtaking.

3 Thermal Management and Cabin Environment

Coupling of flow and heat transfer and predicting such multiphysics phenomena is an important issue in CFD. In the automotive applications, such problems appear in vehicle thermal management in an engine room, or in the indoor thermal environment. In the case of natural convection in which buoyancy dominates the flow, some sophisticated turbulence models are required for better prediction. In addition to heat convection, radiation and even conduction must be taken into consideration for the total thermal management. Reproduction of a solid body surface in detail is indispensable for the better prediction of heat transfer, and surface geometry of targets is usually complicated both in an engine room or a vehicle cabin. Accordingly, applications

of CFD to this category go back not so long a way compared with the vehicle aerodynamics. The history began in the late 1980's when a supercomputer was available. Especially recently, with the advent of new energy systems such as the hybrid electric system or the fuel cell, importance of CFD in the field is going to be more important than ever.

In addition to the thermal treatment, we need additional advanced numerical techniques for rotary machines such as a radiator fan or a blower fan for air conditioning. Physical modeling of a radiator as a porous media is also an important issue to properly predict the flow rate coming into the engine room through the front grille. The latest topic in the thermal management in an engine room is the consideration of the outer external flow around a vehicle for the inner simulation. The state of the art of simulations made with LBM is shown in Fig. 3 [6].

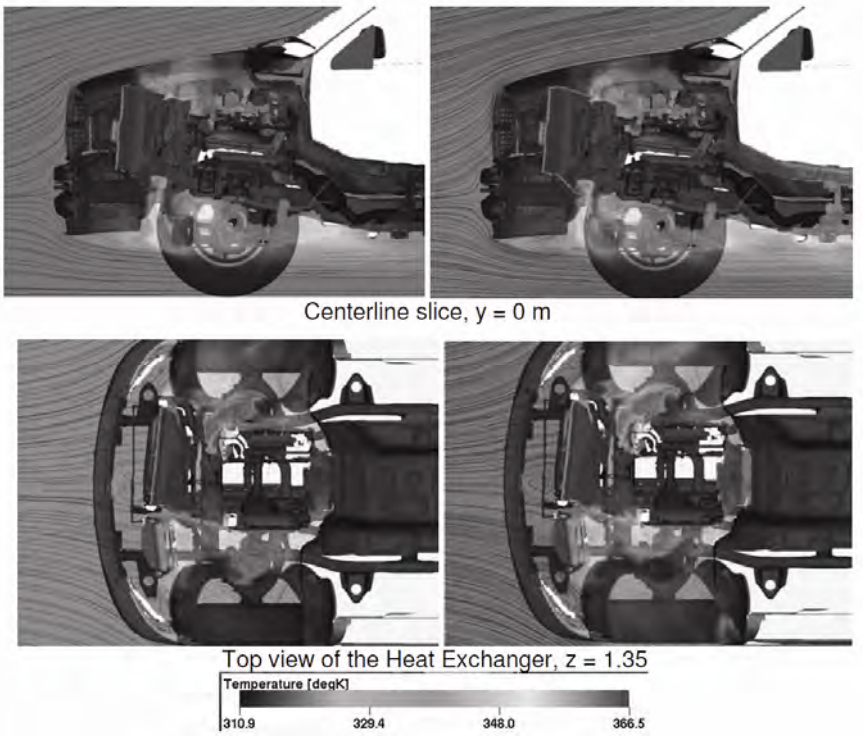

Fig. 3. Thermal management of an engine room with LBM: Temperature distributions with-out (left) and with (right) hot surface conditions (reprinted with permission from SAE Paper 2007-01-0100 ©2007 SAE International).

To exert a greater effect of air conditioning performance from the limited capacity, the assessment of the cabin thermal environment is conducted by

CFD. In such a simulation, radiation and solar insolation strongly affect the total environment. Fig. 4 shows the flow and heat transfer predicted by a RANS method, which indicates the effect of radiation on the total temperature profiles on the surface of the human model [7].

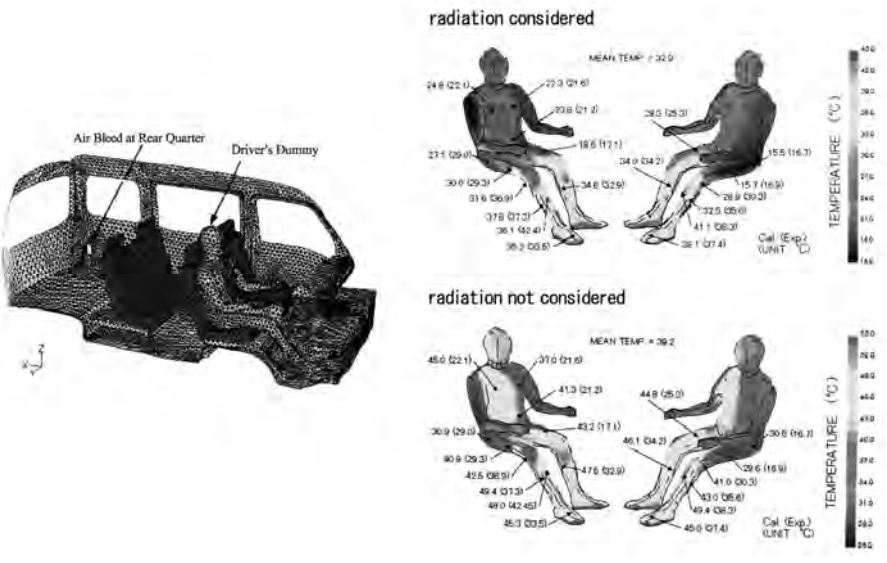

Fig. 4. Comfort assessment for the indoor environment considering heat radiation.

In addition to such difficulty in treating the physical condition, biological problems arise in the cabin CFD. For thermal comfort evaluation, the goal is to predict accurately the surface temperature of the human body, which is strongly affected by the biological heat balance inside the body. Thus a sophisticated heat transfer model for humans must be constructed. We need further progress concerning this matter.

In addition to the integrative objects mentioned above, CFD for elemental targets are also popular in this field. Fig. 5 shows a result for an air conditioning duct with very complicated geometry [8], which contains six ventilation nozzles, four in the dashboard and two in the B-pillars, four nozzles to the floor, one main defroster and two side defrosters. Total of about three million meshes are employed for RANS simulation using a commercial code. Fig. 5 shows the fraction of total flow rate through each branch of the air distribution system, which indicate that CFD shows relatively good agreement with experimental measurements.

Prediction of frost or moisture condensation patterns in a cabin or related equipments is also of great concern. We have to treat phase change in some situation. Fig. 6 shows an example of moisture and natural convection simulation inside a headlamp with complicated geometry [9]. The simulation con-

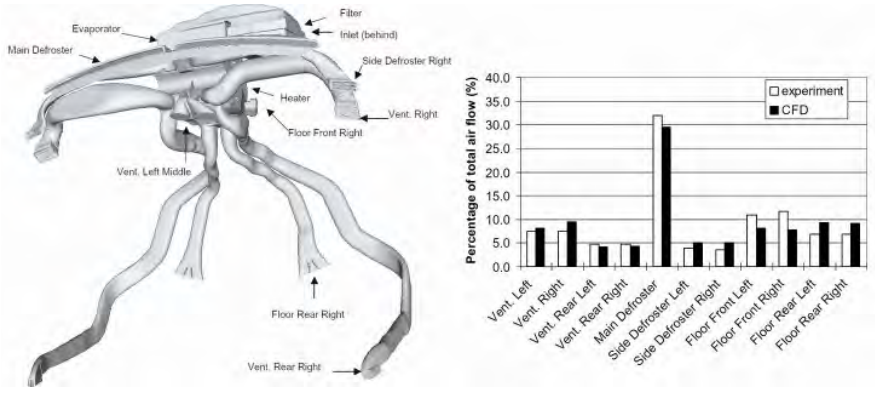

Fig. 5. Duct simulation for the air ventilation and conditioning system (reprinted with permission from SAE Paper 1999-01-1200 ©1999 SAE International).

siders radiation as well as moisture transfer resourcefully by applying a newly developed technique for the treatment of solid fluid inter-face. As shown in Fig. 6, CFD well predicts the moisture condensation pattern observed in the experiment.

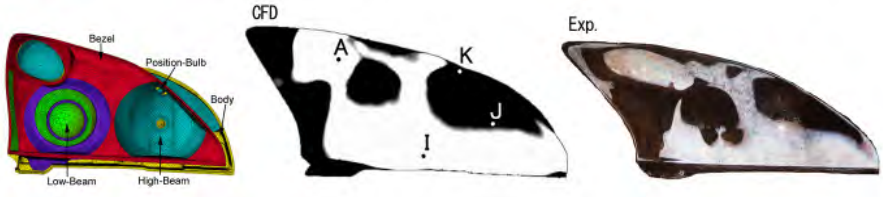

Fig. 6. Moisture and natural convection simulation inside an headlamp: Front view of the numerical mesh and the moisture condensation after 20 min (reprinted with permission from SAE Paper 2005-01-1449 ©2005 SAE International).

4 Internal Combustion Engine

Present IC (Internal Combustion) engines have been drastically changed more than ever. Owing to a combination of a turbo-charger, EGR (Exhaust Gas Recirculation), common-rail injection system, DPF (Diesel Particulate Filter) and electric engine control system, the performance of diesel engines has been much improved. At the same time, the engine system has become very complicated and needs an optimized control. Now, a diesel has to reduce exhaust gas emissions as low as a gasoline engine and also the cost. On the other hand,

a gasoline engine has to improve thermal efficiency as much as a diesel even followed by some cost up. Application of CFD in this category is relatively new, because we have to treat cavitation, two phase flow with phase change and chemical reaction, as well as the complicated geometry. The targets of CFD for IC engines are categorized to the following three topics: simple gas flow, fuel supply, and reacting flow.

In the gas flow simulation, air charging system, EGR system, VVA system and in-cylinder flow control are targeted. Especially in the VVA (Variable Valve Actuation) system, the optimization of open/close valve timings and valve lift amount are carried out by CFD.

The fuel supply and mixture formation processes is relatively challenging, because we have to consider cavitation with erosion or the gas-liquid two-phase flow phenomenon. In most cases, the treatments of interfaces between liquid and gas phases, surface tension, turbulence at its interface and phase change phenomenon must be well modeled numerically [10, 11]. Especially, as cavitation is a very rapid phenomenon, calculation stability is quite bad. It is a big issue what kind of calculation scheme and technique should be used. The in-nozzle flow CFD is useful not only for the prediction of cavitation and erosion but also for boundary conditions at the nozzle exit for the calculation of spray inside the cylinder [12]. The mixture formation inside the cylinder is also important. The Lagrangian method of DDM (Discrete Droplet Model) that treats droplets by grouping them into several thousands parcels is widely used.

The evaporation process is modeled in a phenomenological way based on many experimental results. The mixture formation inside a cylinder depends on both convective flow and turbulent diffusion. As the in-cylinder gas motion is very complex and strongly unsteady, a standard turbulence model such as a k-model is not necessarily appropriate. Moreover, cycle-to-cycle flow variation exists in an engine flow field. To resolve this, an application of LES is strongly expected [13, 14].

Reacting flows are the most advanced field in the last years in the modeling of flow and chemical reactions. The demand of predicting chemical reactions became quite strong since a new combustion technology of HCCI (Homogeneous Charge Compression Ignition) has been introduced. In HCCI, the ignition timing must be controlled precisely, which is achieved by controlling many items spatially and temporally, such as EGR, fuel concentration, gas temperature and gas pressure. This is actually very difficult using conventional map-control systems, instead, model-based control that needs CFD is used [15]. Predicting the ignition onset timing is also an important issue, and chemical elementary reactions must be solved. However, the reaction mechanism is too complex to solve for an actual engine in 3D at the moment. In the near future, the prediction ability of ignition onset timing as well as other physical properties will be improved enough for practical use.

The flame propagation process of a spark ignition engine varies from cycle to cycle. In order to design a production engine, the cycle-to-cycle variation

should be reduced. Figure 7 shows calculated results [14] of flame surface density using LES for four consecutive engine cycles. This information will be quite useful for the engine design.

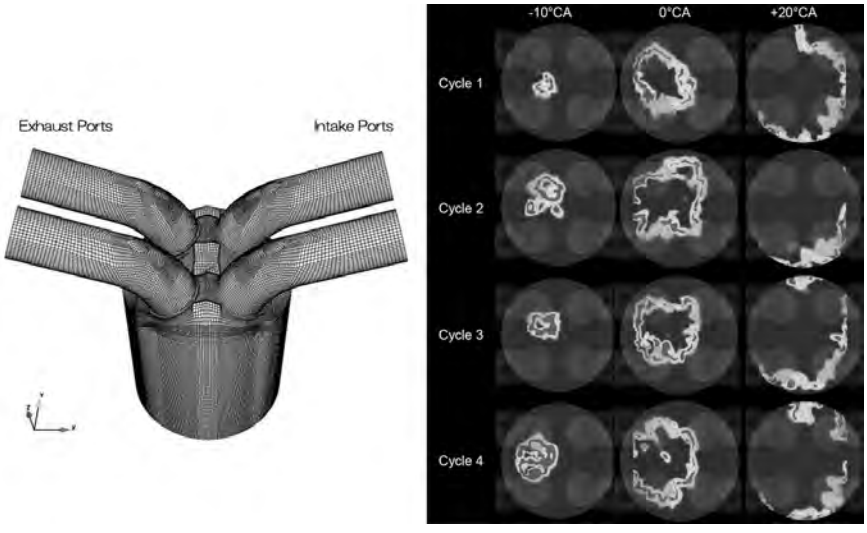

Fig. 7. LES of flow and combustion in an IC engine: the flame surface density at three crank angles for the 4 cycles (reprinted with permission from SAE Paper 2007-01-0151 ©2007 SAE International).

5 Aeroacoustics

Notorious aeroacoustics relating to vehicles is: wind noise generated by the A-pillar and door mirror, wind buffeting noise generated by a sunroof, or fan noise generated by a radiator fan or an air conditioning fan. If the target aerodynamic sound is supposed to be generated at low Mach numbers condition around the source object, far-field sound can be estimated from the Lighthill-Curle's equation, which can be solved separately from the flow simulation. The typical aeroacoustics such as the wind noise or the fan noise can be treated in this manner. Under this assumption, the time history of the pressure distribution on the solid surface is solved by CFD to predict the wind noise. In fact, if we can estimate the source of the noise through CFD, it is going to be a valuable tool for aeroacoustic problems. However owing to the relatively high computational cost for the unsteady 3-D simulation, its history has just begun.

Even though the mathematical method for the noise prediction itself has already been matured, we have to treat the numerical method for flow sim-

ulation more carefully to properly capture the broad spectra of turbulence fluctuation. Unsteady simulation methods such as LES [16] or the Lattice Boltzmann Method (LBM) will be promising for this purpose. Fig. 8 shows a computational analysis of underbody wind noise sources using LBM [17]. The predicted fluctuating pressure level for the 400 Hz 1/3 octave band shows good qualitative agreement with experimental measurements.

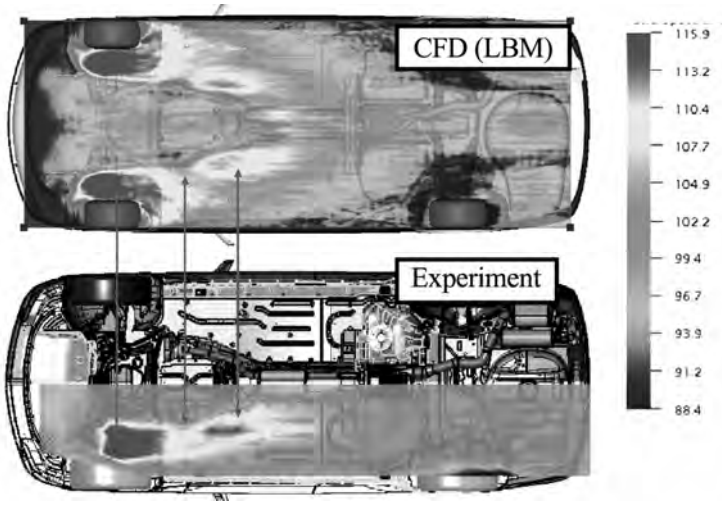

Fig. 8. Underbody wind noise predicted by LBM: 400 Hz 1/3 octave band (reprinted with permission from SAE Paper 2007-01-2400 ©2007 SAE International).

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Performance Upgrading of Hydraulic Machinery with the Help of CFD

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Summary In the developed countries the installation of new hydro electric power stations is nowadays very difficult and in many cases impossible. Here the upgrading of old power stations through replacement of critical components is the right measure to considerably increase the production of electricity by use of renewable resources. The development of such improved and more powerful components, most of all the turbine runner, is today possible based on numerical flow simulation and other modern CAE-tools. More than 50 % of old power plant installations have operational problems such as cavitation erosion, vibration of the structure due to vortices at off-design operation or severe noise. As an example the numerical engineering is described, that was carried out in order to upgrade a low head small hydro electric power station in Germany to increase power production by 30 % and to avoid cavitation erosion in the turbine runner. The new components have been installed and successfully put to operation. Now the turbine is performing well and is running surprisingly smooth.

1 Modernization of Old Hydro Electric Power Stations

Francis turbines are the standard type of hydraulic turbines used in the range of 50 to 500 m head. In total all over the world roughly 85 % of the hydraulic turbo machines are of the type Francis. The biggest hydroelectric Power plants such as Itaipu in the South of Brazil as well as Three Gorges Dam in China are equipped with Francis Turbines. But also for lower heads down to a few meters Francis turbines can be and already are successfully used.

Fig. 1 shows a Computer representation of a low head small hydro twin Francis turbine in southern Germany. Numerical analysis was made in order to find out what could be improved with the old machine that was built in the 1920s. In fact the two old runners were damaged seriously over the years

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of operation due to cavitation erosion, photograph in Fig. 2 shown below. Furthermore, the question was whether it was possible to increase the power output not only with improved efficiency but by increasing the discharge at full load in order to generate more electrical energy than before.

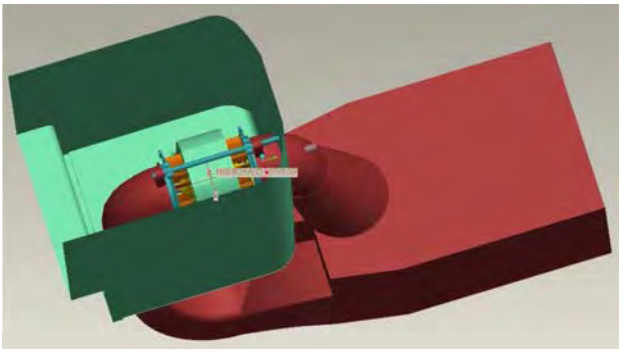

Fig. 1. Low head small hydro Francis turbine.

The task was quite ambitious because the machine had some special construction features, for instance, Fig. 1:

- no spiral casing,
- two runners on one shaft,
- two draft tubes converging into one outlet.

Therefore the question was not only, how to find a good solution to replace the existing runners in order to avoid cavitation erosion, but also to increase the output. First of all, it was to find out whether the other components of the machine were in good condition or not. As a consequence 3D flow simulation was carried out through the components of the existing machine, in fact through:

- the intake and the distributor,

Fig. 2. Cavitation erosion on the old runner.

- the runner,
- the bends and draft tubes.

In addition 2D analysis was performed to control the global data as well as the main dimensions of the turbine components. This was of special importance for the development of a replacement runner with less cavitation and increased energy production.

2 Analysis of Turbine Components

There were some doubts that the shape of the intake would lead to an acceptable quality of the flow in the distributor. It is clear, that if the flow distribution around the runner is far from being constant along the circumference, then rough running of the turbine would be the consequence. These doubts were justified due to the fact that the existing intake has a 90 degree step so that the incoming flow must separate from the edge, forming vortices in front of the machine, Fig. 3.

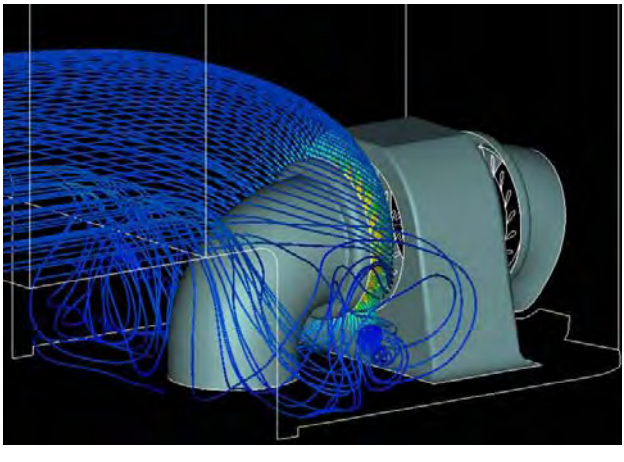

Fig. 3. Flow at turbine intake for best efficiency.

However, it was surprising how low the disturbance at the location of the turbine distributor in fact was. Fig. 4 shows the flow inside the guide vanes at mid span of the blades.

The flow velocities are indicated through colors, blue means very low flow, red means high flow velocities (here 8 m/s). The region in red forms nearly a circle, which means that the fluid entering the turbine runner is close to be perfectly distributed in terms of through flow as well as in terms of swirl. This gave confidence that a successful modernization of the existing power station

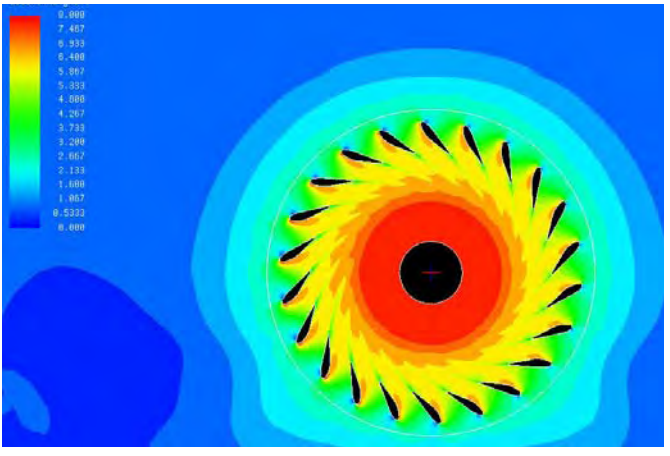

Fig. 4. Flow at the turbine intake and the wicket gate at mid span.

through replacement of important components with a new design was really possible.

It was known that the bends at both sides downstream of each runner could be a problem because there is no deceleration of the flow between runner outlet and the bend. However, with the help of some guiding profiles the turning of the flow inside the bend could be considerably improved leading to an acceptable flow pattern for the rest of both draft tubes.

3 Preliminary Design of a New Runner

Normally, when upgrading an existing old machine, the guide vanes as well as the runner are to be investigated and, in case it is necessary to replace these components to achieve the goals, a change in the construction has to be made. In order to get an idea how the new construction can look like, the Euler equation of turbo machinery can be used:

$$u_1\, c_{u1} - u_2\, c_{u2} = q\, H.$$

Using this equation it easily can be found that the existing contours lead to pretty strange blade shapes. Instead, by streamlining the flow channel and changing the radii of the leading edge as well as the trailing edge of the blading, much better blade shapes can be found, Fig. 5.

For the design point the following data were fixed: head $H = 10\,m$, discharge $Q = 10\ m^3/s$, runner speed $n = 214\ rpm$.

The runner speed had to be kept as before because the same generator should be used for the first time after modernization before the new one was ordered and installed. According to the above design condition the main dimensions were derived: $D_1 = 1{,}56\ m$, $D_2 = 1{,}65\ m$, $B_o = 0{,}52\ m$.

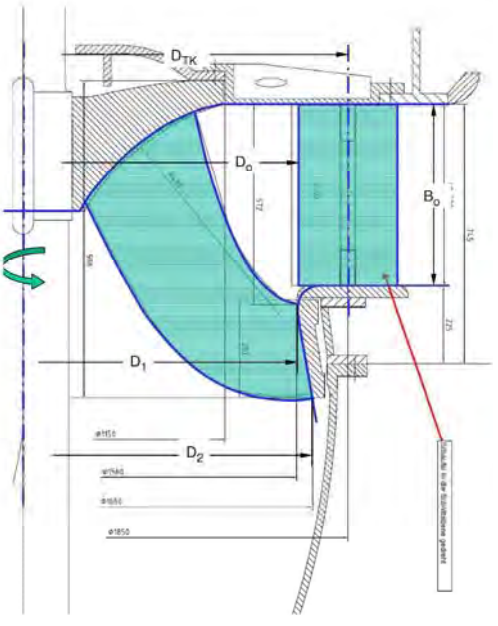

Fig. 5. Estimation of the new meridional contour by use of Euler's equation for turbo machinery.

Because the calculated angles are flow angles when using Euler's equation, the blade angles, that have to be used to define the final runner geometry, must be different to the first estimation. This difference between flow angles and blade angles must be found by using CFD.

4 Analysis of the Existing (Old) Runner

According to best engineering practice in the refurbishment and upgrading of old hydro electric power stations, the following steps have first been followed:

- assessment of the old runner geometry,
- based on this, creation of a numerical model for the old runner,
- flow simulation according to the old design condition,
- correlation of the results with observation, performance as well as cavitation erosion, if any.

The assessment of the old runner geometry was carried out using photogrammetry. The wetted surfaces were derived and based on this, the numerical model of the runner was created to perform the flow simulation. The result of the simulation shows clearly low pressure regions for the old runner at blade leading edge adjacent to the runner band, Fig. 6. As for many old runner

designs in Francis turbines, leading edge cavitation is the consequence, when the pressure is below vapor pressure, which correlates well with the erosion of the material observed on the old dismantled runner.

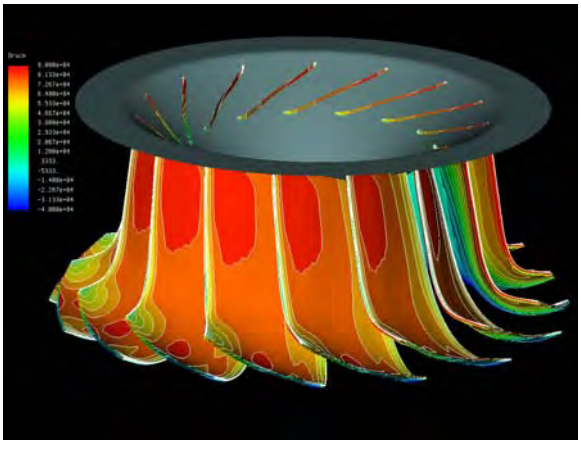

Fig. 6. Pressure distribution on the old runner blades at the inlet.

This is shown in Fig. 7. Cavitation at the runner inlet is likely to be the reason for the erosion that destroyed completely some parts of the blade leading edge, white circle.

This erosion is roughly the same at all blades of the old runner. The corresponding pressure distribution along the blade profile close to the band is given in Fig. 8. On the pressure side of the blade, the lowest pressure is at the leading edge.

Over some 20 % of the blade length there is no difference in pressure on both sides of the blade. Therefore, in this region the blade lift is zero, and the resulting torque is zero as well. This cannot lead to highest hydraulic

Fig. 7. Cavitation erosion at the blade's leading edge.

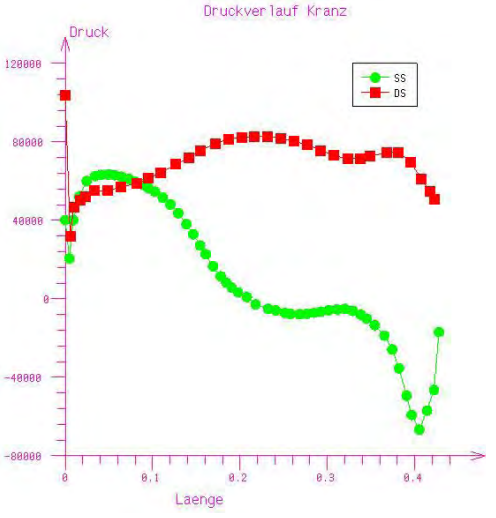

Fig. 8. Pressure on the blade close to the band, leading edge left. Ordinate: pressure, abscissa: chord length, SS: suction side, DS: pressure side.

efficiency. On the suction side of the runner the pressure distribution is shown in Fig. 9. This result correlates again quite well with the erosion as can be seen in Fig. 7. Note that the low pressure region is close to the trailing edge of the runner blades. In this region the cavitation starts to develop. The corresponding erosion of the material can only be downstream of this area, where the pressure rises up to values above vapor pressure.

In order to measure the improvement with the modernization, the performance of the old turbine was measured in the power station before the works were started.

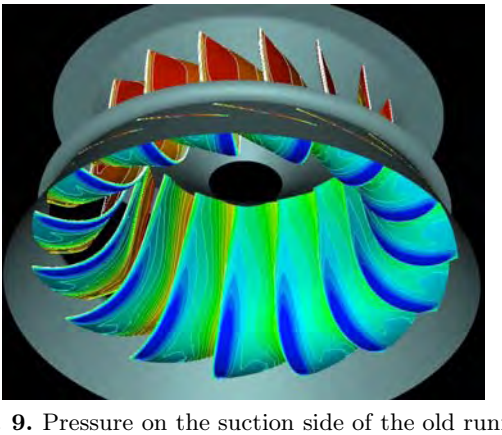

Fig. 9. Pressure on the suction side of the old runner.

Fig. 10 indicates the improvement which could be achieved with the modernization as well as the upgrading of the turbine. The graphic shows the turbine output depending on the discharge through the turbine. The discharge is regulated through different openings of the wicket gate. The data given for the power output are values produced at the outlet of the turbine generator. This means that all hydraulical, electrical as well as mechanical losses are included.

Prior to the upgrading of the turbine the maximum power output at full load was roughly 1200 kW. Now, after modernization, the power output is as much as 1600 kW. This is equivalent to an increase of nearly 30 % of the turbine power at full load operation. This shows clearly the potential for upgrading of old hydro electrical power stations, which are some 50 years old or more.

In addition, the operation of the turbine is remarkably smooth. It is well known that for Francis turbines smooth running can only be achieved in a certain range of operation around the point of best efficiency. Surprisingly, with the new design, the turbine is running smoothly from part load to full load.

5 Optimization of the New Runner

In modern hydraulic engineering for the development of a replacement runner, the approach is usually based on numerical flow simulation [1]. However, CFD is important, but only one part of the whole design process [2]. In total one has to:

- create the runner geometry (parametric design),

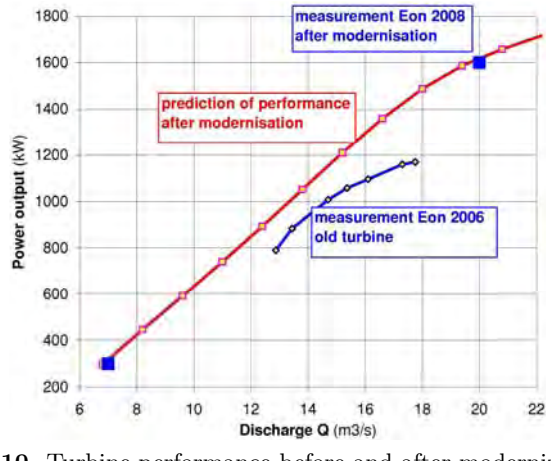

Fig. 10. Turbine performance before and after modernization.

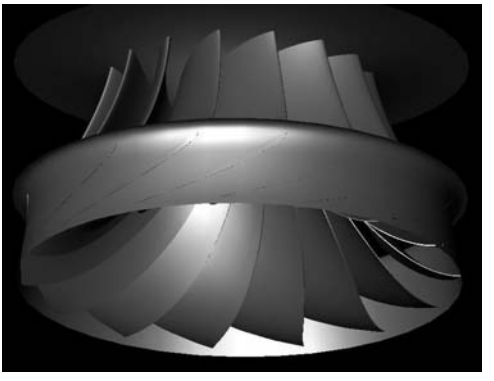

Fig. 11. Final runner design.

- generate the computational mesh automatically,
- specify (correct) boundary conditions,
- perform the flow simulation,
- visualize the important computation results in detail,
- summarize the main results to decide whether
- continue or stop.

Experience shows, that integration of all these parts is essential and one key for success [3]. Especially for low head turbines a good runner design is not easy to develop. A great number of steps has to be carried out not only to achieve the desired performance and hydraulic efficiency, but also to minimize cavitation inception at critical flow regimes [4]. In addition one has to minimize vibrations caused by rotor-stator interaction as well as those vibrations caused by draft tube vortex formation at off-design conditions.

The final runner geometry for the actual project is shown in Fig. 11. Typical for such a modern design is the curved shape of the blade trailing edges. This is in contrast to the old design philosophy, were the outlet edge of the runner blades was radial in any case.

What has been achieved in terms of pressure distribution on the runner blades can be seen in Fig. 12. Over a great portion of the profile length the blade loading is nearly constant. This is important in particular at the tip profiles near the band, because at the greater radii most of the runner torque is produced. Nevertheless, a small low pressure peak on the suction side at the blade's leading edge is still left, which is caused by the strong turning of the through flow at the runner inlet.

Comparison of Fig. 12 with Fig. 8 shows clearly the improvement against the old runner. The rear loading of the old blade is completely avoided.

Not to forget, that the operating conditions for the two figures are different. The pressure distribution in Fig. 8 corresponds to a considerable smaller

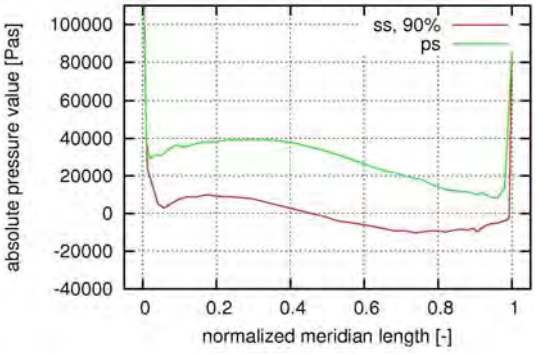

Fig. 12. Pressure distribution on the runner blade at the band, leading edge left.

discharge as for that distribution shown in Fig. 12. This indicates in addition a big step forward with the new runner design.

6 Parametric Runner Design

The new runner was optimized intuitively in a virtual reality environment [5]. Based on a set of parameters corresponding to the hydraulic data given by the power plant as well as to the geometrical data given by the existing turbine, the runner geometry is generated and the computational meshes are produced. Then the flow simulation is carried out according to the given operating condition for the turbine in an automated way. Within the same process the visualization is made so that the reaction of the flow on the change introduced to the runner geometry can be studied straight forward.

To give an impression of the shape of the new runner blades, the conformal mapping of three selected profiles is shown in Fig. 13 for the blade profiles at hub, mid span and at the band. Since this is a low head installation, the curvature of the blade profiles is low. However, the rotational speed as well as the meridional position of both the blade leading and trailing edge have an influence on the blade shape and in particular on the curvature of the blades.

In this sense it might be interesting to compare the preliminary dimensions and blade position shown in Fig. 5 with the final design after the complete numerical optimization. To do this the new runner is shown in Fig. 14 with the view from the inlet. The outlet cannot be shown in this representation.

It turns out that the shape of the preliminary blade leading edge fits quite well with the final runner design, [6]. This positive feedback is pretty important because in a typical project for rehabilitation or upgrading of an old power station one of the first questions is, whether or not a good solution is feasible.

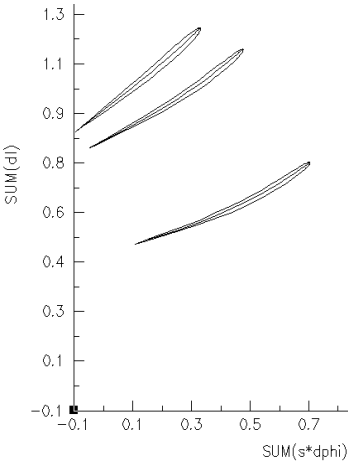

Fig. 13. Conformal mapping for the new blade profiles at the hub, mid span and band, from top to bottom.

7 Conclusion

After installation of the new components the first turbine is now in operation for a couple of months. The old generator is still in use with the consequence that, due to the limit of the existing generator, the maximum power is now limited to 1600 kW. The predicted potential of the old turbine could be realized, according to Fig. 11. As a result the performance of the turbine could be increased by more than 30 % due to the modernization measures. Also important is that the operation of the turbine is now remarkably smooth within the whole operating range from closed guide vanes to full open. This is quite unusual because the experience shows for Francis turbines for part load as well as for full load more or less rough running mostly because of vortices in the draft tube or some noise due to cavitation.

This example shows the great potential of increasing the production of electricity on the basis of renewable energy resources through upgrading of

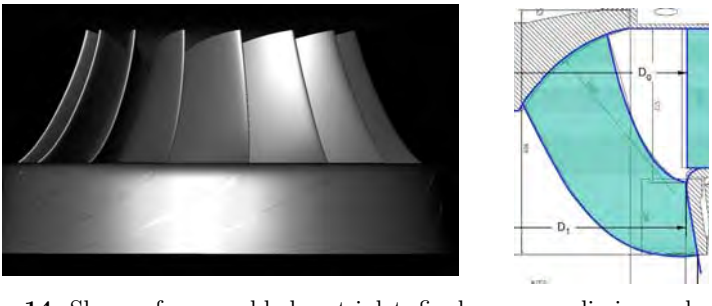

Fig. 14. Shape of runner blades at inlet, final versus preliminary design.

old hydro electric power stations. Especially in the developed countries the installation of new dams on rivers as well as reservoirs in the mountains is nowadays very difficult and in many cases impossible. In the old days the development of hydraulic turbines and pumps was made on the test stand, and only in few cases the design was going to be perfect. Nowadays with the upcoming numerical tools, it is possible to detect the weak parts of the existing designs. Combined with new materials now it is possible to put the old power station to their physical limit.

However, only the big companies have the equipment as well as the experienced personnel to perform a successful modernization. The engineering process is difficult, time consuming and therefore expensive. This is the reason why even in big companies upgrading engineering is only made for big hydro electric power stations, when the power output is above 20 MW up to the biggest turbines of 700 MW. For small and medium hydro power typically in the range from 500 kW up to 5 MW, the business is made by small and medium companies, and these companies are too small to develop tailor-made solutions in order to improve existing power stations.

Here universities play an important role because they develop and are using state of the art numerical tools for simulation as well as optimization. For the project described above, the hydraulic engineering was carried out at IHS, University of Stuttgart, the realization was made by Stellba Hydro, a small company in Baden-Württemberg, and the power plant operator is the great utility E.on. After the successful upgrading of turbine 1, these days the modernization of turbine 2 within the same power station is under installation.

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Calculating Blast Loads for Civil Engineering Structures

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Summary A brief overview of the state of the art of computing blast loads on civil engineering structures is given. The general problem setting, requirements, main physical phenomena and timescales, as well as suitable numerical methods are described. Several examples show the power of blast loads calculations for civil engineering structures.

1 Introduction

Explosions remain the most frequently used form of terror attack. They represent a low-tech, cheap, abundantly available resource that produces the desired destructive, psychological (mainly fear and rage), publicity (monopolization of news), economical (disruption of travel, commerce, investment and consumption) and political (destabilization) effects.

The amount of explosive used can vary considerably, from $10^{-1}kg$ for airplanes to $10^{4}kg$ for the more spectacular building attacks. Given the increasingly unstable international situation, the remarkable willingness of individuals to commit suicide, as well as the abundant availability of explosive materials, the number of worldwide attacks has increased in recent years. Outside crisis regions (e.g. war zones), a major attack ($> 10^{3}kg$ of explosive) has occurred every 6-12 months.

For buildings, the physical damage includes window breakage, disruption of amenities and services (water, gas, telephone, air conditioning, etc.), and loss of structural integrity (cracks, progressive collapse). Most of the casualties

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are due to glass shards flying into rooms at high speeds (timescale: tens of milliseconds), and building collapse (timescale: seconds).

From a civil engineering point of view, the design of structures is certified by building norms that consider the following static and dynamics loads: gravity (weight, water, contents), wind, vibration due to machinery, as well as earthquakes. Currently buildings do not require any form of certification for blast loads. This implies that most buildings have no inherent 'design for blast survivability' (e.g. in the form of a delayed or gradual collapse), and will remain highly vulnerable for the foreseeable future.

At present, the most effective means of protecting structures are given by standard low-tech options: restriction of access (safe perimeter zone with the ensuing disruption of traffic, comfort, etc.), screening of any material entering the safe zone close to the building, indoor walls and shatter-proof windows.

In order to assess the vulnerability of a given building or place, design for blast survivability, place cameras and sensors, as well as legislate building standards, it is imperative to know the maximum possible damage an explosion can cause. This, in turn, requires an accurate assessment of the pressure loads a blast will produce on a building.

A considerable amount of experimental and numerical work has been carried out in this field over the last three decades. While many dispersed journal publications exist, the proceedings of the Military Application of Blast Simulators (MABS) [32], Shock Wave [44], Shock and Vibration [43] and International Symposia on Detonation [9] provide a good overview.

Many groups are actively developing, improving and applying CFD codes for the assessment of blast loads on civil engineering structures. We mention, without any claim of completeness, the groups at ARA in Albuquerque, NM [16], SAIC/GMU in McLean, VA [4, 5], Cranfield University (UK) [42, 40], EMI (Germany) [17], Gramat/Marseille (France) [34], St. Petersburg [47] and Japan/China [15].

2 Physics

Let us consider the physically relevant phenomena present during a typical explosion. The explosive is detonated and chemical reactions ensue that liberate an enormous amount of energy in a timescale of microseconds. The shock wave produced by this energy then travels through the surrounding medium, weakening, in open air, as a function of the distance from the origin to the third power (r^{-3}). The timescale for the shock propagation phase, also known as diffraction phase, is of the order of a second. For very large blasts one can also identify a drag phase, where the detonation products continue expanding and the loads on structures are produced by form or viscous drag. This drag phase can extend for several seconds. For most civil engineering structures the bulk of the destruction occurs due to shock loading during the diffraction phase.

From a numerical point of view, the accurate treatment of all chemical reactions is beyond current hardware capabilities. Given the high variability of explosive materials, as well as their susceptibility to handling and storage conditions, it is questionable if such a detailed treatment would be of use for daily production runs. Instead, most engineering calculations use simplified burn models and combine these with equations of state (EOS) in order to arrive at descriptions that capture the main physical phenomena: jump in the p, ρ state when detonation occurs with the assumption of a subsequent isentropic expansion.

Thus, the physically relevant phenomena are well described by the compressible Euler equations, given by:

$$\mathbf{u}_{,t} + \nabla \cdot \mathbf{F}^a = \mathbf{S}, \tag{1}$$

$$\mathbf{u} = \{\rho \ , \ \rho v_i \ , \ \rho e\}, \quad \mathbf{F}^a_j = \{v_j \rho \ , \ v_j \rho v_i + p\delta_{ij}, \ v_j(\rho e + p)\}. \tag{2}$$

Here ρ, p, e, v_i denote the density, pressure, specific total energy and fluid velocities in direction x_i respectively. The sources $\mathbf{S}$ may be given by external forces, such as gravity or radiative energy deposition, or may originate from the interaction with particles from a second phase (e.g. dust). This set of equations is closed by providing an equation of state (EOS). For a polytropic gas, the EOS is simply :

$$p = (\gamma - 1)\rho e_i = (\gamma - 1)\rho[e - \frac{1}{2} v_j v_j], \tag{3}$$

where γ, e_i are the ratio of specific heats and the specific internal energy. In general, the equation of state will be of the form $p = p(\rho, e_i)$. For high explosives (HE), a common EOS is the Jones-Wilkins-Lee (JWL) EOS, given by:

$$p = A\left(1 - \frac{\omega}{R_1 v}\right) e^{-R_1 v} + B\left(1 - \frac{\omega}{R_2 v}\right) e^{-R_2 v} + \omega \rho e, \quad v = \frac{V}{V_0} = \frac{\rho_0}{\rho}. \tag{4}$$

The burn front is determined either from the the detonation velocity v_d (so-called 'programmed burn') or it is determined from local pressures, densities and temperatures (so-called 'forest fire burn') [33].

3 Numerics

Any spatial discretization via finite difference, finite volume or finite element methods of the Euler equations will yield a discrete system of the form:

$$\mathbf{M} \cdot \mathbf{u}_{,t} = \mathbf{r}(\mathbf{u}), \tag{5}$$

or, in index notation:

$$M^{ij}\hat{u}^j_{,t} = C^{ij}\mathcal{F}_{ij} = r^i. \tag{6}$$

Here, $\mathbf{M}, \hat{u}^j, C^{ij}, \mathcal{F}^{ij}$ denote the mass/volume-matrix, vector of unknowns, edge-coefficients for fluxes and edge-fluxes respectively (for cell-based finite volume techniques, replace 'cell' by 'face' in what follows). Given that no implicit time-marching scheme has shown the ability to propagate shocks accurately over many elements/cells in one time step, only explicit schemes are employed. In most cases, multistage Runge-Kutta schemes of the form:

$$\mathbf{M}\left(\mathbf{u}^{n+i} - \mathbf{u}^n\right) = \alpha_i \ \Delta t \ \mathbf{r}(\mathbf{u}^{n+i-1}), \quad 0 < i \leq k, \quad \alpha_i = \frac{1}{k-i+1} \tag{7}$$

have been used. We can now define the flux functions and limiters used, and then proceed to useful combinations that optimally combine speed and accuracy for the class of problems considered here.

3.1 Fluxes and Limiters

For the standard Galerkin approximation we have

$$\mathcal{F}_{ij} = \mathbf{f}_i + \mathbf{f}_j, \tag{8}$$

i.e. an equal weighting of fluxes at the end-point of an edge. This (high-order) combination of fluxes is known to lead to an unstable discretization, and must be augmented by stabilizing terms to achieve a stable, low-order scheme. The resulting flux is often referred to as a 'consistent numerical flux'. The physically most appealing flux of this kind is obtained from the exact solution of the Riemann problem, leading to the so-called Godunov solver:

$$\mathcal{F}_{ij} = 2f(\mathbf{u}^R_{ij}). \tag{9}$$

Here $\mathbf{u}^R_{ij}$ is the local exact solution of the Riemann problem to the Euler equations, expressed as $\mathbf{u}^R_{lr} = Rie(\mathbf{u}_l, \mathbf{u}_r)$. In order to achieve a higher order scheme, the amount of inherent dissipation must be reduced. This implies reducing the magnitude of the difference $\mathbf{u}_i - \mathbf{u}_j$ by 'guessing' a smaller difference of the unknowns at the location where the Riemann flux is evaluated. The assumption is made that the function behaves smoothly in the vicinity of the edge. This allows the construction or 'reconstruction' of alternate values for the unknowns at the middle of the edge. The additional information required to achieve a scheme of higher order via these improved values at the middle of the edge can be obtained in a variety of ways:

- Through continuation and interpolation from neighboring elements [6];
- Via extension along the most aligned edge [49]; or

- By evaluation of gradients [50, 30].

The last option is the one most commonly used, but carries a considerable computational overhead: 15 gradients for the unknowns in 3-D can account for a large percentage of CPU time.

The inescapable fact stated in Godunov's theorem that no linear scheme of order higher than one is free of oscillations implies that with these higher order extensions, some form of limiting will be required. For a review of these, see [46]. It is important to note that this form of limiting is done **before flux evaluation**, and that, strictly speaking, it should be performed with characteristic variables. We also remark that many limiters were derived for 1-D shock problems (and/or steady transonic shock problems), which are not indicative of shocks encountered in 3-D blast problems (see Figure 1). This is an area where considerable work is still required, as most current limiters tend to 'clip' exceedingly the sharp shock profile shown in Figure 1 b).

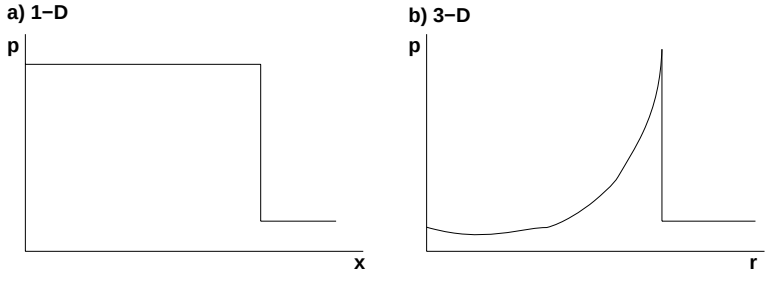

Fig. 1. Typical shock profiles.

Summarizing, a typical Godunov-based scheme has five main cost components:

- Gradient-based reconstruction of higher order approximations to the left and right states;
- Transformation from conservative to characteristic variables;
- Limiting;
- Transformation from characteristic to conservative variables;
- Solution of the exact Riemann problem.

In the sequel, we will enumerate possible simplifications to each of these cost components.

Transformation between conservative and characteristic variable can be avoided by limiting based on the conservative variables. Most production codes use this option.

The solution of the **exact Riemann problem** can be avoided by the use of **approximate Riemann solvers** that retain as much of the physics as possible [21, 41, 38, 14, 48, 31]. They may be written abstractly as:

$$\mathbf{u}_{lr}^{AR} = ARie(\mathbf{u}_l, \mathbf{u}_r). \tag{10}$$

A widely used solver of this class is the one derived by Roe [41], given by:

$$\mathcal{F}_{ij} = \mathbf{f}_i + \mathbf{f}_j - |\mathbf{A}^{ij}|(\mathbf{u}_i - \mathbf{u}_j), \tag{11}$$

where $|\mathbf{A}^{ij}|$ denotes the standard Roe matrix evaluated in the direction d^{ij}. Note that, as before, reducing the magnitude of the difference $\mathbf{u}_i - \mathbf{u}_j$ via reconstruction and limiting leads to schemes of higher order. A further possible simplification can be made by replacing the Roe matrix by its spectral radius:

$$\mathcal{F}_{ij} = \mathbf{f}_i + \mathbf{f}_j - \mid \lambda^{ij} \mid (\mathbf{u}_i - \mathbf{u}_j), \quad \mid \lambda^{ij} \mid = \mid v_{ij}^k \cdot S_k^{ij} \mid + c^{ij}, \tag{12}$$

where v_{ij}^k and c^{ij} denote edge values, computed as nodal averages, of the fluid velocity and speed of sound respectively, and S_k^{ij} is the unit normal vector associated with the edge. This can be considered as a centered difference scheme plus a second order dissipation operator, leading to a first order, monotone scheme. We will denote this scheme as 'central/2'.

Limiting may be avoided by using a **sensor function**:

$$\mathcal{F}_{ij} = \mathbf{f}_i + \mathbf{f}_j - \mid \lambda_{ij} \mid \left[\mathbf{u}_i - \mathbf{u}_j + \frac{\beta}{2} \mathbf{l}_{ji} \cdot (\nabla \mathbf{u}_i + \nabla \mathbf{u}_j) \right], \tag{13}$$

where $0 < \beta < 1$ denotes a (pressure) sensor function of the form [39]:

$$\beta = 1 - \frac{|p_i - p_j + 0.5\ \mathbf{l}_{ji} \cdot (\nabla p_i + \nabla p_j)|}{|p_i - p_j| + |0.5\ \mathbf{l}_{ji} \cdot (\nabla p_i + \nabla p_j)|}, \tag{14}$$

and $\mathbf{l}_{ji} = \mathbf{x}_j - \mathbf{x}_i$. For $\beta = 0, 1$, second and fourth order damping operators are obtained respectively. Several forms are possible for the sensor function β [36]. Although this discretization of the Euler fluxes looks like a blend of second and fourth order dissipation, it has no adjustable parameters. This scheme, denoted as 'central/2/4', is of little use close to shocks, but works well for smooth regions of the flow.

3.1.1 FCT: Limiting After Flux Evaluation

Limiting after flux evaluation is the key idea inherent to all FCT schemes [20]. If we focus on high order schemes of the Lax-Wendroff/Taylor-Galerkin family, the high and low-order increments may be written as:

$$\mathbf{M}_l \Delta \mathbf{u}^h = \mathbf{r} + (\mathbf{M}_l - \mathbf{M}_c) \Delta \mathbf{u}^h \quad , \quad \mathbf{M}_l \Delta \mathbf{u}^l = \mathbf{r} + c_d (\mathbf{M}_c - \mathbf{M}_l) \mathbf{u}^n. \tag{15}$$

Here $\mathbf{M}_l, \mathbf{M}_c$ denote the diagonal (lumped) and consistent mass-matrix, and $c_d = O(1)$. Subtracting these two equations yields the antidiffusive edge contributions:

$$(\Delta \mathbf{u}^h - \Delta \mathbf{u}^l) = \mathbf{M}_l^{-1} (\mathbf{M}_l - \mathbf{M}_c)(c_d \mathbf{u}^n + \Delta \mathbf{u}^h). \tag{16}$$

Note that no physical fluxes appear in the antidiffusive edge contributions. This may also be interpreted as: advance the physical fluxes with extra diffusion, thus assuring transport, conservation, etc. Thereafter, perform the antidiffusive step to enhance the solution as much as possible without violating monotonicity principles [23, 24, 18, 19]. The simplicity of the antidiffusive edge contributions for this class of scheme makes it both fast and very general, and has been one of the main reasons why this scheme has served the CFD community for more than 15 years without major alterations, in particular for the shock-object interaction problems considered here.

Maximizing Efficiency

Most blast-structure interaction problems tend to be CPU-intensive. For this reason a considerable amount of effort has been devoted to maximizing efficiencies. We enumerate the main techniques that have proven expedient:

3.2.1 Modified Fluxes for Runge-Kutta Steps: Given that any Runge-Kutta solver for first-order hyperbolic equations allows for larger Courant-numbers with increasing stages, an interesting alternative is to evaluate stages $1 : k-1$ in a k-stage scheme using inexpensive (albeit inaccurate) fluxes, and only employ the expensive, accurate flux evaluation for the last stage. Simple schemes that allow inexpensive flux evaluations are given by central, central/2 and Taylor-Galerkin. Schemes of this kind have been used successfully in the past [21, 8] for the class of shock propagation problems considered here. In the majority of cases 2-stage Runke-Kutta schemes were considered (i.e. $k = 2$). Using a purely central scheme for the first stage implies the risk of overshoots. The use of the 'central/2' scheme for the first stage implies the risk of more dissipation in the solution. For some recent results, see [29].

3.2.2 Modified Fluxes in Smooth Flow Regions: An observation made for many flow fields is that the regions of shocks and contact discontinuities only constitute a small fraction of the overall computational domain. It is in this relatively small region that the sophisticated, accurate and expensive schemes are required. In smooth flow regions, one could use less expensive 2nd order schemes such as central/2/4. This idea has been used repeatedly, particularly for the more elaborate (and expensive) solvers flows [10, 22, 29]. Note that the gradients are available, as they are required for limiting.

3.2.3 Deactivation in Quiescent Regions: For many blast problems, large regions remain quiescent during a considerable portion of the run. This is especially true for point-blasts. At the beginning, when high pressures and densities are present, the time steps are accordingly very small. This implies that during many time steps, regions away from the blast origin do not need to be updated. Quiescent regions are detected by evaluating differences of density, momenta and energy. If any of these exceeds a preset tolerance, the edge/face/element is marked as active.

3.2.4 Adaptive Mesh Refinement: Adaptive mesh refinement presents a particularly well suited option to reduce memory and CPU requirements for shock propagation problems. The gains achievable as compared to uniformly refined grids easily exceed 1:10, of magnitude, and in some cases approach 1:100. This should come as no surprise, as the regions that require refinement only occupy a small percentage of the total volume. To date, production codes have used simple h-refinement and coarsening, allowing only one level of refinement per mesh change. This allowed the construction of extremely fast adaptive refinement modules, that require only 20% of the total CPU time even for cases with simple EOS and a mesh change every 5 (explicit) time steps [25, 47, 27].

4 Engineering

Under 'engineering' we summarize best practices that have emerged over the years.

4.1 Initiation From Detailed 1-D/2-D/Axisymmetric Runs
In order the save CPU and improve accuracy, it is convenient to carry out the initiation of the detonation using 1-D (for ground blast) or 2-D/axisymmetric (for above-ground blast) codes. These codes will run 1-2 orders of magnitude faster, and by saving their results one can create a database of initializations. For a given scenario, one then finds the closest distance to the ground or a wall, determines if a 1-D or 2-D/axisymmetric initialization can be employed, if the HE material and amount already exists in the database or if it has to be calculated, and then proceeds to obtain the initialization. This 1-D or 2-D/axisymmetric initialization file is then interpolated to the 3-D mesh, and the 3-D run proceeds as long as required.

4.2 Successive Interpolation
In order the save CPU and improve accuracy, it is also convenient to 'stage' shock runs using successively larger domains as the blast wave propagates. A series of grids is build at the beginning of the run. Two options are possible: change the CAD definition (from small region to large region) and mesh, or use the overall CAD definition and simply increase the element size quickly away from the regions of interest. Sensors are then placed on the boundary of each domain/region. Once the arrival of the shock wave is sensed, the next mesh in the series is read in, the results are interpolated and the run continues. This modus operandi has worked very well over the years, and many important runs have been carried out employing it.

5 Examples

In this section we include two typical examples. The aim is not to show detailed comparisons to experiments, which have been conducted copiously in the past.

5.1 Nairobi, Kenya: This attack was one of the largest and most visible in recent years. A powerful bomb was detonated close to the American embassy in 1998. The immediate task of the CFD runs conducted was to back trace the amount of explosive based on the window damage observed. This run was the first to reach 500 Mtets (tet = tetrahedral) in a fully adaptive, transient setting, and was carried out on a multiprocessor SGI O2000 machine using successive interpolations. All runs were initiated from detailed axisymmetric detonation runs. The results of one of the runs is shown in Figure 2.

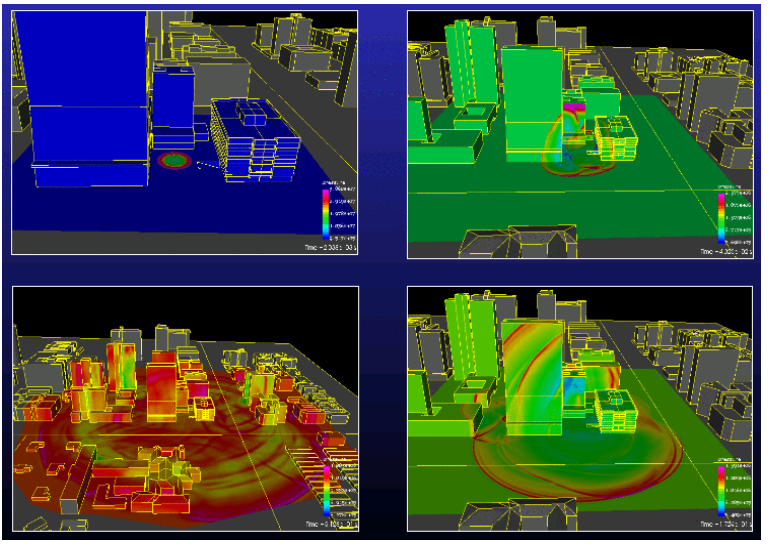

Fig. 2. Blast in city.

The successively larger domains are clearly visible. The adaptive refinement of the mesh can be seen in Figure 3.

5.2 Market Square: This run is typical of vulnerability assessment studies. The building under consideration is shown in Figure 4 left. One layer of refinement was specified wherever the physics required it. The pressures and grids obtained at the surface and a plane at a given time are shown in Figure 4. The mesh had approximately 60 Mtets.

5.3 Financial Center: This run is again typical of vulnerability assessment studies. The financial center under consideration is shown in Figure 4a. One layer of refinement was specified wherever the physics required it. The pressures obtained at different times are apparent from Figures 5 and 6. Note the presence of many reflected shocks, leading to successive pressure loading on the surfaces. This run clearly demonstrates that for complex geometries

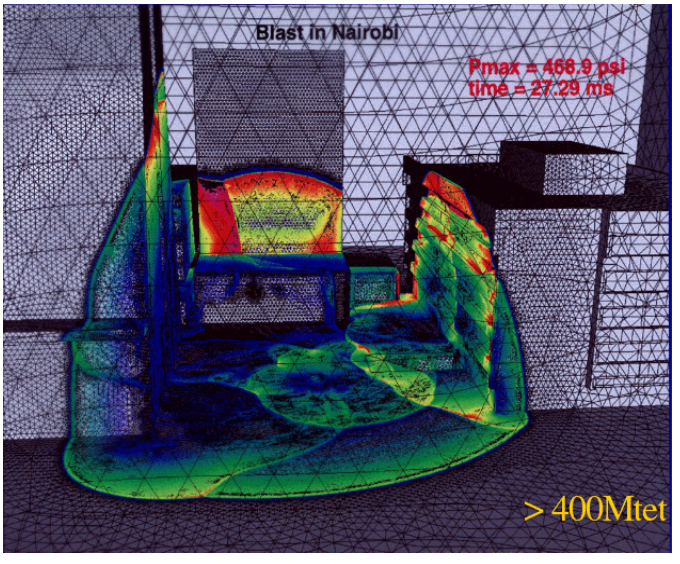

Fig. 3. Blast in city (detail showing adaptive refinement).

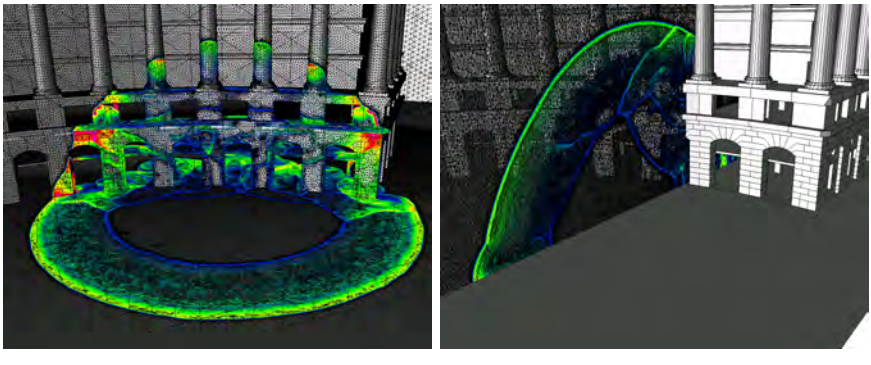

Fig. 4. Mesh and Pressure on Surface and Plane Cut.

and/or urban settings only first-principles, 3-D CFD codes can yield meaningful results.

6 Conclusions and Outlook

This paper has given a brief overview of the state of the art for the calculation of blast loads on civil engineering structures. The general setting, requirements, main physical phenomena and timescales, and suitable numerical methods were described.

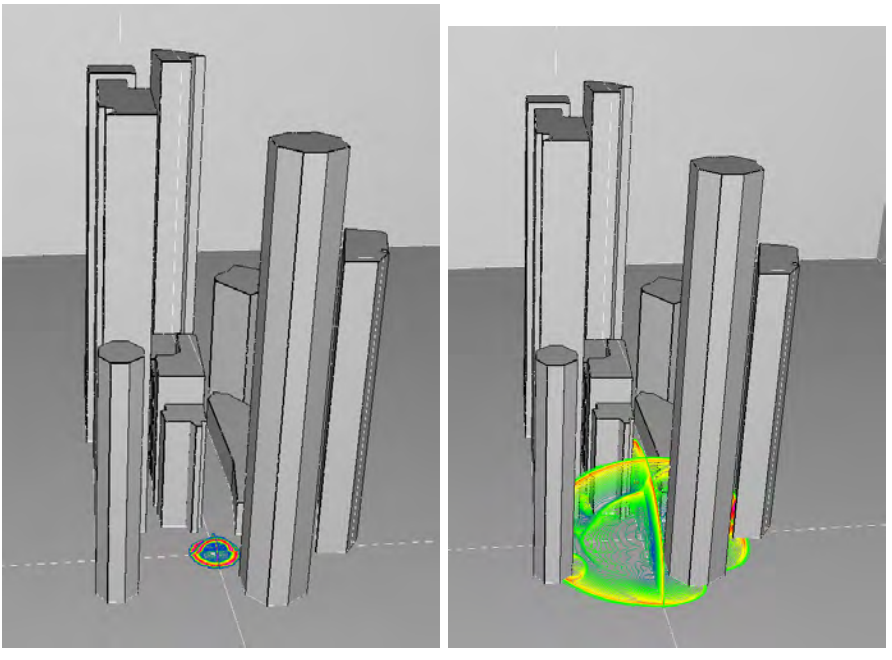

Fig. 5. Pressure at $T = 0.0$ $msec$ (left) and $T = 0.1$ $msec$ (right).

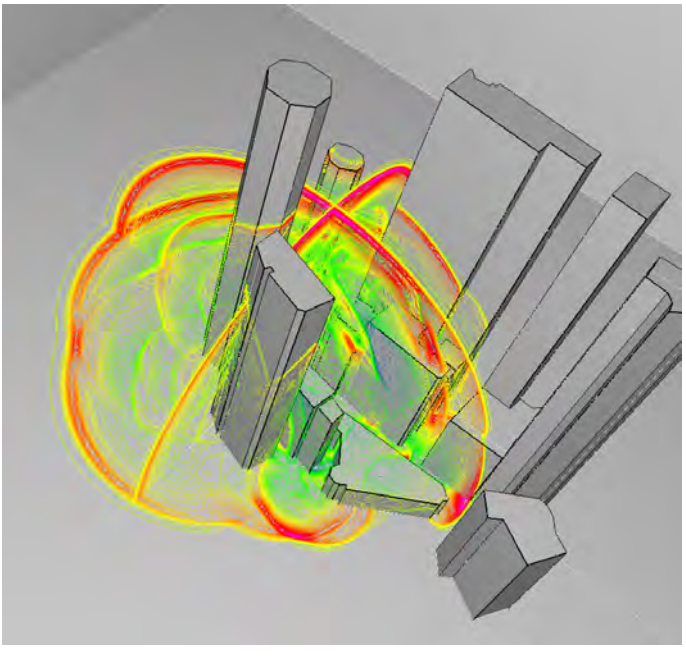

Fig. 6. Pressure at $T = 0.4$ $msec$.

While most of the paper has concentrated on the calculation of pressure loads, it is clear that a comprehensive capability must encompass fully coupled fluid-structure interaction. Work in this area has been going on for more than a decade [26, 28]. Suffice it to say that the uncertainties encountered in flow simulations pale in comparison to those found in structural dynamics simulations: the description of glass, steel and concrete failure, reinforcement bars, beam joints and many other structural aspects will require a concerted experimental and numerical effort to arrive at reliabilities that approach those currently available for the flow codes.

7 Acknowledgements

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Numerical Modelling of Technical Combustion

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Summary This contribution gives a short overview over modern numerical combustion modelling. Numerical simulation of combustion is a multi-scale problem, because the specific issues of fluid mechanics and chemical reaction systems accumulate. There exist a large variety of combustion models for different flame types, which are more or less universal. For some turbulent reacting flows, existing methodologies are acceptably accurate, and have justifiable computational cost. Depending on the expected answers of numerical simulation, substantial advances are required and have to be worked out.

1 Introduction

Technical combustion is characterized by the interaction of chemical reactions, fluid- and thermodynamics. Therefore, a wide range of phenomena has to be considered ranging from e. g. turbulence, chemistry of ignition and incomplete combustion to formation of pollutants and soot, including processes as pyrolysis, heterogeneous reactions, spray formation and evaporation. Boundary conditions are widely varying with respect to pres-sure, preheating, thermal load and are governed by flame stability, thermo-acoustics, heat transfer by convection and radiation, flame/wall interactions, catalytic effects and safety aspects.

In recent years, the capability of Computational Fluid Dynamics (CFD) codes expanded drastically with respect to numeric algorithms and implementation of complex processes and computer capacity has been expanded substantially. Nevertheless, numerical simulations of combustion are difficult, because the specific problems of fluid mechanics and chemical reaction systems accumulate. A crucial problem e. g. is the handling of the highly non-linear chemical reaction rates.

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This contribution gives a short overview over modern numerical combustion modelling. For a deeper insight some basic additional literature is quoted: turbulence (Hinze (1959), Wilcox (1998), Pope (2000)), combustion basics (Williams (1988), Turns (2000)), combustion modelling (Libby et al. (1994), Peters (2000), Poinsot et al. (2001)), numerical methods (Patankar (1990), Oran et al. (1987), Fox (2003)).

2 Strategies for Numerical Simulation of Combustion

In general, numerical combustion implies the calculation of the conversion of chemical species as well as the calculation of fluid flow and transport processes that supply molecular mixed substances. Therefore, the simulation of combustion demands the solution of the balance equations for mass, momentum, species and energy as well as additional relations for the thermodynamic state and the thermo-physical properties. The different principles and strategies for the calculation of these balance equations have to be combined in numerical combustion which is the most challenging task in this field. In addition, different boundary conditions arise from the flame types to be considered which are classified roughly in Fig. 1 into premixed and diffusion flames under laminar or turbulent flow conditions.

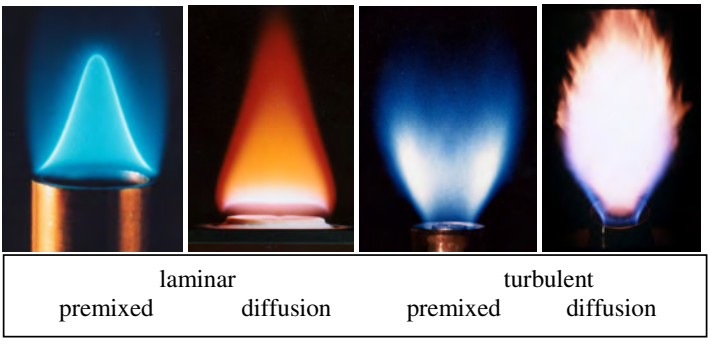
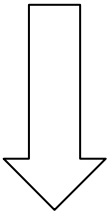
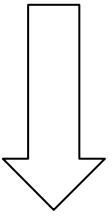


Fig. 1. Flame types defining boundary conditions for numerical simulation of combustion.

2.1 Calculation of the Flow Field

For the calculation of multidimensional fluid flow different methods with various levels of detail exist. The most common methods are listed in Table 1. The more universal the method is, the larger is the computational effort. Besides that, there are numerous specialized methods which are only applicable to distinct flow problems.

Table 1. Methods for the calculation of fluid flow

Universalism	Method	Effort
	1. Solving potential equations	
	2. Solving Euler-Equations	
	3. Solving the Reynolds-averaged Navier-Stokes Equations (RANS- or URANS-approach)	
	4. Solving the Space-filtered Navier-Stokes Equations (LES: Large-Eddy-Simulation)	
	5. Solving PDF-transport equations	
	6. Solving of the Navier-Stokes Equations (DNS: Direct-Numerical-Simulation)	
	7. Calculation of molecular motion and collisions (e. g. Lattice-Boltzmann-approach)	

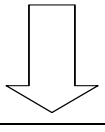
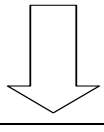
2.2 Modelling of Chemical Reactions

The numerical simulation of chemical reactions can be carried out on different levels of simplification, Table 2. The coarsest approach is given when using formal conversion rates (level 1). In contrast, the calculation by "Electronic Structure Theory", "Statistical Mechanics Method", "Group Additivity method", or "multi-frequency Quantum Rice-Ramsperger-Kassel" (QRRK) method imply all chemical effects (level 4). The usage of a detailed reaction mechanism (level 3) implies the knowledge of elementary reactions from experiments or calculations of level 4.

The aim of reduction is to simplify a detailed mechanism to the reactions which characterize the chemical system by the properties under consideration (e. g. temperature, fuel consumption rate, concentrations of main species or intermediates, flame propagation speed). Mainly four methods are used for the reduction of mechanisms, all making use of asymptotic principles: global kinetics, lumping methods, semi-empirical approaches and dynamic procedures (e. g. intrinsic low dimensional manifold method, ILDM (Maas et al. (1992)), computational singular perturbation, CSP (Lam (1985)), genetic algorithms (Elliott et al. (2004)).

The applicable level of complexity in fluid flow calculations and chemical reactions is restricted by the available computer capacity. Even if the increase of computer power continues as in the last decades, the level required for a detailed description of both, chemistry and fluid flow, will be reached, if at all,

Table 2. Methods for the calculation of chemical reactions

Universalism	Method	Effort
	1. Formal conversion rates	
	2. Reduced reaction mechanisms	
	3. Detailed reaction mechanisms based on elementary reactions	
	4. Calculation of statistical quantum mechanics	

in the very far future. Therefore, e. g. simulation of turbulent combustion must make a judicious balance between how much the computer power is put into the complexities of flow and how much into the complexities of chemistry. The only alternative to calculate technical systems is the abstraction from physical/chemical processes by models.

3 Some Basic Properties

The description of combustion processes comprises the evolution of numerous chemical and thermo-physical properties in space and time. To reduce the variables of interest it is preferable to introduce some basic quantities that describe the entire process from a more global point of view.

Flame speed In premixed flames the reaction zone propagates normal to itself into the homogeneous mixture of fuel and oxidizer with the burning velocity or flame speed S. For a planar laminar flame the laminar flame speed S_l is a thermo-physical property. In contrast, the flame speed S_t of a turbulent flame depends on the local, instantaneous properties of flow and turbulence. The determination of the turbulent flame speed is one of the important unresolved problems in premixed combustion and matter of actual experimental, theoretical and numerical research (see e. g. Driscoll (2008)). The flame speed as a global property reflecting the conversion of fuel in a large network of chemical reactions can be related to the source terms in the balance equations for species.

Mixture fraction f For the description of mixing in non-premixed combustion the scalar variable mixture fraction f is used. In general, it can be defined as the normalized mass fraction of one or more chemical elements (i. e. carbon and hydrogen). As the mixture fraction is a conserved scalar it changes only due to diffusion and convection but not due to reaction.

Reaction progress variable q From the view point of a formal description of the conversion from fuel/oxidiser to products it is helpful to introduce a progress variable which may be defined as a normalized temperature or a normalized product mass fraction, respectively. It has the value zero in the unburned mixture (cold, only educts) and the value one in the burned state (hot, only products). The purpose of introducing one or only few reaction progress variables is to re-duce the amount of variables for which balance equations have to be solved. The balance equation for the progress variable reads:

$$\frac{\partial(\rho\theta)}{\partial t} + \nabla(\rho\,\overrightarrow{u}\,\theta) = -\nabla\left(\overline{\rho}\frac{\nu}{Sc}\cdot\nabla\theta\right) + \rho\cdot\dot{\omega}_\theta. \tag{1}$$

The main task of combustion modelling then reduces to the treatment of the source term $\dot{\omega}_\theta$ on the right hand side of eq. (1) which can also be related to the flame speed.

Turbulence Turbulent combustion is encountered in most practical combustion systems as rockets, internal combustion or aircraft engines, industrial

burners and furnaces. Turbulence alters the flame structure, increases the mixing rate and may enhance the global conversion rate of species. In extreme cases turbulence inhibits conversion completely, leading to flame quenching. On the other hand, the flow and its turbulence structure are induced by heat release from the combustion reactions.

Turbulent combustion implies a large range of both length and time scales for both turbulence and chemical reactions. A basic concept for turbulent combustion models is based on the physical principle that the prob-ability of the interaction of scales decreases with the extent of scale separation. Diagrams defining regimes of premixed or non-premixed turbulent combustion in terms of scale separation have been proposed by Borghi (1985) and Peters (2000). Almost all turbulent combustion models explicitly or implicitly assume scale separation.

Scale separation of the fluid flow in turbulent combustion is based on the eddy-cascade hypothesis. Large eddies break up into smaller eddies until the smallest eddies disappear due to viscous forces. The length scales of these turbulent flows range from the size of Kolmogorov eddies l_η up to the size of the integral length scale lt of the large, energy containing eddies. In technical applications l_t is typically one order of magnitude smaller and l_η typically three orders of magnitude smaller than the size of the flow system. The length scales of flames range from the thickness l_f of the fuel consumption layer inside laminar flames up to the overall size of large turbulent flames or furnaces. The interaction of length scales can be related to the ratio of the thickness of the fuel consumption layer l_f to the Kolmogorov length scale l_η and is called the Karlovitz number $Ka \sim l_f/l_\eta$.

Length scales of turbulent reacting flows Corresponding to the length scales – via a characteristic flow velocity – there exist time scales, accordingly. The time scales of the turbulent flow range from the life time of the fine grained Kolmogorov eddies τ_η up to the characteristic life time τ_t of the energy containing large eddies. For chemical reactions time scales range from very small time scales (formation of radicals) up to large time scales (e. g. formation of NOX), and, therefore, many time scales exist, that are able to interact with those of turbulence, Fig. 2.

However, there are many circumstances where only a limited range of chemical and turbulent time scales are involved and, moreover, the overlap of these ranges is small. Assuming that the typical time scale of heat release τ_c is the largest one of all chemical reactions of interest, scale separation then can be captured using the Damköhler number which is the ratio of the times scales of heat release to that of turbulence: $Da = \tau_c/\tau_t$.

The time scale of heat release depends mainly on the kind of fuel. Combustion, i. e. molecular reaction, requires molecular mixing provided by dissipation on the smallest scales of turbulence. The smallest time scales of turbulence are dependent on the turbulent Reynolds number and the type of flow. For small and large Damköhler numbers, time scales of heat release are sepa-

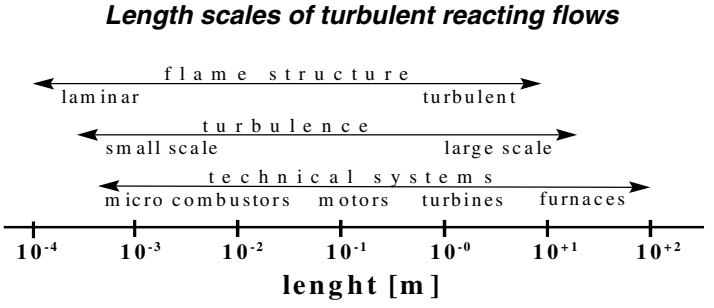


Fig. 2. Length scales of turbulent reacting flows.

rated from those of mixing in the inertial sub-range. This simplifies modelling significantly.

In industrial application, non-gaseous fuels are most commonly employed. The phase change of such fuels introduce additional time scales (spray atomization and evaporation, gasification of solid fuels), which usually are larger than the relevant chemical time scales.

4 Numerical Simulation of Combustion

Numerical simulation of laminar flames is of wide interest because these configurations allow for a detailed comparison between experiments, theory and computation. That is why validation of reaction kinetics is possible here. Moreover, laminar flames play an important role as basic elements of combustion models for turbulent flames. However, numerical simulation of laminar flames is state of present art so that the focus is on turbulent combustion in the following.

The description of turbulent combustion processes may be achieved using a variety of numerical methods. Four levels of turbulent reacting flow computations are distinguished: RANS, LES, DNS and PDF-methods. Fig. 3 shows a photograph of a turbulent non-premixed flame. The details of the flame front captured by the different modelling strategies and the resulting temperature at a distinct position in space are shown on the right.

For RANS and LES-modelling the instantaneous balance equations are filtered in time and space, respectively. All variables (e. g. the reaction progress variable θ) are subdivided into a resolved part and an unresolved part:

$$\theta(\overrightarrow{x},t) = \overline{\theta}(\overrightarrow{x}) + \theta'(\overrightarrow{x},t). \tag{2}$$

The filtered balance equation for the reaction progress eq.(2) reads:

$$\frac{\partial(\overline{\rho}\widetilde{\theta})}{\partial t} + \nabla(\overline{\rho}\,\widetilde{\overrightarrow{u}}\,\widetilde{\theta}) = -\nabla\left(\overline{\rho}\frac{\nu}{Sc}\cdot\nabla\widetilde{\theta}\right) - \nabla\overrightarrow{q} + \overline{\rho}\cdot\widetilde{\dot{\omega}}_\theta, \tag{3}$$

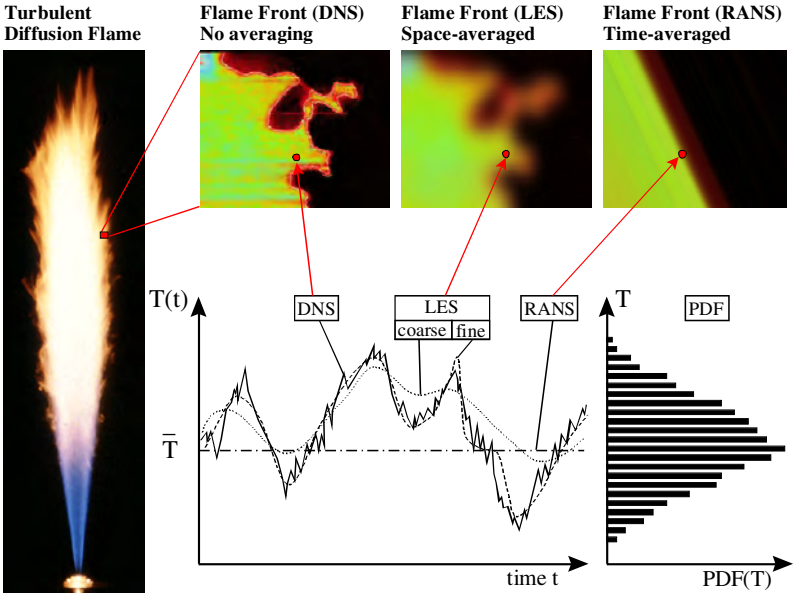


Fig. 3. Evolution of shape and temperature of the local flame front in a turbulent flame brush due to different modelling strategies.

where '~' denotes the Favre-averaging defined as $\widetilde{\theta} = \overline{\rho\theta}/\overline{\rho}$. The treatment of the unresolved flux $\overline{\vec{q}}$ and the source term $\widetilde{\dot{\omega}}_\theta$ depends on the turbulence and combustion model, respectively.

4.1 RANS-Modelling

The balance equations for RANS (Reynolds-Averaged-Navier-Stokes) techniques are obtained by time-averaging the instantaneous balance equations. The rule for the time-filter is:

$$\overline{\theta}(\vec{x}) = lim|_{t_1 \to \infty} \frac{1}{t_1} \int_0^{t_1} \theta(\vec{x}, t) dt, \tag{4}$$

where the time t_1 has to be large versus the typical time scales of turbulence. For a statistically steady state jet flame as shown in Fig. 3 the predicted temperature at a given point is constant corresponding to the time-averaged temperature $\overline{T}$ at this point. The filter for the ensemble averaging (or phase averaging) over different realizations (or cycles) for periodic flows like those found in piston engines leads to the URANS (Unsteady-Reynolds-Averaged-Navier-Stokes) concept:

$$\overline{\theta}(\overrightarrow{x},t) = \frac{1}{t_1}\int_0^{t_0+t_1} \theta(\overrightarrow{x},t)dt. \tag{5}$$

Here, the time t_1 has to be larger than the turbulent time scales and smaller than the overall time scale of the transient process (or periodic variations). Hence, $\overline{\theta}(\overrightarrow{x},t)$ includes only the deterministic parts of the turbulent flow. The filtering leads to unclosed terms (turbulent fluxes $\overrightarrow{q}$ of momentum, energy, species and reaction progress, e. g. $\overline{\rho}\,\overrightarrow{u''}\theta''$) for which additional rules (turbulence models) are required. The simplest approach is to use a gradient transport assumption. For the flux of the reaction progress it reads:

$$\overrightarrow{q} = \overline{\rho}\left(\widetilde{\overrightarrow{u''}\theta''}\right) = \frac{\mu_t}{Sc_t}\cdot\nabla\widetilde{\theta}, \tag{6}$$

where Sc_t is the turbulent Schmidt number. The main task of turbulence modelling is the provision of the turbulent eddy viscosity μ_t and the main task of combustion modelling is the treatment of the time-averaged source term $\widetilde{\omega}_\theta$ of the progress variable, eq. (3), or the time-averaged consumption rates of species, respectively. The time-averaged source terms cannot be calculated using the time-mean species concentrations $\overline{Y}_i$ and temperature $\overline{T}$, because reaction rates are highly nonlinear: $\widetilde{\omega}_\theta(Y_i,T) \neq \widetilde{\omega}_\theta(\overline{Y}_i,\overline{T})$. Combustion models can be distinguished with respect to their capability to treat premixed or non-premixed combustion, or both. Other distinctive features are the details of the chemical mechanism or the assumptions for the time-scale or length-scale separation.

Models based on the flame front geometry (premixed flames) All model approaches of this type describe the kinematics and the topology of the flame front of turbulent premixed flames. The basic assumption is the existence of length scale separation between the flame front and the turbulent eddies. The thickness of the flame front is considered to be small against the size of the smallest vortices of turbulence ($Ka < 1$). All models of this type make use of the turbulent burning rate S_t. For the calculation of the geometry of the flame front mainly three different, but mathematically equivalent, strategies are pursued:

- *G-equation* or level-set approach, Peters (1999).
- Averaged flame front surface density $\bar{\Sigma}$ (area of flame front per volume) and the laminar flame speed: $\widetilde{\omega}_\theta = \bar{\Sigma}\cdot\rho\cdot S_l$, Bray et al. (1986), Gouldin et al. (1989), Cant et al. (1990), Mantel et al. (1994).
- Flame front winkling defined as the ratio of the surface of the turbulent flame (folded laminar flame) to the projected area normal to the propagation direction, Weller et al. (1990), Lipatnikov et al. (2001). With some assumptions the model reduces to an expression incorporating ("Turbulent Flame speed Closure" or TFC, e. g. Driscoll (2008)).

Models based on the flamelet/scalar dissipation approach (diffusion flames) Fast chemistry permits the de-coupling of turbulence and chemistry and leads to models based on the scalar dissipation/flamelet approach

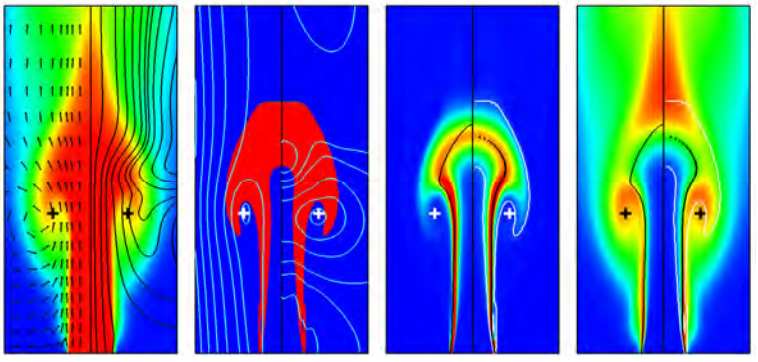


Fig. 4. URANS calculation ($k-\varepsilon$ turbulence model and TFC-combustion model) of a pulsated premixed turbulent jet-flame (stoichiometric methane/air mixture. Nozzle diameter: 26 mm, time-mean velocity: 24 m/s, frequency: 150 Hz, thermal load: 40 kW). 2-D slices from left to right: mixture fraction; flame volume, consumption rate of methane and temperature. The crosses mark the centres of the flow induced large scale coherent ring vortices appearing at each acceleration phase of the pulsated flow (TCP-EBI (2007)).

(Peters (1986), Peters (1993), Bray (1987)). The scalar dissipation rate χ has the dimension of an inverse time (like strain) and may be interpreted as the inverse of a characteristic diffusion (i. e. mixing) time. Flamelet models explicitly assume length scale separation between the thin and short laminar scales of reaction and the larger scales in the inertial sub-range of turbulence. In this case, the turbulent flame can be handled as an ensemble of laminar flamelets. The decoupling of turbulence and chemistry allows the inclusion of detailed chemistry. Using the flamelet concept splits the combustion problem into two sub-problems:

- The mixing problem to provide the time-average mixture fraction $\bar{f}$ and some of its higher statistical moments in space and time.
- The flame structure problem, where the local mixture fraction f and scalar dissipation rate χ are used to construct all flame variables (species mass fractions and temperature).

It is generally agreed, that the flamelet concept is applicable in the range of large Damköhler numbers and small Karlovitz numbers. These conditions are satisfied in many practical situations. However, there are some open questions referring to the incorporation of aspects like heat loss (due to radiation or convection), transient effects, preferential diffusion and non-equilibrium chemical kinetics.

Conditional Moment Closure (diffusion flames) An alternative to the flamelet approach is the concept of Conditional Moment Closure (CMC) (Klimenko et al. (1999)). The consideration is, that the fluctuations of the reactive scalars are accompanied by fluctuations of mixture fraction. Conse-

quently, the reactive scalars are conditioned on the mixture fraction. Closure is obtained by neglecting the difference between the local concentration of the reactive scalar and its conditional average. This approach is applicable to premixed turbulent combustion, with conditioning on the progress variable.

Linear Eddy Model Another approach to account for non-equilibrium chemistry in turbulent combustion is the Linear Eddy Model (LEM) (Kerstein (1992)). Molecular mixing is simulated on a one-dimensional domain embedded in a turbulent flow. The evolution of the reactive scalar field then is described in one dimension due to a system of parabolic equations. The scalar field is integrated into a stochastic sequence of instantaneous, statistically independent "rearrangement events". Each event may be viewed as representing the effect of an individual eddy on the scalar field. Both processes are performed at the finest scales of fluid property variations in physical space, which makes this method computationally expensive.

4.2 Modelling Using PDF-Transport Equations

If turbulent mixing is relatively fast or the chemistry is relatively slow (Damköhler number < 1) there is no time-scale separation. In this case PDF-approaches are claimed (Bray et al. (1977), Borghi et al. (1986), Borghi (1988), Bray et al. (1991)). The Probability Density Function (PDF) of a variable determines the probability (or frequency of occurrence) for the value of a variable to be in a certain interval (see Figure 3). A general statistical description of turbulent reacting flows with premixed, non-premixed and partially premixed combustion, is the application of PDF-transport equations (Dopazo (1994)). There are numerous approaches of using and solving PDF-transport equations including of velocity, reactive scalars and other properties into a joint PDF. Because of the high dimensionality of the joint PDF transport equation the numerical solution with finite-volume and finite-difference techniques is not attractive. Therefore, virtually all implementations of PDF-methods use Monte-Carlo simulation techniques (Pope (1981)). These methods employ a large number of virtual particles. The state of the particle, from which the PDF is reconstructed, is described by its position and velocity and by the values of the reactive scalars that it represents as a function of time. The main draw-back of Monte-Carlo methods is that they suffer from a statistical error which decreases only slowly with the number of particles. A typical number for moderate grid sizes is 100 particles per cell.

In PDF-transport equations all on-point processes such as convection and chemical reactions appear in closed form. Multi-point processes such as diffusion have to be modelled. The predictive capability of PDF-methods for turbulent combustion depends on the quality of the models that can be constructed for the unclosed terms. For chemically reacting flows the molecular mixing term is the most difficult to model.

Models based on presumed probability density functions PDF methods may be employed in a hybrid way for treating unclosed terms in the

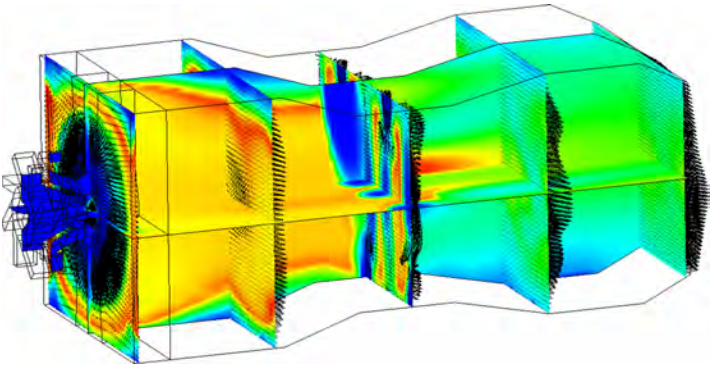


Fig. 5. RANS-Calculation ($k-\varepsilon$ turbulence model and JPDF-combustion model) of the combustion chamber of an aero-engine gas-turbine (length: 0.1 m). Shown is the temperature field with additional velocity vectors (TCP-EBI (2007)).

RANS or LES. E. g., the time-mean consumption rate can be calculated by multiplying the instantaneous consumption rates by the joint PDF of each basic variable (e. g. for θ and f):

$$\widetilde{\dot{\omega}}_\theta = \int_0^1 \int_0^1 \dot{\omega}_\theta \cdot P(\theta)P(f)df\,d\theta. \tag{7}$$

Within this approach the usage of multi-step chemical reaction kinetics is possible. The benefit is, that this approach enables to describe the mean consumption rate of fuel in a closed form.

Instead of calculating the PDF, a coarser, but faster way which penetrates into industrial application is the use of presumed PDF's. There, the principal form of the PDF (typically a Gaussian- or Beta-PDF) is stated.

4.3 LES-Modelling

For deriving the basic LES equations the instantaneous balance equations are spatially filtered with a filter size of Δ, which usually is the size of the grid. The objective of LES is to compute the larger structures of the flow field (typically structures larger than the mesh size) whereas the smallest eddies are modelled using subgrid closure rules (employing length-scale separation). For the jet flame of Fig. 3 LES would resolve the low-frequency variations of temperature. The finer the grid, the more frequencies are captured. The rule for the space-filter yielding the resolved part of the progress variable $\overline{\theta}$ (s. eq. (2)) is:

$$\overline{\theta}(\overrightarrow{x},t) = \int_{Vol} G(\overrightarrow{x},\overrightarrow{x}',t)\cdot\theta(\overrightarrow{x}',t)d\overrightarrow{x}'. \tag{8}$$

G denotes the filter function, $\overrightarrow{x}$ the position vector and $\overrightarrow{x}'$ its deviation. The unresolved flux of the filtered balance equation can be modelled using a gradient transport assumption:

$$\overrightarrow{q} = \overline{\rho}\left(\widetilde{\overrightarrow{u}\theta} - \widetilde{\overrightarrow{u}}\,\widetilde{\theta}\right) = \frac{\mu_t}{Sc_t} \cdot \nabla\widetilde{\theta}. \tag{9}$$

The sub grid eddy viscosity μ_t has also to be modelled, e. g. due to Smagorinsky (1963)). Review papers are given by e.g. Lesieur et al. (1996) and Moin (1997).

Compared to RANS simulations LES simulations are more expensive. Usual simplifications, which can be applied by RANS as symmetry conditions or two-dimensional flows, cannot be retained. The solution has to be time-dependent, even for statistically steady-state flows. Thus, to gain knowledge on the usually required time-mean quantities, an additional thorough statistical evaluation has to be performed. Compared to DNS there is in principal no restriction to the Reynolds number. But at least, the integral length scale has to be resolved. In practical simulations, laminar flame fronts cannot be resolved on the computational mesh. The problem for combustion is to get the space-filtered reaction rate $\widetilde{\dot{\omega}}_\theta$. The chemical limit depends on the subgrid scale model. Combustion modelling based on LES is an actual field of research. Several concepts of modelling combustion in the RANS context have been transferred to the subgrid scale of LES, both for premixed and non-premixed flames (presumed shape beta function subgrid PDF, Pierce et al. (1998), Branley and Jones (1999), G-equation, Im et al. (1997), flame surface density model, Boger et al. (1998), CMC, Kim et al. (2005), linear eddy model, El-Asrag and Menon (2007)).

In the future the use of LES will certainly increase because it is able to eliminate inaccuracies of the RANS models and gives a more realistic view to turbulent combustion.

Fig. 6. LES-calculation of a double-concentric, swirling flow (Re = 81000). The surfaces of equal averaged pressure indicate the existence of coherent structures leading to flame pulsation and noise emission (TCP-EBI (2007)).

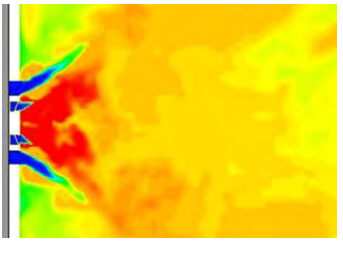


Fig. 7. LES-calculation of a double-concentric, premixed swirling burner (Re = 90000, fuel: methane, thermal load 250 kW). Shown is the instantaneous temperature indication the dominant role of the inner recirculation zone (TCP-EBI (2007)).

4.4 DNS-Modelling

Direct numerical simulation (DNS) is based on the direct solution of the instantaneous balance equations (Navier-Stokes-Equations) without any turbulence model (Moin et al. (1998)). All turbulent scales are explicitly determined and their effects on combustion (including molecular mixing) are captured by the simulation. For the flame of Fig. 3 DNS would predict all time variations of temperature.

The available computer capacity restricts the calculation in two ways. The first condition results from the fact, that the length scale of the smallest eddies (Kolmogorov scale) decreases with the Reynolds number of the flow. Accordingly, the number of required grid nodes increases. For technical applications there are at least three orders of magnitude between the size L of the flow system and the mesh size Δ needed to resolve the smallest scales. In 3D this would result in at least 10^9 grid points. Therefore, DNS is still out of reach as a method to predict isothermal turbulent flows for practical engineering applications (high Reynolds number) for many years to come. Actually, practical simulations of isothermal flows are restricted to Reynolds numbers in the order of one thousand.

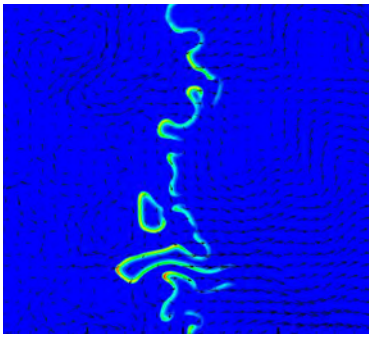


Fig. 8. DNS-calculation using detailed chemistry of the interaction of a premixed lean H2/air flame with a turbulent flow field (size of domain: 40x40 mm, Re = 340). Shown is the consumption rate of hydrogen with velocity vectors. Turbulence generates curvature, strain and quenching on the flame front (TCP-EBI (2007)).

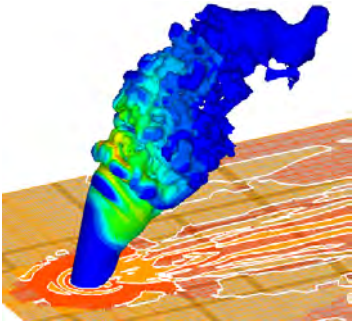


Fig. 9. DNS-calculation of a jet-in-crossflow configuration, Re = 650 and velocity ratio R = 3.3. The crossflow comes from the left. Shown is the reaction rate of a chemical reaction with Da = 0.5 colored by the averaged fluctuations of the same quantity (TCP-EBI (2007)).

The second condition is imposed by the proper resolution of the flame structure in the case of reacting flow. The thickness of the inner fuel consumption layer of a laminar flame is typically of the order of 0.1 mm. If this length is discretized by 10 cells, a grid of 1000^3 cells would yield a box size

of about 10 mm. A complete numerical simulation of the three-dimensional balance equations describing a chemically reacting flow and including multi-species transport, realistic thermodynamics and complex chemistry for technical combustion systems is far out of reach.

Therefore, the calculation of reacting flows is limited to small flow regions or requires additional restrictions as low Mach number, simple chemical systems or reduction of dimensionality in space. However, these restrictions can be used to understand basic mechanisms by isolating a specific phenomenon. DNS has allowed detailed studies of regimes of combustion, flame structures under interactions with turbulent eddies, extinction processes, pocket formation, influence of heat losses, wall interactions, ignition and flame kernel growth. Many basic problems may be considered with DNS and the results may then be used to improve specific sub-models. DNS has offered a new way to investigate flame/turbulence interactions and significant progress has been achieved both for models and fundamentals of turbulent combustion (Poinsot (1996)). DNS is an extremely valuable research tool gaining much more impact in the future.

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Kinetic Modeling and Simulation of Environmental and Civil Engineering Flow Problems

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Summary In this contribution the authors address recent advances of modelling and simulating flow problems related to Environmental and Civil Engineering using Lattice-Boltzmann methods (LBM) and present results documenting the potential of this kinetic approach. After a short introduction to theoretical aspects of the method, we address extensions of the basic LB ansatz to model turbulent, thermal and multiphase flows, free surface flows and bidirectional Fluid-Structure-Interaction. All simulations were done with the LBM research prototype software Virtual Fluids [16], a transient 2D/3D-code offering adaptive hierarchical Cartesian grid refinement, massive parallelization and multi-physics capabilities. The simulation of a simplified debris flow problem is based on the coupling of the flow solver with an external physics engine.

1 Introduction

Reliable analysis and prediction of flows related to Civil Engineering and the Environmental sciences by computational models is still a very challenging task for scientists and engineers as well, although substantial advances have been made both in developing mathematical descriptions (usually as partial differential equations, PDEs) as well as in the field of numerical, algorithmic and hardware related issues. The main reasons for the ongoing difficulties in this area are due to the fact that most real life problems in this area are coupled multi-scale multi-physics problems which require great care in decoupling the different aspects and scales of the problem and in developing reliable abstract large-scale models with a relatively small number of degrees of freedom (DOF). In addition, the proper definition of boundary and initial conditions is often

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difficult, even for rescaled experiments as important dimensionless quantities of the problem cannot be matched sufficiently.

The basic model equations for transport problems are characterized by material derivatives (change in time combined with advection), diffusive and source terms. Yet, the weight of the corresponding terms may drastically change for various applications implying a qualitatively different dynamic behaviour of the model and the need to utilize specific numerical methods to discretize the equations efficiently. In this sense, it is advantageous to use model families which are sufficiently general to represent these different behaviours as model parameters and where approximate solutions are accessible with ideally simple but efficient numerical schemes. One approach in this direction is offered by so-called Lattice-Boltzmann models which will be discussed in the remainder of this paper. The extensive literature provided should enable the interested reader to dive more deeply into the subject than a short paper as this may hope to achieve.

2 A Short Introduction to Lattice-Boltzmann Modelling of Navier-Stokes Problems

In the last two decades LBM methods have matured as an interesting alternative to discretizing macroscopic transport equations such as e.g. the Navier-Stokes equations or systems of PDEs describing coupled transport problems such as Fluid-Structure-Interaction (FSI), Multiphase, free surface, thermal and turbulent flows. Overview articles and general introductions can be found in e. g. [4, 41, 26, 10, 34, 48, 19, 63] and the references therein.
The Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v}\nabla f = \Omega \tag{1}$$

describes the dynamics of a probability distribution function f of particles with a microscopic particle velocity $\mathbf{v}$ under the influence of a collision operator Ω. Macroscopic quantities such as fields of density, flow velocities, energy or heat fluxes could consistently be computed as moments of ascending order from the solution f, but obtaining the solution for macroscopic problems is mostly as difficult as unnecessary as long as one is not interested in rarified gases or flows with non-vanishing Knudsen numbers. For the flow problems under consideration here, eq. 1 can be drastically simplified by discretizing the microscopic velocity space ($v \rightarrow \{\mathbf{e}_i, i = 0, \ldots, b\}$) and by using a simplified collision operator [5]. This results in a set of PDEs called the discrete Boltzmann equations

$$\frac{\partial f_i}{\partial t} + \mathbf{e}_i \nabla f_i = \Omega_i = -\frac{1}{\tau}(f_i - f_i^{eq}), \tag{2}$$

where τ is a microscopic relaxation time determining the time scale f_i approaches a suitable equilibrium function f_i^{eq}. A straight forward Finite Difference discretization for this set of PDEs results in the Lattice-Boltzmann equations [41]

$$f_i(t + \Delta t, \mathbf{x} + \mathbf{e}_i \Delta t) - f_i(t, \mathbf{x}) = \Omega_i(t, \mathbf{x})). \tag{3}$$

More elaborate collision operators will improve the scheme in terms of accuracy and stability (see e.g. [12, 13]). In the asymptotic limit $\Delta t \to 0, \Delta x \simeq |\mathbf{e}_i \Delta t| \to 0$ it can be shown [8, 30] that the first moments of f_i namely the hydrodynamic pressure $p \propto \sum_i f_i$ and the flow velocity $\mathbf{u} \propto \sum_i f_i \mathbf{e}_i$ are solutions of the incompressible Navier-Stokes equations and thus the microscopic scheme 3 can be utilized to compute corresponding approximate solutions of this macroscopic equation(s) once suitable f_i^{eq} have been chosen and the kinematic viscosity has been identified as a linear function of τ. Appropriate hydrodynamic boundary conditions for the distribution functions are discussed in [35, 6, 21, 23]. An interesting feature of the LB approach is that the vectors $\mathbf{e}_i \Delta t$ span the unit cell of the numerical grid. This coupling of the physics model (the set of the microscopic velocities $\mathbf{e}_i$) and the numerical disretization has some consequences for grid refinement which have to be taken into account [15, 11, 42]. A more elaborate LB-model has been successfully used for benchmark computations indicating that the LB scheme has its merits both in terms of numerical and computational accuracy [17].

3 Extensions of LBM for Coupled Problems

3.1 Turbulent Flows

The extension of LB methods to model turbulent flows follows two lines. The first approach incorporates standard turbulence models such as LES [32, 14, 60] or RANS approaches [51] into the LB framework (where the additional transport equations can be treated in the spirit of [20, 47]). Alternatively, kinetic modelling of turbulence is being investigated [9, 3]. For a standard Smagorinsky LES the turbulent viscosity can be computed from the strain rates $S_{\alpha\beta} \equiv \frac{1}{2} \left(\partial_\beta \, u_\alpha + \partial_\alpha \, u_\beta \right)$, according to

$$\nu_t = C_s^2 h^2 \|S\|, \tag{4}$$

where C_s is Smagorinsky's constant. An interesting feature of the LBM is that strain rates can be computed locally from the non-equilibrium part of the distribution function

$$S_{\alpha\beta} = -\frac{3}{2\rho(\tau_v + \tau_t)} \sum_i e_{i,\alpha} e_{i,\beta} (f_i - f_i^{neq}), \tag{5}$$

where τ_v and τ_t are the dimensionless relaxation rates corresponding to the molecular and turbulent viscosity. From eqs. 4 and 5 the turbulent viscosity $\nu_t \propto \tau_t$ can be computed as a local (nodal) quantity.

As an example problem we chose the flow around two adjacent cooling towers. It is well known that the structural stability of clusters of neighbouring cooling towers can severely be affected by resonance phenomena induced by vortex coupling (e.g. the collapse in Ferrybridge, England, 1965). For realistic cases we have $Re = \mathcal{O}(10^8)$ which is presently beyond the computational limit of LES simulations. Yet, as the transient behaviour is of primary interest we assume that the LES approach will still give reasonable insight at $Re = 10^5$. The system consists of $\approxeq 5 \times 10^8$ DOF which were iterated for $\approxeq 3 \times 10^5$ time steps (corresponding to 20 minutes realtime). The simulation took about 120 h on twenty cores of a 1.4 GHz Opteron Cluster. During the last quarter of the simulation time we recorded the drag forces on both towers. Their power spectrum depicted in Fig. 1 clearly shows substantial differences for the two buildings which require further analysis and ideally experimental validation.

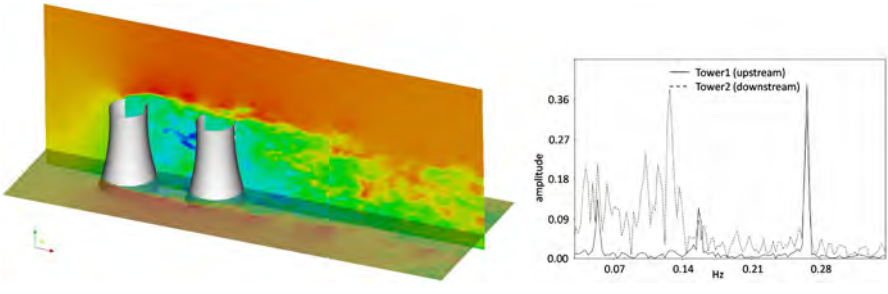

Fig. 1. 3D-LES simulation of flow around two cooling towers: a) snapshot of downstream velocity b) power spectra of drag force for both towers.

3.2 Multiphase Flows in Porous Media

Environmental flows are not only associated with high Reynolds numbers. In soil physics one is interested to predict subsurface multiphase flow which is typically governed by capillary effects. Multiphase flow models based on discretizations of the Navier-Stokes equations are described e.g. in [40, 57]. LBM methods for multiphase flows are described in [24, 44, 50, 56, 38, 55]. These approaches have proven to be especially effective for pore scale simulations [2, 1] which are based on tomographic reconstructions of the pore space [31]. Fig. 2 shows a reconstructed soil probe and an isosurface indicating the interface between air and water. The simulation required approximately 10^{10} DOF.

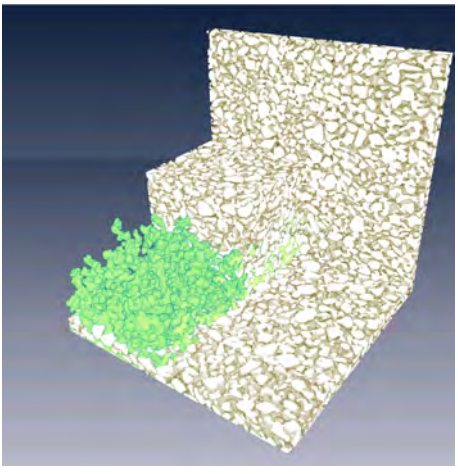

Fig. 2. Multiphase flow simulation in a reconstructed porous medium.

3.3 Free Surface Flows and Fluid-Structure-Interaction

Environmental flows often include free surfaces and Fluid-Structure-Interaction (FSI) (e.g. wave impact on infrastructure, debris flow or windload on bridges). Recent advances in FSI can be found e.g. in [27, 58, 7] and the references therein. The extension of the LBM for FSI is discussed in [33, 46, 45, 18]. Free surface flows have been treated with LBM in [22, 52]. The free-surface approach used in this work employs a Volume of Fluid approach for the advection of the fluid fraction variable and is described in [29]. A computational example of a wave impact on a cylinder is given in Fig. 3. The simulated drag force on the cylinder matches the experimental results to $\approxeq 10\%$. The simulation time for this 3D-case with 2×10^7 DOF is approximately 3 h on a fast PC.

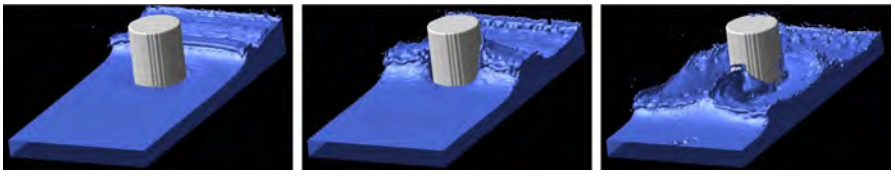

Fig. 3. Free surface flow simulation of wave impact on a cylinder.

A combination of free surface flows and FSI simulated by a Finite-Element approach is described in [61, 62]. As a preliminary model to capture the main features of debris flow we coupled the LBM code to a physics engine [28] which computes the rigid body dynamics. Fig. 4 shows a simple case where a stack

of bricks is being destroyed by the wave impact. A more detailed study is on the way and will be subject to a forthcoming publication.

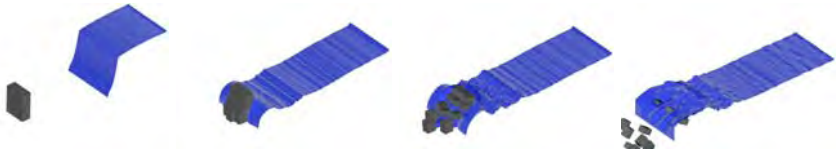

Fig. 4. 3D-LES free surface simulation of wave impact on a stack of bricks.

3.4 Thermal Flows

During the last decade different approaches for the simulation of thermal driven flows using the LB method have been developed [59, 49, 15, 39, 36]. Energy-conserving multispeed thermal LB equation models (TLBE) use a larger set of discrete velocities than the standard method [41] to include temperature. A better way is to use hybrid thermal LB models (Hybrid TLBE), i.e. an explicit coupling between an athermal LBE scheme for the flow part and a separate transport equation for the temperature equation. Most of these approaches were tailored to simulate nearly incompressible flows covered by the Boussinesq limit [43, 25, 36, 37].

A hybrid scheme was developed by Lallemand and Luo in [36] by coupling the energy mode of the athermal LB model [12, 13, 34] to the temperature field. A model for thermal low Mach number *compressible* flows for large density variations has been developed in [53]. The flow field is solved by the multi-relaxation time LBM and the equilibrium moments are modified to obtain the correct equations for large density variations. The temperature equation is solved by a separate Finite Difference scheme.

Based on a similar approach as described in [60] the thermal simulation of an atrium is depicted in Fig. 5. Two openings with reference pressure couple the building climate to the atmosphere. External radiation through the translucent roof heats the faces inside the building which leads to a recirculation regulating the internal temperature.

4 Conclusion and Outlook

The LBM has considerable potential as a modelling and simulation ansatz for real life problems in Civil and Environmental Engineering and is a vibrant field of research. Its explicit numerical approach allows a straightforward coupling to other models representing structural dynamics or radiation and an efficient parallel implementation. Especially the use of special purpose hardware [54] is expected to deliver the accuracy of 3D transient transport simulations without the use of expensive supercomputers.

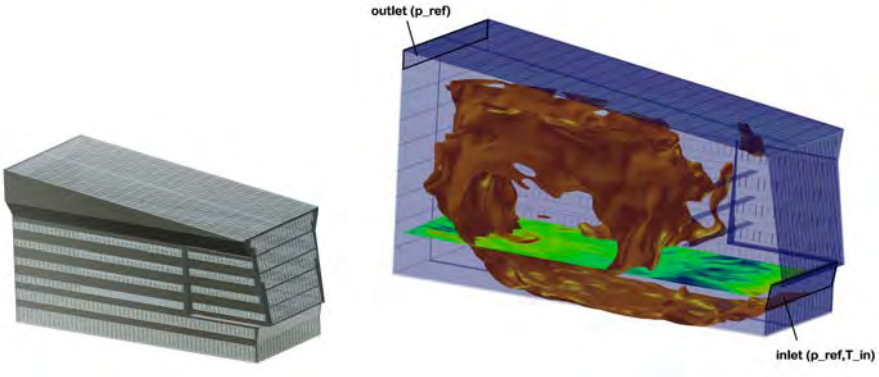

Fig. 5. Thermal comfort simulation inside a large office building; left: CAD-model, right: orthoslice of velocity magnitude and 20° Celsius isosurface.

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CFD in Process Engineering

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Summary Process engineering focuses on the design, operation and maintenance of chemical and material manufacturing processes. As in other disciplines, CFD has attained a certain maturity in order to analyze and optimize these processes. Besides convective, turbulent and diffusive transport of mass, momentum and energy, CFD in process engineering has to account for several other complexities such as multi phase fluids including phase changes, the kinetics of chemical and biological conversion, unknown material and thermodynamic properties, among others. The paper presents a selection of applications, where classical CFD techniques as well as new developments such as the lattice-Boltzmann technique are utilized.

1 Introduction

Process engineering is often used as a synonym for chemical engineering and focuses on the design, operation and maintenance of chemical and material manufacturing processes. Within an industrial value chain, process engineering is located in between the recovery of raw materials and manufacturing of finished products. Thus, it directly and substantially contributes to the economic success in many industries, e.g. in material technology, chemistry, life science and biotechnology.

Mechanical process engineering shall be understood as an application of mechanical and fluid-dynamical principles to the conversion of matter by the effect of mechanical action. Basic building blocks are crushing, agglomeration, mixing, separation and conveying of materials. *Thermal* process engineering denotes the application of thermodynamics with a focus on distillation, extraction and adsorption. In *chemical* process engineering or reaction engineering the focus is on conversion processes using chemical reactions and is therefore strongly linked to chemistry. A major issue in chemical process engineering is to scale up from laboratory scale experiments to production scale processes. A

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further branch is *bioprocess* engineering emphasizing conversion due to biological processes such as fermentation. These processes are usually characterized by ambient pressure, low temperature (20-50^{o}C) conditions and low reactions velocities but high selectivity. *Nano-particle technology* is often regarded as a new area of process engineering.

From a fluid dynamical point of view, basic building blocks in process engineering are the convective (also turbulent) and diffusive transport of mass, momentum and energy in one or multi phase fluids including phase changes. Additional complexity arises from the kinetics of chemical and biological conversion processes, unknown material and thermodynamic properties as well as further transport phenomena such as radiation in high temperatures processes.

As other fields of technology, process engineering benefits significantly from modelling and simulation as a mean to optimize existing processes and to design new ones. At a large or plant scale, stationary or dynamical system simulations based on flow sheet models have become widely used tools. The key to success in applying these methods is a sound understanding of the process fundamentals. This can be achieved by the development and analysis of experimentally verified process models. Here, CFD may be used as a complementary measure to improve the formulation of such models. Additionally, CFD allows to assess and to optimize process details. The importance of CFD in process engineering is in the meantime widely acknowledged and the topic is adopted by various technical committees such as ProcessNet[1]. Textbooks with focus on CFD in process engineering are available, see e.g. [1].

In the following section, basic aspects of the modelling of fluid flows in process engineering are outlined. This survey includes widely used methods based on continuum assumptions as well as more recent developments such as the lattice-Boltzmann methods. Subsequently, based on selected examples, perspectives of CFD with regard to process engineering are presented. This selection is far from being complete or representative for the entire field of process engineering.

2 Modelling Complex Fluids

The major challenge of using CFD in process engineering is due to the complexity of the fluids under consideration [1]. In contrast to other fields of fluid dynamics, modelling of the momentum transport in a single phase flow field alone is not sufficient, even though this is often challenging enough. In order to correctly predict the yield and selectivity of a conversion process, additionally homogeneous and heterogeneous chemical or biological reactions have to be considered. Their exact kinetics may be quantified only for a limited number of reactions and only if the reactions pathways are knows. Besides, the conversion strongly depends on mixing, in particular at a micro scale, which in turn

[1] www.processnet.org.

requires appropriate turbulence models. The mass transport is determined not only by convective and turbulent effects but additionally by various forms of molecular transport, such as ordinary and thermal diffusion [2].

In the energy balance, additional contributions due to chemical heat release or due to radiation [3] have to be considered. Finally, chemical and mechanical processes very often comprise multi-phase flows. Examples are the transport, conversion, separation or deposition of solid particles in liquids or gases, the phase separation of immiscible fluids or the phase change e.g. in sono-chemical reactors due to cavitation. These phenomena challenge existing models such as Euler-Lagrange techniques in case of highly loaded particulate flows or in case of interactions between particles at nano scale. For the details of the aforementioned phenomena, the reader is referred to text books such as [1, 4], where some of the most important phenomena are addressed in a comprehensive way.

3 Top-Down and Bottom-Up Approach

At a continuum level, the transport of mass, momentum and energy along with the above mentioned conversion processes is usually modelled using conservation equations (e.g. Navier-Stokes), closure assumptions and mostly empirical model assumptions such as reactions rates. This *top-down* approach finally leads to a set of nonlinear, second order partial differential equations which may be solved together with suitable boundary and initial conditions in an approximate way. Suitable techniques such as finite volume or element methods are in the meantime well documented [5, 6] and are therefore not outlined here. For industrial purposes, a vast number of commercial programs is available. Some of them provide special purpose models tailored for particular applications in process engineering, such as fuel cell or catalytic converter design.

Beside these traditional CFD methods, in the past years, the *lattice gas cellular automata* (LGCA) and *lattice Boltzmann Methods* (LBM) have attained a certain maturity and subsequently challenged other methods of computational fluids mechanics in many areas, in particular in process engineering. In that context, traditional methods of CFD are understood to include all numerical schemes that aim to solve the Navier-Stokes equations using some finite approximations. In contrast to that, the LBM may be derived from a *bottom-up* approach. From a gaskinetical, i.e. microscopic, point of view, the movement of a fluid may be considered as the propagation and collision of molecular particles. The modelling of this motion may be carried out on several levels, starting with the Hamilton equation of a set of discrete particles. Since this approach prohibits itself because of the large number of molecules to be considered in a real fluid, several attempts have been made to simplify this picture by extracting only the essential criteria required to model e.g. the motion of a Newtonian fluid. In that context, the lattice gas automata may

be seen as an abstraction of the fluid making use of the fact, that mean quantities of the gas may be correctly described by a significantly reduced number of molecules. If one additionally applies discrete velocities and a simplified dynamic of collisions one arrives at the lattice gas automata.

The FHP automata, named after [7], was a first successful attempt to construct a discrete model to compute the motion of a Newtonian fluid. Although this approach seems promising, there are problems due to spurious invariants and random noise in the solutions. In particular the problem of noise, which is due to the discrete nature of the method, can be overcome by applying the idea of McNamara and Zanetti [8], who replaced the discrete particles by their distribution functions. In fact, this approach may be viewed as an approximation of the Boltzmann equation, where the velocity space is discretized with few degrees of freedom. The complicated collision term is replaced by a simple relaxation term based on the Bhatnagar-Gross-Kroog approximation and the Boltzmann H-theorem, i.e. if a Maxwellian equilibrium velocity distribution exists. Further technical details of this method may be found in [9]. From the computational point of view the above approach is interesting as it resembles a simple finite difference scheme applied to a first oder (in time and space) equation in diagonal form. This extremely simplifies the design of a numerical scheme. However, finally the solution of the Navier-Stokes equations with second order accuracy in the limit of low Mach numbers is recovered, as can be shown by applying the Chapman-Enskog procedure.

The approach presented above is just the basic version of the LBM. Many improvements have been designed in order to improve the method's range of applicability, see e.g. the review article of Chen and Doolen [10]. For various applications, particularly in chemical and process engineering, the convective and diffusive transport of energy and species are of key importance. Thermal models have been proposed by [11, 12], reaction diffusion problems have been investigated e.g. by [13, 14]. The simulation of multi-phase flows and immiscible fluids are subject to several investigations where the LBM provides interesting alternatives to model particle interaction, surface tension etc. In modelling suspensions of particles, the interactions of the fluid and particles may be treated by dicretizing and mapping moving particles in a Lagrangian sense [15]. Models for turbulent flows have been adapted from classical LES (large eddy simulation) approaches, as applied to the Navier-Stokes equations. Alternatively, two-equation models have been proposed by e.g. [16].

4 Simulation in MOVPE Reactor Design

The metal organic vapor phase epitaxy (MOVPE) is an important step in manufacturing electronic devices such as semiconductors or optoelectronic components by depositing thin layers of metal-organic compounds such as GaN or AlN on a wafer. In further production steps, electronic circuits are manufactured using etching techniques. There is an increasing demand in

optimizing existing deposition techniques and in designing new processes, e.g. by using new precursor systems. The goal is to improve the quality of the deposited layers and to improve efficiencies of the process. In that context the numerical simulation plays an increasing role in order to predict the influence of process parameters on the deposition, if validated physical and chemical models are available. Besides that, the numerical simulation allows to shed some light on the underlying physical and chemical processes and thus, to improve the understanding and validation of models.

At a reactor scale the process is modelled based on conservation equations of mass, momentum and energy together with suitable models and parameters to describe homogeneous and surface chemical reactions, thermodiffusion and radiation. More details regarding the modelling may be found in [17]. Figure 1 shows an industrial reactor and Fig. 2 the computed temperature distribution inside the reactor for different radiation models.

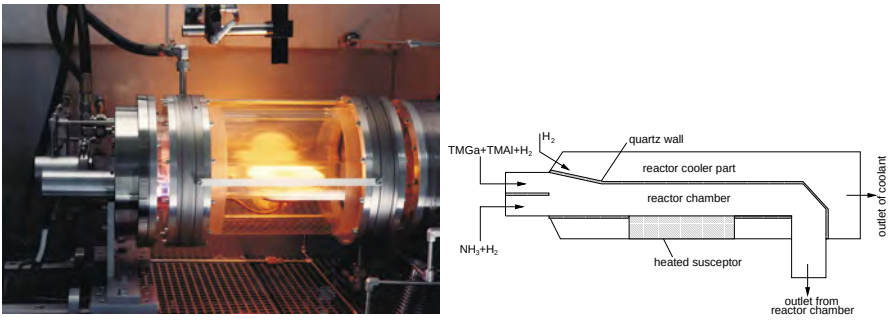

Fig. 1. Aixtron AIX200 RF reactor and sketch of the reaction chamber with cooling part.

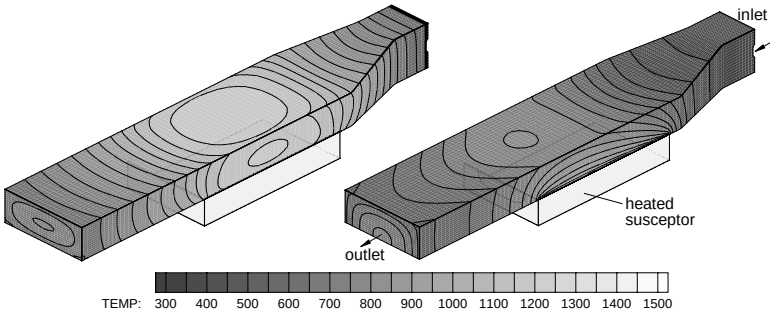

Fig. 2. Temperature distribution at the reactor chamber walls taking into account the radiative heat transport mechanism (left) and neglecting this mechanism (right).

In order to elucidate the accuracy of predicted deposition rates of metal-organic compounds along the surface of the susceptor, a comparison with experimentally obtained growth rates is presented in Fig. 3 for different inflow rates of the precursor (case A and B). More details regarding the sensitivity of model parameters with respect to the prediction of engineering properties such as growth rates are discussed in [17, 18].

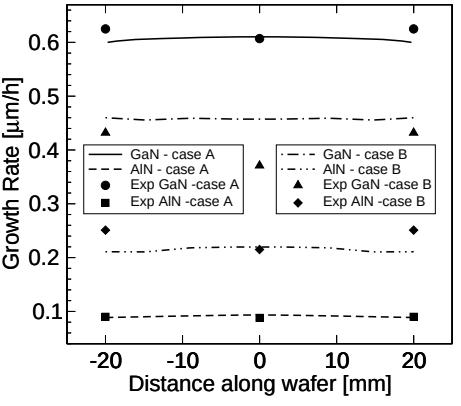

Fig. 3. Comparison of the experimental and numerical growth rates for GaN and AlN.

The challenge with respect to the modelling of the transport phenomena and of the chemical conversion processes is, that for new precursors basically no information regarding thermodynamic and transport properties and chemical kinetics is available. The reaction pathways can only be estimated or quantified by experiments. In a joined project between researchers from fluid mechanics, inorganic and computer chemistry[2], ab-initio simulations at atomistic scales were performed in order to determine these data and to provide the input for process simulations at the reactor level. Thus, a reactor model was validated which was completely based on numerical simulations.

5 Applications of LBM

In chemical industries, packed beds and porous media are frequently used as reaction, separation or purification units. The design of these devices is usually based on pseudo-homogeneous model equations with averaged semi-empirical model equations such as dispersion and mass-transfer correlations. The design concepts based on these models fail if local flow phenomena such as channelling effects become dominant. Therefore, several attempts have been made in order

[2] Within the collaborative research project DFG SPP 1119.

to improve these models. However, new design methodologies are required if no or insufficent empirical data are available. Lattice Boltzmann methods can be used to directly simulate the flow field in these configurations together with chemical reactions and diffusion effects. This allows to analyse in detail the hydrodynamic effects, e.g. the channelling due to inhomogeneous void space distributions and other flow anomalies and to quantify their influence on the prediction of the bulk conversion and selectivity of the reactor. The lattice Boltzmann method has been chosen mainly because of its ability to model highly complex geometries.

The *direct* numerical simulation of flows through packed beds uses a digitized image of the structure under considerations. This may be obtained from computer tomographic data of a real probe of the material or by synthetically generated geometries. Following the marker and cell approach, this geometry can easily be transferred to the uniform, Cartesian mesh, which is typically used in lattice Boltzmann methods. Due to the low memory requirements of these methods, meshes with several million elements may easily be used to capture the geometric details, Fig. 4.

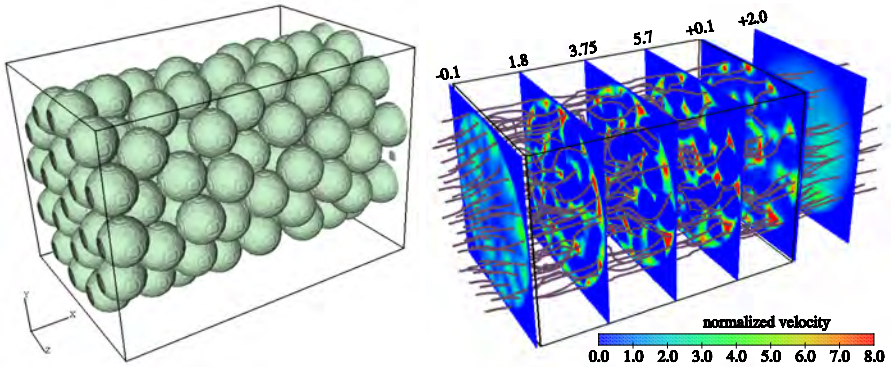

Fig. 4. Image of the packed bed structure generated synthetically (left) and velocity distribution from LBM simulation (right).

The Reynolds number based on the particle diameter is $Re \approx 10$. The structure consists of particles, randomly distributed in a confining cylinder with a diameter ratio (cylinder/particle) of 5. The computational domain is discretized with $150 \times 150 \times 750$, i.e. more than $16 \cdot 10^6$ elements. In order to obtain a converged steady state solution, about $40,000$ propagation (= iteration) steps were necessary for the present laminar flow conditions, which took about $2h$ CPU time on six NEC SX-5e shared memory processors.

The above approach allows to analyse transport phenomena in more complex geometries such as porous media including reaction or diffusion phenomena. Again, this requires the detailed representation of the geometry of the media. Here, a three-dimensional x-ray computer tomography is used to provide

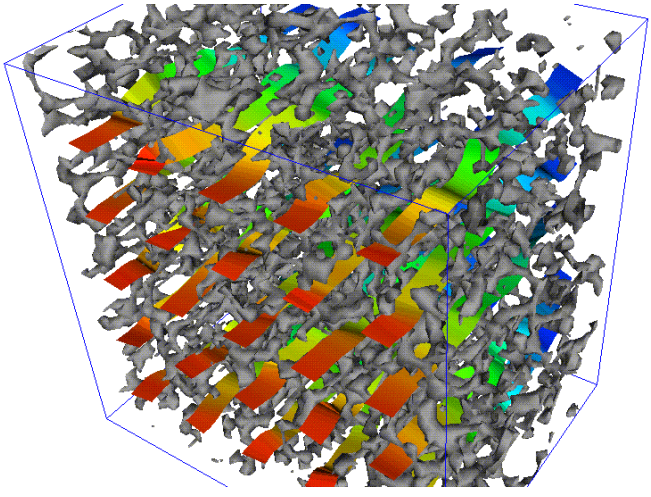

Fig. 5. Snapshot of the structure and the flow in a porous media. The geometry is obtained from a computer tomographic scan of a ceramic, foamlike structure. The flow is calculated with the LBM for $Re \approx 1$.

a 3D *bitmap* of the geometry. Figure 5 shows a detail of this medium together with stream-ribbons to show the tortuosity of the flow. In order to analyse more quantitatively the flow and dispersion in porous media, the transport of a passive scaler may be simulated, as presented in [9]. From such numerical experiments, dispersion coefficients may be obtained which are parameters in system simulation tools.

6 Conclusion

Computational fluid dynamics has to be considered as a useful tool to investigate flow and conversion phenomena in process engineering, as has been shown in the present contribution for two different devices and using different numerical tools. This demonstrates, that CFD may be used on the one hand as a tool with predictive capability, even in situations were numerous empirical and uncertain parameters enter into the models. This allows process engineers to analyze and optimize existing devices. On the other hand, CFD allows to provide parameters that may enter into process models at a system scale.

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Computational Electromagnetics

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Summary The progress during the past forty years of computational electromagnetics in the time domain is summarized. Contributions from the computational fluid dynamic community to this scientific discipline are highlighted. The impact of characteristics-based formulations, high-resolution algorithm development, and concurrent computational techniques has alleviated two fundamental limitations in computational electromagnetics. This knowledge sharing has opened new avenues for basic research and practical applications for electrical engineering and interdisciplinary computational physics.

1 Background

All electromagnetic phenomena are described fully by the Maxwell equations in the time domain [1, 2, 3]. However in practical application, a wide range of numerical methods was developed for physical phenomena according to where their dominant frequencies occur: in the Rayleigh, resonance, or optical region. Therefore computational electromagnetics (CEM) has a tiered structure for analyzing physical phenomena over frequency spectra. The predictive techniques fall naturally into two general groups according to the ratio of wavelengths and the characteristic length of the investigated problem. The collective modeling and simulation tools include the asymptotic method, method of moment, time-domain method, and the more recent development of the hybrid technique [4]. As a group this methodology has been extremely productive for telecommunication, micro-strip patch antenna design, wide-band communication, microwave diagnostic technology, and electromagnetic signature analysis.

In optical region applications, the most efficient modeling and simulation tool is the asymptotic approximation – ray tracing. This technique is based on physical optics, physical theory of diffraction, or a combination of both. The scattered far field is derived from the induced surface current by physical

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optics integration [3, 5]. The methodology is highly specialized for antenna design and radar signature application but it can't describe the electromagnetic field structure. Again in some applications, the electromagnetic phenomena are best analyzed in the frequency space. This formulation is derived by either the separation of variables technique or by the Fourier transformation. The transformed partial differential governing equations are an elliptic system. A very large group of numerical methods for solving the frequency-domain formulation is collectively called the method of moment (MoM). For the frequency-domain method, the fast multi-pole algorithm has demonstrated a greater computational efficiency by reducing the arithmetic operation count [4]. In turn, the computational efficiency gain enlarges the application envelope of MoM methods from the resonance approaching the optical region. These groups of specialized methodology using either asymptotic theory or MOM in the frequency domain will not be elaborated further in here.

2 Maxwell Equations in the Time Domain

Computational electromagnetics (CEM) in the time domain is built on the time-dependent Maxwell equations. The fundamental equations of electromagnetics were established by James C. Maxwell in 1873 and experimentally verified by Heinrich Hertz in 1888 [1]. This approach represents the most general formulation for electromagnetic phenomena in the tier-structured CEM technology. The time-dependent Maxwell equations consist of the Farady's induction, generalized Ampere's and two Gauss's divergence laws. Together with the associated initial values and boundary conditions they constitute hyperbolic partial differential equations. For the hyperbolic system of equations, all associated eigenvalues are real; the initial values will propagate continuously along the characteristics to infinity. Unfortunately, numerical solutions in discrete space must be obtained on a truncated computational domain. This approximation unavoidably leads to the creation of artificial boundaries. Improperly specified value on this boundary is known to induce spurious wave reflections. This numerical artifact leads to erroneous accumulation of radiation energy and unrealistic wave modulation even though the computation is stable [2, 5].

A widely adopted numerical algorithm of CEM in the time domain is the characteristics-based formulation [3, 5]. For scattering simulations of arbitrary electric shapes, the combination of this algorithm together with the unstructured grid technique has been proven to be the most effective. This type of data connectivity is also found to be compatible for parallel computing using the domain decomposition strategy. Additional numerical efficiency can also be derived from implicit schemes that remove the conditional-stability constraint imposed by explicit methods. The rich heritage of computational fluid dynamics (CFD) has provided an in-depth knowledge for computational electromagnetics. The first-order curl differential system reflects the coupled and

mutually orthogonal features of electric and magnetic fields. This peculiar behavior is clearly revealed by the instantaneous electromagnetic field structure of a simple pulsating dipole depicted in Figure 1.

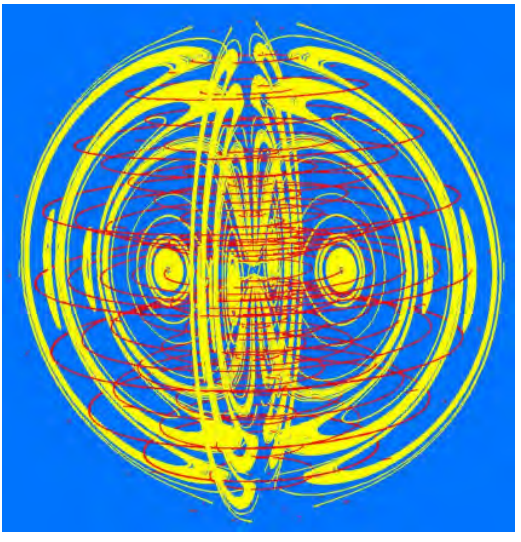

Fig. 1. Oscillating electric dipole.

In this figure the magnetic field is depicted in red and the electric field is given in yellow traces. The mutually perpendicular formation of the electromagnetic field is clearly displayed.

Associated with this attribute the time domain approach also incurs a numerical efficiency constraint imposed by numerical accuracy requirement. In discrete space, the fundamental and absolute numerical resolution requirement for wave motion is the Nyquist frequency limit [6]. In essence, a minimum of two discretized points per wavelength is necessary to achieve a physically meaningful simulation. There is, at least, an order of magnitude disparity between current capabilities of the most commonly adopted second-order numerical schemes and the utmost resolution achievable [7]. For three-dimensional simulations, the potential of algorithmic improvement towards the absolute resolution ceiling is over a thousand-fold. This theoretical limit also defines the upper bound of practical application in either the frequency spectrum or the physical dimension in which a transient phenomenon can be simulated.

In 1966, Yee led the pioneering effort for computational electromagnetics in the time domain by solving the time-dependent, two-dimensional Maxwell equations. Yee's outstanding contribution to CEM can be summarized in two aspects: First, by his insight in electromagnetics by using the staggered grid description to couple the electric and magnetic fields. Second, he adopted the leap-frog scheme to minimize the dispersive numerical error. An ever in-

creasing range of engineering applications in broad bandwidth and dynamic electromagnetic events has been realized by noted contributions from Taflove, Umashankar, Cangellaris, Shankar, Luebbers, Malloney, and Shang among many others [2, 3, 9, 10, 11, 12, 13].

In the middle 1970's, Taflove and his collaborators conducted the first grid-based time-integration for a two-dimensional electromagnetic wave interaction until it reaches the sinusoidal periodic state. Three-dimensional simulation for electromagnetic wave absorption by complex, inhomogeneous biological issues was also accomplished by his team. Most of the numerical simulations employed uniform Cartesian coordinates along with staircase boundaries to approximate the surface of a structure that did not align with the coordinates [2]. In 1981, Mur published his second-order accurate absorbing far-field boundary condition and removed the concern of computational stability [14]. Shortly afterwards, CEM expanded applications to electromagnetic wave scattering to compute the near fields, far fields, and the radar cross-section (RCS) for two-dimensional and three-dimensional configurations [2]. Rapid progress has expanded the application envelope in the next few years to simulate waveguides, cavity structures, antennas, and picosecond optoelectronic switches [2, 9].

Transition of CFD techniques to CEM started in the later 1980's. Anderson [15], Shankar et al [10, 16], Goorgian [17], and Shang [3, 11, 12, 18] were active in the knowledge transfer. During that time frame, the hypersonic flow investigation invigorated the basic research for nonequilibrium dissociation and ionization phenomena of high-temperature gas. The moving charged particles of the ionized gas create an electromagnetic field and introduce an additional diffusion mechanism for momentum and energy transfer. The two entirely different areas of research of CFD and CEM have a common interest, namely to acquire a better analytic capability for describing the electromagnetic field. Meanwhile it was also critical for the CFD community to open a new avenue to interdisciplinary endeavor. Therefore, it is natural and logical to leverage the basic knowledge among CFD and CEM to achieve synergetics. The fundamental idea of flux-splitting methods for solving hyperbolic systems of equations, body-conformal curvilinear coordinate transformation, implicit numerical algorithms, as well as finite-volume and finite-element methods were floating easily between CFD and CEM communities. Especially for the electromagnetic field of RCS prediction, the main concern is the appropriate treatment of incident and scattering wave propagation from a reflecting surface. The elimination of non-physical reflecting waves from artificial outer boundary is a paramount issue and can be alleviated by the theory of characteristics.

Computational electromagnetics in the time domain has become an effective tool for electromagnetics research. However, the maturation of this technology for design and evaluation was hampered by the fundamental problem of well-posed computational boundary conditions, numerical resolution, and data processing efficiency. Some of these issues remain even today as the challenges to time-dependent computational electromagnetics.

A key dilemma of CEM is the initial value and boundary condition problem that must be solved on a truncated physical domain with a finite size of computer memory. The limitation was remedied earlier by the absorbing far-field boundary condition of Mur [14] and later by the perfectly matching layer (PML) of Berenge [19]. In 1995, Shang et al [11, 12] formally derived the characteristics formulation for the time-dependent, three-dimensional Maxwell equation on generalized curvilinear coordinates. In the characteristic-based formulation, the no-reflection far-field boundary condition is readily achievable by imposed vanishing incoming flux vector components. The effectiveness of the characteristic formulation is demonstrated by the numerical simulation of the near-field, microwave radiation from a rectangular pyramidal horn in Figure 2.

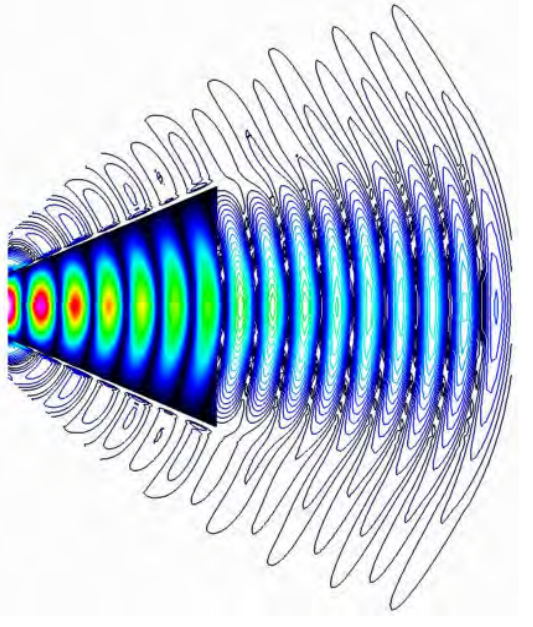

Fig. 2. Microwave transmitting from a pyramidal antenna.

In this figure the transmit wave is the principal transverse electric mode, TE1,0, at a frequency of 12.56 GHz with a wavelength of 2.398 cm, and the aperture of the antenna has a dimension of 3.05 by 3.64 wavelengths. The far-field boundary condition for this numerical simulation is placed just a few wavelengths from the exit of the antenna. The graph is presented at the time frame in which the transmitting wave front has just passed through the outer computing domain. The contour of electrical intensity exhibits no detectable distortion of any reflected waves from the computational boundary.

3 Current Status of CEM

The limitation of computational efficiency for practical application by frequency-domain and time-domain methods has been alleviated by the high performance multi-computers (parallel computers). The concurrent computing significantly reduces the wall-clock time of data processing. From research efforts in porting CEM programs to multi-computers, a speedup by three orders of magnitude for the data processing rate on a thousand-node multi-computer is realizable [9, 20, 21]. It is well-known that balancing work load and minimizing inter-processor communication are essential to use multi-computers effectively. A frequently overlooked requirement for efficient parallel computing on a RISC (reduced instruction set central process unit) system has been identified from the programming paradigm on mapping numerical procedures for solving time-dependent Maxwell equations. The cache memory and the memory hierarchy utilization emerge as an equally critical element for high concurrent computing performance [20, 21].

More importantly, the distributed and the shared-distributed memory systems can now accommodate a far larger number of unknowns than were attainable just a few years ago [20]. This increased capacity expands the frequency range and complexity of physics that can be practically simulated. A solid illustration can be observed by a validating comparison of solutions of the Maxwell equations in the time and the frequency domain. Figure 3 depicts the RCS predictions by the time-domain and frequency-domain method (MOM).

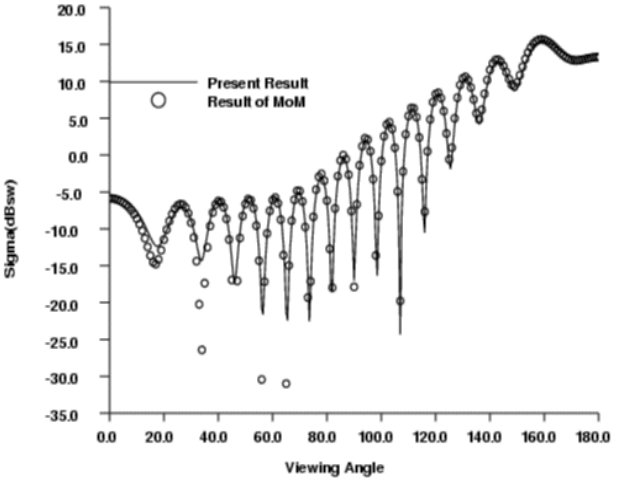

Fig. 3. Validating comparison of RCS of an ogive cylinder with an incident wave of 4 GHz.

The incident electro-magnetic wave is transmitting parallel to the axis of an ogive cylinder at a frequency of 4 Giga Hertz. The bi-static electromagnetic signature is given in the unit of decibel per square wavelength (dBsw) and is a function of the direction of the observation point relative to the propagation direction of the incident field. The radar cross-section is the ratio of the scattered and incident electric or magnetic fields at a large distance from the scattering body [22]. The agreement is excellent between results of different numerical methods in dBsw over a dynamic range of 50. The disparity in all lobes is less than a tenth of one dBsw, and the maximum discrepancy only appears the nulls of the HH polarization computation. The numerical results were obtained on a 120-node Cray T3E multi-computer system with a parallel computational efficiency of 93.7% [20]. In more recent CEM simulation, this kind of parallel computing efficiency is routinely achievable and the performance on multi-computers becomes truly scalable [3, 9].

The rapid data processing rate on a massively parallel system through a superior scalable performance has shown the realism for future real-time simulations. In 1998, a path finding CEM electromagnetic signature simulation using a total of 34.5 million grid cells was demonstrated [3]. The numerical simulation requires an unprecedented problem size of more than 192 million unknowns. On a 258-node SGI Origin 2000 system, the data processing rate is estimated to be about 24.32 Gflops [3, 5]. Using an unstructured gird approach to solve the identical problem, a perfect load balancing was easily achieved and the issue of scalability to operate on a greater number of computing nodes and a higher data processing rate was also demonstrated [20, 21]. The lesson learnt from this research effort is that the unstructured grid technique must be introduced to CEM in the time domain for versatile applications. However, a dispersive preserving and low dissipative procedure must also be introduced to achieve acceptable numerical accuracy [7, 23].

For telecommunication and navigation, high-frequency wave packets are required to propagate over a long distance without significant phase error and amplitude modulation. However in time-dependent calculations, the truncation error of a numerical result is manifested in dissipation and dispersion. The accumulated numerical error during a sustained period of calculation or in an extensive computational domain may lead to a situation where the wave modulation and phase errors become unacceptable [5, 17]. In principle, the numerical accuracy can be improved either by refining the mesh point density or by adopting a high resolution numerical procedure. The former approach is always limited by the available computing capacity, and, when a huge amount of computing resource is required, the simulation ceases to be a viable engineering tool. The more fundamental approach of devising a reliable high resolution numerical procedure for complex configurations that can expand the application range of CEM is much more appealing.

All known finite-difference or finite-volume computational procedures have a fixed range of wave numbers in which the numerical results will contain the least dispersive and dissipative errors. The desired feature of a numeri-

cal scheme may be derived from optimization in Fourier space [24, 25]. The Fourier analysis of numerical approximations for hyperbolic equations is readily available, and has been extensively used in algorithm research [26]. The numerical resolution is quantified by the Fourier analysis in terms of the normalized wave number. In applications, the quantification is measured by the grid-point density per wavelength, and has a direct correlation to the wave number. However, this criterion will become insufficient when the computational domain contains inhomogeneous media with a wide range of characteristic impedances. This occurrence simply reinforces the fact that all numerical schemes have a limited wave number range for accurate computations. Figure 4 offers an example for this contention; when a transverse microwave propagates at a frequency of 12.56 GHz through a rectangular waveguide in which a thin plasma sheet is trapped by an externally applied magnetic field of 0.9 Tesla.

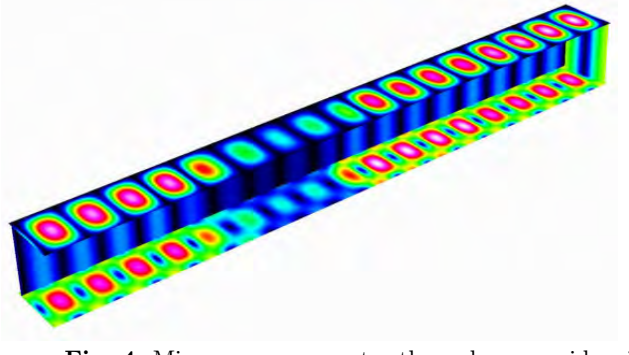

Fig. 4. Microwave propagates through waveguide with different media.

In this composite presentation, the electric and magnetic field intensities are projected on the top and bottom sidewall of the waveguide respectively. It is observed that the distortion of the propagating microwave is significant and extends beyond the plasma sheet thickness of 2.5 wavelengths.

The advance in high-resolution numerical procedures seeks an algorithm that needs a small stencil dimension and yet maintains a lower level of dispersive and dissipative error than conventional numerical schemes. The compact-difference method based on Hermite's generalization of the Taylor series possesses this unique feature [24, 25]. The basic high-resolution differencing formulation is a spatially central implicit procedure for evaluating the derivatives of dependent variables. The stencil of this identical formulation can degenerate into a three-point, fourth-order scheme – the well-known Pade's formula. A sixth-order scheme can also be recovered by assigning a coefficient to the recursive formula and the formula is now supported by a five-point stencil [25]. Both the fourth- and sixth-order scheme combined with a four-stage Runge-Kutta scheme for time integration are conditionally stable, when ap-

plied to the one-dimensional model wave equation. The fourth- and sixth-order scheme has allowable Courant-Friedrichs-Levy (CFL) numbers of 1.63 and 1.42 respectively [21, 22].

In the finite-volume approximation, the compact-differencing formulation is used mainly in the reconstruction process [23]. The distinction between the cell-averaged and the cell-interface values is critical in the finite-volume approach for preserving high-order accuracy. The basic approach employs a primitive function for describing the variation in a cell-averaged data array [27]. This set data is first integrated from boundary to boundary to develop the primitive function. Then the reconstructed data at the cell interface is generated by differentiation [23, 27]. The substantially improved numerical resolution of the compact difference scheme over that of the conventional second-order algorithm is seen by the L2 norm comparison in Figure 5.

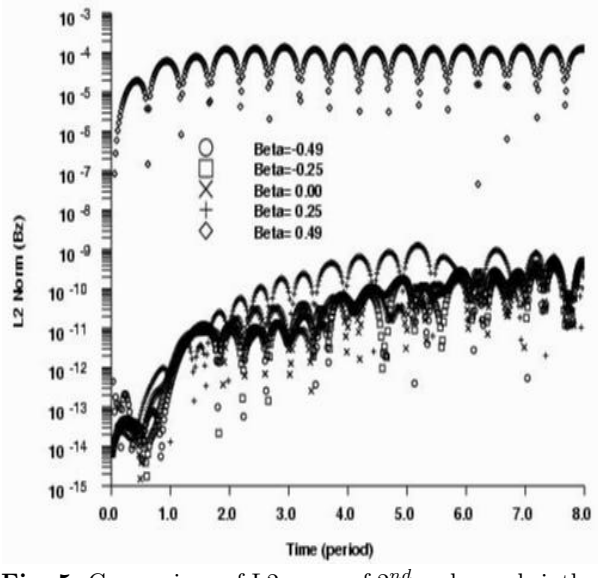

Fig. 5. Comparison of L2 norm of 2^{nd}-order and sixth-order schemes with low-pass filter.

When the high-resolution algorithm is applied to solve the simple wave equation, the numerical scheme reduces the numerical error by six orders of magnitude in comparison with the conveniently second-order method.

An undesirable feature of compact-difference schemes is the time instability during the integration process over a long period [28]. Although these high-order schemes are stable in the classical sense, however numerical results frequently exhibit a non-physical growth in time. Time instability is incurred by a positive and real eigenvalue component of the discrete operator matrix [7]. This component of eigenvalue will dominate the numerical results after a

long period of evolution. The numerical instability is usually manifested in the form of spurious high frequency Fourier components of the numerical solution. A low pass filter is ideal to eliminate undesirable high frequency Fourier components without affecting the remaining components of the numerical solution [23]. In essence this numerical filter eliminates the Fourier components that are unsupportable by the grid point density used. Furthermore, the adopted spatial filter only modifies the amplitude but not the phase relationship among all Fourier components of the solution. The spectral function of a symmetric numerical filter contains no imaginary part and has the ideal low pass amplitude response [23, 26]. Nevertheless, a sustained research for a numerical algorithm that possesses a spectral-like resolution must be maintained for the modeling and simulation technology.

4 Concluding Remarks

The assessment of computational electromagnetics in the time domain indicates that high-resolution numerical algorithm research and high performance parallel techniques are the pacing items for sustaining this scientific discipline. On RISC-based multi-computers, cache utilization, and matching problem memory size with the number of computing nodes emerge as important considerations for high performance parallel computing. For the purpose of load balancing on a multi-computer, the unstructured grid numerical algorithm offers a parallel computing performance superior to the traditional structured grid approach.

The compact-difference formulation has reduced the required grid point density per wavelength by a factor of 3.2 from the bench mark second-order methodology. This improvement has substantially expanded the practical CEM application range for three-dimensional simulations. Unfortunately, the expanded stencil dimension also required a transitional differencing operator to bridge the gap between the interior domain and the boundary. This transitional operator becomes the source of computational instability. A low-pass filter was developed to effectively control an undesirable time instability feature of compact-difference schemes. An innovative numerical algorithm of spectral-like numerical resolution is still needed for further CEM development. At the present, spectral difference methods for unstructured grids based on the Gauss quadrature are under development. This new approach may lead to the long awaited technical advancement in high-resolution procedures.

To improve aerodynamic performance of high-speed flight, a new physical dimension form of plasmadynamics for momentum and energy transport becomes evident. Computational magneto-aerodynamics may offer new insight and new capability to improve performance of hypersonic vehicles. A key element of this technical requirement is integrating computational electromagnetics in the time-domain with computational fluid dynamics together

with computational chemical kinetics. The impact of this interdisciplinary endeavor may open a new scientific frontier.

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Computer Modelling of Magnetically Confined Plasmas

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Summary Magnetic plasma confinement research poses multifaceted requirements for computational modelling. The determination of plasma equilibria, the prediction of their global stability, the physics of plasma heating, the estimation of the energy losses out of the plasma and the interaction of the energetic plasma with the walls require all support by modelling, using distinct approaches. In particular, the quantitative analysis of turbulent energy transport was for a long time exclusively based on semi-empirical approaches. In the last decade, however, ab-initio plasma models have become progressively more realistic. The contribution reports highlights and trends of this development since the de-classification of fusion research, and describes the components of a numerical tokamak[1], expected to become, concomitantly with the burning plasma experiment ITER, the main research tool of the fusion science community.

1 Introduction

The needs of thermonuclear fusion research have traditionally been a strong driver of computer modelling. A net energy gain from the reaction of the two hydrogen isotopes deuterium and tritium depends on producing a sufficiently dense, thermal plasma with ion temperatures T_i in the 10 keV range and confining it over a sufficient time τ_E, so as to satisfy a Lawson-type criterion [1] for $n_e T_i \tau_E$ ($\cong 5{\times}10^{21}$ $m^3 keVs$), with n_e the electron density. Two very distinct approaches have emerged for peaceful applications: impulsive compression, driven by Lasers or fast particle beams [2, 3], with subsequent inertial confinement of the burning plasma on a nanosecond time scale, or quasi-stationary magnetic confinement of a plasma initially heated up within

[1] The topomak is a toroidal chamber with magnetic coils as plasma confinement device.

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some tens of seconds. The two lines have inspired also very different code developments, with the inertial fusion effort profiting strongly from the conceptual proximity to military applications. We will concentrate in the following on the magnetic confinement approach and the progress of modelling in it during the last five decades.

The most advanced toroidal confinement system, the tokamak [4] owns part of its early success to the fact that little computational sophistication is needed to design and operate a simple device, using the Joule heating intrinsically associated with its toroidal current. Plasma confinement is due to the superposition of toroidal and poloidal fields producing axisymmetric flux surfaces in the form of nested tori. The complexity arises with the need to optimize its configuration and to explore the limits of its performance. Figure 1 shows a schematic view of the plasma vessel and of the magnetic flux surfaces of a modern divertor tokamak (ASDEX Up-grade).

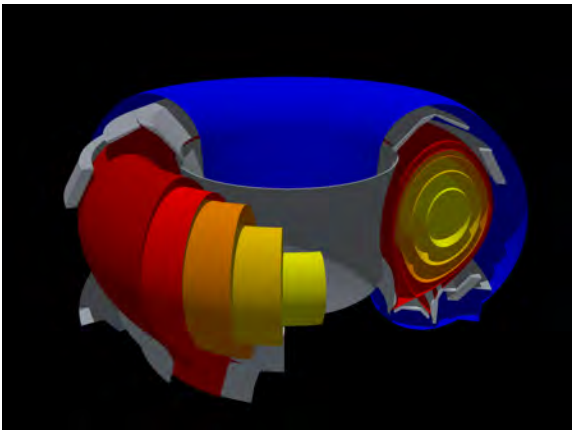

Fig. 1. Plasma vessel and flux surfaces of a modern tokamak.

The plasma pressure is balanced by the magnetic tension of field lines and the gradient of the magnetic pressure. The magnetic field provides also a very effective thermal insulation perpendicular to flux surfaces and allows to maintain a temperature difference between the core (the yellow region) and the boundary (defined by the flux surface with a separatrix in the poloidal cross-section) of several keV over a distance of half a meter. Also the international fusion test facility ITER, to be built as a joint enterprise by the EU, Japan, Russian Federation, USA, China, South Korea and India in Cadarache (France), follows this design principle. It will be the first magnetic confinement device to rely on plasma heating by nuclear reactions, and is expected to produce, by thermonuclear fusion, 10 times more power than externally supplied to it for heating the plasma.

Very advanced modelling tools were finally needed to quantitatively interpret and extrapolate the response of the plasma to powerful heating, and to understand and possibly control the nonlinear consequences of several instabilities. The advance of computational fusion science was of course ultimately limited by the pace of hardware and algorithm development, but reflects also strongly the changing needs of a continuously advancing experimental program. We classify in the following these developments into three phases, concluding with an outlook. Typically the needs of the tokamak program have signed the pace of the developments and, except where specifically indicated, we refer to this configuration.

2 Early Modelling Efforts

After theoretical arguments had emerged at the beginning of the 1970s that non-circular plasma cross-sections should have significant performance advantages, "equilibrium" codes, relating the externally applied magnetic fields to the plasma shape, were first needed. The conjecture was that such equilibria would allow stable plasma operation over a larger parameter range, and therefore also codes, testing these equilibria for linear stability, were needed. Finally one had to solve some balance equations in the form of 1-d time-dependent diffusion equations for particles, temperatures and current densities to relate the observed profiles to the sources and sinks – in the latter including impurity radiation. As it became soon evident that transport coefficients based on laminar, collision-induced diffusion were generally optimistically low, ad-hoc coefficients with little theoretical justification were used to account for unexplained, turbulence-induced losses.

Joule dissipation in a plasma rapidly decreases with temperature and hence additional heating methods are needed to approach the fusion-relevant 10 keV range. Several such heating methods were developed with great success in the 1980s, concomitant with modelling tools for the associated power deposition in the plasma. The increased heat fluxes highlighted the problem of plasma-wall interaction and the resulting wall damage and impurity influxes. For this purpose the divertor concept (Fig. 1) had been incorporated into the new devices, and a distinct new modelling discipline: divertor and scrape-off layer codes, emerged.

The increased heating power could also push tokamak discharges to limits of the sustainable ratio of plasma pressure to magnetic field pressure ($\beta = 2p\mu_0/B^2$). Extensive work with magnetohydrodynamic stability codes identified a relatively simple and universal expression for these ultimate limits, which was verified in impressive form by many dedicated experiments [5] . Below these limits, however, the actually achieved values of plasma temperature and pressure were determined by turbulent transport, and no significant progress was made in the theoretical understanding of the latter. An empirical and rather crude approach was adopted to extrapolate this transport –

measured by the global energy confinement time τ_E (= plasma energy/applied heating power) to future planned devices: a power law fit to the very extensive data base produced – in later versions [6] – by up to a dozen, different size tokamaks.

2.1 Emerging Fields of the 1980s

In the early 1980s powerful additional heating methods became available in the form of neutral beam injection and different wave heating schemes. The increase in the power deposited in the plasma exasperated the problem of impurities, which are produced by plasma-wall contact, and – if penetrating into the plasma core – produce radiative energy losses and dilute the potentially fusion-reacting species. Two experiments were constructed to test at high heating powers the so-called "divertor" idea: to displace, by proper design of the magnetic field, the first plasma-wall contact into a separate chamber, relatively distant from the plasma. They demonstrated not only the feasibility of this concept, but one of them discovered also that the divertor could also lead to a dramatic reduction in the turbulent energy losses [7]. This initiated a complete conversion of the tokamak construction programs towards divertor equipped devices, but also motivated a large, dedicated modelling effort.

Divertor tokamaks, as shown in Fig. 1, maintain axisymmetry, but the plasma region in direct wall contact cannot be treated even approximately by 1-d models. In fact the extend of the scrape-off layer (SOL) beyond the flux surface separating closed and open field lines (the "separatrix") is determined by the competition of parallel and perpendicular transport. Whereas along field lines the plasma flow is essentially gasdynamical and can, in principle, become also supersonic, plasma convection perpendicular to field lines, both within and perpendicular to flux surfaces is dominated by slow drifts and diffusion. Likewise, heat conduction is extremely fast along field lines, but several orders of magnitude lower perpendicular to them. Neutral particles are important – they are the source of the plasma – but are weakly coupled to the plasma, practically do not collide among each other and have to be described by a Monte-Carlo approach. Impurities have to be included in a very comprehensive way, often by treating the individual ionisation stages as separate, but interacting species, and accounting also for the radiative energy losses.

The geometry of the problem is complex, as can be seen from Fig. 1, and coordinates following the magnetic field configuration have a singularity on the separatrix. Modelling of this region is a multi-physics problem, and the codes [8, 9, 10] which have emerged from this effort include also packages describing the surface physics effects of the interaction of hydrogen and impurity ions and atoms with the wall, and detailed packages for the atomic physics. Like for transport codes in the plasma core, their basic limitation lies in the unsatisfactory description of the turbulent transport perpendicular to the flux surfaces. In the SOL region this is further aggravated by the fact that

fluctuations in density and temperature are not universally small compared to the background values, and that intermittency and the irregular ejection of "blobs" of plasma often play a central role. At present these models therefore have only a modest predictive value, but play an essential role in correlating and interpreting the very extensive and diversified diagnostic measurements in the plasma edge region.

Several methods of plasma heating – ITER will incorporate three of them, and is contemplating a fourth – have successfully been brought to maturity. Their physics is generally quite well understood and their performance can be predicted by ab-initio models. For the case of low (tens of MHz) frequency electromagnetic wave heating, however, these models become computationally quite demanding. The basic wavelength is not negligible compared to the device dimensions, while at the same time essential physics (absorption, mode conversion, reflection) happens over spatially very localized regions and involves only a fraction of resonating particles, whose orbits have to be tracked across the relevant interaction region. In the most widely used code [11] the electric wave field is decomposed into separating Fourier components in toroidal, and coupled ones in poloidal direction, with a finite element representation in the direction perpendicular to the flux surfaces. The requirements become progressively more demanding with the size of the modelled device, and application of this code to ITER-like devices or its extension to higher frequency, shorter wavelength heating schemes has become only possible now by massive parallelisation of calculations even for an individual toroidal mode. (A realistic heating antenna spectrum excites several toroidal modes, but their parallel treatment is trivial).

The above modelling developments were essentially driven by the needs of the tokamak. An alternative toroidal confinement geometry – the stellarator – has the principle advantage that it does not require a toroidal current flow in the plasma for the production of nested, closed flux surfaces, is intrinsically stationary (the tokamak requires a transformer to induce these currents, or at least expensive additional systems to drive them by appropriate momentum input to electrons or ions) and not prone to sudden, instability driven disruptions of the plasma current. It gains these advantages at the cost of a substantially more complex coil geometry. Even more fundamental is the fact that by dropping a symmetry (the axial one) particle orbits lose one rigorously conserved constant of motion (the generalised toroidal momentum) which in a tokamak ensures, in the absence of collisions and fluctuations, the confinement of particles to closed surfaces.

It was a dramatic step forward that Boozer [12] formulated the theoretical constraint on 3-d magnetic field configurations to ensure a similar benign orbit behavior as in tokamaks and that Nührenberg [13] succeeded to identify, by numerical studies, actual stellarator plasma shapes satisfying these criteria. This was a major computational break-through, strictly linked to the arrival of systems of the Cray-1 performance class. To arrive from this at the design of a stellarator experiment, substantially narrowing the performance gap to

the then existing tokamaks, required to create the 3-d equivalents to most of the above-mentioned codes. Three-dimensional plasma equilibria cannot be simply found by the solution of a single partial differential equation, but require, by some procedure, the identification of 3-d stationary states of the total potential energy under suitable conservation constraints. Such codes [14] typically start from a given shape of the bounding plasma surface; identifying subsequently the external coil shapes producing these equilibria is, like in the tokamak case, not a well-posed problem, requiring regularisation procedures [15]. Due to the 3-d nature, the linearized analysis of MHD instabilities cannot make use of a separation into non-interacting toroidal modes.

Collision driven ("neoclassical") transport for weakly collisional plasmas – a field that can be largely treated analytically in tokamaks – depends critically on the collision-free particle orbits, and can easily exceed, in stellarators, the turbulent transport found in tokamaks of comparable size. Its computation is therefore a very demanding discipline, with a large practical impact on experiment design. Codes developed for its analysis followed either a Lagrangian approach to particle motion (Monte-Carlo codes) or an Eulerian description of phase space. From the above it is evident that the design of a stellarator requires a computational effort literally of higher dimension than that of a tokamak.

Figure 2 shows a conceptual picture of the plasma surface of the first stellarator experiment designed, incorporating all the above considerations (W7X) and of the complex shape of the magnetic field coils required to form it. This experiment, presently under construction in Greifswald, Germany, should drastically narrow the performance gap to present-day tokamaks, but is, in particular, also a milestone of computational physics.

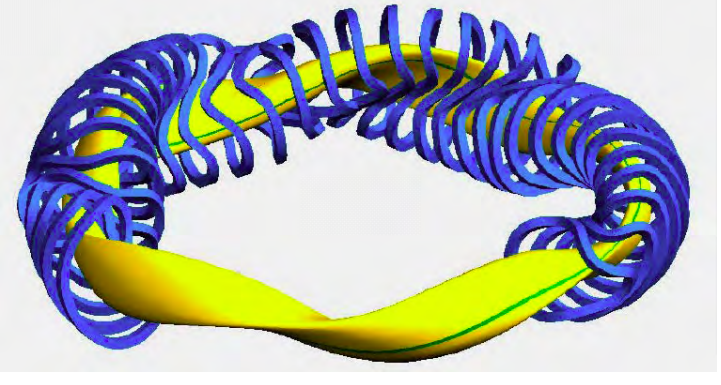

Fig. 2. Plasma surface and coil system of an optimized stellarator (W7X).

2.2 On the Way to a Numerical Tokamak

So far, the performance prediction of magnetic confinement experiments has been nearly exclusively empirically. Even for the W7X stellarator, where numerical calculation played an unprecedented role in the layout, the large computational effort concerned mainly items which in a tokamak are either uncritical, or can be calculated with relatively simple models. This empiricism based approach was adequate, as the performance target of all these devices (including ITER) are still essentially scientific, but becomes progressively more costly and risky with each new and larger generation of experiments.

Since the mid-1990s, however, confidence has been rapidly growing, that ab-initio modelling of tokamak – and, subsequently also stellarator – performance will be able to accurately explain ITER results and to fix the parameters of its successors. Apart from the past and expected future growth of computer power, and the algorithmic improvements of general-purpose routines (e.g. parallel matrix solvers), this is mainly due to the growing conviction that a plasma model has been identified containing all the necessary physics affecting turbulence in fusion devices, and that this plasma model can be implemented with sufficient accuracy on upcoming computers to quantitatively explain the associated energy and particle transport. This high expectance in computational modelling has, moreover, also spread to other areas of fusion physics, so that the vision of a numerical tokamak, consisting of a complete ab-initio model of the plasma core as a design tool for future fusion power plants, is becoming credible.

As reactor relevant plasmas are nearly collision-free and turbulence can also include magnetic fluctuations, the most general model would require a time-dependent description of the distribution function in three geometrical and three velocity space coordinates, plus the full set of Maxwell's equations, simplified only by the neglect of displacement currents. Some, usually well justifiable simplifications render the problem of transport-inducing turbulence, however, more tractable. The most important one is the gyro-kinetic model, which reduces the phase space by averaging over the very fast gyro-motion of particles, while taking properly into account the possible spatial variation of electric and magnetic fields over the spatial scale of the circular gyro-orbit.

The second starts from the observation that the most important effect of magnetic field perturbations concerns the components perpendicular to the equilibrium field, which allows to consider only one component of the vector potential. Furthermore, the extremely strong anisotropy of magnetized plasmas implies a very long scale length for all perturbations along field lines. Using magnetic coordinates with one coordinate line aligned with the magnetic field allows to translate this into a much reduced resolution requirement in one coordinate direction. Finally, fluctuations are usually small compared to the background quantities, suggesting a splitting of the distribution function into a smooth distribution F_o and a perturbation δf, reducing thereby e.g. in particle-in-cell (PIC)-based methods the statistical noise.

Kinetic equations can be treated either in an Eulerian or a Lagrangian framework, while the field equations, coupling the particles require a spatially fixed grid. Nevertheless the complexity of geometry and of particle orbits appeared to favour a particle-following, Lagrangian approach, and the early gyrokinetic turbulence simulations used PIC-Codes. Following the pioneering efforts of Jenko and Dorland [16], Eulerian (also called continuum or Vlasov-) codes, based on a fixed grid in velocity space have established themselves as at least competitive, and at present comparable efforts are invested in the two lines of development. Also a hybrid (semi-Lagrangian) approach has been employed to combine the advantages of a fixed grid in velocity space with the use of particle trajectories as characteristics.

Depending on parameters (ratios of electron to ion temperatures T_e/T_i, gradients of T_e, T_i and of electron density, collisionality, β, ratio of gyro-radius to gradient length, structure of the magnetic field) different instabilities drive the turbulence and necessitate, in particular, different sophistication in the treatment of the electrons. A broad and relevant range of cases is covered by conditions where the smallest perpendicular space scale is of the order of the ion gyro-radius ρ_I whereas the fastest time-scales are set by electron thermal motion or by the (roughly comparable) Alfvén wave propagation along field lines.

Much of the underlying physics can be gathered from calculations covering only the spatial domain of a flux bundle less than 100 ion-gyroradii across in both radial and poloidal directions. In this case artificial (usually periodic) boundary conditions have to be applied to the fluctuating quantities, both within a flux surface, but also at the radial boundaries. The latter assumption is mathematically consistent with a local approximation to the background parameters neglecting their variation across the computational region. Such models cannot give, however, full information about the scaling of turbulent transport with the ratio of a/ρ_i across the regime covering present medium ($a/\rho_i \cong 200$) to large ($a/\rho_i \cong 400$) size devices and onward to ITER ($a/\rho_i \cong 800$) and therefore a move to global simulations is everywhere ongoing.

Typically Lagrangian models can easily work on a global scale, but have more difficulties refining the physics model and controlling statistical noise, whereas Eulerian models are pioneering more complete physics model, but are proceeding more slowly to a global coverage. All gyrokinetic turbulence simulations are computationally extremely demanding undertakings as is manifested, for example by their inclusion into the Grand Challenges of the US Department of Energy initiative on Scientific Discovery Through Advanced Computing (SCIDAC) [17].

Fig. 3 left and right, taken from a local simulation with a Eulerian Code [18], illustrate one of the most important and universal results of gyrokinetic simulations, for a situation dominated by ion temperature gradient (ITG) driven turbulence. The figures show two time-slices referring to the initial development of the instability and a later phase of saturated turbulence. Per-

turbations are always aligned with the screw-shaped magnetic equilibrium field and have a larger amplitude on the outer side of the torus.

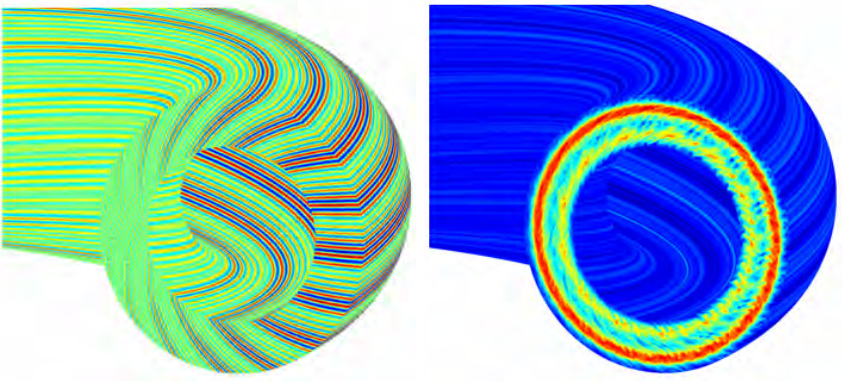

Fig. 3. Nonlinear evolution of an instability driven by the temperature gradient of the ions. Left: linear phase of the mode, right: nonlinear evolution, affected by the formation of poloidal (zonal) flows.

Initially they tend to develop radially elongated streamers, which are very effective in mixing plasma across the magnetic surfaces (left). The emerging turbulence itself, however, drives sheared zonal flows in poloidal direction, which have a shorter radial wavelength, and tear apart these elongated structures. Numerical simulations therefore, after some time (a few hundreds of units of the characteristic time $L_\perp/C_s$, defined by the radial gradient length and the ion sound speed), settle down to a quasi-stationary state (right), with a significantly reduced transport compared to the initial overshoot. Such turbulence simulations have succeeded capturing many features of the experimentally observed energy and particle transport.

The effects of finite extent of the ion-gyro radii can also be captured by a fluid model (called "gyro-fluid") [19, 20], which however, in the weakly collisional case has to resort to ad-hoc assumptions to provide a fluid closure along magnetic field lines. If the latter is properly chosen, a good agreement with the gyrokinetic models can be reached even regarding the core regions of plasmas. In particular, however, gyrofluid codes are the current state of art regarding the simulation of turbulence in the more collisional edge zone of the plasma, where geometry effects and boundary conditions are of dominating importance, and fluctuation amplitudes are comparable to the background values.

At present, more than a dozen codes for the simulation of turbulence in toroidally confined plasma are in continuous development. This multitude of models and algorithms is justified by the ambitiousness of the task – quantitative ab-initio modelling of turbulent transport – and the large savings that will result from a reliable model for the dimensioning of thermonuclear power plants. It is necessary, however, also to establish the credibility of the outcome,

as direct, unambiguous proof of the results by experimental measurements is still limited in extent. Therefore, from the very beginning a significant effort has been placed on the bench-marking of all these codes, starting with the definition of the "Cyclone" test case [21], which has since then been studied with each relevant code. For clearly defined conditions, such tests usually result in a 10% agreement among the participating codes [22] for the predicted turbulent fluxes.

In the modelling of large scale, magnetohydrodynamic instabilities the interest originally was only in their prevention by a careful mapping of the linearly stable plasma conditions. It was subsequently recognized that unstable modes exist, which result only in a cyclic rearrangement of profiles and are compatible with an overall quasi-stationary discharge behavior. They can, however, influence the global energy confinement or the heating efficiency, or can be associated with pulsed heat loads to vessel structures and require therefore a nonlinear model for their full cycle. In some cases it has been demonstrated or is expected that feedback-control can significantly extend the operational range of tokamaks beyond the linearly stable regime. Finally, disruptive instabilities of the plasma current – expected to be rare, but design-base events in a fusion power plant – are potentially associated with large heat loads and electromagnetic forces onto the vessel structures that need reliable extrapolation from present devices.

These necessities and trends have given new impetus to the development of nonlinear, global MHD codes to describe such large scale, large amplitude perturbations. Many aspects are tied to the question of fast reconnection of magnetic field lines, and a strong link exists therefore to the areas of space and astrophysical MHD modelling, including the common use of a test model [23]. Two large, parallel code developments are taking place in the US, both involving several institutes, and both coordinated within a common project [24, 25] and two, less comprehensive models also in the EU [26, 27]. Contrary to turbulence simulations, the emphasis in this case is on significant changes in the magnetic topology, a global treatment of the whole plasma, and the generally longer characteristic time scale of the dynamics. In addition to the severe problem of anisotropy (which is aggravated by the fact that the large topological changes make the use of magnetic coordinates difficult), the large spread of the potential time-scales require the elimination or the implicit treatment of the fastest wave motions. The most common solution to this problem is the addition of a semi-implicit operator to the equation of motion [28, 29].

In some applications – notably the disruptive termination of tokamak discharges – one wants to model quite realistically the contact of the plasma with the 3-d structure of the walls, including the passage of electric currents into them. Other areas require an extension of the usual resistive MHD model by two fluid effects (to treat the smaller scale effects important for reconnection), additional current drive terms arising at low collisionality from the particular nature of particle orbits in toroidal geometry (the so-called "bootstrap" current) and the electromagnetic coupling of the plasma to the suprathermal

particles described below. The two US code developments are therefore true multi-physics efforts, with different terms and packages – depending on the specific application – added to the core of the resistive MHD equations.

Plasma heating often is associated with the presence of fast ions, injected originally as neutrals from the outside, or accelerated by wave resonance processes, or – as final goal – produced by thermonuclear fusion reactions. These fast particles can influence the macroscopic stability of the plasma through both their gradients in geometrical and velocity space. In particular, fusion-α particles have at birth a velocity larger than the Alfvén velocity, and can resonantly interact and destabilize otherwise weakly damped plasma modes through the spatial gradients of their distribution function. Depending on the further nonlinear growth and interaction of these modes, they could lead to a significant loss of fast particles, reducing thereby the efficiency of the thermonuclear plasma heating, and causing localized heat loads on the plasma vessel.

Fast-particle driven modes in different contexts have been studied on existing experiments in some detail, but the combination of isotropy and super-Alfvénic velocity associated with fusion-α particles will be novel on ITER. As their effect will be of critical importance for the self-heating of a fusion reactor they are becoming a new focal point of computational modelling. Already the linear stability analysis, requiring a spatial coverage of the whole plasma and a detailed description of the particle distribution function is a challenging problem, which, in particular due to the resonances in frequency leads to a difficult, non-standard eigenvalue problem. Early codes in fact used a simplified, perturbative approach, in which the eigenfunctions of stable, ideal MHD modes were used to compute only (complex) corrections to the frequency arising from kinetic effects. When the energy content of fast particles becomes a significant fraction of the plasma energy, however, new modes can arise, which have no correspondence in the ideal MHD spectrum, and are hence not captured by this approach. Latest-generation codes therefore treat fast particles and MHD effects on an equal footing, solving the linearized equations either as an eigenvalue or initial value problem, or scanning the response of the system to an external excitation by an antenna with variable frequency [30, 31, 32]. To determine the actual losses associated with these effects requires of course a nonlinear model, including the interaction of different modes, the modifications to the distribution function and ultimately also the nonlinear modifications to the magnetic perturbations. Also this work has started, albeit so far with simplified models [32, 33].

3 Future Trends

The ultimate aim of fusion plasma theory is ambitious: to provide a model for the plasma core of a fusion reactor that can be incorporated into design codes for a power plant. This comprehensive model – sometimes termed "numerical

tokamak" (or stellarator, respectively) – has to include modules covering all the above areas in an integrated form taking into account their mutual interaction. The confidence is quite high that in most of these areas we have adequate physics models at hand, and know – in principle – how to include them into the codes. We still have to drop, however, some simplifying assumptions in their implementation, include more realistic geometries and extend the region in space and time covered by the simulations. Fortunately in most areas, the computational effort required scales strongly with size, so that models developed and tested for present-day experimental devices during the next ten years will find the computer power ready to run with ITER parameters once the latter starts operating.

Prior to their combination in integrated models, we expect from the improved and extended codes the solution of a number of well-defined enigmas. The most important one regards the sudden improvement in energy confinement observed at high enough heating powers in divertor tokamaks [7], evidently associated with the suppression of turbulence in a narrow layer close to the plasma boundary. This transition from L (low) to this H (high) confinement regime is a highly reproducible bifurcation phenomenon, with dramatic consequences: it gives rise to a doubling of the plasma energy content, which in a deuterium-tritium plasma would be associated with a 4-fold increase in fusion power. It is expected that this phenomenon will spontaneously show up also in turbulence simulations with a sufficiently realistic model, and achievement of this would be viewed as the Holy Grail of fusion plasma theory. A second, similarly universal, and equally unexplained phenomenon is the appearance of a density limit in tokamaks [34], which is not observed in an analogous form in stellarators [35].

The integration of codes dealing with different aspects of tokamak operation is a growing necessity and task forces have been created explicitly for this task. A unification in efforts will, however, also arise form the fact that increasing computing power allows codes created for one purpose to extend their applicability to other areas. Simulations with codes originally developed for "micro"-turbulence cover increasingly larger regions of the total plasma, whereas nonlinear codes for macroscopic MHD instabilities improve the physics models and the spatial resolution. A case in point for this kind of convergence are studies of edge-localized magnetic perturbations ("ELMs"). They share some characteristics with global MHD instabilities, but are restricted to a small fraction of the plasma close to the boundary, and are presently treated, in parallel efforts by both turbulence [20, 36] and macroscopic MHD codes [25, 27].

The most significant trend in magnetic fusion research is, however, the general acceptance that first-principle based modelling will substitute the empirical and semi-empirical approaches used in the past [6] for the performance extrapolation to next-generation devices. This is documented by the consideration of fusion related model developments as one of the grand challenges of computational physics, but, for example also by the decision of the EU and Japan to include a dedicated high performance computing centre into their

joint "Broader Approach" effort towards fusion energy production, accompanying the construction of ITER.

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Frontiers in Computational Geophysics: Simulations of Mantle Circulation, Plate Tectonics and Seismic Wave Propagation

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Summary Recent progress in geophysical modelling of global plate tectonic, mantle convection and seismic wave propagation problems is reviewed, while paying particular attention to novel adjoint methods for the efficient inversion of seismic and tectonic data. Observed is that the continuing growth in high performance and cluster computing promises the crossing of long standing barriers in the simulation of first-order geophysical phenomena.

1 Introduction

Geophysics differs from other scientific disciplines in its focus on processes one can neither repeat nor control. Examples include the nucleation of an earthquake as brittle failure along faults, or the dynamic processes of ductile (creeping) flow in the earth's interior which give rise to plate tectonics and the endogenic (internally driven) geologic activity of our planet. The inherent experimental limitations and the indirect nature of our observations explain in part why there is such a remarkable impact and success of high-performance computing (HPC) in this field. And indeed many a geophysical observable are only interpretable through the use of sophisticated modelling tools.

Another reason for the prominence of HPC lies in the recent crossing of long standing thresholds in capacity and capability computing. This allows us today to implement models having in excess of 1 billion grid points. The development makes it feasible for the first time to overcome in three dimensional (3D) models the great disparity of length scales which characterizes important geophysical phenomena: an earthquake rupturing a fault segment over a distance of some 100 km while emanating seismic energy throughout the planet (10,000 km), or the peculiar nature of plate tectonics with deformation

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concentrated along plate boundaries of 10-100 km width separated by plates of dimension 1,000-10,000 km serve as example. Before we address challenges and recent successes in global geophysical modelling, let us take a brief look at the gross structure and inherent dynamic time scales of our planet.

The earth's interior is complex, consisting of three distinct regions. Starting from the outside there is first the cold lithosphere, which is dominated by brittle behaviour. It then follows the solid mantle, which deforms slowly over geologic time by a mechanism known as ductile creep. Finally near the earth's centre there is the (mostly) liquid core. As a result of convective and other forcings, all three regions are in motion, albeit on different time scales. On the longest time scale solid state convection (creep) overturns the mantle once in about every 100-200 million years [8]. This overturn is the primary means by which our planet rids itself of primordial and radioactive heat.

Tectonic processes operate on shorter time scales, up to a few million years or so. They include rapid variations in plate motions, which are revealed by the recent arrival in the earth sciences of highly accurate space geodesy techniques, such as the global positioning system GPS [11].

On still shorter time scales of perhaps 1-1000 years convection of the liquid iron core generates the earth's magnetic field through a complicated dynamo process that probably operated throughout much of earth's history [18]. Only recently have geophysicists been able to study dynamo action in sophisticated magneto-hydrodynamic models of the core. We will not concern ourselves with these models and refer to the recent review by [15]. On a time scale of hours to seconds both the core and the mantle are traversed by seismic sound waves, and seismologists are now turning to computer models to study seismic wave propagation through our planet [21].

2 Mantle Flow and Circulation Modelling

The mantle comprises approximately 70 % of the earth's volume and convects with surprising vigour. Its thermal Rayleigh number, estimated at 10^6 to 10^8 [10] exceeds the critical value at which convection begins by a factor of 10^3 to 10^5, yielding flow velocities of 1-10 cm/year and an upper thermal boundary layer (known as plates) of thickness of 50-100 km depth. The advent of powerful computers allows us to resolve the flow in realistic 3D spherical geometry, and a number of high-resolution, parallelised mantle convection models are now available. The models have provided crucial insight into key parameters governing the behaviour of global mantle flow, such as the effects of mantle phase transitions, a depth-wise increase in viscosity and the partitioning of internal (radioactive) and external (core derived) heating, [37, 6, 41, 35].

Mantle convection can mathematically be modelled by a coupled system of three equations, see e.g. [29, 35], describing the conservation of mass, momentum and energy. These differ from the standard Navier-Stokes system of convection driven fluid dynamics in that respect that due to the high Prandtl

number (on the order of 10^{24}) inertial terms in the momentum equations can be dropped. This reflects the creeping nature of the flow. Note also that for similar reasons Coriolis and centrifugal forces may safely be neglected.

Mass conservation is a constraint on the velocity field of the Stokes problem, and the coupled system of mass and momentum conservation, after discretization by standard techniques like finite-element and finite-volume approaches, gives rise to a saddle-point problem, which one solves for a velocity field satisfying the divergence-free condition. Most mantle convection codes adopt Uzawa-type algorithms for this purpose, see e.g. [1], often employing conjugate gradients for the outer and multigrid for the inner iteration. Multigrid employs a hierarchy of nested computational grids, so that near-and far-field components of the momentum balance are effectively solved at once. We show the nested structure of the icosahedral grid adopted in the Terra code [7] as an example in Fig. 1.

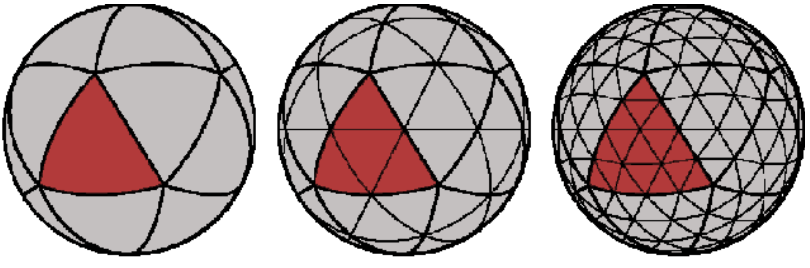


Fig. 1. Three successive mesh-refinements of the icosahedral grid.

Similarly one often treats the energy equation through mixed finite volume, finite difference methods for the advected and conducted heat flux. The Péclet number of the mantle is large (in the range of 10-100), that is heat transport in the mantle is controlled primarily by advection outside of thermal boundary layers. This makes finite volume methods, which are conservative and easily adapted to unstructured meshes, an effective solution approach.

It is common to use the term *circulation* to describe the motion of the mantle, in analogy to the general circulation of the oceans and atmosphere. A number of mantle circulation models (MCMs) have been constructed recently, [8, 4, 27], and a representative MCM at high numerical resolution (about 100 million grid points) is shown in Fig. 2. MCMs differ from traditional convection models in that they include geologic information on the history of subduction [8]. This allows them to make explicit predictions on the large-scale thermal structure of the mantle, which is an essential component if one wants to assess the force balance of plate motion.

In general MCMs compare well with tomographic mantle models, [33], which constrain earth structure from independent seismic observations. MCMs suffer, however, in a fundamental way from lack of initial condition informa-

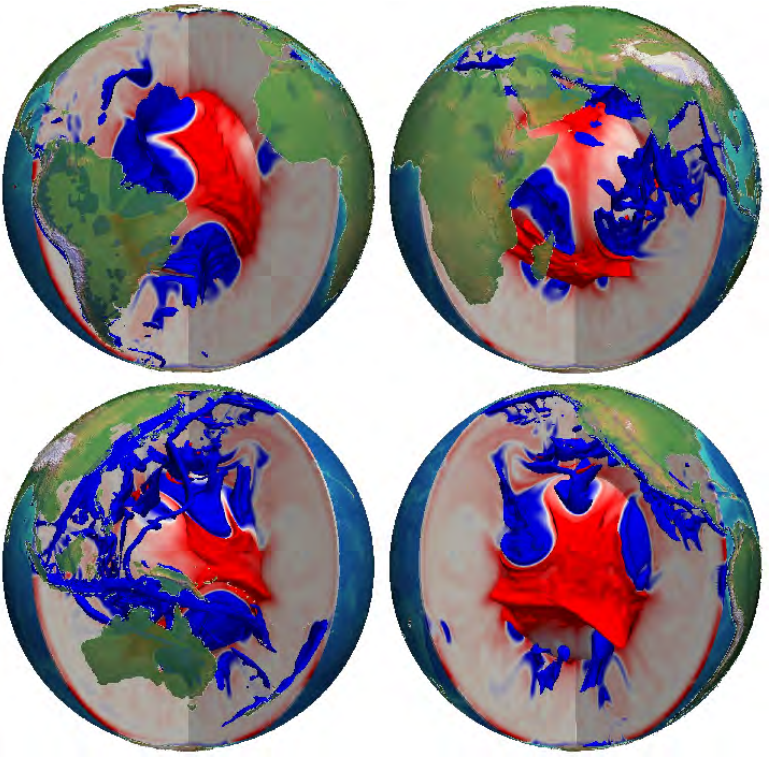


Fig. 2. 3D representation of temperature variations in a high resolution Mantle Circulation Model (MCM), see text. Shown are four cross sectional views from 35 (upper left), 125 (lower right), 215 (lower left) and 305 (upper right) degrees longitude. Continents with colour-coded topography and plate boundaries (cyan lines) are overlain for geographic reference. Iso-surfaces of temperature are taken to be at -600 and +400 Kelvin. The +400 iso-surface was clipped in the uppermost 500 kilometers in order to allow views into the mantle underneath the mid-ocean-ridge systems which span large parts of the oceanic upper mantle. The colour-scale is saturated at -400 and 400 Kelvin. About 100 million numerical grid points are used, providing a grid point spacing of at most 20 km throughout the mantle, sufficient to resolve the convective vigor of global mantle flow.

tion. The difficulty becomes more challenging the further back in time one wants to model the evolution of mantle buoyancy forces, say over the past 10-100 million years. Lack of initial condition information is a problem shared with circulation models of the ocean and the atmosphere.

To overcome the initial condition problem one must formulate a large scale fluid dynamic inverse problem. Essentially one seeks optimal initial conditions that minimise, in a weighted least squares sense, the difference between what a mantle convection model predicts as mantle heterogeneity structure and the heterogeneity one actually infers from, say tomography. This class

of problems is known in different contexts as e.g. *history matching* or *variational data-assimilation*, meaning that model parameters are inferred from a variational principle through the minimisation of a cost function F. The necessary condition for a minimum of F, that the variation $\nabla F = 0$, leads to the usual mantle convection equations coupled to a corresponding set of so-called *adjoint equations*.

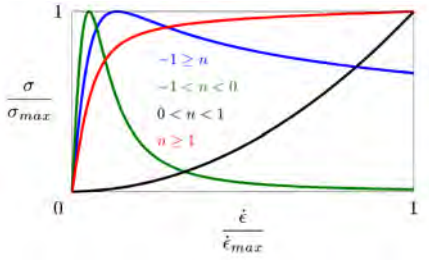
The adjoint equations, which have been derived recently, [5, 23], together with large-scale simulations showing that flow can be inferred back in time for at least 100 million years, are nearly identical to the forward model except for forcing terms. Unfortunately adjoint modelling of global mantle flow at realistic convective vigour comes at a heavy computational price. Weeks to months of dedicated integration time are needed to solve this class of problems even on some of the most powerful parallel machines currently in use. Such resources, however, are coming within reach of topical PC-clusters dedicated to capacity computing [29].

3 Plate Tectonics and Boundary Forces

A long persistent challenge in geophysics is the computational treatment of plate tectonics, because it is difficult to simulate shear failure along plate boundaries. One strategy, developed more than 30 years ago, models known plate structures and their influence on mantle flow by specifying regions that move in a plate-like manner, [9, 30, 14]. An alternative approach adopts highly non-linear (non-Newtonian) viscous creep, strain-rate weakening rheologies, and viscoplastic yielding, [43, 36, 31].

In [28] Moresi and Solomatov explored the effects of strongly temperature-dependent viscosity combined with a plastic yield stress: the former causes the cold upper boundary layer (lithosphere) to be strong, while the latter allows the boundary layer to fail locally in regions of high stress. The success of this *ductile* approach to plate tectonics, measured through a so-called *plateness*, is evident when one applies exotic rheologies with an extreme form of strain softening. One such rheology, where both viscosity and stress decrease with increased strain rate, is known as *self-lubrication*, see [2]. We summarise its essence in Fig. 3. Unfortunately, self-lubrication requires the use of power-law exponents ranging between -1 and 0 (see Fig. 3). These values do not agree with laboratory experiments of ductile deformation performed on olivine, which find n in the range 2 to 5, see e.g. [24].

The challenge to develop plate-like behaviour in convection models reflects the difficulty to account for brittle failure and reactivation of pre-existing faults in the uppermost cold region of the lithosphere. The high strength in the upper part of the lithosphere expresses the resistance of rocks at low temperature to break, or slide past each other when already faulted. Experimental results indicate a simple linear relationship to parameterise this behaviour, where shear stress is proportional to the effective normal pressure through a



$$\sigma(\dot{\epsilon}) = \nu(\dot{\epsilon}, T, z) \cdot \dot{\epsilon}$$
$$= A \cdot (\gamma + \dot{\epsilon}^2)^{\frac{1-n}{2n}} \dot{\epsilon} e^{\frac{B+Cz}{T}} \cdot \dot{\epsilon}$$

$$\sigma(\dot{\epsilon}) \propto \dot{\epsilon}^{\frac{1}{n}} \quad \text{for} \quad \dot{\epsilon} \to \infty$$
$$\sigma(\dot{\epsilon}) \propto \dot{\epsilon} \quad \text{for} \quad \dot{\epsilon} \to 0$$

Fig. 3. Generalised power law rheology, where the stress σ is proportional to the strain rate ϵ through a viscosity ν that depends on temperature T, strain rate and depth, where A, B, C, γ and n parameterise the dependence. Note that so-called *self-lubrication* rheology arises only for a narrow and unphysical band of power law exponents ranging from -1 to 0, which is not observed for geologic materials.

friction coefficient. Geodynamicists have introduced weak zones at the surface of mantle convection models in an attempt to account for brittle failure in the lithosphere [9]. The logical development of this approach is the inclusion of discontinuities directly into the computational grid and the representation of faults through contact-element interfaces. This has been done, for example, in the modelling work of Zhong and Gurnis [42] and the global neo-tectonic model of Kong and Bird [26].

Today the neo-tectonic models have reached a high level of maturity allowing them to account for surface topography, regional variations of lithosphere density and thickness according to either Pratt or Airy isostatic compensation, the thermal regime of the lithosphere – based on heat flow measurements and crustal radioactive decay – and for realistic plate configurations [32, 3]. The models typically use finite-element formulations to solve the equations of mass and momentum conservation in the Stokes limit that we have seen before, and compute the instantaneous force balance and associated plate velocities. The use of finite elements makes it feasible to implement empirical, depth-dependent rheologies of the lithosphere to account for ductile as well as brittle deformation. We show the computational grid from the global lithosphere model of Kong and Bird [26] in Fig. 4.

A first-order result in plate tectonic modelling is the recent explanation of the plate motion change off-shore of South America (see Fig. 5). For the Nazca/South America plate margin a variety of data indicate a significant decline (by some 30%) in convergence velocity over the past 10 million years. The ability to consider past as well as present plate motions provides important constraints for our understanding of the plate tectonic force balance, because changes in plate motion are necessarily driven by changes in one or more driving or resisting forces. By explicitly coupling MCMs, which provide estimates on the mantle buoyancy field, to neo-tectonic models Iaffaldano, [20, 19], shows that the recent topographic growth of the Andes is a key factor controlling the long-term evolution of plate motion in this region.

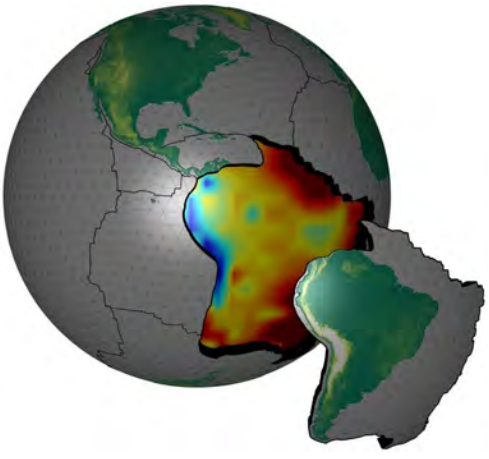


Fig. 4. Grid of a global neo-tectonic SHELLS model coupled to a global mantle circulation model (see text); colours represent temperatures (red=hot, blue=cold) at a depth of 200 km below the surface.

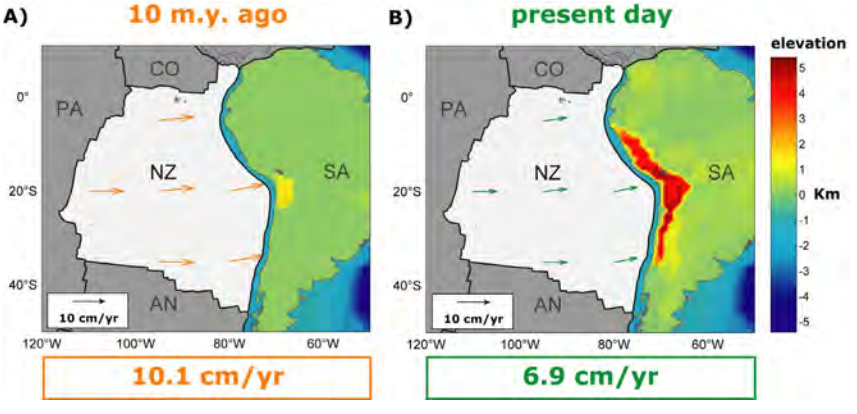


Fig. 5. Computed velocity for the Nazca plate (NZ) relative to the South America plate (SA) from global plate motion simulations. The topography of the South America plate from numerical simulations is shown together with a color bar. Plate boundaries are in black, coastlines in gray: A) for 10 million years ago we compute a convergence rate of 10.1 cm/yr with the topography of the South America plate inferred from geological indicators, B) for present day we compute a convergence rate of 6.9 cm/yr with the topography of the South America plate from the ETOPO5 database. 4 km of topography lifted up over the last 10 million years can account for the slow down of the Nazca plate.

Further supporting evidence for the dominant effect of Andean topography on plate boundary forcing along the Nazca/South America margin comes from gravity and stress field measurements, [34, 17, 44]. Heidbach, Iaffaldano, and Bunge [16] show that these independent observables can also be reproduced with the coupled models.

4 Seismic Wave Propagation

In seismology there has been a gap between observations and theory for several decades in that the quality and quantity of observations far exceed the traditional methods of seismic modelling. Although the existing tomographic images of the mantle have greatly contributed to our understanding of the planet's dynamics, the inversions of seismic observables usually involve substantially simplified forward models, namely ray theory and finite normal mode summations. Ray theory is only applicable to the arrival times of high frequency waves, therefore significantly reducing the amount of exploitable information. Conversely normal mode approximations rely on smoothly varying structures and long period waveforms, resulting in a limitation of resolution.

The fact that today's computational power is sufficient to accurately solve the wave equation in realistic earth models [22, 25] is prompting new efforts to replace the approximate ray-theory and normal mode forward models by the exact forward model of full seismic wave propagation, and to invert for seismic waveforms with shorter periods. The expectation is that the resulting increase of exploitable information will translate into an increase of resolution especially in regions poorly sampled by seismic rays.

In analogy to the efforts of using adjoint theory in geodynamics, adjoint methods are explored in seismology. The approach allows us to compute the derivative with respect to the parameters by combining the synthetic forward wavefield and an adjoint wavefield governed by a set of adjoint equations and adjoint subsidiary conditions. This concept was introduced by Tarantola [38, 39] into the field of seismology. Recently, the adjoint method was used in the context of finite-frequency traveltime kernels [40] and regional seismic models [12, 13]. It is expected that these models will yield great improvements in the imaging of earth structures.

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Solar System Plasmadynamics and Space Weather

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Summary This paper describes progress in computational plasmadynamics applied to the prediction of "space weather" – the study of how conditions on the sun lead to transients in the solar wind, which in turn affect Earth's magnetosphere, ionosphere and thermosphere. The progress is based on advances in algorithms, parallel computing, and a software framework that couples the multi-physics and multi-scale modules necessary to model this challenging and important problem.

1 Introduction

The solar corona is so hot, at more than one million K, that in regions of open magnetic field it undergoes a transonic expansion, filling all of interplanetary space with a supersonic magnetized plasma flowing radially outward from the Sun. This flowing plasma is called the solar wind. As it passes Earth, it interacts strongly with Earth's magnetic field, severely compressing the field on the dayside of the Earth, and drawing it out into a long, comet-like tail on the nightside. The confined region of Earth's magnetic field is called the Earth's magnetosphere. "Space weather" is the study of the conditions on the Sun and how they affect the solar wind, which in turn affects Earth's magnetosphere, ionosphere, and thermosphere. Space weather can influence the performance and reliability of space-borne and ground-based technological systems, and can endanger human life or health.

Significant temporal variations of solar wind speed at the orbit of Earth occur due to the rotation of solar wind structures. Such variations can also be produced by the transient ejection of mass and magnetic field from the solar corona: coronal mass ejections, or CMEs. Indeed, the most severe storms experienced in the Earth's space environment are driven by exceptionally fast CMEs that exhibit a strong southward magnetic field component through-

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out a significant fraction of their volume. These very fast CMEs, which are ejected from the corona at speeds of more than 1000 km/s, also drive strong magnetohydrodynamic shocks. These shocks are efficient producers of energetic particles. Of course, a very fast CME is only effective in producing a severe geomagnetic storm when it is directed towards the Earth, and this fact presents a problem for those attempting to predict space weather.

The solar wind not only confines the terrestrial magnetic field within the magnetospheric cavity, but it also transfers significant mass, momentum, and energy to the magnetosphere, as well as to Earth's ionosphere and upper atmosphere. One dramatic consequence of this interaction between the solar wind and the magnetosphere is the production of a variety of complex electric current systems. These range from a sheet of current flowing on the boundary between the solar wind and magnetosphere, to an enormous ring of current flowing around the Earth in the inner magnetosphere, to currents flowing throughout the ionosphere and connecting along magnetic field lines to magnetospheric currents systems.

Another result of the solar-wind/magnetosphere interaction is the production of highly energetic particles that are stored in the magnetosphere and precipitated into the upper atmosphere. Both the electric currents and the energetic particles can have severe consequences for a number of human activities, all the way from the ground to space. It is the variation over time of these electric current systems and energetic particle populations in the geospace environment that modulates the consequences for human activities, and that is consequently the source of what is referred to as space weather.

A CME and its interaction with the magnetosphere is illustrated in Figure 1. The magnetic cloud generated by the CME approaches the magnetosphere in the top frame. In the bottom frame the cloud interacts with the magnetosphere and generates stronger magnetospheric current systems and larger, more energetic magnetospheric particle populations, a phenomenon which is called a geomagnetic storm. During magnetic storms the magnetospheric topology is significantly modified and large transients are generated. As solar activity increases, the frequency of CMEs is substantially increased, and the severity of space weather is concomitantly increased.

2 Modelling the Solar Wind

2.1 The Governing Equations

The solar wind can, in much of the region between Earth and the Sun, be modelled as an ideal, non-relativistic, compressible plasma. The governing equations in this region are the ideal magnetohydrodynamic (MHD) equations, which consist of conservation of mass, momentum and total energy, combined with an evolution equation for the magnetic field. In MHD, the total energy includes kinetic, internal and magnetic energy, the momentum equation includes the Lorentz force in addition to the pressure gradient, and the energy

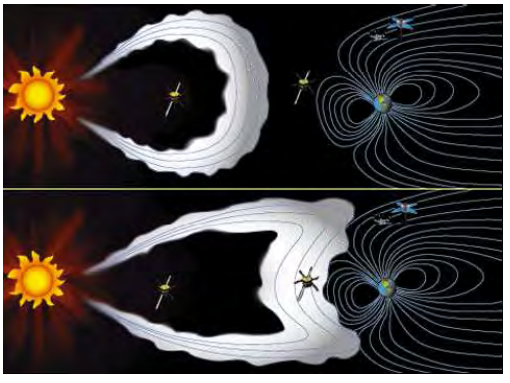

Fig. 1. Schematic representation of the interaction of the magnetosphere with an expanding magnetic cloud.

equation includes Joule heating. This system of conservation laws is of a form that Godunov denoted as "partially symmetrizable" [Godunov(1972)]. This partial symmetrizability arises from the constraint that the divergence of the magnetic field starts and remains zero.

The partially symmetrizable formulation of the ideal MHD equations is formally not fully conservative. Terms proportional to $\nabla \cdot \mathbf{B}$ appear in what would otherwise be a fully symmetrizable divergence form of a system of conservation laws [Harten (1983)]. It is therefore important that $\nabla \cdot \mathbf{B}$ be as close to zero as possible. Enforcing this constraint numerically, particularly in shock-capturing codes, can be done in a number of ways, but each way has its particular strengths and weaknesses. Tóth has published a numerical comparison of many of the approaches for a suite of test cases [Tóth (2000)].

The MHD eigensystem arising from the ideal MHD equations leads to eight eigenvalue/eigenvector pairs. The eigenvalues and associated eigenvectors correspond to an entropy wave, two Alfvén waves, two fast magnetoacoustic waves, two slow magnetoacoustic waves, and an eighth eigenvalue/eigenvector pair that depends on the specific form of the ideal MHD equations being solved. This last wave (which describes the jump in the normal component of the magnetic field at discontinuities) has a zero eigenvalue when the equations are written in divergence form, and an eigenvalue equal to the normal component of the velocity, u_n, in the partially symmetrizable form [Powell (1994)]. The expressions for the eigenvectors, and the scaling of the eigenvectors, are more intricate than in gasdynamics [Roe and Balsara (1996)]. However, once the more intricate eigensystem and the need to control $\nabla \cdot \mathbf{B}$ have been accounted for, modern high-resolution schemes used in gasdynamics can be modified to be applied to ideal MHD.

2.2 Resolving Disparate Scales

For typical solar-wind flows, length scales can range from tens of kilometers in the near-Earth region to the Earth-Sun distance (1.5×10^8 km), and timescales can range from a few seconds near the Sun to the expansion time of the solar wind from the Sun to the Earth ($\sim 10^5$ s). The use of adaptive mesh refinement (AMR) is not only extremely beneficial, but a virtual necessity for solving problems with such disparate spatial and temporal scales. AMR schemes such as those developed by Berger [Berger and Saltzman (1994)] and Quirk [Quirk and Hanebutte (1993)], can be applied to the solar wind problem. A self-similar data structure, shown in Figure 2, can help ensure good scalability on parallel machines.

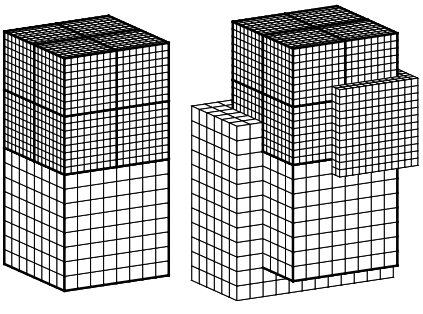

Fig. 2. Left: self-similar blocks used in parallel block-based AMR schemes. Right: self-similar blocks illustrating the double layer of ghost cells for both coarse and fine blocks.

The computational cells are embedded in regular structured blocks of equal sized cells. The blocks are geometrically self-similar and consist of $N_x \times N_y \times N_z$ cells, where N_x, N_y, and N_z are even, but not necessarily all equal, integers. Typically, blocks consisting of anywhere between $4 \times 4 \times 4 = 64$ and $12 \times 12 \times 12 = 1728$ cells are used (see Figure 2). Solution data associated with each block are stored in standard indexed array data structures. It is therefore straightforward to obtain solution information from neighboring cells within a block.

2.3 Parallel Performance

This parallel block-based AMR scheme achieves very high performance on massively parallel architectures. The underlying upwind finite-volume solution algorithm, with explicit time stepping, has a very compact stencil and is therefore highly local in nature. The hierarchical data structure and self-similar blocks make domain decomposition of the problem almost trivial and readily enable good load-balancing, a crucial element for truly scalable computing. A natural load balancing is accomplished by simply distributing the blocks equally among the processors. Additional optimization is achieved by

ordering the blocks using the Peano-Hilbert space filling curve to minimize inter-processor communication. The self-similar nature of the solution blocks also means that serial performance enhancements apply to all blocks and that fine-grain parallelization of the algorithm is possible. The parallel implementation of the algorithm has been carried out to such an extent that even the grid adaptation is performed in parallel. The scaling on various architectures is shown in Figure 3.

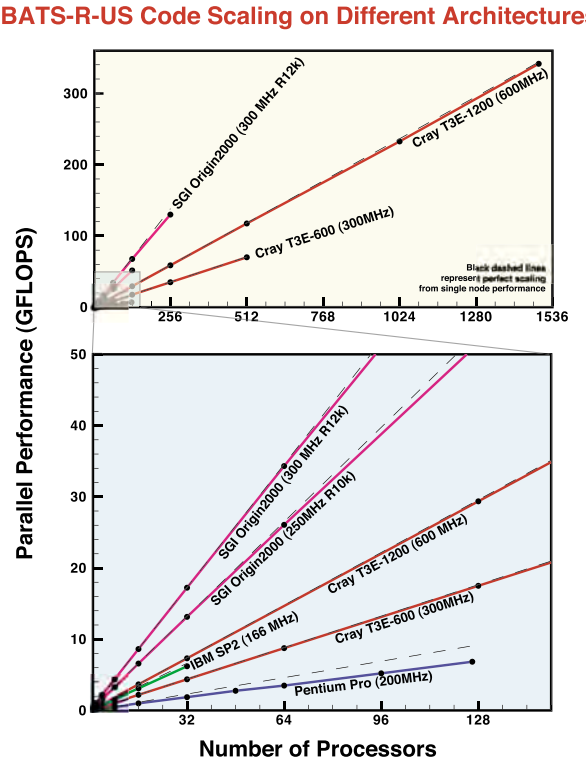

Fig. 3. Parallel speedup of MHD code on various architectures. Black dashed lines represent perfect scaling from single node performance.

A number of time-stepping algorithms have been implemented in the AMR MHD solver. The simplest and least expensive scheme is a multistage explicit time stepping, for which the time step is limited by the CFL stability condition. An unconditionally stable fully implicit time stepping scheme [Tóth et al. (1998)] has also been implemented. The second-order implicit time discretization (BDF2) [Bank (1985)] requires the solution of a non-linear system of equations for all the flow variables. This can be achieved by the Newton-Krylov-Schwarz approach: a Newton iteration is applied to the non-

linear equations; a parallel Krylov type iterative scheme is used to solve the linear systems; the convergence of the Krylov solver is accelerated with a Schwarz type preconditioning. The resulting implicit scheme requires about 20-30 times more CPU time per time step than the explicit method, but the physical time step can be 1,000 to 10,000 times larger. This implicit algorithm has a very good parallel scaling due to the Krylov scheme and the block by block application of the preconditioner.

3 A Space-Weather Modeling Framework

The parallel, adaptive ideal MHD solver described above is an important piece of a space-weather model. However, ideal MHD is not the appropriate model in the near-Earth and near-Sun regions. Separate models for specific regions of the Sun-Earth environment are necessary, and they must be coupled to the ideal MHD solver in order to model space weather.

The Space-Weather Modeling Framework (SWMF) aims at providing a flexible and extensible software architecture for multi-component physics-based space weather simulations, from the low solar corona to the upper atmosphere of the Earth. The SWMF is described more fully in several articles [Tóth et al.(2005)] and the SWMF web site (http://csem.engin.umich.edu/SWMF).

The modules that currently comprise SWMF are:

- Solar Corona (SC),
- Eruptive Event Generator (EE),
- Inner Heliosphere (IH),
- Solar Energetic Particles (SP),
- Global Magnetosphere (GM),
- Inner Magnetosphere (IM),
- Radiation Belt (RB),
- Ionosphere Electrodynamics (IE),
- Upper Atmosphere (UA).

The modules are coupled together by the framework, through a control module. The control module determines the overall time-stepping of the code, the parallel decomposition of the models, the initiation and termination of the model runs, and the saving of restart files of the models. This involves code that determines when the coupling should occur, how it happens, grid interpolation, message passing between different components, and synchronization of the model runs to allow for a physically meaningful coupling. The SWMF uses a component architecture (Figure 4), with each component created from a physics module by making some minimal changes and by adding two relatively small units of code: a wrapper, which provides the standard interface to control the physics module; and a coupling interface, to perform the data exchange with other components. Both the wrapper and the coupling interface are constructed from building blocks provided by the framework.

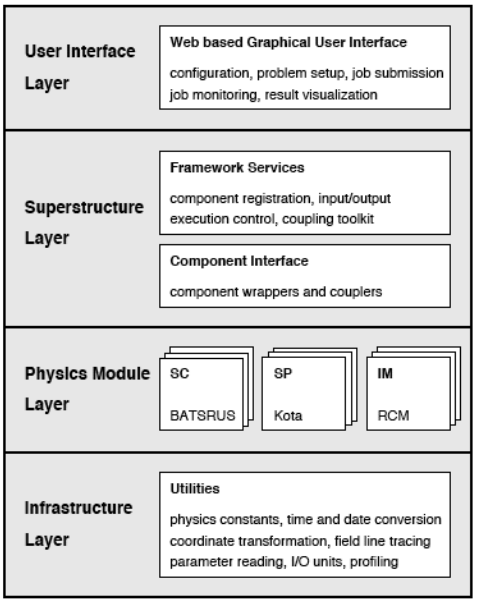

Fig. 4. The Architecture of the Space-Weather Modeling Framework (SWMF).

4 Representative Results of the Coupled Model

A real test of the SWMF is the calculation of an energetic CME, its propagation, and its interaction with the Earth's magnetosphere. One of the most energetic CMEs observed was the October 28, 2003 event, commonly referred to as the Halloween storm. The Solar Corona and Inner Heliosphere modules provided an initial, rotating solution consistent with solar-surface observations from that time. These modules, based on the parallel adaptive MHD solver described above, were run with 2.5 million cells, as small as $3 \times 10 - 3R_{\odot}$, in the Solar Corona, and more than 16 million cells, ranging from $0.25R_{\odot}$ to 4 $R_{\odot}$, in the Inner Heliosphere region (where $R_{\odot}$ is the solar radius). The Eruptive Event Generator was used to initiate a CME, with the location, orientation and strength set to match observations. As the solution was advanced in time, the CME grew and propagated towards Earth.

The interaction of the CME with Earth's magnetosphere and upper atmosphere were calculated by the Global Magnetosphere, Inner Magnetosphere, Ionosphere Electrodynamics and Upper Atmosphere models. Figure 5 shows a representation of the magnetosphere at 08 UT on October 29, 2003, as computed by SWMF. The simulation captured the large ring current and the high pressure associated with it, thanks to the drift physics model in the Inner Magnetosphere module.

Comparisons between simulation results and satellite observations are shown in Figure 6. The three satellites are: Cluster, which was in the day-

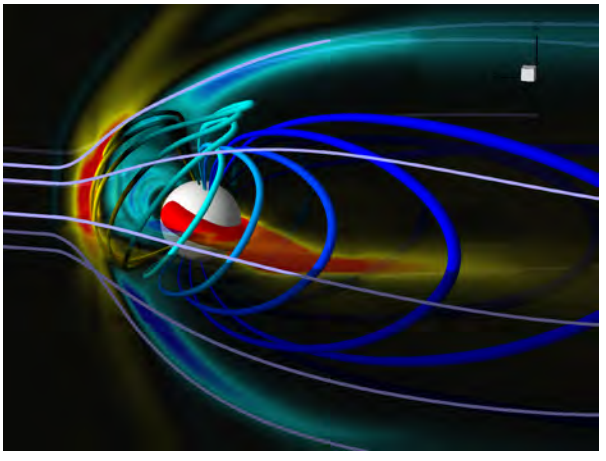

Fig. 5. 3D structure of the magnetosphere during the main-phase of the October 29-30, 2003 storm. The colored cylinders show the last closed magnetic field lines, while the black cylinders indicate solar-wind stream-tubes around the magnetosphere. The color contours on the planes are electric current density. The 100 nPa pressure iso-surface that intersects this boundary is also shown.

side magnetosphere; Polar, which was near the northern cusp; and GOES-10, which was behind the Earth at geosynchronous orbit. The results show that the simulation reproduces the observations in the dayside magnetosphere and in the cusp region extremely well. The agreement with Cluster and Polar is very good. In the closed field line region behind Earth the agreement is reasonable but there are several important features that are missed by the simulation. On the positive side, the simulation reproduces the Bz component, and thus captures the motion of the magnetopause. However, the transient feature around 2300 UT is missed by the simulation.

5 Concluding Remarks

The ability to model and predict space weather is extremely important in protecting satellites, astronauts, and even ground-based systems that are affected by upper atmosphere disturbances. The complex multiscale, multiphysics nature of the problem makes development of a software framework for these simulations a multi-person, multi-year effort. Early results from these models represent a good start towards the overarching goal of first-principles-based modelling of space weather.

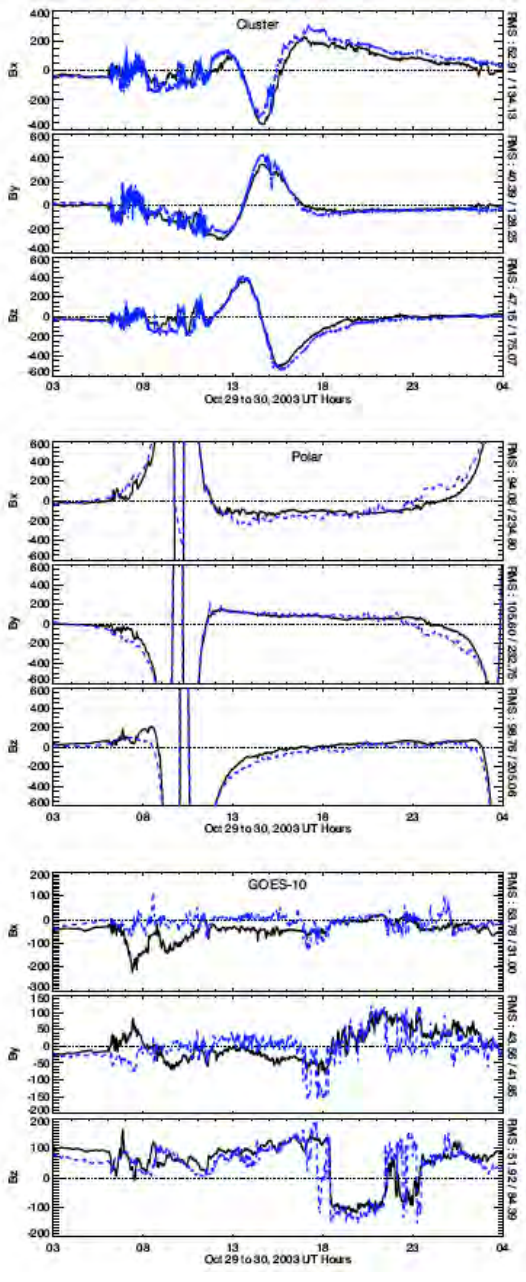

Fig. 6. Comparison of the magnetic field measured by the Cluster, Polar and GOES-10 satellites (blue) with simulation results (black) for the October 29-30, 2003 storm.

Acknowledgments

Many people were involved in the development and application of the space-weather modeling framework detailed here. Some of the key players are: Darren De Zeeuw, Tamas Gombosi, Kenneth Hansen, Ward Manchester, Aaron Ridley, Ilia Roussev, Igor Sokolov, Quentin Stout, Gabor Tóth.

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Numerical Fluid Dynamics in Astrophysics

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Summary The matter of astrophysical objects (*e. g.,* a star or a galaxy) can often be approximated as a gas or fluid, *i. e.,* the equations of fluid dynamics are adequate to describe the astrophysical phenomena. Hereafter, for simplification, the word fluid will be used as a synonym for both fluid and gas. Because most astrophysical conditions are inaccessible in the laboratory, and as astrophysical fluid motion may occur on time scales long compared to the life span of humans or deep inside astrophysical objects, numerical simulation is the only means to study such fluid motion. In this respect numerical simulations play a more important role in astrophysics then in most other branches of physics: astronomers are passive 'observers' of what Nature decides to show them. The study of astrophysical fluid flows is further complicated by the effects of self-gravity, which must be considered in many astrophysical flow problems, by the enormous range of length scales and time scales to be covered in the simulations, and by a variety of other physical effects which must be taken into account frequently. The latter include radiation transport (of photons or neutrinos), heat conduction, radiative cooling, ionization and recombination of atoms, magnetic fields, energy generation by thermonuclear reactions, flow velocities near the speed of light, and strong gravitational fields.

1 Newtonian Flows

In most astrophysical applications both, Newtonian hydrodynamics and Newtonian gravity are excellent approximations because the characteristic velocities are far below the velocity of light c and the gravitational potential is much less than c^2. This includes the dynamics of planets and of most stars (excluding neutron stars and black holes), the flows observed in the interstellar and intergalactic gas (excluding relativistic jets), and even the formation of structures in the Universe on large scales where the flow of matter is well described by Newtonian physics in a co-moving system of coordinates, and

E.H. Hirschel et al. (Eds.): 100 Vol. of 'Notes on Num. Fluid Mech.', NNFM 100, pp. 409–420.
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General Relativity only enters through a homogeneous and isotropically expanding background.

In astrophysics usually the geometry of the boundaries of the fluid flows is not an issue because we deal with either open boundaries or with periodic boundaries if certain sub-volumes of large systems are under consideration. Therefore either finite-volume schemes on structured static or adaptive grids or smoothed-particle hydrodynamics (SPH) are the methods of choice for numerical simulations.

In the past years SPH has become very popular for cosmological simulations for several reasons. As we know from astronomical observations the Universe today is dominated by 'Dark Energy', a smoothly distributed form of energy with negative pressure, possibly the energy of a quantum vacuum, and by 'Dark Matter', some form of weakly interacting particles that behave like a collision-less gas or dust. Both components account for 96% of the energy density of the Universe today, and to find out their very nature is subject of intensive research. Because the dark components of the Universe are best simulated by an ensemble of N particles interacting by gravitation only, it makes sense to model the Baryonic gas by 'smoothed particles' also. A second reason is the fact that during most of the evolution of galaxies and clusters of galaxies hydrodynamic instabilities or shocks play a minor role, but large density contrasts and complicated 3D structures form because of the dust-like nature of the Dark Matter. Of course, this situation can best be handled by Lagrangian hydrodynamics and, thus, by SPH. We will discuss the results of recent simulations of that kind later in Sub-Section 1.1.

On the other hand, for many problems in astrophysics self-gravity is less important and the time evolution of the objects is governed by hydrodynamics. In those cases the fact that almost always the objects are huge but the viscosity of the matter they are made of is kind of 'normal' results in huge Reynolds numbers, typically of the order of 10^{12} to 10^{15}. Therefore the equations one has to solve are the Euler rather than the Navier-Stokes equations, and turbulence becomes a crucial issue. The methods that are commonly used are very similar to those of other fields of computational fluid dynamics: explicit or implicit finite volume schemes combined with means to handle large gradients of physical quantities such as density, velocity or chemical composition, 'adaptive-mesh refinement' (AMR) being an example. However, whenever turbulence is important AMR may not be the best choice since turbulence, not limited to some boundaries as in many terrestrial systems, is volume filling thus erasing the advantages of AMR. Therefore 'large eddy simulations' (LES) have become a more popular method in astrophysical applications in recent years, an example being presented in Sub-Section 1.2.

1.1 Flows in Cosmological Structure Formation

Galaxies and clusters of galaxies, and their distribution in a particular large-scale pattern of filaments and voids known as the 'Cosmic Web', grew out of

tiny fluctuations in the matter density present in the primordial universe after the Big Bang. These fluctuations were gravitationally unstable; over time they were amplified by self-gravity, and eventually collapsed in a highly non-linear process to all the objects we see around us today. The precise nature of the initial fluctuations has been established with great precision through observations of the cosmic microwave background anisotropies (e.g. [18]), so that cosmological structure formation becomes an initial value problem *par excellence*. Given sufficiently powerful numerical techniques, simulations can accurately predict the complex non-linear outcome of the initial conditions of the standard cosmological model, and hence bridge 13 billion years of cosmic evolution. Comparison with the real universe at the present epoch then provides for crucial tests of the cosmological paradigm.

One of the surprises modern cosmology has found is that most of the matter in the Universe is dark, and consists of weakly interacting, non-baryonic elementary particles that have yet to be discovered in the laboratory. These particles behave as a *collisionless fluid*, subject only to forces from the collective gravitational potential. Such a system obeys the Poisson-Vlasov system of equations (i.e., the collisionless Boltzmann equation plus gravity) and can be best treated with a Monte-Carlo approach where the dark mass is discretized in terms of particles. Individual particles in this N-body method randomly sample the phase-space of dark matter and follow characteristics of the underlying system of equations. A crucial strength of this method is that it can comparatively easily cope with the large dynamic range and the geometric complexity that results from the gravitational clustering process, where bound objects with central density contrasts in the range of 10^6 to 10^7 times the mean background density form abundantly throughout the volume, and then hierarchically merge to build ever larger structures.

Ordinary baryonic matter only amounts to about one sixth of the total matter. Thanks to its typically very low densities and low velocities relative to the speed of light, the baryons behave as an ideal gas and can be accurately described by the Euler equations on cosmological scales. As the treatment of dark matter as particles is without alternative, it is very popular in this field to represent the gas with particles as well, based on the smoothed particle hydrodynamics (SPH) approach (see Monaghan 1992 for a review). In this mesh-less formulation of Lagrangian hydrodynamics, fluid properties and hydrodynamic forces are estimated by adaptive kernel-interpolation over a set of neighboring particles. As a result, SPH offers an *automatic* adjustment of its spatial resolution to the local density, so that the highest resolution is achieved right at the center of galaxies, where it is needed most. Also, the method is Galilei-invariant and free of preferred directions, both important advantages for simulations of cosmological structure formation, where the fluid motion can often be highly supersonic relative to the rest frame of the universe. Furthermore, the representation by particles simplifies the calculation of the gravitational field, as the same N-body solver can be used at matching accuracy for both mass constituents.

These advantages explain the popularity of SPH in this area, even though the method also has serious drawbacks. It requires an artificial viscosity to capture shocks, and due to the inherent smoothing effects of the kernel interpolation technique, shocks and contact discontinuities are smoothed out over several mean particle spacings. Perhaps more importantly, numerical effects in SPH can stabilize contact discontinuities against fluid instabilities such as the Kelvin-Helmholtz instability, provided the density contrast is large enough ([1], but see [15]).

In Figure 1, we show an example of a simulation of the formation of a cluster of galaxies, carried out with SPH. The panel on the left-hand side shows the dark matter distribution, the panel in the middle the projected gas density, and the panel on the right the temperature field at the present epoch. Clearly visible is the clumpy nature of the collisionless dark matter, which shows a large abundance of substructures in the cluster. These are the remnants of galaxies that have fallen into the cluster during its formation and now orbit in the cluster potential. In the gas distribution, only the most massive lumps that have fallen in most recently have managed to hold on to some of their gas. However, these gas clumps are in the process of being disrupted, as evidenced by bow shocks, tails of stripped gas, and the presence of contact discontinuities that separate cold and hot gas phases.

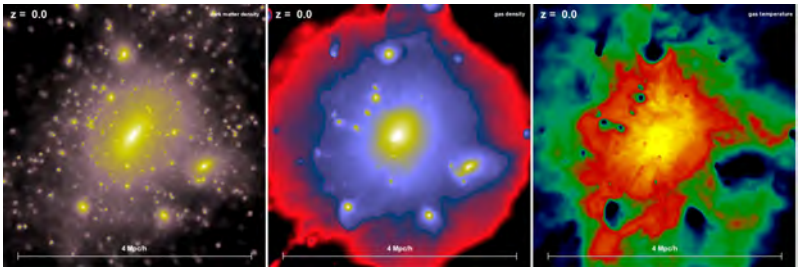

Fig. 1. A cluster of galaxies formed in an SPH simulation of cosmological structure formation. The panel on the left shows the collisionless dark matter, the middle panel gives the projected gas density, and the panel on the right shows the corresponding gas temperature map.

Ultimately, hydrodynamic processes convert the kinetic energy of the infalling matter to heat that then supports the gas in virial equilibrium against further collapse under self-gravity. The temperature field shows that the cluster is filled with a hot plasma of relatively homogeneous temperature of several $10^7\,K$, with some signs of fluctuations induced by the residual gas motions, which may have in part turbulent character. This hot plasma emits copiously in X-rays, which is the prime target of X-ray astronomy. Such hydrodynamic simulations are therefore very important for interpreting observations of clus-

ters of galaxies, and for calibrating the use of X-ray clusters as cosmological probes.

A quite different application of SPH in galaxy formation is shown in Figure 2. Here two spiral galaxy models are collided on the computer, a process that eventually leads to a merger of the galaxies and the formation of a new, morphologically transformed galaxy, an elliptical galaxy.

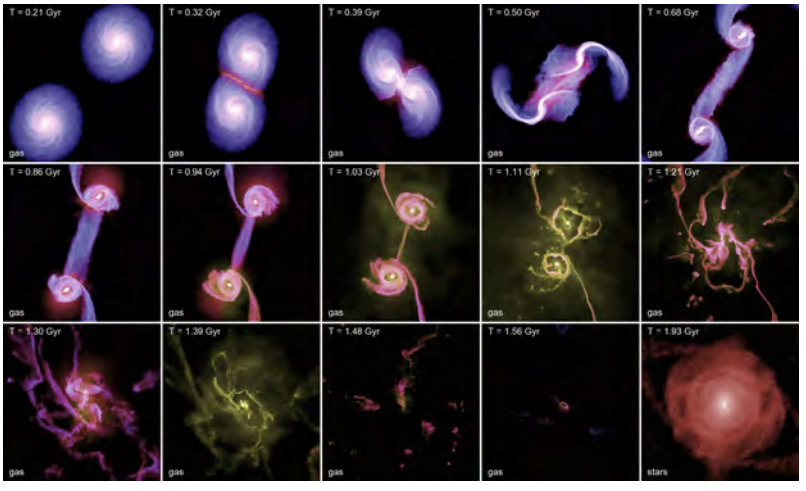

Fig. 2. Time evolution of a galaxy merger simulation carried out with SPH. The individual panels show the projected gas density in a prograde equal-mass encounter of two spiral galaxies. Gravitational tides during the merger funnel gas to the galaxy nuclei, where it fuels quasar activity. The energy feedback by the growing supermassive black holes expels much of the gas, leaving behind a gas-poor elliptical galaxy (last panel) whose stellar system quickly reddens due to a dearth of young stars.

SPH is especially useful for such calculations thanks to its effortless ability to treat vacuum in large parts of the simulated volume. Of particular interest in such galaxy mergers is how much gas is driven by gravitational tidal forces into the nuclei of the galaxies. There the increased gas density can produce a luminous starburst. Furthermore, it is now well established that supermassive black holes are lurking in the centers of most if not all galaxies. Accretion of gas onto such a central black hole will be fueled by the merger-induced gas inflow, making the black hole grow rapidly and shine as a quasar. The simulation depicted in Figure 2 models this accretion physics by a sub-resolution model and accounts for energy deposition by the quasar in the galaxy nucleus [6]. Eventually, this energy pressurizes the central gas to the extent that it expels most of the gas in a pressure-driven outflow. This terminates the starburst and further black hole accretion, such that a comparatively gas-poor elliptical galaxy is left behind that shows very little residual star formation, similar to what is observed.

1.2 Thermonuclear Supernova Explosions

Some stars end their lives with a powerful explosion which can destroy them completely. Usually, these explosions are accompanied by a dramatic increase of the light output from what was the star. If such an event occurs sufficiently close to us, it can be observed even with the naked eye. Only a few such events were ever so bright, and they were called 'novae' ('new' stars) by ancient astronomers. We now differentiate between mild (in relative terms!) surface explosions (novae) and the very bright explosions that mark the sudden end of a star's life, and call the latter 'supernovae'. This is a well-deserved name because for a few weeks, a single supernova can emit almost as much light as a whole galaxy, even though a galaxy contains about a billion stars.

Over the past few years a certain sub-class of supernovae, commonly named 'Type Ia', has received considerable attention, not only among astronomers but also from the public. This sub-group is the brightest and most homogeneous among all supernovae: their light curves are all very similar, and so are their spectra at all phases. Therefore it is tempting to use them as cosmic distance indicators and, in fact, they have become a standard tool to measure cosmic distances out to several 10^9 light years, i.e., many of these supernovae exploded when the Universe was half its present age [13, 17]. Therefore the question arises if these very distant stellar explosions are the same which we observe in great detail in our cosmic neighborhood, and this question can only be answered once we understand them.

There is clear evidence that type Ia supernovae are the thermonuclear disruptions of white dwarf stars with a mass slightly higher than the Sun and radii comparable to the radius of the Earth. Thermonuclear fusion of carbon and oxygen is thought to supply the necessary energy and, therefore, the computational problem is very similar to simulations of chemical combustion of turbulent pre-mixed flames [9]. The equations that have to be solved are the reactive Euler-equations of fluid dynamics in three dimensions, for a general equation of state, plus a system of ordinary differential equations to deal with nuclear reactions, the Poisson equation for self-gravity, and a model of small length-scale turbulence to compute the propagation of nuclear 'flames' into the unburned carbon-oxygen fuel. As in many technical applications, the latter is done by describing the flame by a level-set function moving with the velocity of the turbulent velocity on the grid scale. For thermonuclear supernovae this is an excellent approximation since the width of the flame as well as of the reaction zone is tiny in comparison to the size of the star or even the integral scale of turbulence: a fraction of a millimeter and several kilometers, respectively. The effective speed of the flame on the scale of the numerical grid is calculated from the sub-grid scale model of the turbulent velocity fluctuations, again an excellent approximation in the limit of strong turbulence, encountered in the huge Reynolds-number flows in a supernova.

The up to now largest computations of Type Ia supernova explosions used 1024^3 grid points, about 80 Gigabytes of memory and around 500,000 proces-

sor hours on an IBM Power 4 supercomputer per simulation. The simulations were 'parameter free' in the sense that only physical degrees of freedom, i.e., the composition of the white dwarf and the ignition conditions had to be fixed, parameters expected to be different from supernova to supernova [16].

The results of one of these simulations are shown in Fig. 3 which displays a sequence of snapshots of the nuclear-fusion layer. Due to heat conduction the flame burns from a large number of ignition spots (shown in the enlarged box) near the center of the white dwarf star outward. This proceeds with velocities lower than the local sound speed and is termed deflagration.

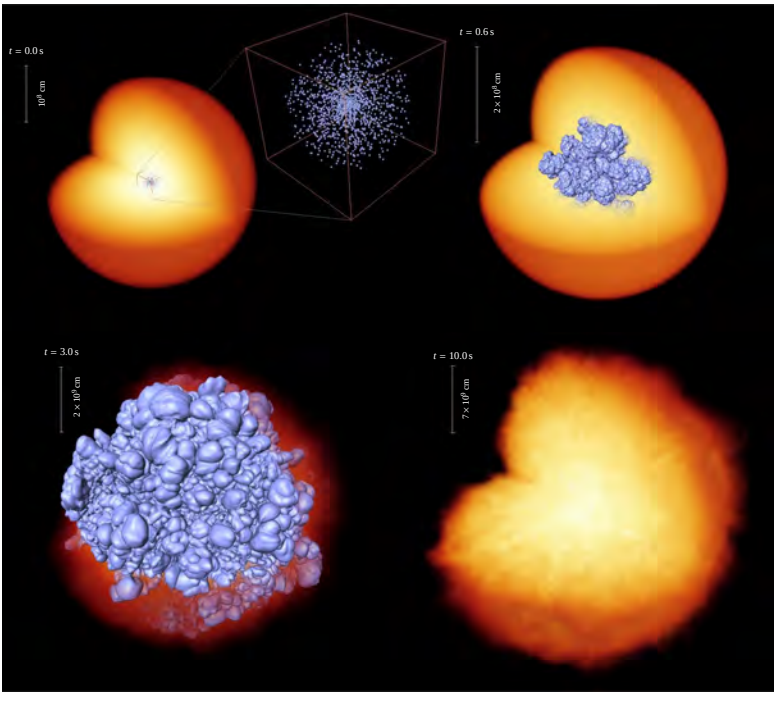

Fig. 3. Evolution of the thermonuclear supernova explosion simulation. The zero level set associated with the thermonuclear flame is shown as a blue isosurface and the extent of the white dwarf (WD) is indicated by the volume rendering of the density. The upper left panel shows the initial set up and the close-up illustrates the chosen flame ignition configuration. The subsequent two panels illustrate the propagation of the turbulent flame through the WD and the density structure of the remnant is shown in the lower right panel (from [16]).

Some SN Ia models assume a transition of this flame propagation mode to a supersonic detonation driven by strong turbulent velocity fluctuations at later times. The models discussed here are based on the pure deflagration model.

Deflagration flames burning from the center of the white dwarf star outward leave hot and light burnt material behind. The fuel in front of it is, however, cold and dense. This results in a density stratification inverse to the gravitational field of the star, which is therefore unstable. Thus, blobs of burning material form and ascend into the fuel. At their interfaces shear flows emerge. These effects lead to strong swirls. The resulting turbulent motions deform the flame and thus enlarge its surface. This increases the net burning rate of the flame and leads to the energetic explosion. The last snapshot is at a time when burning has already ceased. Large parts of the star are burnt in the explosion and expand strongly. The configuration has lost its initial symmetric shape.

The supernova model presented here is the first simulation leading to an explosion strength and an amount of burnt material that come very close to the observed values. Details of such numerical models will be analyzed in future investigations. They will allow to assess the models on the basis of synthetic light curves and spectra which can be directly compared with observations.

2 Relativistic Flows

Some astrophysical phenomena require a relativistic formulation of fluid dynamics. A special relativistic formulation must be used if the flow velocity reaches a significant fraction of the speed of light, or if the internal energy of the fluid becomes comparable to its rest mass. General relativistic effect must be considered for flows in strong gravitational fields which exist near compact objects like neutron stars or black holes, and are encountered in the formation or merging process of neutron stars and black holes.

2.1 Special Relativistic Flows

An important difference between Newtonian and (special) relativistic fluid dynamics is the presence of a maximum velocity, *i. e.,* the speed of light, in the latter case. Another major difference with classical hydrodynamics stems from the role of tangential velocities. In relativistic calculations the components of the flow velocity are coupled through the presence of the Lorentz factor in the equations. In addition, the specific enthalpy also couples with the tangential velocities, which becomes important in the thermodynamically ultra-relativistic regime. This gives rise to numerical complications [11].

In classical numerical hydrodynamics it is easy to recover primitive flow variables (density, velocity, and pressure) from conserved ones (rest mass density, momentum, and total energy). In the relativistic case, however, this recovery is much more involved (see *e. g.,* [11]). As state-of-the-art special relativistic hydrodynamic codes are based on numerical schemes where the conserved quantities are advanced in time, it is necessary to compute the

primitive variables from the conserved ones several times per numerical cell and time step making this procedure a crucial ingredient of any algorithm.

The application of high-resolution shock-capturing (HRSC) methods have caused a revolution in numerical special relativistic hydrodynamics (SRHD). These methods satisfy in a quite natural way the basic properties required for any acceptable numerical method [11]: (i) high order of accuracy, (ii) stable and sharp description of discontinuities, and (iii) convergence to the physically correct solution. Moreover, HRSC methods are conservative, and because of their shock capturing property discontinuous solutions are treated both consistently and automatically whenever and wherever they appear in the flow. As HRSC methods are written in conservation form, the time evolution of zone averaged state vectors is governed by some functions (the numerical fluxes) evaluated at zone interfaces. Numerical fluxes are mostly obtained by means of an exact or approximate Riemann solver although symmetric schemes can be also implemented. High resolution is usually achieved by using monotonic polynomials in order to interpolate the approximate solutions within numerical cells. Solving Riemann problems exactly involves time–consuming computations, which are particularly costly in the case of multidimensional SRHD due to the coupling of the equations through the Lorentz factor. Therefore, as an alternative, the usage of approximate Riemann solvers has been proposed.

Special relativistic astrophysical flows are encountered in (galactic) microquasars, active galactic nuclei and gamma-ray bursts (see *e. g.,* [11]). All three phenomena involve highly collimated supersonic outflows (jets), which are thought to form as a consequence of mass accretion onto a central rotating black hole. General relativistic effects seem to be crucial for a successful launch of the jet. In the commonly accepted standard model of jets in extragalactic radio sources associated with active galactic nuclei [4] flow velocities as large as 99.9% of the speed of light (Lorentz factors $\lesssim 20$) are required to explain the apparent superluminal motion observed at parsec scales in many of these sources. Although magneto hydrodynamics (MHD) and general relativistic effects seem to be crucial for a successful launch of the jet, purely hydrodynamic, special relativistic simulations are adequate to study the morphology and dynamics of relativistic jets at distances sufficiently far from the central compact object (see *e. g.,* [12]). Observations of gamma-ray bursts and gamma-ray burst afterglows imply collimated outflows with Lorentz factors up to ~ 100. Nowadays, such ultra-relativistic flows can be successfully and accurately simulated with codes based on HRSC methods (see Fig. 4).

2.2 General Relativistic Flows

The simulation of relativistic flows involving strong gravitational fields and relativistic speeds requires the integration of the general relativistic fluid equations and the numerical solution of Einstein's field equation if the space-time metric changes due to the flow. Such situations are encountered in accretion flows onto compact objects like neutron stars or black holes, in the formation

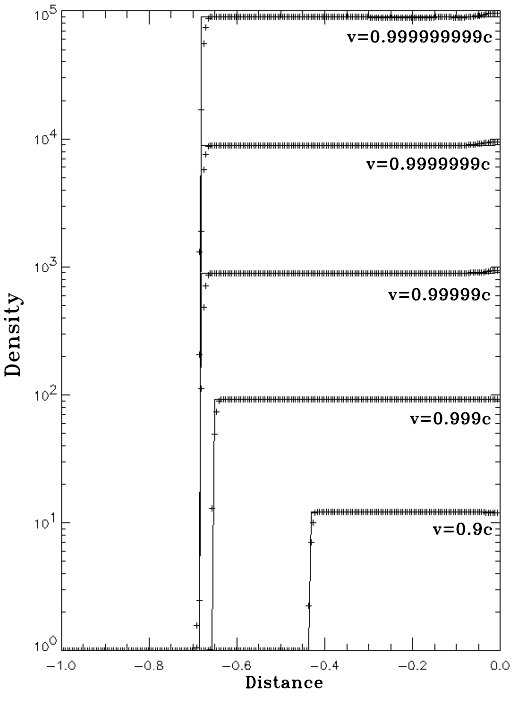

Fig. 4. Performance of the HRSC code GENESIS for the relativistic planar shock reflection problem on an equally spaced grid of 401 zones at $t = 2.0$ (only the left half of the grid is shown!). Solid lines represent the exact solution while symbols refer to numerical values (from [2]).

or merging process of neutron stars and black holes, and most likely during the formation process of relativistic jets and gamma-ray burst outflows.

Up to now only a few attempts have been made to extend HRSC methods to general relativistic hydrodynamics (GRHD) (for a review see [7]), all of which are based on the usage of linearized Riemann solvers. An interesting and powerful procedure exploiting the developments in the field of special relativistic Riemann solvers in GRHD was proposed by [3] and implemented by [14]. It relies on a local change of coordinates at each zone interface such that the space-time metric is locally flat. Any special relativistic Riemann solver can then be used to calculate the numerical fluxes, which are then transformed back into the curved space-time. As the transformation to an orthonormal basis is valid only at a single point in the space-time, but the use of Riemann solvers requires the knowledge of the behavior of the characteristics over a finite volume, the use of the local Lorentz basis is, however, only an approximation.

In the case of dynamic space-times, the equations of relativistic hydrodynamics are solved on the *local* (in space and time) background solution provided by the Einstein equations at every time step [7]. The solution of the Einstein gravitational field equations and its coupling with the hydrodynamic equations is the realm of *Numerical Relativity* (see, *e. g.,* [10]).

The inclusion of magnetic fields which are of importance, *e. g.,* for the gravitational collapse of a magnetized stellar core to a neutron star or a black hole (Fig. 5), requires a general relativistic magneto hydrodynamics (GRMHD) code.

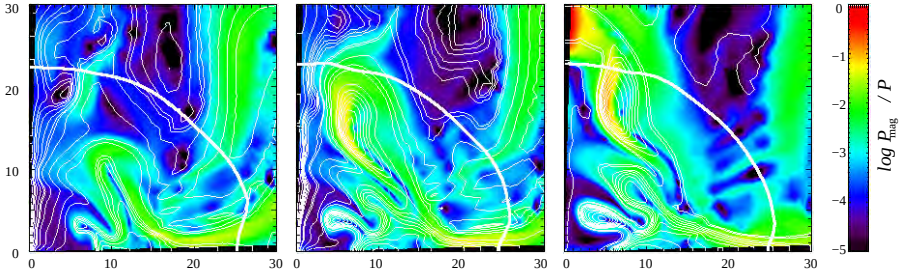

Fig. 5. Development of the magneto-rotational instability in an axisymmetric GRMHD simulation of the collapse of a magnetized rotating stellar core. The middle (right) snapshot is taken 2.5 ms (5 ms) after the left one. Shown are the ratio of magnetic pressure to thermal pressure (color coded), poloidal magnetic field lines (thin white), and the location of the neutrino-sphere (thick white). Axis labels are in units of km (from [5]).

The non-trivial task of developing such a code is considerably simplified by the fact that due to the high electric conductivity of the dense stellar plasma one must only consider ideal MHD. As magnetic fields are divergence free, numerical schemes are required which maintain this constraint during the evolution. Only recently developed GRMHD codes are able to simulate flows in a *dynamic* space-time (see *e. g.,* [8]).

3 Concluding Remarks

Computational fluid dynamics will remain a major tool in astrophysics in the years ahead. Grand challenges that await solutions include the formation of stars and planets, a full understanding of stellar explosions, astrophysical jets and accretion disks, and the formation and evolution of galaxies and clusters of galaxies. Recent progress in some of these fields was demonstrated in this contribution. However, solving the radiation-(magneto)-hydrodynamic problems ultimately will need supercomputers with several hundreds of Teraflop/s sustained performance (which may become available in the next decade) as well

as the development of new numerical tools. In any case, significant progress towards the understanding of all these exciting questions can be obtained already by reducing the dimensionality of the simulations assuming approximate symmetries or by simplifying the physics of the models, as was done in the examples discussed here.

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Multigrid Software for Industrial Applications - From MG00 to SAMG

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Summary In this article, we review the development of multigrid methods for partial differential equations over the last 30 years, illuminating, in particular, the software question. With respect to industrial software development, we will distinguish "optimal" multigrid, multigrid "acceleration" and "robust" multigrid. Surprisingly, not geometric multigrid but algebraic multigrid (AMG) finally brought the breakthrough. With the software package SAMG, which is based on block-type AMG, systems of partial differential equations can be treated efficiently also. Finally, we outline how SAMG is used for industrial applications.

1 Introduction and Historical Remarks

Today, multigrid is accepted as the most efficient approach for the solution of certain classes of partial differential equations (PDEs), in particular elliptic boundary value problems. One should therefore expect that many commercial software packages for the solution of PDEs be based on the multigrid principle. Surprisingly, this is not the case: To our knowledge there is no commercial software package available which could claim to rely on "classical" multigrid in a strict sense. What are the reasons for this situation? In this paper we will try to give an answer to this question. It will turn out that a more differentiated consideration is needed in order to describe and understand the role the multigrid principle is playing in modern software development.

In our review, we will go back to the late 1970s and then discuss what has happened over the last 30 years of multigrid development. Since there is a vast amount of literature on multigrid, we restrict ourselves to citing mostly several survey papers as well as some recent papers on multigrid for industrial applications (see Section 6, in particular). Surveys include [2, 23] for more general iterative solvers, and [35, 30, 29, 4] for "classical" geometric multigrid

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and/or algebraic multilevel techniques. For introductions to multigrid, refer to [38, 35, 34], for instance.

Some historical remarks and an outline of this paper Multigrid started in the 1960s with studies on Poisson-like PDEs in 2D by Fedorenko and Bakhvalov. But only Achi Brandt recognized the practical potential and the high efficiency of multigrid in the 1970s. Much happened in the late 1970s and the early 1980s: Based on theoretical considerations, multigrid was reinvented independently by Wolfgang Hackbusch in 1975/1976 (compare [12]). At the same time, Johann Schröder and Ulrich Trottenberg had developed the "total reduction method" in 1973-1976 [24, 25], which is a special multigrid variant. Around that time, software development was also started: In 1977 Ulrich Schumann organized the – second – GAMM-Workshop "Fast Solution Methods for the Discretized Poisson Equation" (see also the contribution by C. Weiland and E. H. Hirschel in Part I of this book). Most of the software programs submitted to this workshop were based on cyclic reduction and FFT type methods, like the Buneman algorithm; only the total reduction based program TR2D01 – which turned out to be one of the fastest solvers – had some multigrid features already.

The "First European Conference on Multigrid Methods" (Köln 1981) brought the multigrid breakthrough. The idea of *"optimal" multigrid* was introduced and became accepted, see **Section 2**.

However, we will see that the original idea of optimal multigrid (in the 1980s) was soon replaced in practice by an idea which we would like to call the *multigrid acceleration approach*, see **Section 3**. Later on (in the 1990s), the acceleration approach was generalized and the term *robust multigrid* was introduced, see **Section 4**.

The idea of *algebraic multigrid* (AMG, see **Section 5**) had already been introduced by Achi Brandt in the (early) 1980s. Although John Ruge and Klaus Stüben had already published the first reasonable AMG code (AMG1R5) in 1985, only in the mid 1990s did industry and software houses become interested in AMG. Substantial work for extending AMG to PDE systems started around 2000 (see [4] and references given therein) and is still an ongoing process. Progress being made for several important classes of industrial applications is briefly summarized in **Section 6**.

2 The Beginning: Optimal Multigrid

In the 1970s, multigrid evolved. At the beginning of that decade, multigrid was essentially unknown. At the end of the decade, multigrid had become mature and – at the same time – quite popular. This was due to the fact, that Brandt's ideas and papers had been recognized by the numerical community and Hackbusch's theory had become well-known. Trottenberg's numerical group had combined total reduction methods with multigrid ("MGR" methods) and thus shown that multigrid was not only a very general and

effective numerical principle but could also be used to construct extremely fast algorithms for very special problems (like the Poisson equation in rectangular domains). An important event in this respect was the "Conference on Elliptic Problem Solvers" held in Santa Fe in 1980 [26]. There, the multigrid community and the more traditional elliptic solver community met, and the generality *and* efficiency of multigrid became clear. At that conference, the two codes MG00 (for Poisson-like equations with Dirichlet, Neumann or Robin boundary conditions), in rectangular domains, see [13] and MG01 (for Poisson-like equations in general bounded 2D-domains) were made available.

Both programs realized the goal of "optimal" multigrid. Here, the term optimal addresses the goal of tailoring the multigrid "components" to the problem at hand in such a way that one obtains a "textbook efficiency".

In order to explain what is meant by "components" and "textbook efficiency", let us roughly describe the general multigrid algorithmic structure (for Poisson-like boundary value problems). Multigrid makes use of *smoothing* procedures (traditionally relaxation-type iterations), in order to reduce the high frequency error components. The low frequency error components are treated by means of the *coarse-grid correction*. Algorithmically, this means that a hierarchy of grids is used and the ideas of smoothing and coarse-grid correction are used recursively. On all grids smoothing steps are performed; only on the coarsest grid is the corresponding equation solved. The *transfer* between the grids is done by *restriction* operators (from fine to coarse) and by *interpolation* operators (from coarse to fine). On each coarse grid, an analog of the fine grid equation is used (*coarse-grid equation/operator*). In its original form, multigrid is an iterative process, in which each iteration step consists of the components described above and is characterized by the *type of cycle* ("V"- or "W"- or more complicated types). Here, smoothing, the number of smoothing steps per multigrid cycle, restriction, interpolation, coarse-grid equation, solver for the coarsest-grid equation, and cycle type are the so-called multigrid components which have to be chosen adequately. If they are specifically tailored to the problem at hand, we would expect a "textbook efficiency". In the case of Poisson-like equations, for instance, this means convergence factors of ≤ 0.1 per multigrid cycle and a computational effort comparable to just a few finest-level smoothing steps per cycle.

We would claim that the two program packages MG00 and MG01 were the first multigrid codes which were not just experimental, academic programs but fulfilled industrial software standards. These codes were indeed used in many contexts, they have been included in PDE program libraries (like ELLPACK, NAG, IMSL), and several industrial applications were treated by them.

Based on MG00 and MG01 developments, several research groups, for instance of Brandt and Trottenberg, tried to conceive and realize multigrid software packages which would give "the textbook efficiency" for large classes of PDEs. The LiSS package (compare [35]) was an attempt of this type, but it was (mainly) restricted to 2D problems, and had a more experimental, academic character than a commercial intention.

3 Making Compromises: Multigrid Acceleration

In parallel to the early attempts to conceive an "optimal" multigrid software package, several software developments made use of multigrid ideas and techniques in order to improve and speed up *existing* codes. In accordance with [27] we would like to call this approach *multigrid acceleration*. A typical example for this approach is to start from a classical iterative single-grid (= one-level) algorithm (like SOR) on a given – fine – grid. The idea is, based on this given grid, to construct a coarse grid structure and a corresponding (coarse) grid hierarchy, typically by standard coarsening (i.e. doubling the mesh size in all directions, on each grid level). Instead of the single-grid algorithm, a standard V- or W-multigrid cycle is used in which the single-grid iteration plays the role of the smoothing procedure now. Often this simple approach may work, since many of the classical iterative single-grid methods have reasonable smoothing properties. In addition, it may be useful to introduce certain smoothing parameters, since one now is more interested in optimal smoothing than in optimal single-grid convergence [27, 13].

This multigrid acceleration approach has been used in the context of several software developments. One prominent code which can be regarded as based on the acceleration idea is the code [14] of Antony Jameson. Here a Runge-Kutta-type iteration (introducing an – artificial – time dependency) is used for smoothing with multiple parameters. The code has gained much attention and was used very intensively; it was also the starting point for the FLOWer development in the German Aerospace Center DLR.

Still, one has to be aware of the fact that these codes do not exhibit the textbook multigrid convergence (and neither do they claim to do so). In [35] it was shown, for example, that the multi-parameter Runge-Kutta approach is not at all optimal for simple scalar equations where one can do much better with more sophisticated smoothing procedures. And in [27] examples were given in which anisotropies or stretched grids make the classical point-wise iterative single-grid methods totally inefficient for smoothing, so that one has to switch to line- or plane relaxation [35] if standard coarsening is maintained.

One even more basic disadvantage of the multigrid acceleration approach as described above is that the given original grid has to have some regularity for the construction of a reasonable and useful coarse-grid hierarchy. In case of a block-structured finite-difference or finite-volume based grid, a natural coarsening usually is feasible (doubling the mesh size should be a possible coarsening strategy). If we have, however, an unstructured (perhaps automatically generated) finite-element grid, the construction of a coarse grid hierarchy may become difficult and will at least be technically cumbersome, since complicated interpolation techniques have to be provided.

However, also the following approach is a kind of multigrid acceleration: The given, original code may contain parts (modules) which can be separated from the rest of the code. In implicit or semi-implicit discretization approaches, for instance, one will have to solve large systems of discrete equations, and for

these parts – in particular, if they are compute-intensive – multigrid acceleration may be very useful.

Also certain formulations of the continuous problem – which then are reflected by the discretization – give rise to a quasi semi-implicit character: The pressure correction formulation in computational fluid dynamics, or the IMPES (implicit in pressure, explicit in saturation) approach in oil-reservoir simulation are examples.

In any case, the idea of multigrid acceleration is one way to speed up existing software and – of course – also an option for a new software design. It has played a role since the 1980s and is still of interest, in particular in combination with algebraic multigrid (AMG).

4 The Idea of Robust Multigrid: Towards AMG

In addition to the idea of optimal, problem-tailored multigrid, the idea of robust multigrid came up in the 1990s: a kind of multigrid, in which the components are not specifically optimized to the problem at hand, but defined in such a way that large classes of problems are addressed. Robustness in this understanding then, of course, implies that optimal efficiency is not achieved.

Operator-dependent interpolation and/or "Galerkin" coarse-grid operators are the key components of robust multigrid approaches. For smoothing, ILU-type methods were recommended (see [35]) since they seemed to be more robust, for example in the case of anisotropies, than traditional pointwise relaxation-type smoothers.

Whereas multigrid originally was considered as a particularly fast and general *solver*, the robust approach instead regarded multigrid as a *preconditioner* in the context of Krylov subspace methods (compare [35]). Whereas classical multigrid reduces high frequency error components on fine grids by use of suitable smoothing procedures and low frequency error components by use of the coarse grid correction, certain isolated error frequencies may well be treated (cancelled) by Krylov (CG, GMRes, BiCGstab) acceleration.

Still, again no real multigrid software package with commercial intentions did appear. The UG package [1], a quite general platform for the numerical parallel solution of PDEs, supporting unstructured grids and adaptive grid refinement, was regarded more as a multigrid based toolbox for academic purposes.

However, the combination of operator-dependent interpolation and Galerkin coarse-grid operators with an algebraic construction of coarse "grids" (= coarse levels) and the use of multigrid as a preconditioner have leveraged the widespread usage of *algebraic* multigrid.

5 Algebraic Multigrid (AMG)

A few historical remarks on AMG have already been given in Section 1. In the following, we will summarize general AMG developments for scalar PDEs as well as for systems of PDEs. We start with a brief discussion on the differences between geometric and algebraic multigrid.

5.1 Algebraic Versus Geometric Multigrid

AMG extends the two fundamental multigrid principles – smoothing and coarse-grid correction – to a fully algebraic setting. All (geometric) multigrid components such as smoothing, coarsening, restriction, interpolation, and the coarse-level operators, have an algebraic analog and play a similar role as in geometric multigrid. In both approaches, error components which cannot be diminished by the coarse-level correction process should efficiently be reduced by the smoothing process and vice versa. However, the way in which an efficient interplay between both processes is achieved, constitutes the conceptual difference between the geometric and the algebraic concept.

In the geometric case, a hierarchy of grids is *predefined*; the coarsening process and the interpolation operators are fixed and kept as simple as possible. Consequently, for an efficient interplay between smoothing and coarse-grid correction, *the smoothing process has to be adjusted to the pre-defined grid hierarchy* to achieve good convergence. For anisotropic PDEs, for example, one has to use line/plane relaxation if standard coarsening is kept; whereas pointwise relaxation is adequate in the case of "semicoarsening".

In AMG it's the other way round: AMG only knows $Av = b$, the original linear system to be solved, at least in a purely algebraic setting. In particular, a suitable coarse "grid" (coarse level) – hierarchy – is not known a priori. In contrast to the geometric approach, a preferably simple smoothing process (typically pointwise Gauss-Seidel relaxation) is fixed in AMG, and AMG's main task is then to build up a suitable, problem-dependent hierarchy of levels including all necessary transfer operators as well as coarse-level operators *automatically* and *algebraically* by solely using information contained in the matrix A. Of course, this coarse-level correction process has to be adjusted to the smoother for good overall efficiency.

5.2 AMG for Scalar Partial Differential Equations

Two main classes of AMG methods are known today, namely classical AMG and aggregation- or agglomeration-based AMG.

Classical AMG (see [30, 29] and references given therein) is known to provide very efficient and robust solvers or preconditioners for large classes of matrix problems $Av = b$, an important one being the class of (sparse) linear systems with matrices A which are "close" to being M-matrices. Problems like this widely occur in connection with discretized scalar elliptic PDEs. In

such cases, classical AMG is very mature and can handle millions of variables much more efficiently than any one-level method. Since explicit information on the geometry (such as grid data) is not needed, AMG is especially suited for unstructured grids both in 2D and 3D.

AMG's coarsening process is directly based on the connectivity pattern reflected by the matrix, and interpolation is constructed based on the matrix entries. Restriction is simply defined to be the transpose of interpolation, regardless of whether the matrix to be solved is symmetric or not. The Galerkin coarse-level matrix for level $n+1$ is then computed as

$$A_{n+1} := \left(I_{n+1}^{n}\right)^{T} A_n I_{n+1}^{n}$$

with I_{n+1}^{n} being the interpolation from level $n+1$ to n, starting from level 1 which represents the original matrix equation $Av = b$.

Aggregation- or agglomeration-based AMG (see [36] and also the references given in [29, 4]) differ from classical AMG in the way coarse-level variables and interpolation formulas are constructed. Aggregation means splitting the set of variables into disjoint subsets (the "supernodes" or "macro variables"), for each of which a constant interpolation formula is constructed. This approach yields a simple-to-compute Galerkin operator as well as sparse coarse-level operators for the hierarchy constructed. Interpolation in the case of agglomeration-based AMG is also piecewise constant. However, agglomerates are sets of neighboring finite elements glued together. Here, variables on the interfaces of elements belong to more than one agglomerate. Their interpolation is just the "average interpolation" of the surrounding agglomerates. For both, aggregation- and agglomeration-based AMG, smoothing of interpolation [36] can be used in order to increase the quality of interpolation and thus the robustness of the overall method which is especially necessary for matrices stemming from second-order discretizations.

Classical AMG with *aggressive coarsening* [30], roughly characterized, is a(nother) means of providing a compromise between the robustness of interpolation of classical AMG and the "small" coarse levels and sparse coarse-level operators resulting from aggregation-based AMG.

5.3 AMG for Systems of PDEs

In practical applications, a variety of PDE systems whose numerical properties can differ drastically has to be solved. Relevant systems often consist of diffusion equations with additional convection, drift (migration) or reaction terms. The individual PDEs are often of first order in time (if time-dependent) and of second order in space. They can be nonlinear and/or strongly coupled, the latter normally enforcing a "fully coupled" solution approach, that is, a simultaneous solution for all physical functions involved. Typical approaches implemented in modern (industrial) simulation packages consist of an implicit discretization in time and space, a Newton-type method to treat the nonlinearities and direct and/or iterative one-level methods to solve the arising systems

of linear equations. The corresponding matrices are large, sparse, frequently ill-conditioned, often not symmetric positive definite, and usually far from being M-matrices. Hence, these matrices do not exhibit the properties that the "scalar" AMG approaches mentioned above principally rely on. Still, the goal is to replace or enhance the linear solver(s) integrated into the packages by multigrid approaches.

In the past, several ways to generalize existing AMG approaches have been investigated, and there is still an ongoing development of new AMG and AMG-like approaches. For a detailed review, we refer to [4]. In the following, we will briefly summarize corresponding popular developments.

5.4 Function-Based (or Unknown-Based) AMG

The historically so-called unknown-based approach, already proposed in early papers on AMG (see [22]), is very similar to scalar AMG except that all "unknowns", i.e. *scalar* physical functions of the PDE system to be solved, are treated separately. To be more specific, coarsening and interpolating the variables of the n-th function is strictly based on the submatrix of A reflecting the couplings of the (variables of the) n-th function to itself. In particular, interpolation to any variable i involves only coarse-level variables corresponding to the same function i belongs to. The Galerkin matrices, however, are usually computed with regard to all functions.

The essential conditions for function-based AMG to work are that, for each function, the submatrix of A reflecting the couplings of this function to itself is close to being an M-matrix and that smoothing results in an error which is smooth separately for each function. Advantages of function-based AMG are then that it can easily cope with anisotropies which are different between the different functions and that functions can be distributed arbitrarily across mesh points. This simple approach works quite efficiently for some important applications, for instance from linear elasticity. However, it will become inefficient if the cross-function couplings are too strong, as is the case for most PDE systems (compare Section 6).

5.5 Point-Based AMG: A General Framework

Clees [4] developed a flexible framework for constructing so-called point-based AMG approaches (based on classical AMG) to solve various types of strongly coupled PDE systems. Point-based AMG operates on the level of points rather than variables as do scalar and function-based AMG. Typically, points are physical grid nodes (in space). However, it is only relevant whether there are (disjoint!) blocks of variables (corresponding to different functions) which may be coarsened, maybe also interpolated, simultaneously.

In order to coarsen A, a so-called primary matrix P is constructed, with the number of points as its dimension. Its entries can be seen to result from a "condensation" of the point-coupling matrices (each of which representing

the couplings of the variables of a point to the variables of another point) to scalar values of P so that the resulting P reflects the couplings between the points reasonably well. A "scalar" coarsening process is applied to P, and the resulting coarsening transferred to all functions. Note that this is different from function-based AMG where each function is associated with its own hierarchy. Many different variants for P and the interpolation are possible (compare Section 5.6). Note, however, that a reasonable choice of components (if possible) strongly depends on the application at hand (compare also Section 6).

5.6 Linear Solver Libraries Based on Multigrid

Among the most prominent, up-to-date software libraries or environments for practical use, substantially containing multigrid methods, we want to mention the commercial SAMG [4, 31] and the research codes Trilinos ML [11], Hypre BoomerAMG [18], and UG (see Section 4).

Particularly SAMG is used for many industrial applications. It consists of the three main strategies mentioned, namely the classical scalar AMG approach, and in addition the two approaches for systems of PDEs and similar problems, namely function- and point-based AMG. In point-based AMG, coarsening can be based on several norms, coordinates, or submatrices of A. Three types of interpolation are integrated for point-based AMG, the so-called single-unknown, multiple-unknown and block-interpolation. Moreover, SAMG features different smoothers, including several ILU-type variants, and different accelerators, namely CG/BiCGstab, and restarted GMRes (compare [23]). Development of automatic, adaptive solver and parameter switching strategies, in particular for ILU-type smoothing, are in progress; for first very promising results, see [5, 6]. SAMGp [16] is SAMG's MPI-based parallel version.

Whereas BoomerAMG contains parallel classical AMG techniques, Trilinos ML is based on parallel smoothed aggregation. Both BoomerAMG and ML offer certain geometric multigrid techniques as well as special AMG methods for edge finite-element discretizations of the curl-curl formulation of the Maxwell equation. Both are part of large packages providing different smoothers and accelerators.

6 Industrial Applications

Navier-Stokes equations. Multigrid in several flavors is commonly used in computational fluid dynamics (CFD), ranging from pure research to the major industrial simulators. For the system of Navier-Stokes equations, we can find both segregated as well as coupled solution approaches in the literature. In a segregated approach, scalar PDEs are solved. Geometric as well as algebraic multigrid for this application is discussed, for example, in [35, 30].

More and more, the Navier-Stokes system is solved fully coupled in CFD simulators. For instance, the old approach [20] (integrated into the TASCflow code, now ANSYS CFX) can be characterized as a non-smoothed agglomeration AMG method suitable for matrices arising from an implicit finite-volume discretization of the 3D Navier-Stokes equations. It employs an ILU smoother. Coarsening is based on the strength of pressure coefficients, similar to a pressure-based point-based SAMG approach.

Other non-smoothed aggregation/agglomeration-type approaches for Navier-Stokes systems can be found in [37] and references given therein. The main differences of the approach [37] (integrated into the FLUENT code, now part of ANSYS) compared to [20] are that an augmented Navier-Stokes system, consisting of five equations for the 3D case, is solved, and that [37] employs block-Gauss-Seidel smoothers.

Recently, in [17] a point-based SAMG approach has been developed for the hybrid spectral / finite-element code SFELES for direct numerical simulation of turbulent flow, which allows simulation of 3D unsteady incompressible flows with planar or cylindrical geometries of arbitrary complexity. The potential of this method is demonstrated for large-scale applications.

Ground water and reservoir simulation. AMG techniques are also well-established in (industrial) ground water and oil&gas reservoir simulation. Common AMG approaches, solving scalar pressure-based systems, can be found in [33, 8, 3], for instance. The recent [28] gives a survey on AMG methods for reservoir simulation.

Recently, in [32, 15, 5], several new SAMG-based methods for the PDE systems arising in oil&gas reservoir simulation have been presented and their performance demonstrated for a series of standard model problems as well as real-life reservoir applications. A very promising method for the coupled solution of the arising systems, an automatic and adaptive solver and parameter switching technology [5], employs a pressure-based point-based AMG approach with ILU-type smoothing.

Linear elasticity. Appropriate extensions of the aggregative and also the agglomeration-based AMG methods (taking care of the "rigid body modes") are very suitable for industrial finite-element discretized linear elasticity problems, as has been discussed in [36, 19], for instance. Also function-based AMG can be quite efficient for typical elasticity applications arising in practice (see [21, 4], for instance).

Semiconductor process and device simulation. Methods and results for industrial applications in semiconductor process and device simulation are presented and discussed in [10, 9, 7, 4], showing that SAMG's function- or point-based approaches yield efficient solution processes for three very different and important types of PDE systems arising there, namely Lamé equations (linear elasticity), reaction-diffusion(-convection) and drift-diffusion (-convection-reaction) systems.

Electromagnetic compatibility (EMC) and Maxwell equations. New, AMG-based methods for solving special industrial EMC problems have been presented in [6], for instance. Here, Maxwell's equations are discretized by a so-called partially equivalent electrical circuit (PEEC) method, leading to special circuit simulations. The resulting matrices can be quite dense. Applications in the time and frequency domain, the latter leading to complex-valued matrices, can be solved, even for large frequencies. However, the methods are still in their infancy. They make use of an automatic and adaptive solver and parameter switching technology which is similar to the approach [5].

Trilinos ML and also BoomerAMG offer AMG methods specially developed for certain "classically" discretized Maxwell formulations, see Section 5.6.

Some further applications. Algebraic multigrid methods are also used in several other application areas. For *casting and molding*, featuring linear elasticity and Navier-Stokes systems, AMG methods (most often based on SAMG) are used in the world-leading simulation packages. In *circuit simulation*, classical AMG methods (based on or similar to SAMG) are already used in several industrial codes for power grid applications, for instance. Also in analytical placement problems (*circuit layout*), AMG methods can be found. Recently, research on SAMG's point-based methods for *electrochemical machining and plating*, featuring Navier-Stokes and drift-diffusion-convection-reaction systems, has started with first very promising results.

7 Outlook

In our opinion, a pragmatic increase of robustness and applicability constitutes the principal trend in multigrid-based solver development. Among the main directions of AMG research and development shall therefore be the following:

- automatic and adaptive solver and parameter switching techniques (extending [5, 6] for instance),
- in particular, adaptive ILU-type smoothers with "smart" (re)ordering,
- appropriate combinations of techniques from algebraic multigrid, multi-level ILU, reduction, and multi-frontal direct solvers towards a general multi-level framework based on approximate Schur complements,
- deflation and other "Krylov recycling" methods (compare [15], for instance),
- parallelization for modern cluster and multi-core hardware architectures.

Strongly coupled PDE systems, comprising more and more physical effects and quantities, have to be solved in many practically important applications. Hence, solver development should especially profit from more "physically oriented" enhancements.

And geometric multigrid? Will it play a role only in academia in the future? We expect that it will find its commercial niches. And when, finally, fully

dynamic adaptive local grid refinement techniques are recognized by software houses as an important option, geometric multigrid may have its renaissance.

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Computer Science and Numerical Fluid Mechanics – An Essential Cooperation

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Summary The role of computer science in application fields such as computational fluid dynamics has been underestimated for a long time. However, with a growing complexity of application scenarios as well as numerical algorithms and hardware architectures, the need for sophisticated methods from computer science becomes more and more obvious. Just think of the visualization of the in general very large data sets resulting from numerical simulations, parallelization and load balancing in particular in combination with the upcoming multicore architectures and petascale computers, code verification and software engineering for large and highly complex software codes, and, of course, the efficient implementation of classical numerical algorithms which are typically data-intensive and, therewith put a big challenge on data storage and data access concepts. We focus on the last point in this contribution and show two examples in more detail, where computer science contributes to more efficient simulation environments: in the memory management for adaptive space-tree grids and, second, in the field of partitioned fluid-structure interactions.

1 Introduction

Traditionally, as in other fields of computational science and engineering (CSE), computer scientists have hardly been among the key players in numerical fluid mechanics. This is mainly due to the fact that modelling and classical algorithmics have dominated the field for years. Although the (super-)computer had always been associated with computer science, there was a widespread feeling that the intellectual challenge was over, once the algorithmic, i. e. numerical, scheme had been found. The remainder was considered as mere programming – maybe tedious, but nevertheless more or less technical.

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In the meantime this picture has changed. The notion of the simulation pipeline or simulation loop identifies more key stages in a successful simulation cycle: implementation, exploration and visualization, validation, and embedding. Obviously, all of them involve core issues of computer science: efficient implementation today means hardware and, in particular, cache awareness as well as parallelization, scalability, and multi-core capabilities; visualization reaches far beyond "colorful fluid dynamics", since computing turns more and more to a data- and, thus, insight-driven mind set involving sophisticated techniques of information extraction, analysis, and rendering. Post and Votta claim in a key publication in "Physics Today" [27] that "Computational Science needs a new paradigm" and request the introduction of code verification; the PITAC report 2005 [5] identifies the software issue as the future bottleneck of simulation, putting hardware and algorithmic challenges in the shade. Users, from academia as well as from industry, want to integrate simulation tools into process chains and call for flexible, modular software concepts allowing for lean interfaces, organizational concepts, and an efficient work flow management. All these are, to a large extent, computer science topics, Fig. 1.

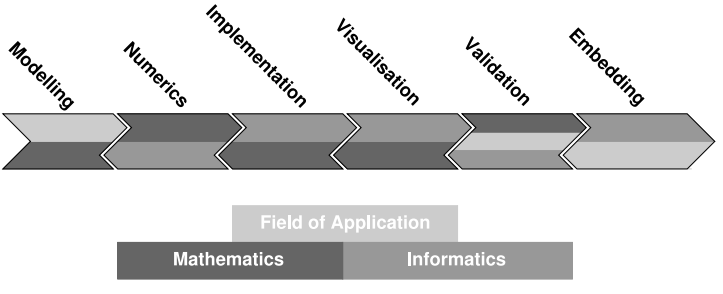

Fig. 1. The simulation pipeline and its stages, involving input from mathematics, informatics, and the respective field of application.

What is true for the above-mentioned newer stages of the simulation pipeline also holds for classical numerical algorithmics. Since, along with and in addition to the increasing complexity of hardware architecture, more and more complex algorithmic schemes have been introduced (think of grid adaptivity or multilevel methods, e. g.), a profound understanding of the interplay of hardware, compilers, and implementation is essential if the task is to develop an efficient simulation code. In view of high accuracy requirements and more and more complex applications (think of multi-physics problems, e. g.), it is obvious that efficiency is a precondition for a code to be applicable for realistic simulations, and it is obvious that the notion of efficiency goes far beyond the classical $O(h)$-type considerations.

The purpose of this article is to provide and discuss a few examples of where and how computer science can fruitfully contribute to computational fluid

dynamics. Obviously, the numerical simulation of fluid flow is a complicated and time-critical task, and the both effective and efficient organization of such complex tasks is at the core of computer science. As in other applications, we usually have a lot of degrees of freedom to choose how to organize our work. Some of these degrees of freedom are completely hidden to the user and, thus, often underestimated in terms of their influence on software performance. Others such as the user interface are very visible to the user, in contrast. Between these two evident layers of a software system – the hidden layer and the visible user interface – there may be additional ones with possible contributions of informatics and with a significant influence on the algorithmic concepts of the software.

For each of them, certain design principles or design patterns have to be applied to end up with a "good" simulation code. Of course, many of these design patterns have been adopted by scientists from the fields of application. However, many techniques are that sophisticated but, nevertheless, vital due to the ever growing size and complexity of application codes and due to the high requirements in terms of extensibility, reusability, and flexibility, that it is preferable that this part of the work is done by specialists. We give a few examples for design principles, some of which are discussed in the remainder of this paper more extensively:

1. Most programs – as far as they are not simple enough to be completely understood by everyone – need an elaborate user interface which has to be adaptable to the knowledge and expertise of the user.
2. As multi-physics applications such as fluid-structure interactions are more and more in the focus of numerical simulations, efficient and flexible techniques for coupled simulations using two or more independent codes become more and more important. Hereby, the main design principle is to keep logically independent components independent also in the actual implementation of the whole problem solving environment.
3. The high computational demand of applications and the upcoming of multi-core processors require the parallelization of the respective codes. For large software packages as those nowadays commonly used for almost all science and engineering applications, it is mandatory to do this parallelization in a platform-independent way to avoid unaffordable implementation overheads. This would be impossible without modern tools such as MPI (Message Passing Interface) or OpenMP.
4. For data-intensive applications such as fluid dynamics, memory access has turned out to be a severe bottleneck. It keeps the performance of the respective software usually below ten or even one per cent of the hardware's peak performance. Thus, the memory architecture of modern computers has to be taken into consideration during algorithm design and implementation.

Of course, these four items do not cover all the informatical potential in fluid flow simulation. They are just examples for possible contributions. In the following sections, we will describe two of them together with one exemplary solution method, each. Section 2 picks up item 4 and presents the cache-aware realization of data structures and data access in a flow solver. In Section 3, we refer to item 2 and propose a software environment for the simulation of fluid-structure interactions based on a partitioned approach, that is using two already existing and independent solvers for the flow and the structure part. Finally, some conclusions will close the discussion.

2 Memory Management for Adaptive Space-Tree Grids Based on Stacks

A very general design principle influencing the algorithmic approach of a fluid solver is to check first which component of the solution process is the bottleneck that needs most of the computing resources. Then, we try to find an approach where this part is solved efficiently. In this section, we apply this principle to the choice of a computational grid of our flow solver.

Looking at different possibilities, we make the following observations: unstructured tetrahedral grids can be adjusted easily to complex boundaries. On the other hand, the construction of the grid in the interior of the domain is computationally costly. Second, we have to explicitly store relations between the components of the grid (elements, faces, edges, nodes). Third, the refinement process in case of adaptive grids is non-trivial in three dimensions and really complicated in the four-dimensional case (time-dependent problems with grids varying in time). And fourth, identifying a grid hierarchy to be able to apply efficient multigrid techniques, e. g., also induces quite some overhead.

In contrast, structured Cartesian grids are cheap: the location and correlation of nodes, edges, faces, and elements is known or computable on-the-fly and, thus, does not require memory space. Second, the finite difference, finite element, or finite volume stencils have a simple structure which remains the same all over the interior of the domain. Third, the refinement of a hypercube is straight-forward in all dimensions and a grid hierarchy is inherently given. On the other hand, the handling of complex boundaries is a challenge for regular grids. Achieving a good accuracy at the boundary requires special software components for the constructions of the stencils at the boundary.

If we summarize these aspects with the eyes of a computer scientist, that is in view of complexity, we observe that – except for very coarse grids – most of the grid points are interior points and much less points are on or neighboring the boundary. The ratio gets even worse with increasing mesh resolution. Thus, following the mentioned design principle, we have to use the variant where the interior is as cheap as possible. This means, we have to chose structured Cartesian grids. However, we must not restrict to regular grids not

to harm another design principle: changes in one part of the domain should not influence other parts. If we apply this principle to the local grid resolution, it is obvious that grid adaptivity is necessary. Fig. 2 gives an illustration of the three possible grids mentioned: An unstructured grid, a regular Cartesian grid, and an adaptive Cartesian grid in two dimensions. A three-dimensional adaptive Cartesian grid for a complex geometry is displayed in Fig. 3.

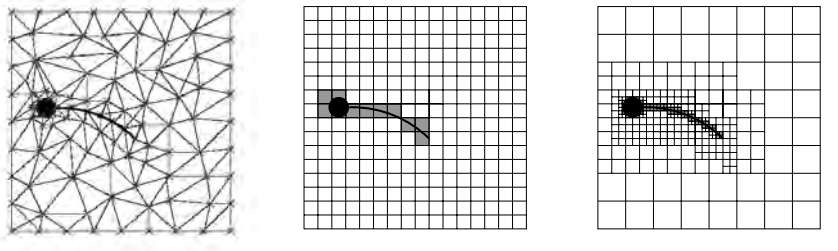

Fig. 2. Two-dimensional grids describing the geometry of a fluid-structure benchmark [17] at a certain state: Unstructured grid (left), regular Cartesian grid (middle), and adaptive Cartesian grid (right).

The construction of the adaptive Cartesian grid from Fig. 2 is based on space-trees, the data structure used in computer science for adaptively refined Cartesian grids. Space-trees are widely used in computer graphics and data bases. But also for engineering applications, this concept recently turned out to be very competitive [1, 26, 14, 15, 10, 3].

However, often only the combination of basic approaches exploits the whole potential of a concept. This is the case also for space-trees. They can be combined with another basic structure in computer science, the space-filling curves [29]. From a mathematical point of view, space-filling curves are a surjective continuous mapping of the unit interval $[0; 1]$ to a compact d-dimensional domain with positive measure. The relation of this theoretical concept to space-trees becomes obvious if we consider the construction principle of a particular class, the recursively defined self-similar space-filling curves. These curves are the result of an infinite refinement process. As the refinement geometrically corresponds to a space-tree refinement, the intermediate states of this process (called iterates) can be used to define an ordering of the elements of a space-tree. Fig. 3 shows an iterate of the two-dimensional Peano curve in an adaptively refined space-tree grid.

If we evaluate the stencils in a grid in this order, memory access stays very local [34, 13]. If we use Peano curves, we can even further enhance the memory access pattern by using a third basic concept, the stack. Stacks can be considered as the most basic collection data types and turned out to be useful in many fields of computer science. They allow for only two operations: `put` a datum on top of the stack and `pop` a datum from the top of the stack.

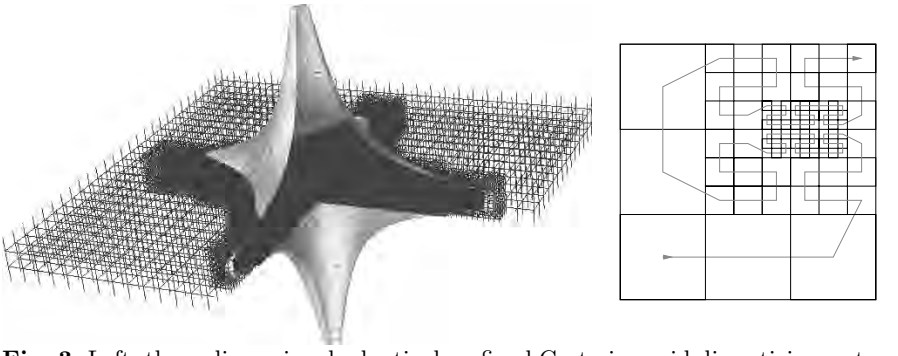

Fig. 3. Left: three-dimensional adaptively refined Cartesian grid discretizing a star-shaped computational domain. Right: iterate of the two-dimensional Peano curve defining an ordering of the cells of an adaptively refined space-tree grid.

To explain why this is useful, we first compare the way how data are usually read and written in a numerical algorithm to the way they are handled using stacks. Usually, data are stored in a random access memory (RAM) with named memory cells. Named variables stay at the same memory location during the program run. If a variable is read and not changed, the value does not have to be written back to the memory cell because it is still up-to-date. In contrast, if a program uses stacks as data structures, the programmer has to ensure that the variables which are needed are on top of one of the stacks because only the top of the stack is accessible by the program. As a consequence, these variables usually can not stay at the same memory location during the whole program run. Instead, they have to be moved from one stack to another, in general. Note that writing back a value to another stack usually can be done in parallel with the next step of the algorithm. So this additional action does not cause overheads in terms of computational time in a clever implementation. The main advantage of the stack concept, however, is caused by the fact that in a straight-forward implementation of stacks in a RAM, the memory access always stays local. Only a move to direct neighbours in memory is allowed, jumps are not possible. This results in an excellent cache performance.[1]

Fig. 4 shows the construction principle for the stacks in the case of a Jacobi solver on a two-dimensional regular Cartesian grid with degrees of freedom located at the grid vertices. In this case, we need only two stacks plus one input and one output stream.

The first stack implementation of a multigrid finite element solver on adaptive space-tree grids was implemented in two dimensions by Günther [14, 15]. He used eight stacks – independent on the refinement depth of the grid al-

[1] If a stack was implemented in hardware, the memory access would even improve as the address calculation would be obsolete. Only moves to neighbour cells would have to be designed in hardware.

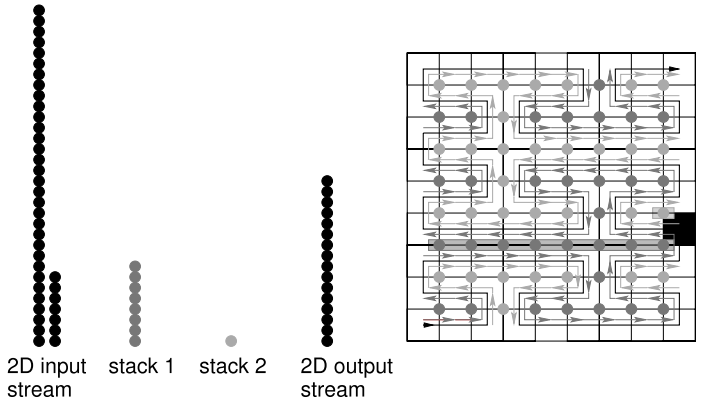

Fig. 4. The stack concept for a two-dimensional regular grid with nodal data. Dark and light grey denote the two stacks used. The current cell is marked and the current vertex data on the stacks are highlighted grey.

though multilevel hierarchical data are involved. Pögl [25, 15] generalized the approach to three dimensions using 28 stacks. In the meantime, the strategy was improved by Weinzierl (to be published). Only $2d + 2$ stacks are used in the d-dimensional case.

To measure the contribution of the stack concept to the performance of our codes, we consider the L2 cache-hit rates which are not the only but a very important ingredient for a high performance application [11]. For all applications and in all versions of our code, we achieve cache-hit rates clearly above 98 % [14, 15, 25, 20, 31, 22, 23, 9]. Such high hit rates are not at all trivial for PDE solvers. As an example, [32] gives the hit rates for data to be found in the L2-cache or higher as 83 % for a standard implementation of a red-black Gauss-Seidel solver on a 1024×1024 grid. Even a cache-optimized version of this solver achieves only a hit rate of 97.1 %.

As already mentioned above, another advantage of the method is the fact that it is extremely economical in memory usage. It was shown by Pögl for the implementation of a Poisson solver in a general three-dimensional region, that the geometry description and the structure of the refinement require only two bits for every grid point. Actually, this is really very low compared to conventional finite element implementations where the refinement structure and also the description of the geometry requires a complicated and memory-consuming data structure, leading to memory requirements in the range of several kBytes for unstructured grids, in particular. Because data are read and written in a structured and sequential way in our stack concept, we can even store all data up to a short buffer containing currently needed cut-offs of the stacks on a disc instead of in the RAM without loosing efficiency in terms of runtime [25]. For a test run of a $1000 \times 1000 \times 1000$ regular grid 40 GByte

disk space and one Gbyte RAM are sufficient which is usually available on a PC.

To finish this section, we mention that the method described here is also useful in other fields of numerical programming. Matrix multiplication, one of the most basic routines in numerical linear algebra, can be implemented very efficiently, if the matrix elements are ordered by a Peano space filling curve [2]. As in the case of PDE solvers, jumps in the memory space for the matrices do not occur, resulting in an excellent cache performance. A recent optimized implementation on modern multi core processors turned out to be faster in most cases than the optimized competing BLAS-routines [16].

3 Fluid-Structure Interaction

We already mentioned that it is an important design principle to keep logically independent parts of a problem also independent in the actual implementation. This notably holds for the partitioned simulation of multi-physics problems such as fluid-structure interactions. The principle of such a partitioned simulation is simple: we take two existing solvers for the fluid and the structure part of the domain and connect them via a suitable coupling component. The advantages of this approach are simplicity, flexibility, and reusability of existing and established codes. However, we have to be very careful in designing the coupling component or, to be more precise, we have to avoid direct mutual dependencies between the solvers or between the solvers and the control of the whole coupled simulation. Otherwise, we lose flexibility to a great extent.

The nowadays most commonly used software for the coupling of several codes is `MpCCI` [18, 12]. It has been developed at the Fraunhofer Institute for Algorithms and Scientific Computing (SCAI) as a successor of `GriSSLi` [4]. It provides the user with functions supporting the exchange of data between the codes and even includes several interpolation procedures to realize the mapping of data between the (typically non-matching) computational grids of the involved solvers.[2] Such, it strongly facilitates the coupling of codes and, in particular, enables the programmer to realize the coupling in a platform-independent way, which is a great success. However, the implementation of the coupling control, that is the choice of the coupling strategy (explicit/implicit, single-/multilevel,...), has to be implemented in the respective solver codes. This entails the drawback that at each replacement of one or both solvers, this coupling control has to be re-implemented, which is error-prone, time-consuming, and annoying. For some sophisticated coupling strategies such as multigrid coupling, the implementation of the coupling strategy in one of the

[2] For special cases such as higher-order elements used in one of the involved solvers, of course also the interpolation of data can not be performed with functions provided by `MpCCI` but has to be re-done in a problem-adapted way.

solvers is even hardly impossible since, here, not only a data-exchange but a real control is required, possibly demanding re-starts of the solvers with changed settings (grid resolution, e. g.). In addition, it is obvious that black-box solvers can not be used, neither.

To overcome these drawbacks, the coupling environment FSI❄ce has been established in a cooperation between computer scientists and civil engineers at the Technical University Munich [7, 8]. Fig. 5 shows the different concepts of `MpCCI` and FSI❄ce: while, in the case of `MpCCI`, the interpolation is done in the coupling component and the coupling control in one or both solvers, it is vice-versa if we use FSI❄ce: we implement the interpolation in the solvers and realize the actual coupling control in FSI❄ce.

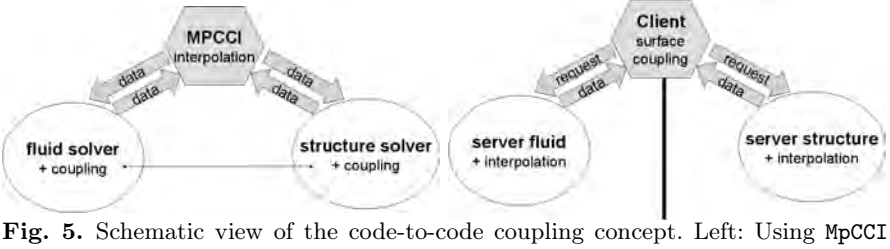

Fig. 5. Schematic view of the code-to-code coupling concept. Left: Using `MpCCI`. Right: using FSI❄ce.

To see how this restores the flexibility and component-independence, we have to explain two central aspects of the concept of FSI❄ce a little more in detail:

1) **The client-server approach:** FSI❄ce acts as a client with the two solvers as servers that receive input data and jobs from the client. That is, the whole steering of the simulation is performed by FSI❄ce. Thus, we can implement arbitrary coupling strategies ranging from simple explicit schemes over implicit and multilevel schemes [6, 33] to reduced order models [30] or even methods solving a third equation at the coupling surface (as typically done in monolithic schemes).
2) **The central surface mesh:** The exchange of data is not performed directly between the solvers, but, instead, via a third grid, the central surface mesh. This central mesh is a triangulation of the coupling surface that is the boundary between fluid and structure and acts as a kind of separator between the computational grids of the involved solvers, Fig. 6. Since each of the solvers maps its surface data to or gets updated surface data from the central surface mesh, the data mapping procedures that have to be implemented in the solvers do not at all depend on the partner solver. Such, we can freely exchange a solver without any changes of the remaining components. For standard cases, interpolation functions between solver grids and the central surface mesh will of course be provided as library functions, e. g., in the future.

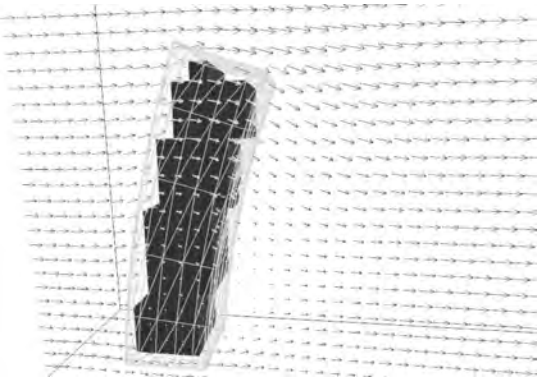

Fig. 6. Central mesh used by FSI❄ce for the description of the surface of a flexible beam in simple fluid-structure scenario together with the representation of the flexible beam in a fluid solver using Cartesian grids in combination with an Eulerian approach. Dark arrows: fluid velocities. Light arrows: Forces acting on the beam in the representation on the fluid grid.

A third aspect of FSI❄ce concerns the efficiency of the coupling. As this contribution is engaged in computer science, we concentrate on efficiency not in the numerical sense but in the sense of complexity of the algorithm: the most costly part of the coupling is the data mapping between solver grids and central mesh. For the interpolation of data, we have to determine neighborhood relations between the elements of the central mesh and those of the solver grid. In the ideal case, this would be done with a cost growing linearly with the size of the coupling surface. To achieve this, FSI❄ce uses sophisticated octree-algorithms [24, 8]. Octrees are a special case of the space-trees described in Section 2. The principal idea behind these algorithms is to use inheritance within the underlying tree of grid cells. Such, for example only those triangles of the central mesh intersecting a father cell have to be examined to find out which triangles intersect the son cells. Table 1 shows that we in fact get a linear growth of computing time in dependence on the number of grid nodes of the fluid solver grid at the coupling surface. The dependence of the number of triangles of the central surface mesh is even weaker.

Applications for fluid-structure simulations cover a wide range. Just think of interactions between elastic wings and the surrounding air, of skyscrapers and towers under different wind conditions, coastal fortifications exposed to heavy waves, inflation of parachutes or airbags, movement of ships or oil platforms, and many others. Fig. 7 shows an example of a scenario happening on the micro-scale but still on the scale of continuum mechanics. The channel with oscillating diameter displayed in the figure is a cut-off of one pore of a kind of sieve which serves as a continuous and parallel device (called drift ratchet) for the separation of microscopic particles according to their size [19]. Such

Table 1. Computing times for the determination of neighborhood relations between triangles of the central surface mesh in FSI❄ce and the nodes of a Cartesian fluid grid in dependence of the resolution of the two grids. The computations were performed on a Pentium M 1.6 GHz processor.

#triangles central mesh	# surface nodes fluid grid	computing time (sec)
8,000	75,514	0.7
8,000	305,394	2.6
8,000	1,227,986	10.1
32,000	1,227,986	14.3
128,000	1,227,986	17.4

a separation of particles plays an important role in life sciences (sorting of macromolecules, e. g.).

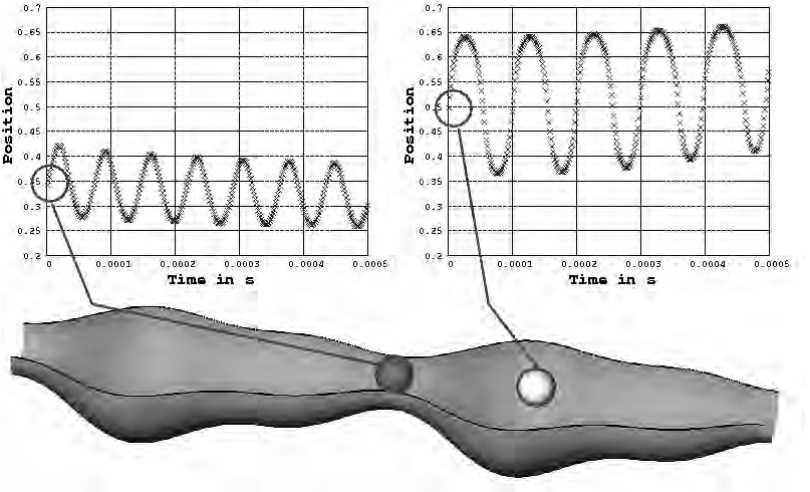

Fig. 7. Simulation results for the transport of microscopic particles in a pore of the drift ratchet [21]. Circle: starting position. Crosses: positions in subsequent time steps. The displayed frequency is the pumping frequency of a pump inducing a to-and-fro movement of the fluid in the pores.

Figure 7 shows the basic effect, a long-term 'drift' of a particle in a pore whereas the direction of this drift depends on parameters such as particle size or frequency with which the fluid with the resolved particles is pumped through the sieve forward and backward in an oscillating manner. The idea of the drift ratchet has been shown to work experimentally [28]. However, further computational studies have to be done to understand the detailed processes and, finally, to be able to optimize input parameters such as pore geometry and pumping amplitude or frequency for specific applications.

4 Conclusion

In Computational Science and Engineering, the role of informatics has been frequently considered to be restricted to computers and a rather technical programming task. For the example of CFD, this contribution aims at highlighting two organizational and conceptual design patterns developed and optimized in computer science, but of huge benefit for state-of-the-art flow simulations. Although arisen in an implementation context, they turned out to be highly interwoven with the other stages of the simulation pipeline and to have a strong impact on code performance.

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Commercial CFD in the Service of Industry: The First 25 Years

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Summary This paper traces the development of Computational Fluid Dynamics (CFD), from its beginnings in the second half of the 20th Century to the present time with special emphasis on the evolution of the market for commercial codes. A discussion is provided on the reasons behind the current 'success' of commercial CFD packages and the present issues concerning the everyday use of CFD in Industry are examined. An attempt is made at providing some perspectives for its future deployment.

1 Introduction

The equations of Fluid Mechanics are a set of coupled non-linear partial differential equations known as the Navier-Stokes equations, which defy treatment by analytical methods except for a few relatively simple situations. CFD is a branch of Fluid Mechanics which deals with the solution of these equations on digital computers. Unfortunately, at moderate or high Reynolds numbers, direct solutions are not possible even on the most powerful digital computers which exist today. Therefore, CFD solves 'averaged' equations which are 'closed' by employing 'physical models' or 'hypotheses', such as turbulence models (examples include the Boussinesq hypothesis, two equation k- models, Reynolds stress models and sub-grid scale models in Large Eddy Simulation), and, as the case may be, models for turbulent combustion (prescribed probality density function (pdf), Monte Carlo based pdf transport models) and numerous others for a variety of physical processes such as heat, mass and momentum transfer between phases in multi-phase flow, radiation heat transfer, surface chemistry and so on. Because of this, CFD is often employed hand in hand with laboratory experiments and field data to arrive at successful engineering design and development solutions.

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2 Brief History and Background

Perhaps one of the most important milestones in the evolution of modern Computational Fluid Dynamics is the formation of group T-3 at the Los Alamos Scientific Laboratory in 1958. Most the numerical methods that are used today, such as the Particle-in-Cell, Marker-and-Cell, Arbitrary-Eulerian-Lagrangian methods as well as the k-model for turbulence have their roots in the models developed at Los Alamos in the period 1958-1967 [Johnson, 1996]. A second important milestone is the work of Spalding and co-workers at Imperial College London between mid-1960's and late 1970's, where applications to combustion problems were at the focal point. Their work led to very significant advances in both numerical techniques such as the SIMPLE algorithm and also in physical models such as Eddy-Break-Up model of combustion and the refined form of the k-turbulence model which is widely used even today [Spalding, 1999]. Mean-while, the First AIAA CFD conference held in Palm Springs in 1973 paved the way for the introduction of CFD into the aerospace industry and provided the impetus for the development of a broad class of techniques for compressible flow.

2.1 The First 10 Years

In spite of the very limited computing resources that were available during the 1970's and early 1980's, academic interest in CFD and the increasing awareness of it in the engineering community led, in the early part of the 1980's, to the emergence of general purpose, commercial CFD products such as PHOENICS from CHAM Ltd., FLUENT from Fluent Inc., and FIDAP from Fluid Dynamics International, Inc.

The inability to get support from the Imperial College in London for the commercialization of his CFD codes was one of the driving reasons for D. B. Spalding to form CHAM Ltd in 1974. CHAM initially developed and sold niche CFD codes to Industry. However, maintaining multiple CFD codes did prove to be troublesome, so in 1980 CHAM began to consolidate the functionality of its many codes into a single one called PHOENICS (Parabolic, Hyperbolic or Elliptic Numerical Integration Code Series). At the same time that CHAM released PHOENICS, a group of researchers at Sheffield University, UK led by J. Swithenbank obtained financial support from a New Hampshire based technology consultancy company Creare to develop the first versions of the FLUENT code. FLUENT became commercially available in October 1983. A third early player in the commercial CFD arena was FIDAP (Fluid Dynamics Analysis Package), developed by M. Engelman which was commercially available at the end of 1982.

Commercial CFD products in the early 1980's were of both Finite Volume and Finite Element variety. Problem size was limited to 10,000 cells or elements. Grids were hand made. Solutions were mostly to steady state problems. Finite Volume Methods could accommodate complicated physics,

had fast turnaround times but were largely limited to structured, multi-block meshes. Finite Element Methods on the other hand could represent the geometry faithfully using unstructured meshes, interface with CAD packages, but had slower turnaround times. In so far as computing resources were concerned, supercomputers and mainframes reigned, vector rather than parallel computing prevailed, computational times were the major bottleneck and memory was extremely limiting (Cray XMP 16-32Mb), Perkin Elmer 3205 minicomputer 1 Mb).

Towards the end of the 1980's, other CFD codes entered the commercial marketplace such as in 1989 TASCflow from Applied Scientific Computing, a company founded by G. Raithby and his students in Canada, Flow-3d later CFX from UKAEA with its first sale in 1987, Star-CD from Computational Dynamics, a company founded by D. Gosman and R. Issa in partnership with ADAPCO, a US company based in Long Isand, New York, which became available in 1989.

According to SGI's applications catalog, in the beginning of the 1990's, there were 18 commercial CFD codes competing in a market the size of which was no more than $30 million often making exaggerated claims regarding their capabilities and their competitors lack thereof. The following quotation from Celik [Celik, 1993] is a fair summary of the situation in the commercial CFD market at that time: "*Computational Fluid Dynamics (CFD) has established itself as a viable technique for performing research and solving engineering problems, and when used correctly, can give accurate results for many fairly complex problems. This success has lead to an ever increasing number of journal publications, many code developers and surprisingly many users in industry. Commercial CFD packages are often marketed by claiming that a particular code can solve almost every fluid flow problem, while many users, both in industry and academia, stand aloof from quantitative error measures, instead being dazzled by colorful computer generated output.*"

2.2 The 1990's

During the 1990's, very significant gains in computing power and modeling technology revolutionized CFD analysis. In general, large scale utilization of commercial CFD codes by industry resulted from the dramatic changes which took place in numerical methods, modeling processes, geometric detail and the hardware revolution, all resulting in massive improvements to accuracy and turn-around-time. With this, the profile of the CFD users also changed from researchers who were themselves developers, to engineers at R&D departments who were fluid dynamicists. In this period, workstations and UNIX servers reigned; PC/NT emerged as a viable platform and low end workstations outperformed the super-computers of 1980's (HP K-class/CRAY XMP = 50:1). Parallel processing for faster turnaround with 4-8 processors became typical with the high-end at 64-128. Good scalability was achieved on UNIX and on NT. Computational times became less of a limiting factor.

The 1990's also saw very important advances in CFD technologies which made their way into commercial codes. First and foremost in this category, was the adoption of unstructured meshes into commercial Finite Volume codes. Both automated tetrahedral meshes and unstructured hexahedral meshes – with other element types handling degenerate cell faces – were introduced. Parallelism was built into the foundation of most codes allowing the handling of more realistic simulations. Techniques were introduced to cope with mesh motion and mesh layering/de-layering needed for modeling reciprocating machinery. Powerful algebraic multi-grid methods and coupled solvers allowed CFD to achieve high degrees of computational efficiency and robustness. There was also continuing and ongoing improvement of the many physical models needed for a successful CFD simulation.

An insight into the improvements in the CFD customer's productivity can be gained by tracking the performance of a standard FLUENT benchmark over a period of 10 years (from 1995 to 2005). This shows that during this period, the hardware speed improved by roughly a factor of 100 (following Moore's Law of performance doubling roughly every 18-24 months). In addition, the algorithmic efficiency of the CFD solver also increased by a factor of 3.5 (due to performance tuning of the CPU intensive parts of the code). The main message is that dramatic improvements in CFD code performance has been the result of a happy marriage of hardware gains, improved methods and software engineering. It is anticipated that this performance improvement trend will continue for the foreseeable future as hardware improvements will continue to follow Moore's Law. (To put this in perspective, Kawaguti obtained a solution to the problem of flow past a circular cylinder at a Reynolds number of 40, by working 20 hours per week for 18 months using a mechanical hand calculator in 1953 [Kawaguti, 1953]).

2.3 The Present

In spite of its inherent limitations, commercial CFD has found widespread use not only in industry but also at universities and other research establishments. Although academic institutions continue to be the well-spring for 'models' and 'methods' that are used in commercial CFD, very few academics develop their own CFD software today, and those who do are involved with 'high-end' applications such as DNS or LES. (It can be argued that the widespread use of CFD stimulated the development of better physical models because these could be implemented in CFD codes and hence verified). There are many factors which contributed to this 'success'. One can mention improvements in representing complicated geometries via unstructured meshes, or increased solution speed and accuracy or the development of reliable physical models. But perhaps the most important reason is that the CFD community understood what to expect or not to expect from CFD [Weber et al., 1995]. The following quotation [Pelletier, 1998] provides an excellent example of the changing attitudes towards commercial CFD in the 1990's: "*Commercial CFD has reached*

maturity. Increasing number of industrial companies rely on commercial software to meet their CFD needs. Number of papers in research conferences, presenting new algorithms is on the decline. Even academic code developers are using commercial software to verify their codes. It is no longer possible to teach CFD the traditional way. Instead we should teach our students how to use commercial CFD codes".

In today's market place there are number of commercial codes of both general and special purpose. General purpose codes such as FLUENT and CFX from ANSYS, STAR-CD from CD-Adapco, CFD++ from Metacomp Technologies and CFD-ACE+ from the ESI Group, which embody a wide spectrum of physical models capable of addressing a variety of problems encountered in many branches of engineering. Special purpose codes, on the other hand, are codes which are primarily targeted to vertical applications. These include Flotherm from Flomerics Group and IcePak from ANSYS for electronics cooling applications, Moldflow Corporations code suite for injection molding, Numeca Int.'s Fine/Turbo for the simulation of rotating machinery flows, FIRE from AVL-LIST GmbH for internal combustion engines, Flow-3D from Flow Science for free surface applications, the lattice-Boltzmann solver PowerFLOW from Exa (largely used for low speed external flow modeling) and POLYFLOW from ANSYS for die extrusion and blow molding problems. Today CFD is one of the fastest growing branches of Computer Aided Engineering with a market size of around $500 Million and double digit rates of growth

It is the opinion of the present authors that the first phase of adoption of CFD by industry has been completed in the final decade of the 20th Century. We now have to look to the future.

3 The Next Phase

In the next phase, we shall see CFD tools being used more and more by engineers who are involved in the day to day design of engineering equipment or processes. The following quote from a recent authoritative reference is presented in support of this view: "*In industry, CFD has no value of its own. The only way CFD can deliver value is for it to affect the product. To affect the product, it must become an integral part of the engineering process for the design, manufacture and support of the product. To make CFD an integral part of the Product Development and Support engineering processes, it must get into the hands of engineers who execute these processes. CFD developers and 'expert' users can certainly contribute, but are only a part of the engineering process*". [Johnson et al., 2003].

It can be argued that the idea of getting CFD into the hands of design engineers is not a new one, although perhaps not as a general purpose CFD tool. Two routes which have been tried and tested in this direction are products which are "Application Specific" and tools which are "Organization Specific".

There are many examples of "Application Specific" products that have done very well in the market. These products represent the application specific implementation of general purpose flow solvers. The result is the expansion of users in application niches such as electronics cooling, casting, injection moulding, and electro-magnetics. The commercial success of these products suggests that there is demand for "easy to use" application specific simulation tools. On the other hand, there seems to be only a handful of these niches where the applications are deep enough vertically, at least at the present time, to justify the costs of development, maintenance and support.

Organization specific tools, on the other hand, are templates which have been automated and tailored for specific applications; tailored meaning either out of the box or customizable by experts at customer site. They have to be robust as a tool and amenable to "robust analysis", in the sense that we need to take the human out as a possible source of error and inefficiency. The simulation tool must provide accuracy metrics and sensitivity information. The disadvantage here is that these tools are 'custom' tools which are relatively expensive to maintain.

The above solutions for taking CFD to the design engineering community do not bring anything new to the way we do CFD, except packaging existing technologies in a special way. The challenge for commercial CFD vendors is to get more engineers to use CFD techniques to obtain useful results better and faster. This will require much more than packaging or workflow improvements. CFD usage in the 21st Century will require different paradigms of 'ease of use' than we were used to in the last century, with increasing emphasis on the quality and reliability of results. Certain processes such as geometry acquisition, mesh generation and solution control will have to be automated. Error estimation, interval analysis and design optimization will gain importance.

3.1 Geometry Creation and Mesh Generation

Two of the most difficult issues in CFD for design are those of geometry preparation for analysis and mesh generation. Unfortunately, the CAD packages which are used by industry to generate design drawings pay very little attention to the needs of CFD. Geometries provided by CAD almost always have to undergo tedious operations to arrive at a geometry definition suitable for mesh generation.

Although there is no clear cut answer to the problem of geometry import, one method of tightly integrating with a CAD system is to embed the CFD software directly into the CAD system's graphical user interface (GUI) with CFD-specific GUI panels created within the CAD system. The other approach is to have the CAD and CFD programs operate independently, but share a tight data communication capability between one another. All operations, including meshing, solver setup, solution and post-processing, are performed in the CFD GUI with "behind the scenes" querying of the CAD system. Regardless of whether the CFD solution is delivered as an embedded solution, or as

a distinct application with a tight coupling to CAD, the emphasis is on the automation of pre-processing including geometric de-featuring and cleanup, and automated flow geometry extraction.

At the present moment, the geometry preparation and mesh generation phases of a CFD project can easily consume a large proportion of the overall solution time and hence remain to be the fundamental bottlenecks in industrial CFD. Conventional mesh generation procedures frequently require user intervention to control element aspect ratio, grading and skewness, and to resolve boundary layers. Further, body-fitted hexahedral meshes which tend to be the best meshes for best accuracy on a least number of mesh points, are very labor-intensive to generate. We do have the technology to generate tetrahedral (tet) meshes automatically, but the mesh counts can be considerably larger then the equivalent hex-meshes and the accuracy is not as high. An important consideration in mesh generation for CFD is the accurate resolution of boundary and shear layers. Although it is generally possible to align quadrilaterals and hexahedra with the flow direction in boundary layers if local structured meshes are used in the boundary layers, this is not possible with triangles and tetrahedra. For this reason, hybrid meshes, involving quadrilaterals or hexahedra/prisms in the boundary layer, transitioning to triangles or tetrahedra in the bulk, are a good option. The use of polyhedral meshes which are automatically generated from background tet/hybrid meshes can also lead to a good compromise between accuracy goals and solution economy.

Owing to the fact that the geometry preparation and mesh generation process can be extremely tedious and time consuming, surface wrapping methods (used as a precursor to hybrid mesh generation) and Cartesian meshing approaches, which have the potential of full automation and the capability to cope with geometry defects, are becoming attractive for many applications where engineering accuracy will suffice. Although, boundary layer resolution can always be a problem with Cartesian meshes in arbitrary geometries, approaches such as the Immersed Boundary (IB) methods, which show a lot of promise are becoming available [Mittal & Iaccarino, 2005]. The advantage of the Cartesian grid-based IB method becomes very clear for flows with moving boundaries, as the whole process of re-meshing is averted.

3.2 Numerical Methods

We see a clear trend toward the adoption of "all-speed" methods where the distinctions between high-speed and low-speed formulations and specific linearization methods are becoming indistinct. We also see the increased use of higher order methods for specialized applications such as aeroacoustics. Other trends observed are the mainstream use of solution adaptive methods and dynamic meshing for moving front/boundary problems, and the pervasive use of High Performance Computing resources, described in the following paragraphs.

Solution-based mesh adaptation methods were introduced in commercial codes in the early nineties, the primary driver being the ability to dynamically adapt the mesh to the evolving solution. Solution-adaptive meshes allow optimal use of computational resources because grid nodes (and cells) may be concentrated dynamically in areas of high gradients (and/or large errors) without the topological constraints imposed by structured meshes. In the future, we shall see increasing use of error estimation driving the solution adaption procedures. Error estimation techniques like the error transport equation (ETE) and adjoints/sensitivities are being investigated as potential fully automatic drivers for mesh adaption procedures.

Another evolution in the design of modern CFD codes is the ability to automate the dynamic mesh modification required to handle moving geometry problems in applications such as turbomachinery (pumps, compressors, turbines), mixing tanks, valves, reciprocating machinery (as in internal combustion engines) and many others. Sliding mesh techniques have evolved to handle dynamic rotating machinery problems and, more recently, these methods have been extended to include dynamic mesh movement, remeshing, layering/ delayering required for the effective simulation of time-dependent, moving geometry problems such as in-cylinder combustion and valve opening/closing events.

High Performance Computing (HPC) and parallel computing will continue to be a key enabling technology for successful CFD usage. Dual and quadcore processors are showing good performance and seeing rapid adoption in the CFD user base. Scalability to very large clusters in the range of 1024 cores or more is being driven by customers at the leading edge of HPC, where rapid turn-around time is crucial. It is increasingly easy to reach this size systems, now with quadcore processors showing good scalability and large multicore systems being on the horizon. Problem sizes for large cases are rapidly approaching the range of a billion cells or more which will require truly scalable methods and data structures such that no stage causes a bottleneck in either computing time or memory requirements (includes mesh generation, partitioning, load balancing, dynamic mesh, multigrid solver, file I/O, post processing, etc.).

3.3 Physical Models

The modeling of turbulence still remains a bottleneck in industrial CFD computations, particularly for flows involving separation, strong body forces, and other complexities. Although computationally expensive, Large Eddy Simulation (LES) is rapidly emerging as a viable approach to model challenging applications. Re-solving the near-wall region down to the viscous sub-layer is an expensive proposition since the length and time scales of near wall turbulence become rather small in that region. To overcome this, hybrid approaches which combine RANS and LES are becoming available. Of these models, Detached Eddy Simulation (DES) [Spalart, 2000] has gained widespread usage

in the industrial CFD community [Cokljat, 2002] as are methods bridging unsteady RANS (URANS) and LES using analytical closures – Scale Adaptive Simulation (SAS) [Menter, 2005]. In addition, LES is becoming an especially attractive alternative to RANS in modeling reacting flows. When compared with RANS, LES offers several unique advantages such as the ability to predict free jets, swirling jets, jets in cross flow and buoyancy induced structures more accurately and without the need for adjustable constants. Also, for inherently unsteady simulations such as combustor instability and fire spread, the computational cost of LES does not greatly exceed the cost of unsteady RANS simulations.

Another open area for research is the simulation of multiphase flows. For gas-liquid flows, the resolution of interfaces remains a critical problem. Approaches based on interface tracking, volume of fluid, and level set methods [Shyy et al., 2001] have been proposed. More recently, approaches based on the lattice-Boltzmann equation have begun to appear [Seta et al., 2003]. For gas-solid flows, both discrete and continuum models are available. Two fluid models using the continuum approach are being applied successfully to simulate multi-phase turbulence [Kaufmann, A. et al., 2004]. Recently, discrete element simulations of the granular phase coupled, using empirical drag correlations to gas-phase computations, [Tsuji et al., 1993], are being increasingly employed.

3.4 Other Advanced Technologies

For CFD to be a part of the design process in industry, it must be able to do more than just provide solutions for specific configurations under specific conditions. Well established design methodologies in most organizations expect metrics such as reliability and goodness of solution from the processes they employ. Just like experimental analysis or manufacturing processes, CFD must be able to provide such information. Thus, in addition to providing the solution for a given configuration, we must also be able to supply some estimates about the errors in the solution. Secondly, most numerical solution methods typically start with fully deterministic input data and produce the corresponding output data. However, in real life engineering, there are uncertainties in most input data and the solution methodology must be able to account for this. Thirdly, often in the industrial context, analysis of a specific configuration may not typically be the main goal – instead the problem of interest may be an inverse one, we want to find the input parameters that produce the desired output.

The starting point for producing the desired additional information from a numerical procedure is the calculation of the derivatives of the solution. Methods for producing tangent solutions (i.e., derivative of the entire solution with respect to an input parameter) or solution of the adjoint problem (which can be used to determine the derivatives of a particular output quantity with

respect to all input parameters) have been developed [Jameson, 1988]. Derivatives may be determined with respect to parameters such as boundary/initial conditions, material properties, geometry or the empirical constants of a physical model. These methods can either start with the tangent or adjoint form of the governing differential equations and then discretize them or alternatively they can differentiate or create adjoint analogues of the numerical process; these quantities, in turn, can be used for optimization (e.g. shape optimization). When applied to the discretized forms of the equations, the results from a tangent or adjoint solution can be used to improve the solution process itself by providing guidance for optimal choices of solution control parameters, time-steps, grid point locations and the like [Jemcov, 2004].

4 Concluding Remarks

During the last two decades of the 20th Century, CFD has become a valuable tool in industry as a vehicle for product design and development. This was brought about by dramatic improvements in turnaround time, better accuracy and physical models as well as the ability to represent complicated geometries accurately. Most importantly, the CFD community understood what to expect (or not to expect) from CFD. The next phase of CFD development will involve a large degree of automation, with increased emphasis on reliability, quality and trust to enable more and more engineers to use this powerful tool in their work.

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High Performance Computing in Academia and Industry - An Example for a Private Public Partnership in HPC

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Summary High Performance Computing (HPC) has undergone major changes in recent years [1]. A rapid change in hardware technology with an increase in performance has made this technology interesting for a bigger market than before. These changes have also had a massive impact on the usage of HPC in industry. Changes in architecture have had an impact on how industry uses HPC and for what types of applications. The dramatic increase in performance with a drop in prizes has changed the role of HPC as a tool in industry. The High Performance Computing Center Stuttgart (HLRS) has collaborated with various industrial companies in a private public partnership for high performance computing over the last years. This contribution describes the collaboration and the changes it had to undergo in order to keep track with the changing requirements. The paper further comes up with the most important lessons learned from such a long term collaboration with industry in the field of high performance computing.

1 Introduction

HPC has undergone major changes over the last years. Most of these changes were driven by architectural issues. One can describe the major architectural changes over the last two decades in HPC in short as:

- From vector to parallel: Vector processors have long been the fastest systems available with a huge gap separating them from standard microprocessors. This gap became smaller over the years. Even though vector processors still increase their speed, providing higher performance than microprocessors, single processor speed is no longer the driving force in HPC performance. The key factor is parallelism. Looking at the currently

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fastest systems it is obvious that speed mainly comes from massively parallel concepts. The desire to fully exploit the potential of parallel architectures most recently has resulted in concepts for multi-core and many-core processors [2].

- From customized systems to commodity systems: As commodity processors caught up in speed it became simply a question of costs to move from specialized components to standard parts. As of today the number of companies building customized systems in HPC has been reduced to practically two (Cray and NEC). Every other architecture (with the notable exception of the IBM BlueGene which is a story of its own) is built from commodity parts. As of today experts in the field discuss even the usage of graphics processing units (GPUs) to build HPC systems. These parts are sold in millions of game consoles and are hence cheap.
- From single system to clusters: As systems were put together from standard parts every system could look differently using different parts. There are a number of options for processors (Xeon, Opteron, ...), networks (10GE, Infiniband, Myrinet, ...), and operating systems (Linux, Windows). This diversity went at the expense of loosing the single system look and feel of traditional supercomputers. Management of HPC systems has hence become again a difficult task.
- From standards back to specialized systems: Most recently – as standard processors have run into problems of speed and heat dissipation – new and specialized systems are developed again. The IBM BlueGene system is one example of this development. This development is about to bring architectural development for HPC experts to full cycle.

While these architectural changes unfolded we experienced a dramatic increase both in peak performance and in size of main memory of large scale systems. As a consequence we can solve larger problems and typically we can solve them faster. It should not be ignored, though, that the increasing theoretical speed is not matched by a similar increasing sustained performance. Still, today industrial users can lay their hands on systems that are on the average ten thousand times faster than systems 15 years ago. This is a chance on the one hand but it brings new questions on the other hand. In this paper we present how HLRS has teamed up with industry to bring HPC to industry. We will set out to discuss some of the questions raised by the most recent development and suggest some answers. The problems that come with massively parallel systems and specifically with petascale systems are currently beyond the scope of industrial usage and are discussed elsewhere [3, 4].

2 Dual Use: Academia and Industry

The concept of integration of computational resources into seamless environments has been around for a long time. Seamless usage of compute resources, a

simplified handling of data and users, and the notion of on demand computing are concepts that have long been discussed in academia and industry

With the introduction of the internet, high speed wide area networks and the wide spread use of computers such a vision became possible. In 1999 a new term for this old concept was introduced by Ian Foster and others [5]. They called their approach "Grid" and opened a new wave of research in the field of computational science and engineering. Their basic idea with respect to high performance computing is to make all computational resources available to all potential users. Through the concept of a Grid-middleware complexities that had inhibited the usage of these systems by non-experts were supposed to be hidden. Ease of use should lead to a better usage of systems and better access to systems.

An immediate idea that follows from such concepts is to bring high performance computers out of the academic niche it was mainly used in. There were certainly a number of large companies running HPC systems but then the Grid was supposed to allow creating a pool of resources from all fields (academic and industrial) and make them available to every one (academia and industry) in a simple way. The idea could be described as dual use of HPC resources and became rather popular with funding agencies for some time.

2.1 Potential Advantages

The main advantages of such a dual use are promoted by funding agencies. The discussion currently goes two ways:

- Reduction of costs: The argument goes that when industry can make use of academic computing resources funding costs for academia will go down. Industrial usage can be billed. The incoming funds can be used to at least partially pay for the costs of the HPC system. This reduces costs for funding agencies or helps to increase the size of systems purchased.
- Increased usage: Average usage of academic large scale parallel HPC systems is in the order of 80-85%.This is due to the fact that scheduling of resources can not achieve a 100% usage if resources are kept for large scale simulations. The argument goes that industry could use spare cycles running much smaller jobs. This could be done specifically during vacation time when scientists reduce their usage of systems.

3 A Public Private Partnership Approach

The University of Stuttgart is a technically oriented university with one of the leading mechanical engineering departments in Germany. The university has created a strong long term relationship with various companies in the region of Stuttgart. The most important ones are Daimler, Porsche and Bosch.

The computing center of the university was hence working closely with these companies since the early days of high performance computing in Stuttgart.

The computing center had been running HPC systems for some 15 years when in the late 1980s it decided to collaborate directly with Porsche in HPC operations. The collaboration resulted in shared investment in vector supercomputers for several years. Furthermore the collaboration helped to improve the understanding of both sides and helped to position high performance computing as a key technology in academia and industry. The experiment was successful and was continued for about 10 years.

First attempts of the computing center to attract also usage from Daimler initially failed. This changed when in 1995 both the CEO of Daimler and the prime minister of the state of Baden-Württemberg gave their support for a collaboration of Daimler and the computing center at the University of Stuttgart in the field of high performance computing. The cooperation was realized as a public-private partnership. In 1995 hww was established with hww being an acronym for Höchstleistungsrechner für Wissenschaft und Wirtschaft (HPC for academia and industry).

The initial share holders of hww were:

- Daimler Benz: At the time of the founding of hww Daimler Benz had decided to concentrate all its IT activities in a subsidiary called debis. So debis became the official share holder of hww holding 40% of the company.
- Porsche: Porsche took a minority share of 10% of the company mainly making sure to continue the partnership with the University of Stuttgart and its computing center.
- The University of Stuttgart: The University of Stuttgart took a share of 25% and was represented by the High Performance Computing Center Stuttgart (HLRS).
- The State of Baden-Württemberg: In order to better control the operation of such a high risk partnership the State of Baden-Württemberg – as the controlling institution of the University of Stuttgart – took a share of 25% being represented by the Ministry of Finance and the Ministry of Science.

The purpose of hww was not only to bring together academia and industry in using high performance computers but to harvest some of the benefits of such a collaboration. The key advantages were expected to be:

- Leverage market power: Combining the purchasing power of industry and academia should help to achieve better price/performance for both sides. This should hold both for purchase price and maintenance costs.
- Share operational costs: Creating a group of operational experts should help to bring down the staff cost for running systems. This should be mainly achieved by combining the expertise of a small group of people and by being able to handle vacation time and sick leave much easier than before.

- Optimize system usage: Industrial usage typically comes in bursts when certain stages in the product development cycle require a lot of simulations. Industry then has a need for immediate availability of resources. In academia most simulations are part of long term research and systems are typically filled continuously. The intent was to find a model to intertwine the two modes for the benefit of both sides.

3.1 Prerequisites and Problems

A number of issues had to be resolved in order to make hww operational. The most pressing ones were:

- Security related issues: This included the whole complex of trust and reliability from the point of view of industrial users. While for academic users data protection and availability of resources are of less concern it is vital for industry that its most sensitive data are protected and no whatsoever information leaks to other users. Furthermore, permanent availability of a resources is a must in order to meet internal and external deadlines. While academic users might accept a failure of resources once in a while industry requires reliable systems.
- Data and communication: This includes the question of connectivity and of handling input and output data. Typically network connectivity between academia and industry is low. Most research networks are not open for industry. Most industries are worried about using public networks for security reasons. Accounting mechanisms for research networks are often missing. So, even to connect to a public institution may be difficult for industry. The amount of data to be transferred is another big issues as with increasing problem size the size of output data can get prohibitively high. Both issues have been helped for by increasing speed of networks and a tendency of research networks to open up to commercial users.
- Economic issues: One of the key problems was the establishment of costs for the usage of various resources. So far no pricing for the usage of HPC system existed. The partners had to agree on a mechanism to find prices for all resources that are relevant for the usage of computers.
- Legal and tax issues: The collaboration of academia and industry was a challenge for lawyers on both sides. The legal issues had to be resolved and the handling of taxes had to be established in order to make the company operational.

Sorting out all these issues the company was brought to life and its modes of operation had to be established.

3.2 Mode of Operation

In order to help achieve its goals a lean organization for hww was chosen. The company itself does not have any staff. It is run by two part time directors.

hww was responsible for operation of systems, security, and accounting of system usage. In order to do this work was outsourced to the partners of hww.

A pricing mechanism has been established that guarantees that any service of hww is sold to share holders of hww at cost price minimizing the overhead costs to the absolutely necessary. Costs and prices are negotiated for a one year period based on the requirements and available services of all partners.

hww is controlled by an advisory board that meets regularly (typically 3 times a year). The board approves the budget of hww and discusses future service requirements of the overall company.

The partners of hww have agreed that industrial services are provided by industry only while academic services are provided by academic partners only.

3.3 Discussion of Results

As hww was introduced in 1995 we have a 13 years experience now with the concept. The company was modified, though, over the years. The main modifications are:

- Change of Partners: When Daimler sold debis, the shares of an automotive company were handed over to an IT company. The new partner T-Systems further diversified its activities creating a subsidiary (called T-Systems SfR) together with the German Aerospace Center. T-Systems SfR took 10% of the 40% share of T-Systems. On the public side two further universities were included with the four public partners holding 12.5% each.
- Change of operational model: While initially systems were operated by hww since 2002 a new model was used. Systems are operated by the owners of the systems who now only sell CPU time to hww.

These organizational changes had an impact on the operation of hww. Having replaced an end user (Daimler) by a re-seller hww focused more on the re-selling of CPU cycles. this was emphasized by public centers operating systems themselves and only providing hww with CPU time. The increase in number of partners, on the other hand, made it more difficult to find consensus.

Overall the results of 13 years of hww are positive. With respect to the expected benefits and advantages both of hww and a Grid like model the following is found:

- The cost issue: Costs for HPC can potentially be reduced for academia if industry pays for usage of systems. Overall hww was very positive for its partners in this respect over the last 12 years. Additional funding was brought in through selling CPU time but also because hardware vendors had an interest to have their systems being used by industry through hww. At the same time, however, industry takes away CPU cycles from academia increasing the competition for scarce resources. The other financial argument is a synergistic effect that actually allowed to achieve lower prices

whenever academia and industry merged their market power through hww to buy larger systems together.

- Improved resource usage: The improved usage of resources during vacation time quickly turns out to be a too optimistic view as companies – at least in Europe – tend to schedule their vacation time in accordance with public education vacations. As a result industrial users are on vacation when scientists are on vacation. Hence, a better resource usage by anti-cyclic industrial usage turns out to be not achievable. Some argue that by reducing prices during vacation time for industry one might encourage more industrial usage when resources are available. However, here one has to compare costs: the costs for CPU time are in the range of thousands of Euro that could potentially be saved. On the other side companies would have to adapt their working schedules to the vacation time of researchers and would have to make sure that their staff – typically with small children – would have to stay at home. Evidence shows that this is not happening.

The analysis shows that financially the dual use of high performance computers can be interesting. Furthermore, a closer collaboration between industry and research in high performance computing has helped to increase the awareness for the problems on both sides. Researchers better understand what the real issues in simulation in industry are. Industrial designers understand how they can make good use of academic resources even though they have to pay for them. The potential for such a solution still is high.

4 Future

A number of permanent problems remains and some new problems have shown up. These new problems are mainly related to operational procedures at industry. While 10 years ago industry in the region of Stuttgart was mainly using in-house codes we have seen a dramatic shift towards the nearly exclusive usage of independent software vendor (ISV) codes. This shift has put licensing issues and licensing costs at the center of the discussion.

One of the main other problems is that high performance computing systems increasingly are special purpose systems. With industry increasingly relying on ISV codes the gap between HPC for research and HPC for industry starts to widen. Academia and industry start to use different codes, different hardware and move into different directions for the way they want processing speed to be supplied. Nevertheless further collaboration has its potential.

4.1 Requests From Industry

Besides asking for falling costs for high performance computers the main requests from industry are:

- Ease of use: Industrial users are used to prepare their simulation jobs in a visual environment. When accessing remote HPC platforms they have to use scripts or work at the command line level to submit and manage jobs. This should change and portals for accessing HPC systems are requested.
- Fast know-how transfer: In order to harvest the potential of high performance computers research results and methods have to be transferred into industrial usage as quickly as possible.
- System flexibility: Industrial users would like to chose resources in a flexible way picking the best resources for a given simulation. Again this requires portals that show available results and potentially show the costs for an individual simulation on different available systems.
- Usage flexibility: Instead of planning a year ahead – as is the case in hww today – industry would like to work in a flexible mode. This includes requesting access to resources on a more fine granular time level.

4.2 Know-How Transfer

Know-how transfer in high performance computing is a difficult task. In order to solve a complex simulation problem mathematical methods have to be combined with algorithms from computer science and know how in usage of HPC systems. At the same time all these skills have to be integrated into the commercial environments of independent software vendors. The whole process has to be driven by end user industry.

For the automotive industry the partners of hww have come up with a solution that is extended to the whole industry including automotive manufacturers, automotive supply industry, independent software vendors and researchers in the field. A group of partners form these fields have agreed to form the Automotive Simulation Center Stuttgart (ASCS) which was established March 7th 2008 at Stuttgart. It will bring together all the expertise required to push the know-how transfer from academia to industry in the field of high performance simulations in automotive industry.

4.3 Access to Resources

Access to resources is a critical task. Industrial simulation has long moved from a batch type mode to a more interactive style. Although typical simulations still require several hours of compute time users expect to be able to easily chose the right system and then manage the running job. HLRS has developed an environment (SEGL) that allows to define not only simple job execution but a set of jobs [6]. These jobs can be run on any chosen architecture. They can be monitored and controlled by a non-expert. First results in an engineering environment for combustion optimization are promising [7].

4.4 Visualization

One of the key problems in industrial usage of HPC resources is interpretation of the resulting data. Many of these problems are similar to academic problems. The amount of data is large and three-dimensional time-dependent simulations are a specific challenge for the human eye. For industry we see an increasing need to be able to fully integrate visualization into the simulation process [8]. At the same time industrial simulation always goes hand in hand with experiments. In order to make full use of both methods the field of augmented reality has become important [9]. HLRS has developed a tool called COVISE (COllaborative VISualizaton Environment) that supports both online visualization and the use of augmented reality in an industrial environment [10]. In the future HLRS will integrate SEGL and COVISE to make usage of HPC resources even easier.

5 Conclusion

HLRS has successfully set up hww as a public-private partnership mainly with automotive industry to share HPC resources. Over time a number of problems related with such a partnership have been solved. It has turned out that both sides can benefit from such a collaboration both financially and in terms of know-how transfer. However, the use of public resources by industry brings some new problems to academia which have to be dealt with. Such usage requires new and improved techniques to support the average – typically non-experienced – industrial user. The results of a 13 year collaboration show that we still have to go a long way before we can integrate HPC systems into an industrial design process without problems. It will be even more complex to extend such a process to small and medium sized enterprizes which have so far been widely ignored. With the creation of hww HLRS has made an innovative step back in 1995. Introducing the ASCS in 2008 the next step forward has been taken and will increase both the potential of HPC usage in industry and the capability of HLRS to solve industrial simulation problems.

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Computer Hardware Development as a Basis for Numerical Simulation

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Summary Computers were conceived as a replacement for the mechanical solution of engineering applications using simple calculators. The basic idea of Konrad Zuse and John von Neumann was to automate this process by introducing programmability, i.e. the description of the sequence of execution of individual steps of a longer algorithm including the possibility of result-dependent branches and loops. In this way, a universal calculating tool of enormous power was invented. Today, the solution of engineering applications and the field of numerical simulation are the necessary prerequisites for advances in science, products and services. Computers are even more often used for non-numerical commercial and consumer applications today, which shows the universal applicability of the concept. In the following, this article concentrates on the application of computers for numerical simulation.

1 Computer Organization: The von Neumann Concept and Alternatives

From the basic concept of the programmable computer developed by John von Neumann (compare von Neumann 1945, [1]) and Konrad Zuse (compare Zuse 1993, [3]), it was logical to derive a basic computer organization consisting of four units. The **computational unit** is the place, where instructions are executed. The **main memory** contains both the program with its individual instructions and the data to be executed as well as intermediate and final results. The **input/output unit** is the interface to the human user and also contains peripheral data storage. The **control unit** is responsible for the overall control of the computer. The control unit interprets the individual instructions of the program from memory step by step.

This concept, called the **von Neumann Organization,** is independent of the different possible implementations with different technologies that have

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been used to built-up computers. This basic concept has proved to be so universal, that it has survived the growing complexity of computers from several hundred gate functions to billions of gate functions today. It has also survived the steps from one technology to another: from vacuum tube technology over magnetic core technology to semiconductor technology as the predominant technology today.

Numerous modifications to the von Neumann Organization as the basic execution model for computers have been proposed, such as associative processors, data flow machines, reduction machines and others. Associative processors and data flow machines were an attempt to merge the functions of the computational unit and the main memory and to parallelize data access either by content addressable memories (in case of the associative processor) or by associating properties for execution readiness directly to the data (in the data flow model). In case of the reduction machine, a different programming model of the functional type was modeled into the computer architecture based on the concept of the reduction of a mathematical expression.

All of the alternative execution models proposed were not successful in a broad sense in order to replace the von Neumann Organization. Hence, compatibility in the way how programs are conceived and written as well as executed on the machine today, is a prohibitor for the development of new models, even if they offer solutions to the problem of the "von Neumann bottleneck". This bottleneck is a consequence of the common use of the memory for both data and instructions, leading to the necessity of several memory accesses per single instruction execution for the instruction fetch, fetching the operands and storing the result(s). Today's von Neumann Organizations in standard microprocessors have solved this problem by the use of register-to-register execution models (load-store-architectures), eliminating most data accesses to memory and the introduction of a complex memory hierarchy including several levels of (split) caches for data and instructions.

In general, modifications to the von Neumann Organization have been made concerning the internal structure of the units as well as a parallel arrangement of the units. These modifications are described in detail in the next section. However, they have not changed the von Neumann Organization as a basic execution model.

2 Semiconductor Technology, Moore's Law, Instruction Level Parallelism and Multi-Core Technology

Since about 1965, the development of semiconductor technology and its continuing advances in shrinking the size of the individual basic computer components is the main reason for the success of the computer in all parts of daily life as well as the enormous power of supercomputer systems used for grand challenges such as the numerical simulation of airplanes, climate, weather

or the flow of blood in human vessels, just to name a few. The exponential development of semiconductor technology is best described by Moore's Law: indeed, Gordon Moore predicted in 1965 that the number of transistors available on a single integrated circuit would double every 12 to 18 months (compare Moore 1965, [2]). Shrinking the size of the individual transistor in consequence meant a proportional increase in performance of compute power, reliability and a reduction of production costs.

Figure 1 (courtesy of Intel) shows that the development of microprocessors indeed follows Moore's prediction. In 1971, the world's first microprocessor, the Intel 4004 was introduced with 2300 transistors and a clock rate of 108 kHz. The development today has produced microprocessors with more than a billion transistors and clock rates in the order of 3 GHz and above.

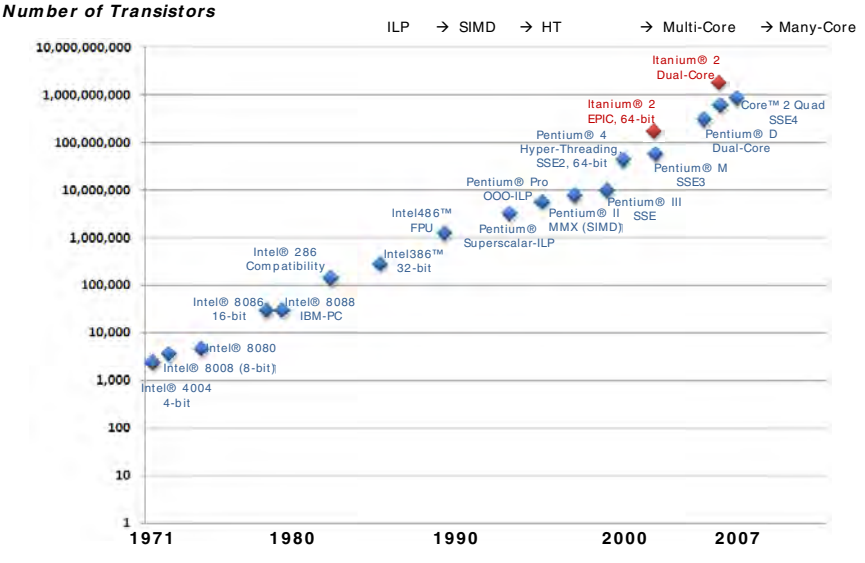

Fig. 1. Development of microprocessor architectures: exponential growth of transistor functions over time and their use for instruction level and multi-core parallelism.

In the history of computer systems, the development of compute power of microprocessors started the upcoming of PCs[1] and workstations in the early 1980s. From then, microprocessors were powerful enough to replace computer systems built from discrete devices. The consequences in the development of computer architectures were more revolutionary than evolutionary. Discrete mainframe computers as well as minicomputers, very successful for more than two decades, have disappeared and been replaced by systems based on microprocessors. In the time of computer architectures built from discrete devices, a large variety of computer architectures existed. In the early times of micropro-

[1] See page 479 for the acronyms.

cessors, the highly integrated semiconductor based counterparts of the discrete architectures were also diverse. There were memory-to-memory architectures, associative architectures, stack machines, register machines, workspace concepts and many other approaches. The value of the software developed, and the wish to port applications in the object program form from one computer to another drove the idea of *binary compatibility.*

Upward compatibility for models in a computer family means that a program that was developed for an earlier model runs without any recompilation in its object form on any later model of the family. This concept was already well known from the mainframe supercomputers, such as the IBM system/360 and /370 and was one of the reasons for the commercial success of these computer families. Regarding microprocessor technology, the trend for compatibility meant that only a small number of microprocessor instruction sets and supporting architectures could survive. Differences in system architecture then mostly came from the way how several microprocessors as well as the memory and IO components were combined into a single system.

As can be seen from Fig. 1, the large number of transistors available on a single microprocessor chip, besides increasing the word length from 4 over 8, 16, and 32 to now 64 bits, was used to support instruction level parallelism. This means that the execution of instructions of a single program is made faster by introducing different types of parallelism between the units of the von Neumann Organization. The first important step was the introduction of instruction pipelining, e. g. the synchronous execution of the machine instruction cycle for several instructions in the program sequence by individual parts of the execution pipeline.

To give an example: a first instruction stores its results in the register file, in parallel to the execution of a second instruction in the arithmetic unit, in parallel to the operand fetching process of a third instruction, in parallel to the operations code decoding of a fourth instruction and the fetching from memory of a fifth instruction. This single example shows that five instructions of a program sequence can be executed in parallel as long as no pipeline obstacles such as branches, accesses to common functional units or data dependencies are available. Of course, the principle is not restricted to a parallelism level of five. Pipelines started with a parallelism level of two with the 8086 in 1978, whereas 20 and more levels can be found in today's microprocessor architectures.

A second important change in the internal structure of the units is the availability of more than one arithmetical unit in a single microprocessor. In the so called *superscalar* arrangement, several instructions of a program may be executed in parallel by superscalar units, if there is no data dependency preventing this parallelization. Control of parallelization in superscalar systems is done by the hardware of the control unit with various mechanisms. The superscalar development started with the integration of floating point coprocessors into the microprocessor chip and continued with the provision of several – mostly specialized – units for fixed point-, floating point- and address calcula-

tion. A next step was taken with the integration of special purpose arithmetic units for graphics support, using the available word length for synchronous parallel operation on a set of pixel data (e. g. 8x8 bits in 64 bit word length) in the way of an array processor (SIMD mode: single instruction, multiple data, compare MMX: multimedia extension in the Pentium II architecture, Figure 1).

Another way to use several parallel arithmetical units is the *very long instruction word (VLIW)* approach, where parallelization is done by the compiler at compile time instead of by the hardware at run-time as with superscalar systems. This approach is also called *EPIC* in Intel's microprocessors using additional run-time hardware to dynamically schedule the parts of the very long instruction word to the arithmetical units for compatibility purposes.

Many additional techniques to circumvent obstacles in case of data dependencies, control flow dependencies and other restrictions have been implemented, such as in-order and out-of-order superscalar processing, branch target caches, branch prediction mechanisms, etc..

The use of transistors for speeding up the execution of a single program by means of different techniques of instruction level parallelism is restricted by the inherent sequentiality or data dependency within a given algorithm. Further speed-up can only be obtained by explicitly parallelizing the algorithm of a single application or by intermixing the execution threads of different applications. This is the basic idea of new forms of parallel coarse grain technologies implemented in the latest microprocessor architectures. With multithreaded processors, the possibility of executing several separate threads in a single processor architecture is supported by the implementation of several separate register files, such that a very rapid exchange in the execution from one thread to another can be obtained.

In the simplest case, first exploited by Intel's Hyper-Threading Technology, one thread executes the application, whereas the second can execute the operating system. Helper threads can even speed-up a single application, e. g. by preloading data and instructions into appropriate caches. Several variants of multithreading exist. Today's microprocessors support up to 16 threads per physical processor. Of course, multithreading hardware must be supported by a multithreading programming environment, where as an example, an optimizing compiler separates parts of a loop execution into separate threads for one single application.

Multi-core and many-core technologies implement a multiprocessor arrangement on a single chip. Several processor cores and their associated cache memories are put onto a single integrated circuit. Different solutions regarding cache architecture have been implemented including separate caches, shared caches and partly shared caches for the cores of a multi-core chip. Today's microprocessors support up to 16 cores, in the future many-core arrangements are expected with more than 128 cores. These are already available for special purpose accelerators in the graphics area.

3 Energy Efficiency as New Optimizing Target

In the past, microprocessor architectures have been developed in order to maximize compute performance. This was obtained by the help of many techniques that use many transistors to predict the behavior of the program as discussed in the section on instruction level parallelism. As each transistor consumes additional power, the power consumption of the overall microprocessor architecture increased directly proportional to the number of transistor functions. Further on, speed-up of microprocessors was strongly supported by increasing the clock frequency. Clock frequency is again directly proportional to the power consumption of the chip. In this way, single chips for microprocessors consume close to 200 watts. Since the reliability of an integrated circuit is indirectly proportional to the operational temperature, cooling is needed. With chips operating in the order of 200 watts, a limit for further power consumption was reached. Therefore, a new optimization for the design of microprocessor architectures appeared: energy efficiency or the metric of *FLOPS per watt.*

The idea of having a number of simpler processor cores that operate at lower clock frequency on a single chip under this optimization goal is more promising than the definition of a single processor with many auxiliary parallelization functions. This fact was the starting point for multi-core and many-core architectures, which are the microprocessor standard today. The question how such coarsely parallel architectures can be programmed by the general user is still open, even though the microprocessor chips are widely available. The general user can only benefit from the experience of the area of high performance computing, where parallel programming has been state of the art for quite some time.

Another contribution to energy efficiency is the use of special purpose hardware or *accelerators.* It is obvious that specialized hardware needs less transistors for the execution of a single application than the general purpose solution, which must always include some sort of redundancy. But the design of special purpose hardware is expensive and must be amortized by heavy use in the application. A good example of special purpose hardware that is heavily used in today's computers is graphics hardware. Indeed, there exist not only specialized functional units within the standard microprocessor architectures such as e. g. MMX and SSE in Intel architectures (compare Fig. 1), but also many microprocessor based systems integrate additional graphic boards to speed-up the execution of games and other types of graphical information. Thus, in most microprocessor architectures interfaces to external accelerator hardware have been integrated. The main obstacle to a broader use of such accelerators is, as in case of many-core systems, the difficulty to program such architectures, and the lack of an efficient general programming model.

4 High Performance Computer Systems for Numerical Simulation

Just as for the development of processor systems depending on technology development, the development of high performance computer systems for numerical simulation went first through the development of special purpose parallel architectures, and uses standard microprocessor components today. The development of HPC system architectures is best described in the TOP500 list[2] (compare Meuer 2008, [4]). It shows that previous to starting the TOP500 list in 1993, special purpose architectures such as SIMD architectures (array processors such as Thinking Machine's Connection Machine), associative processors and vector architectures dominated the market. After 1993, a large number of systems were built as special purpose vector machines of the Cray-type with deep arithmetical pipelines and more than a dozen vector processing units used in a superscalar way, and offering streaming of operations.

From as early as 1995 on, systems based on standard microprocessors dominated the high-end market. This is still true today. The differences in the evolution of the systems were in the use of standard special purpose interconnect structures and the arrangement of memory in shared memory, distributed memory or hierarchical arrangements. Systems consisting of a large number of processors with a special purpose interconnection structure are usually called *massively parallel processor* systems *(MPP).* Systems using standard interconnect structures such as e. g. Ethernet, Infiniband or similar are called *cluster systems.* Systems using a single shared memory are called *symmetric multiprocessor systems (SMP).* Systems with a hierarchical structure consisting of a number of shared memory SMP systems with a distributed overall memory structure are called *constellations.* In the future, the development of vector arithmetic units for microprocessor will bring back vector-oriented processing, however, not as special purpose architectures but rather inside the development of standard microprocessor systems.

Acronyms:

- EPIC: Explicitly Parallel Instruction Computing
- FLOPS: Floating Point Operations Per Second
- HPC: High Performance Computing
- IO: Input/Output
- PC: Personal Computer
- MPP: Massively Parallel Processor
- MMX: Multimedia Extension
- SIMD: Single Instruction/Multiple Data
- SMP: Symmetric Multiprocessor System

[2] http://www.top500.org/

- SSE: Streaming SIMD Extensions
- VLIW: Very Long Instruction Word

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Petaflops Computers and Beyond

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Summary In this contribution, the past technological progress in high performance computer systems is looked back from an architectural view point. Then, major technological challenges and emerging technologies in hardware and software for Petaflops systems are discussed. Those future technologies include device technologies of CPUs, interconnection technologies in hardware, and technical challenges for application development. Finally, two typical projects of Peta-scale computing systems in the US and Japan are introduced to.

1 Technical Progress for 20 Years Since the 1980s

Fig. 1 shows the performance progress of high-performance computers (HPC) since the 1980s. As this figure shows, CPU frequency and performance have increased twice every 1.5 to 2 years following the so-called Moore's law. But the increase of CPU frequency has been recently saturated due to several technical problems such as power consumption and cooling as described in a later section. On the other hand, the aggregate performance of the system has shown an increase by about 10^5 times in these twenty years. This rapid increase of system performance comes from the increase of the parallel degree of CPUs, that is, the parallelization by connecting massive CPUs with a high-speed network. The increase of the parallel degree of CPUs will continue in the future to attain the higher performance of the system. We are facing and will face several technical challenges in the hardware and software development with this higher parallelization of the system.

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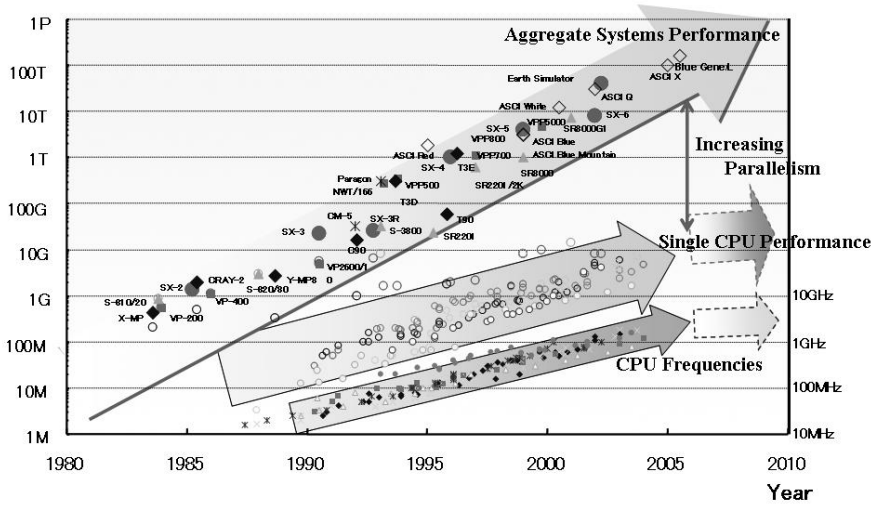

Fig. 1. Performance progress of high performance computers.

Fig. 2 shows the transition of computer architecture in HPC since the 1960s. The CPU architecture in the 1960s was the so-called scalar type in which an instruction handles a single datum, and the system consisted of a CPU connected to a main memory. In this configuration, the optimization of applications owes to the optimization of the compiler, that makes full use of the system or CPU architecture. The application developers were not necessary to know the details of the characteristics of the machine architecture. In the mid 1970s, Cray-1 was developed and introduced. Cray-1 was the first successful vector supercomputer in which a vector instruction processes a bunch of the so-called vector data in a pipelined fashion. The Cray-1 had a high frequency of 80 MHz at that time, high-speed scalar processing, and very high memory bandwidth. Because of such high-speed processing, the Cray-1 showed the extremely high speed of 10 to 100 times compared to the HPCs in those days. The Cray-1 also supported the automatic vectorizing compiler that vectorizes Fortran's DO loops not including data dependencies. In vector architectures, the tuning of applications was easy enough only to make DO loops by avoiding data dependencies. In particular, the fluid dynamics codes ran at very high-speed on Cray-1, because of its vector architecture and high memory bandwidth. The performance of particle codes and structural analysis codes in Cray-1 was not so high as the performance of the fluid dynamics codes, because Cray-1 did not support indirect access functions or list vector instructions.

From the second half of the 1980s to the 1990s, the shared memory parallel processing computers had been developed. These parallel computers supported the parallelizing compiler as well as the vectorizing compiler. Those computers had at most 16 to 32 processors, because the interconnection cir-

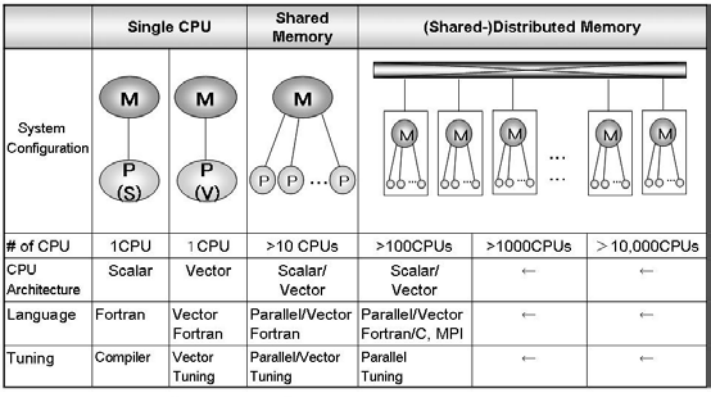

Fig. 2. Transition of HPC architectures.

cuits and wirings between processors and memory limited the number of processors and memory bandwidth of shared memory.

With the rapid progress of semi-conductor technologies and the cost-down of microprocessors, the large-scale parallel processing systems with the shared-distributed memory architecture have been introduced since the 1990s. In this shared-distributed memory architecture, a group of processors sharing the main memory is called a node, and those nodes are connected to each other by a high-speed network. Because each node does not share the main memory, a special consideration for programming is needed. In order to support this architecture, a library called MPI (Message Passing Interface) to exchange messages or data between nodes was introduced.

2 Technical Challenges and Emerging Technologies for Petaflops Computers and Beyond

2.1 Technical Challenges in Hardware

Fig. 3 shows key points required for realizing supercomputers with high sustained performance. The first is to develop high performance CPU (1), the second is to realize high speed data transfer between CPU and memory within a node (2), and the third is to obtain high speed inter-node data transfer (3).

In this section, the trends in advanced semiconductor technology and interconnection technology (within CPU; between CPU and memory; and between nodes) are described.

2.2 Trends of Semiconductor Technology

In the past, it was said that realizing CPU speed-up was heavily depended on the advancement of semiconductor's miniaturization technology. Typical examples receiving benefits from the miniaturization were performance increase

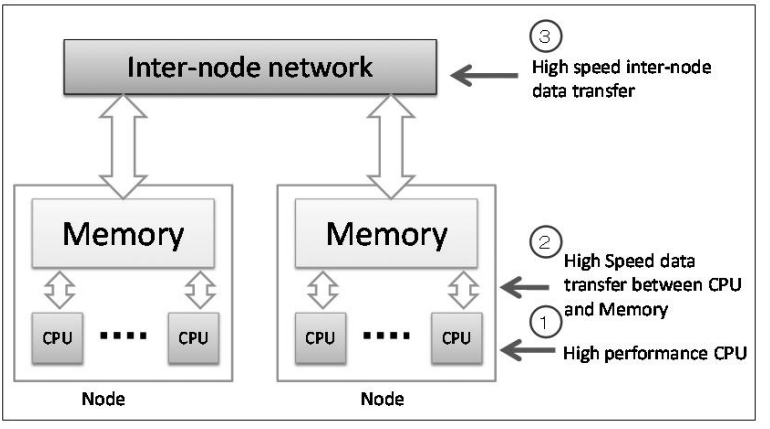

Fig. 3. Key points for realizing high sustained performance.

in transistors, propagation delay time reduction by shortening wiring length, and power reduction. However, since technology node (node: half of the minimum line pitch) was less than 90 nm, the limitation of its miniaturization has become a major concern.

Fig. 4 shows the issues related to CPU speed-up by miniaturization and considered countermeasures. The first issue is an increase of power consumption, which is derived from gate leak currents caused by adopting thin dielectric insulating layers in transistors. The second issue is an increase of wiring delay time. Though miniaturization should theoretically reduce the propagation delay, in reality it increases, because of the increases in coupling capacitance between narrower lines and the increase of resistance, that results from having narrower lines. Because of these backgrounds, further miniaturization has been no longer the case and the speed-up of clock frequency, which was considered as the only way for implementing high performance processors, has also become difficult. In order to cope with this difficulty, several new approaches, such as parallelization by using many cores established in a chip, and wiring delay time minimization within a chip, have been considered as countermeasures.

The first countermeasure is a parallelization which is the way to utilize enormous amount of surplus transistors in a chip. To attain the high performance instead of further speeding-up the clock frequency, so-called "Multi-core" approaches, which adopt not a single processor, but several processors or processor elements in a chip and use them in a parallel fashion, have been researched. Some companies have already shipped quad-core processors. A chip consisting of 80 cores, though for research purposes, has recently been demonstrated. In addition, an approach using GPUs (Graphic Processing Units), designed for a dedicated graphic processing, together with CPUs has become very popular. This is a way applying GPUs as a general purpose usage and

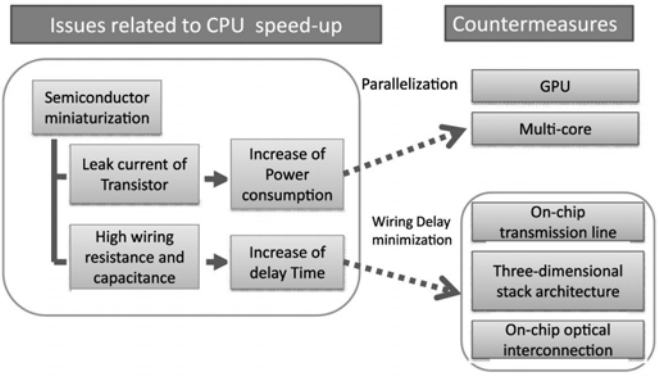

Fig. 4. Issues related to CPU speed-up and countermeasures.

is called GP GPU (General Purpose GPU). For the future, the trends of GP GPU will be powerfully advanced.

2.3 Trends of Interconnection Technology

Trends of interconnection technology within a chip

A number of studies including research on materials and architectures are underway regarding interconnection processes such as interconnection-layer fabrication, insulation-layer, and inter-layer connection. In fact, at the moment, studies are mainly concentrating on material replacement from high resistance to low (Cu), low-permittivity (low dielectric constant k) material development in order to reduce capacitance between lines, and via hole formation to construct vertical metal connections between horizontal interconnection layers. In the field of interconnection technology, research on reducing the connection length is underway. New types of connection, using light or electromagnetic waves, have been proposed for high speed transmission, [1]:

- **On-chip transmission line** A transmission line transmits a signal at the speed of an electromagnetic wave, combining high-speed signal transmission with low power consumption. A differential transmission line, which transmits a signal using the voltage difference between two signal lines, cancels external noise and reduces the amplitude of the signal. Employed for a clock line or a long-distance interconnection, the transmission line will be able to accommodate a higher frequency of processing.
- **Three-dimensional stack architecture** The three-dimensional stack architecture allows multiple Large Scale Integration (LSI) chips to be stacked and connected to each other. So far, both wired and wireless interconnection methods have been studied. Using only vertical interconnection lines, the architecture reduces the propagation delay time when compared to conventional methods. The wired architecture stacks a number of LSI chips on top of one another and connects them, using chip-buried interconnection lines. The chip-buried line carries a signal between the chips.

Pioneering applications of this three-dimensional stack architecture, that have already been constructed, include an artificial retina chip and a vision chip. The wireless method communicates between chips using inductance coupling or via an electromagnetic wave. With inductance coupling, the LSI chips communicate with each other by a magnetic field, using a pair of inductors fabricated on LSI chips. With an electromagnetic wave, the high-frequency wave propagates between LSI chips using transmitting/receiving micro-antennas. This architecture allows data transmission among multiple LSI chips, and is used for simultaneous clock- or data-signal transmission. Incorporating multiple inter-LSI chip interconnections, the three-dimensional stack architecture has the advantage of making parallel data transmission possible. This enables the high-speed communication between a CPU and a memory chip.

- **On-chip optical interconnection** Promising elemental technologies such as a silicon light guide, a photonic crystal, and a polymer light guide have been studied for applying to on-chip optical interconnection. An ultra-fast nano-photodiode (photodetector) has been demonstrated using silicon, and there are plans to apply this technique to a photoelectric transducer, though a compound semiconductor has already been used in this field. A silicon laser transmitting a continuous wave has also been demonstrated, which suggests that a photo device, where communication inside a computer is achieved at the speed of light, could possibly be made commercially available at low cost. The on-chip optical interconnection has advantages that include no interference at interconnection crossings, no cross-talk between high-density signal lines and is expected to be used for clock distribution in order to achieve high-speed processing.

Data transfer between CPU and memory, between nodes

The necessary performance (data transfer performance) of an interconnection technology in ultra high performance supercomputers is predicted as 20 *Gbps* (Giga-bits per second) for each signal in around 2010. To realize such a high performance data transfer, the development of optical transmission technology is essential, because the limitation of electric transmission is considered as 5 to 10 *Gbps* in multi-signal transmission at about dozens of *cm* distance. NEC has developed an optical transmission technology, cooperating with the Tokyo Institute of Technology, for utilization in the next generation supercomputer. They accomplished their initial goal such as "realizing more than 20 *Gbps* transmission performance for each signal" and "realizing high density package with 1000signal."

2.4 Technical Challenges of Application Development

Fig. 5 shows four major points to be considered in parallelization and tuning for application development on massive parallel processing systems. The supercomputers of the Peta-flops or Exa-flops generation will be ultra-massive

parallel computing systems, consisting of several hundreds of thousands to million processors. In order to exhibit the full capability of such an ultra massive parallel system on a specific application, the application must have sufficient parallel degree of more than the number of processors. A fluid dynamics code can generally increase the parallel degree by simply making the mesh size finer, but actually other physical phenomena will have to be considered in most of the applications. Those phenomena different from fluid dynamics will be resolved by different physical models. Inevitably, this will lead to resolving the so-called multi-physics or multi-scale problems.

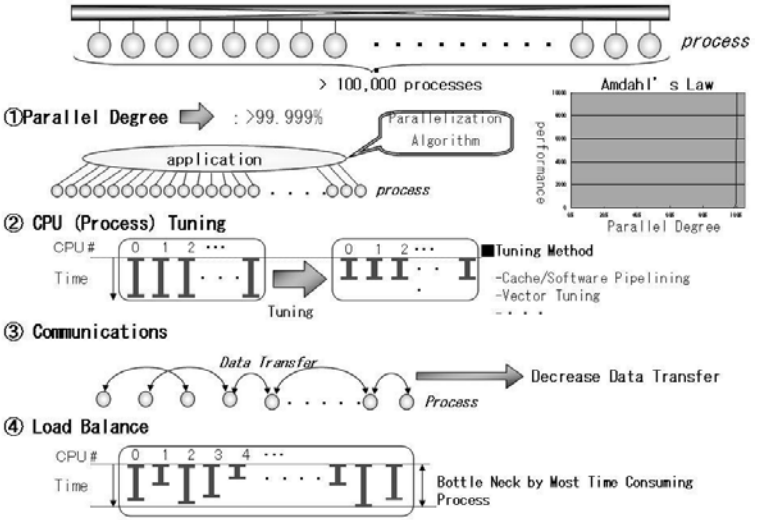

Fig. 5. Parallelization and tuning.

The next important point to be considered for tuning is a CPU or process tuning. This tuning is not limited to parallel processing, but must take much more care of the internal structure of the CPU than before, because the technical limitations have caused more complex structures of CPUs. One of the barriers for speeding-up CPU performance is the memory wall problem. The memory bandwidth has not been increased and will not be increased due to several technical limitations as already described. From an application software view point, the data transfer to/from the memory should not cause the bottleneck of the execution time on the CPU. Users must take care of reducing the required data per arithmetic operation, sometimes called *byte per flop*, as much as possible. To compensate the memory wall problem, a hierarchical memory configuration by a cache memory in the CPU will continue to be employed. A cache tuning, such that data in a cache line read out memory, can be effectively utilized, and the reuse of data in a cache can be made. For speeding-up the arithmetic operations in the CPU, the accelerator of operations like SIMD (Single Instruction Multiple Data) arithmetic units, will

also continue to be developed. The application specific accelerator, such as GRAPE, [2], that has a special arithmetic unit to calculate the force between two materials, will also be adopted to accelerate the arithmetic operations.

The next point to be considered is the communication problem among several hundreds of thousands to millions processors. To fully utilize the power of a system's arithmetic operations, the communication overheads per arithmetic operation must be reduced as much as possible. It is technically very difficult to shorten the latency time including the overhead of communication software in transferring the data from a processor to another processor. It is, therefore, more important to decrease the number of communications by grouping several data to be transferred, even if the amount of data per communication increases. Furthermore, the global data transfer, such that all processors will participate in the communication to get some results like the summation of all processors, must be avoided. This type of processing sometimes results in a serial operation due to the convergence of communications, or consumes most of the processing time for the communication. As a result, the performance increase by parallel processing makes no sense.

The last but not the least important point is the load balance. It is necessary to assign the load, or the amount of processing, to each processor equally by devising dedicated algorithms. Those algorithms will include not only to allocate the number of meshes or particles to be processed to each processor, but also to dynamically pick up and handle the process after each processor finishes a process.

3 Petaflops Projects

3.1 DARPA High Productivity Computing System (HPCS)

The High Productivity Computing Systems (HPCS) project, [3], is sponsored by the Defense Advanced Research Project Agency (DARPA) of the United States Department of Defense, with the goal of completing a prototype system by the end of 2010. The HPCS program is focused on providing a new generation of economically viable, high productivity computing systems for the national security and industrial user community. This program has initiated a fundamental reassessment of performance, programmability, portability, robustness and, ultimately, productivity in the HPC domain. The HPCS program started in 2002 and is now in Phase III, which is focused on completing a prototype system capable of sustaining multiple $Petaflops$ of performance by the end of 2010. IBM and Cray Inc. are the two vendors selected by DARPA to participate in Phase III. In the following, the Cascade system, [4], being developed by Cray is introduced.

The system configuration shown in Fig. 6 is a hybrid computing system which consists of custom compute nodes with multi-threaded and vector capabilities, and commodity x86 processors. These nodes are connected through a high-bandwidth interconnect that enables a globally addressable memory.

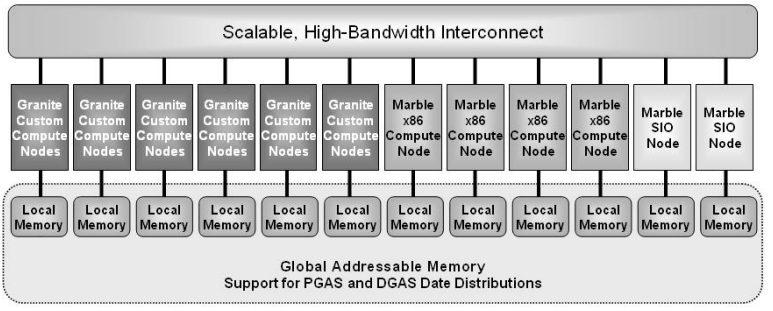

Fig. 6. Cascade system architecture.

The current HPC computers are very unproductive because: 1) it is extremely difficult to write parallel codes in MPI, 2) they lack programming tools to understand program behavior, and 3) significant time and effort to modify codes to fit a particular architecture is needed. Since application codes vary significantly in their requirements, no one architectural approach can fit all codes (one size does not fit all). The Cascade design approach, therefore, is to provide an adaptive, configurable machine, that can match the attributes of a wide variety of applications. Those applications include serial codes, and codes with SIMD data level parallelism or fine grained MIMD (Multiple Instruction Multiple Data Stream) parallelism. To ease the development of parallel codes, the system will support legacy programming models like MPI and OpenMP, improved variants such as SHMEM (Shared Memory Access Library), UPC (Unified Parallel C) and CAF (C-Array Fortran), and the new Chapel language, which provides a Global View programming model.

3.2 The Next Generation Supercomputer Project in Japan

The Japanese government selected the supercomputing technology as one of the key technologies of national importance in "The Third Science and Technology Basic Plan", which is the five year plan started from FY2006. The MEXT (The Japanese Ministry of Education, Culture, Sports, Science and Technology) has launched the Next Generation Supercomputer project, [5], in 2006, based on this governmental basic plan. The system with 10 $Petaflops$ class performance is planned to be complete in 2012.

Although this next generation supercomputer will be developed and widely used for general purpose technical applications such as fluid dynamics, structural analysis, climate modeling, fusion science, and astrophysics, one of the goals of this project is to develop major applications for the life sciences and the nano-technology, called the grand challenge applications. Those grand challenge applications with sustained peta-flops speed on the system are being developed in parallel with the system.

The system architecture was defined after careful study and analysis of several proposed system architectures. The system shown in Fig. 7 is a hybrid general purpose supercomputer consisting of a scalar and a vector unit, in which both units are connected through the front-end unit sharing huge storage units. One of the characteristics of this system is to provide the optimum computing environment for a wide range of simulations by making applications run on suitable units to utilize the computing resources in the most efficient way. The vector unit will run well efficiently for the applications that require higher memory bandwidth and large shared memory such as fluid dynamics and climate modeling codes. The scalar unit will be suitable for running the applications including particle simulation and structural analysis codes.

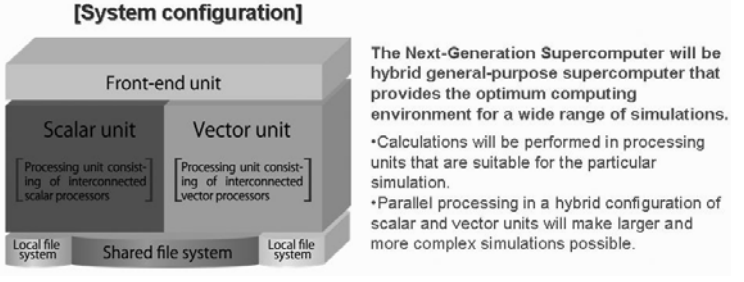

Fig. 7. Configuration of the next generation supercomputer.

The major technical challenges in the system development are to employ the-state-of-art semiconductor technology, to maximize the performance per power consumption, and to configure the highly parallel processing system by the high-speed interconnection network. The conventional programming environment with C, Fortran, MPI and OpenMP, as well as high-speed math-libraries, is planned to be supported.

Acknowledgements

The authors express special thanks to Mr. Mamoru Nakano of Cray Japan, who reviewed the Cascade system part.

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Part VI

Appendix

List of NNFM Volumes

1 Forerunner Volumes

The work of the two editors of this volume at the Institut für Angewandte Gasdynamik[1] of the Deutsche Forschungs- und Versuchsanstalt für Luft- und Raumfahrt[2] (DFVLR, now DLR) at Porz-Wahn near Cologne was largely on the development and application of discrete numerical methods of fluid mechanics in different fields. In the frame of this work several internal publications appeared – with large outside distributions – which can be considered as forerunner volumes of the NNFM series.

The first of these volumes contains contributions to a colloquium on flow processes in gas centrifuges, [1] (see also the third contribution to Part I). The volumes [2], [3], and [5] contain lectures on flow-physics and thermodynamic modelling for numerical aerothermodynamic methods which were developed during general hypersonic research at the institute and in the frame of the German ART programme (Association for Re-Entry Technologies) in the first half of the 1970s. Finally, they include the proceedings of the first two GAMM-Conferences on Numerical Methods in Fluid Mechanics, [4], [6], see the contribution by C. Weiland to Part I.

1. Krause, E., Hirschel, E.H. (eds.): Strömungsmechanische Vorgänge in Gaszentrifugen (Fluid Mechanical Processses in Gas Centrifuges). Contributions to a Colloqium at the DFVLR in Porz-Wahn, May 14, 1970. Internal publication of the DFVLR Institute für Angewandte Gasdynamik, Porz-Wahn, Germany (1970)
2. Hirschel, E.H. (ed.): Transportgrößen in der Strömungsmechanik I (Transport Properties in Fluid Mechanics I). Contributions to a Lecture Series of the DFVLR Institut für Angewandte Gasdynamik in Porz-Wahn, 1971-1972. Internal publication of the DFVLR Institute für Angewandte Gasdynamik, Porz-Wahn, Germany (1972)

[1] Institute for Applied Gas Dynamics.
[2] German Aerospace Research Establishment.

E.H. Hirschel et al. (Eds.): 100 Vol. of 'Notes on Num. Fluid Mech.', NNFM 100, pp. 493–503.
springerlink.com

3. Hirschel, E.H. (ed.): Transportgrößen in der Strömungsmechanik II (Transport Properties in Fluid Mechanics II). Contributions to a Lecture Series of the DFVLR Institut für Angewandte Gasdynamik in Porz-Wahn, 1971-1972. Internal publication of the DFVLR Institute für Angewandte Gasdynamik, Porz-Wahn, Germany (1973)
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5. Robert, K. (ed.): Nichtgleichgewichtsprobleme in der Strömungsmechanik (Non-Equilibrium Problems in Fluid Mechanics). Contributions to a Lecture Series of the DFVLR Institut für Angewandte Gasdynamik in Porz-Wahn, 1974-1975. Internal publication of the DFVLR Institute für Angewandte Gasdynamik, Porz-Wahn, Germany (1976)
6. Hirschel, E.H., Geller, W. (eds.): Proceedings of the Second GAMM-Conference on Numerical Methods in Fluid Mechanics. DVFLR, Cologne, Germany, October 11-13, 1977. Internal publication of the DFVLR Institute für Angewandte Gasdynamik, Porz-Wahn, Germany (1977)

2 NNFM Volumes from No. 1 to No. 100

Listed are all volumes – always with the full bibliographical data – which appeared in the series up to NNFM100. The NNFM label was introduced with Volume 75 in 2001 with the move of the series from Vieweg to the Springer-Verlag.

1. Förster, K. (ed.): Boundary Algorithms for Multidimensional Inviscid Hyperbolic Flows. GAMM-Workshop, Stuttgart, Germany, February 28 and March 1, 1977. Notes on Numerical Fluid Mechanics, vol. 1. Vieweg, Braunschweig/Wiesbaden (1978)
2. Hirschel, E.H. (ed.): Proceedings of the Third GAMM-Conference on Numerical Methods in Fluid Mechanics. DVFLR, Cologne, Germany, October 10-12, 1979. Notes on Numerical Fluid Mechanics, vol. 2. Vieweg, Braunschweig/Wiesbaden (1980)
3. Rizzi, A., Viviand, H. (eds.): Numerical Methods for the Computation of Inviscid Transonic Flows with Shock Waves. GAMM-Workshop, FFA, Bromma, Sweden, September 18 and 19, 1979. Notes on Numerical Fluid Mechanics, vol. 3. Vieweg, Braunschweig/Wiesbaden (1981)
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12. Schönauer, W., Gentzsch, W. (eds.): The Efficient Use of Vector Computers with Emphasis on Computational Fluid Dynamics. GAMM-Workshop, University of Karlsruhe, Germany, March 13-15, 1985. Notes on Numerical Fluid Mechanics, vol. 12. Vieweg, Braunschweig/Wiesbaden (1986)
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