UNDERSTANDING COMPLEX SYSTEMS
Springer: COMPLEXITY

Octavian Iordache

Modeling Multi-Level Systems

Springer

Springer Complexity

Springer Complexity is an interdisciplinary program publishing the best research and academic-level teaching on both fundamental and applied aspects of complex systems - cutting across all traditional disciplines of the natural and life sciences, engineering, economics, medicine, neuroscience, social and computer science.

Complex Systems are systems that comprise many interacting parts with the ability to generate a new quality of macroscopic collective behavior the manifestations of which are the spontaneous formation of distinctive temporal, spatial or functional structures. Models of such systems can be successfully mapped onto quite diverse “real-life" situations like the climate, the coherent emission of light from lasers, chemical reaction-diffusion systems, biological cellular networks, the dynamics of stock markets and of the internet, earthquake statistics and prediction, freeway traffic, the human brain, or the formation of opinions in social systems, to name just some of the popular applications.

Although their scope and methodologies overlap somewhat, one can distinguish the following main concepts and tools: self-organization, nonlinear dynamics, synergetics, turbulence, dynamical systems, catastrophes, instabilities, stochastic processes, chaos, graphs and networks, cellular automata, adaptive systems, genetic algorithms and computational intelligence.

The two major book publication platforms of the Springer Complexity program are the monograph series “Understanding Complex Systems" focusing on the various applications of complexity, and the “Springer Series in Synergetics", which is devoted to the quantitative theoretical and methodological foundations. In addition to the books in these two core series, the program also incorporates individual titles ranging from textbooks to major reference works.

Understanding Complex Systems

Founding Editor: J.A. Scott Kelso

Future scientific and technological developments in many fields will necessarily depend upon coming to grips with complex systems. Such systems are complex in both their composition - typically many different kinds of components interacting simultaneously and nonlinearly with each other and their environments on multiple levels - and in the rich diversity of behavior of which they are capable.

The Springer Series in Understanding Complex Systems series (UCS) promotes new strategies and paradigms for understanding and realizing applications of complex systems research in a wide variety of fields and endeavors. UCS is explicitly transdisciplinary. It has three main goals: First, to elaborate the concepts, methods and tools of complex systems at all levels of description and in all scientific fields, especially newly emerging areas within the life, social, behavioral, economic, neuroand cognitive sciences (and derivatives thereof); second, to encourage novel applications of these ideas in various fields of engineering and computation such as robotics, nano-technology and informatics; third, to provide a single forum within which commonalities and differences in the workings of complex systems may be discerned, hence leading to deeper insight and understanding.

UCS will publish monographs, lecture notes and selected edited contributions aimed at communicating new findings to a large multidisciplinary audience.

Octavian Iordache

Modeling Multi-Level Systems

Springer

Author

Dr. Octavian Iordache
Polystochastic
Pitfield blvd. St. Laurent 3205
H4S 1H3 Montreal
Canada
E-mail: polystochastic@bellnet.ca

ISBN 978-3-642-17945-7 e-ISBN 978-3-642-17946-4

DOI 10.1007/978-3-642-17946-4

Understanding Complex Systems ISSN 1860-0832

Library of Congress Control Number: 2011921006

Typeset & *Cover Design:* Scientific Publishing Services Pvt. Ltd., Chennai, India.

Printed on acid-free paper

9 8 7 6 5 4 3 2 1

springer.com

…his way was to carry his mind into his laboratory, and literally to make of his alembics and cucurbits instruments of thought…

C. S. Peirce

The Fixation of Belief, 1877

Preface

Modeling multi-level complex systems is the object of this book.

Complex systems are assemblies of several subsystems and are characterized by emergent behavior resulting by nonlinear interactions among subsystems for multiple levels of organization.

The complexity of numerous systems is rooted in the existence of many levels of self-organization corresponding to different time and space scales.

There is a need to provide general frameworks able to combine several scales and reality levels of the complex systems in one coherent and transdisciplinary discourse. A challenge for complex systems science and technology is to develop mathematical formalisms and modeling methods able to capture complete systems dynamics by integration of contribution at several hierarchically organized levels. Existing models involve a large number of nonlinear equations, difficult to handle analytically or numerically, and to correlate with real systems behavior. Among the open questions, we mention the definition of relevant parameters and variables to be measured at each scale or level, the study of coupling between different levels, the insufficiency of the algorithmic schema for evolvable or autonomous systems modeling.

The proposed modeling tools for multi-scale and multi-level systems are the polystochastic models, PSM. These characterize systems coming out when several stochastic processes, running at different conditioning levels, are capable to interact with each other, resulting in qualitatively new processes and systems.

Polystochastic models aim to discover and describe new structures and behaviors, which cannot be detected by one level approaches and cannot be reduced to the summation of several levels contributions.

The book is divided in 12 chapters. The chapters 1 to 4 delineate the problems and the methods. The role of multiple levels of reality for different concepts and theories of complexity is highlighted in the first chapter of the book. The relation between levels of reality and categories is emphasized.

Several mathematical methods that have been used in PSM development are briefly presented in chapter 2. This refers to “random systems”, “non-Archimedean analysis”, and “category theory”. Specific concepts as categorification and integrative closure are introduced. Categorical formulation of integrative closure offers the general PSM framework which serves as a flexible guideline for the large variety of research and multi-level modeling problems presented in the book.

Chapter 3 introduces the conventional real-field frame for PSM and some illustrative examples. Chapter 4 leads into the new PSM methodologies. The model categorification method is illustrated. The need of appropriate notions of time and probabilities and of new theoretical concepts is emphasized.

The chapters 5 to 8 are dedicated to case studies relevant to the sciences of nature.

For this part the levels are usually associated to time scales. Chapters 5 and 6 elaborate PSM for mixing and transport in single or multi-compartmental systems while chapter 7 contains a multi-scale study of dispersion and turbulence. Major applications for these chapters range from chemical engineering to pharmacology and environment.

Chapter 8 highlights entropy and entropy production roles for integrative closure conceptual framework. Application concerns entropy production for multi-scale biosystems. Based on different types of causation, new informationl entropy criteria are proposed.

The next four chapters, 9 to 12, outline the potential of the proposed multi-level modeling methods for the domain of system sciences. For this part the levels are conceptual knowledge levels or reality levels associated to categories. Chapter 9 establishes the contact of PSM with formal concept analysis. Applications include enumeration of separation flow-sheets, pharmacology, security management for information technology, and failure analysis. Diagrammatic reasoning using existential graphs is presented in chapter 10. The correlations with pragmatism and studies of continuity are emphasized.

Chapter 11 applied evolvable designs of experiments to pharmaceutical pipeline for drug discovery and development, to reliability management systems and failure analysis for printed circuits.

The connection of the presented PSM methodology with some forward-looking research directions for autonomous systems has been outlined by Chapter 12. Delineated case studies refer to autonomous experimentation, case based reasoning, beliefs desires intentions agents, organic and autonomic computing, autonomous animats, viable systems modeling, and multi-level modeling for informational systems.

Necessary elements of non-Archimedean functional analysis and category theory are presented in appendices.

The case studies analyzed in the book, represent a source of inspiration for emerging technologies in their current transition from adaptive toward evolvable and autonomous systems. They joint also recent trends advocating the convergence of disciplines and the need for transdisciplinary research for complexity. The multi-level modeling is in place at the intersection of sciences of matter as chemistry, life sciences, cognitive sciences, engineering and mathematics.

The PSM methodology presented and developed in this book is successfully confronted with an exciting field of major practical interest and a key area for future investigations, the multi-level complexity.

Contents

List of Figures

List of Tables

Abbreviations

CT-category theory

EDOE-evolvable design of experiment

EG-existential graphs

FCA-formal concept analysis

GL-Galois lattice

NA-non-Archimedean

NBIC-nano-bio-info-cogno

PSM-polystochastic model

RS-random systems

RSCC-random systems with complete connections

RTD-residence time distribution

SDG-synthetic differential geometry

SKUP-states, conditions, operators, possibilities

Chapter 1
Introduction

Abstract. A major property of complex systems is their self-structuring in multiple conditioning levels with different spatial and temporal scales.

Multi-scale and multi-level aspects for modern theories and concepts as: dissipative structures, auto-catalytic systems, catastrophes, synergetics, fractals, artificial life, complex adaptive systems, cybernetics, and biomimetic computation are revealed here.

The topic of multi-level structure of reality and its relation to the study of categories is discussed with emphasize on ontology and pragmatism.

1.1 Multi-level Systems

1.1.1 Levels and Complexity

A complex system is described as a structure or a process involving non-linear interactions among many parts and levels, which displays emergent properties. This means that the aggregate system activity is not derivable from the linear summation of the activity of individual components and that novel structure, patterns or properties arise, from interactions among parts.

A survey of the literature indicates that there is no standard definition of a complex or emergent system. However features such as hierarchy of levels, timescales, emergence, unpredictability, interconnectivity, self-organization, self-similarity, collective behavior, evolvability are focused in complexity studies (Adami 2002, Bar-Yam 1999, Kauffman S. 1995, Mainzer 1996).

Complexity is supposed to come from non-linearity and from a large number of elements with many degrees of freedom and many relationships.

A key property of complex systems is their self-structuring in conditioning levels, each of more or less homogeneous characterization.

Spatial and temporal scales may be associated to conditioning levels.

Self-organization will occur when individual independent parts in a complex system interact in a jointly cooperative manner that is also individually appropriate, such as to generate a new level organization.

Complex systems can be studied at different levels of investigation. For example we can study an industrial installation at the level of molecules or at the level of devices interactions. The number of observation levels is finite. The understanding of complexity changes with the domains of application. Some surveys consider that the complexity level has not an absolute meaning, and it is only a relative notion depending on the level of observation or abstraction. These surveys emphasize a facet of complexity as a relative concept which depends both on the task at hand and on the tools available to achieve this task.

For environmental, industrial or pharmacological systems, despite the fact that numerous physical or chemical processes are identified as complex, more of the conventional ones may be operated in regimes were multi-level complexity properties are neglected. For several centuries, physical and chemical sciences made great steps by experimenting and constructing simplified single level models of complex phenomena, deriving properties from the models, and verifying those properties by new experiments. This approach worked because the multi-level complexities ignored in that models were not the essential properties of the phenomena. It does not work when the multi-level complexity becomes the essential characteristic. In an increasing number of cases the multi-level complexity is not transient or atypical, but it is an intrinsic property of that systems.

Several examples will clarify these aspects of complexity.

Consider the moisture dispersion in soil, a first example inspired from environmental studies. Taking into account only particle movements in the inter-particle space of macro pores, simple stochastic process of moisture dispersion will result. This model corresponds to the one level approach. More detailed studies should be concerned about different levels of the real moisture transport process, after macro pores, successive scales of micro pores, restrictions for flow, and so on. In more developed environmental studies a two-state conditional process valued on the set {“wet”, “dry”}, should be taken into account on daily and on seasonal scale. The basic physical phenomenon, the moisture migration in soil, arrive to be perceived now as a multi-level complex phenomenon in which many interacting processes, at different levels of organization, evolve in a randomly changing environment. The evolvable multi-scale fluid dispersion ecosystem, self-adapting, self-creating the internal and external restrictions, is the object of the PSM studies.

The next example we will consider is the problem of modeling in industrial multi-scale systems (Fraga et al. 2006). Modeling frameworks should incorporate evolvability in order to selectively manipulate the models and to incorporate details and complexity only in those areas of the models which are critical to provide an adequate solution and remove such details and complexity were it is not. Thus we can imagine a multi-level modeling and simulation capability within which the following hold:

- A model consists of a hierarchy of layers or scales of increasing detail, complexity and sophistication, spanning the entire set of length and time scales from molecules to business chains

- Each layer or scale contains a model definition and a number of parameters
- Each layer accepts parameters from below and calculates the parameters required by the layer above
- Evolvability capabilities such as ontology, languages and agents, may be incorporated at any point to define and modify the models, parameters and solutions

Such multi-level architecture should have a number of capabilities as for instance:

- Should be flexible and extensible
- Should provide a rational and consistent basis for multi-scale models
- Should incorporate external modules, models, codes and be integrated with laboratory and plant systems
- Should allow to the user to indicate fitness for purpose
- Should ensure systems evolvability and autonomy in an environment changing at an ever-increasing rate

As another example we will consider the drug action in pharmacological systems.

The pharmacology seeks to develop a global understanding of the interactions between individual physiology and drug action. To develop such an understanding it is necessary to analyze interactions across and between various scales of organization.

The organisms should be analyzed at the levels of organs, tissues, cells or molecules. Drugs are prescribed at the organism level but exert their effect by interacting with their target at the molecular level.

As observed from these illustrative examples, the complexity of systems arises not only from the number of its components or levels but rather from the way these components are interconnected.

Non-linear interactions between different levels and scales represent a characteristic of complexity. Complex systems differ basically from complicated ones. Systems may outline complexity on both structural and on functional level. Structural complexity increases with the number of interacting subunits, the mutual connectedness among them and the degree of interactions of individual subunits. On a functional level, complexity increases with the minimum length of the algorithm from which one can retrieve the full behavior of the system. Complexity in computing science accommodates a hierarchy of conditioning levels depending on the computational time for computer programs or algorithms. The conditioning levels are determined by the structure as well as the degree of coherent cooperativeness among similar modules of the complex system.

1.1.2 Related Concepts and Theories

Since a universally accepted theory of multi-level complexity does not exists, a brief comparison with related theories sharing similar objectives with PSM, and allowing the study of multi-level systems would be of interest.

Prigogine (1980, 1989) and his group (“Brussels School”) have shown that systems far from equilibrium are able to self-organize in a hierarchical way, in

several levels. The equations of dynamics or of thermodynamics are nonlinear and drive to bifurcations. Non-linearity proves to be necessary but not sufficient for complexity. The emergence of hierarchical levels appears to be one of the possibilities. The complex system organizes itself by jumping from an equilibrium state with few hierarchical levels to another equilibrium state with more levels. By this process the system gets more complex. The resulting structures stable in space and time are called "dissipative structures" (Nicolis and Prigogine 1989). Bénard's cells and oscillating chemical reactions have been studied as examples of self-organizing processes.

In relation with the above theory, Eigen and Schuster (1979) focused on the origin of life, the domain where chemical self-organization in levels and biological evolution met. The developed concepts were that of "hypercycle", an auto-catalytic cycle of chemical reactions containing other cycles, and of "quasispecies", the fuzzy distribution of genotypes characterizing a population of quickly mutating organisms or molecules.

In the theory of so-called "catastrophes", Thom studied the mathematics of abrupt jumps from a stable steady state to another stable steady state when a control parameter is varying (Thom 1975). For a critical value of the control parameter, the complex system spontaneously jumps from one equilibrium state to another. The process of self-organization by emergence of new levels can be seen as a hierarchical catastrophe by which a system jumps into more and more hierarchical states. For critical values of control parameters, when a new configuration with new levels appears, the system will select it by stochastic mechanisms Catastrophe theory proposes classifications of the critical behavior of continuous mappings.

Haken (1983) has studied the processes of self-organization by "synergy", that is by cooperative actions of parts of a system. Results concerning the stability of systems with a large number of degrees of freedom corresponding to different levels associated to timescales and concerning the replacing of fast varying variable by time averages have been pointed in "synergetics" theory. Old structures become unstable and break down by changing control parameters. On the microscopic level the stable modes of the old states are dominated by unstable modes. The main principle in synergetics is the "enslavement principle". Due to small differences in initial conditions caused by natural fluctuations, one mode will become the master and enslaves all other modes. As a consequence, just a few order parameters are sufficient to describe the complex system. This seems to be the case in the presented here approach were one basic level induce the convergent behavior of the first, second and third levels.

In the last decades the term "fractal" coined by Mandelbrot (1982) was extensively used to describe the class of objects and phenomena, which display scale-invariance and self-similarity for different levels. Fractal identifies structures in which increasing magnification reveals increasing detail and the newly revealed structure looks the same as what one can observe at lower magnification. It was supposed that many structures and features in nature appear as fragmented and manifest properties of scaling and self-similarity. Notable examples are trees and dendrites, humidity pictures, clouds in a solution, amorphous and porous

materials, branched polymers, diffusion-limited aggregates, percolation clusters, and glasses.

General features of the multi-level organized complex stochastic systems with memory have been revealed for “self-organizing systems” theory (Kauffman S. 1995), “stochastic automata” theory ,“cellular automata” (Wolfram 1994), in “genetic algorithms” theory (Holland 1996), in “artificial neural network” theory (Carpenter and Grossberg 1987) for adaptive resonance theory, in “artificial life” theory (Langton 1989, 1990), in “complex adaptive systems”, “second order cybernetics” (von Foerster 1981) , “autopoiesis” theories (Maturana and Varela 1992), and so on. Multi-level aspects of some of the above enumerated concepts and theories will be briefly presented in what follows.

Kauffman S., (1995) has studied how networks of mutually activating or inhibiting genes can give rise to the differentiation of organs and tissues during embryological development. This led to investigate the properties of multi-level Boolean networks of different sizes and degrees of connectedness. The genetic algorithms introduced by Holland (1996) are parallel, computational representations of the processes of variation, recombination and selection on the basis of fitness that underlay most processes of evolution and adaptation. They have been applied to general problem solving, control and optimization tasks, inductive learning and the modeling of ecological systems.

The “artificial life” approach, tries to develop technological systems such as computer programs and autonomous robots that exhibit life-like properties as for instance, reproduction, swarming, and co-evolution. Based on cellular automata studies, and investigations of self-organized criticality, Langton (1989, 1990) has proposed the general thesis that complex systems emerge and maintain on the edge of chaos, the narrow domain between frozen constancy and chaotic turbulence. The "edge of chaos" idea is a step towards a general definition of multi-level complexity.

Though it shares its subject, the general properties of complex systems across traditional disciplinary boundaries, with cybernetics and systems theory, the theory of “complex adaptive systems” is distinguished by the extensive use of computer simulations as a research tool, and an emphasis on less organized systems, such as ecologies or markets. The "second-order cybernetics” is a theory developed to describe the observed and observing systems (von Foerster 1981). The emphasis on circular, self-referential processes has been continued in Maturana and Varela work on autopoietic systems. The “autopoiesis” that is the self-production denotes the fact that complex systems produce their own components. In that sense they are autonomous or "organizationally closed". For them the environment is merely a source of perturbations that need to be compensated in order to maintain the system's organization (Maturana and Varela 1992).

The “general systems theory” and the study of complex systems in various fields of human sciences testify the wide variety of hierarchical organizations (Klir 1985, Salthe 1985, Ahl and Allen 1996). It is generally accepted that there is a hierarchy of complexity in nature with more or less highly developed levels of organization. A self-organization realizing the most effects with a restricted

number of different parts was considered as the best one. One of the characteristic of the living environment in continuity with ordinary matter is the existence of multiple levels of complexity each of which is relatively homogeneous. The level of nucleic acids in molecular biology gives rise to the level of protein production, which in turn gives rise to that of membrane transport and cytoplasmic organelles that, in turn give rise to cells. Cells cooperatively exchange energy and matter giving rise to organ structure and so on. The architecture in levels is the principle that rules the building of any living systems whatever be its degree of organization. This seems to be also valid for numerous non-living complex systems having a tendency to spontaneously self-organize in hierarchical manner.

Challenging for modern science and technology is to build evolvable, autonomous or creative structures able to perform cognitive tasks specific to the living systems as for instance: data acquisition, transmission, classification and recognition, learning and oversight, computing, autonomy in various conditions, plasticity and creativity. Molecular biology and neuroscience suggest that reversible self-organization in levels, multi-scales for time and space, memory, self-adaptability to stochastic conditions, and multi-phase transition may characterize physical constructions performing cognitive tasks. Following such suggestions from biology "biomimetic" structures have been studied (Cariani 1989, 2001, Mann 1995). In the transition from small molecules to supra-molecular substances and materials, organizing processes play a major role. Small molecular building blocks with known properties lead, in the case of self-assembly processes, to complex aggregates with completely new properties at different scales or conditioning levels. On intermediary scale as the nanometer one, multi-property materials are resulting (catalytic, electronic, electrochemical, photochemical and magnetic). Complementing the experimental research for the hardware of intelligent structures, progresses in software were also reported.

The new field of "biologically inspired computing" is situated at the intersection of several sciences. Successes have been reported in the fields of data communication, control and command, drug discovery, autonomous systems and other. This joints recent trends advocating the convergence of four discipline, nanoscience, biotechnology, information technology and cognitive science known as the NBIC concept (Bainbridge and Roco 2006). This is also close to other initiatives such as organic computing (Würtz 2008) autonomic computing (Kephart and Chess 2003) natural computing (de Castro 2006), and complex systems engineering (Minai et al. 2006).

1.2 Levels of Reality and Categories

The topic of multi-level structure of reality and its relation to the study of philosophical categories and of mathematical categories is certainly not a new one.

Leibniz and Kant are among the philosophers of the past that developed a categorical system for knowledge organization in multiple levels.

More close to our time are the endeavors of Peirce (1931-1958, 1966, 1976), Whitehead (1978) and Hartmann (1952). Modern versions of the theory of levels

of reality were developed by Poli (1998, 2001), Nicolescu (2002), Herre et al. (2006), and Brier (2008, 2009).

Kant derived his categories from the analysis of the logical form of judgments.

He considered the four universal categories: "quantity", "quality", "relation" and "modality" and then divided each category in three.

Peirce proposed a first list of five philosophical categories: "substance"," quality", "relation", "representation" and "being". It should be noted that Peirce wrote about his categories over more than thirty years offering a variety of explanations and developments.

Peirce discarded "substance" and "being" from his initial list of categories and focused only on "quality", "relation" and "representation" which he called in his technical terms "firstness", "secondness" and "thirdness" respectively. They are structurally anologous to "quality", "relation" and "modality" of Kant.

Peirce describes firstness as the mode of being of that which is without reference to any subject or object. Secondness is the mode of being of that which is itself in referring to a second subject, regardless of any third subject. Thirdness is the mode of being of that which is itself in bringing a second and a third subject into relation with each other.

Thirdness brings firstness and secondness into relation with each other, and mediates between them. Thirdness is the mode of being of signs, in that signs mediate relations between their objects and their interpretants.

Firstness may be manifested by "quality", feeling, freedom, or multiplicity. Secondness may be manifested by "relation", action, reaction, causality, reality, actuality, or factuality. Thirdness may be manifested by "modality", representation, thought, continuity, order, unity, or generality. Significant is the close relationship between continuity and thirdness.

Whitehead in his study of process and reality proposed a four categorical architecture which includes "existence", "explanation", "obligation" and "ultimate" category (Heather and Rossiter 2009). Whitehead proposed also an architecture of eight categories, six of which may constitute two Peircean triads, the remaining two being principles for generating more categories. On the physical side Whitehead placed "actual entity" for firstness, "prehension" for secondness and "nexus" for thirdness. On the abstract side, Whitehead had "eternal objects" for firstness, "propositions" for secondness, and "subjective forms" for thirdness (Sowa 2000). It should be noted that the potential correlation between Whitehead and Peirce's categories is still object of studies and controversies (Guarino 2001).

To describe different ontological levels of the world's reality Hartmann (1952) considered a hierarchy of four basic ontological levels "material" or inanimate", "biological or animate", "mind-related or psychological", and "intelligent or spiritual" and emphasized the finite number of sub-levels to be taken into account at any basic level of reality.

Poli advocates the importance of levels or strata in the approaches of formal ontologies and distinguishes three ontological strata of the real world: "material", "mental or psychological" and "social" stratum (Poli 2001). These levels of reality describe different classes of phenomena and are interdependent for example the

social concept of trust depends on social entities which themselves interact in a material world. Levels of reality are characterized by the categories they use, and those categories imply a certain granularity, so that granularity appears as a derived concept.

The ontological theory of levels considers a hierarchy of items structured on different levels of existence with the higher levels emerging from the lower but usually not reducible to the latter, as claimed by reductionism. The mental and the social strata are founded in the material stratum. This means that the categories and entities of the mental and social strata can be reduced to the category of material stratum, but only with a loss of information, so the reverse is not possible. The relation between different strata is significant. Poli has stressed the need for understanding causal and spatiotemporal phenomena formulated within a descriptive categorical context for theoretical levels of reality (Poli 2007).

Nicolescu's (2002) transdisciplinarity approach is based on three pillars: levels of reality, the logic of included middle and complexity. According to the logic of the included middle, in every relation involving two separate levels of experience, there is a third level that belongs simultaneously to both. Complexity is the context in which this level of convergence takes place.

It should be emphasized that the above considerations refer mainly to philosophical categories. An open problem is to highlight the relationship between philosophical categories and mathematical categories. Introducing category theory, MacLane (1971) borrowed the word category from Kant but its concept is different from philosophical concept.

Resorting to a philosophical categories viewpoint means looking for "what is universal", either in general or in some specific domain. We could recognize here the similar claim advanced by mathematical category theory, CT, developed as a foundational theory, based on "what is universal in mathematics". This explains the search for structural analogy of categorical architectures in mathematics, philosophy and other domains.

It results from this brief literature presentation that a large number of concepts, paradigms and theories have been developed in the study of multi-level complexity. These theories are different since the multi-level complexity science problems and methods arises from many sources as for instance, nonlinear thermodynamics, solid-state physics, connectionist machines, cellular automata, artificial intelligence and life, knowledge engineering, cybernetics and systems sciences, mathematics and philosophy.

PSM is proposed as a new modeling tool for multi-level complexity, mainly for evolvable and autonomous systems investigation. The complexity will be portrayed in PSM studies using concepts such as hierarchy and conditioning levels, "real" and "other than real", that is "non-standard", time and probability algebraic frames, categorification methods and integrative closure. Conventional methods, applied in specific ways, joined new ones resulting in a distinct methodology devoted to a domain of highest scientific and technological interest, the modeling of multi-level systems.

References

Adami, C.: What is complexity? Bioessays 24(12), 1085–1094 (2002)

Ahl, V., Allen, T.F.H.: Hierarchy Theory. Columbia University Press, New York (1996)

Bainbridge, W.S., Roco, M.C. (eds.): Managing Nano-Bio-Info-Cogno Innovations: Converging Technologies in Society. Springer Science and Business Media, Berlin (2006)

Bar-Yam, Y.: Dynamics of Complex Systems. Harper Collins, Perseus Books, Reading, MA (1999)

Brier, S.: Cybersemiotics: Why information is not enough. University of Toronto Press, Toronto (2008)

Brier, S.: Cybersemiotic pragmaticism and constructivism. Constructivist Foundations 5(1), 19–39 (2009)

Cariani, P.: On the Design of Devices with Emergent Semantic Functions. Ph.D. Thesis, Binghamton University, New York (1989)

Cariani, P.: Symbols and dynamics in the brain. Biosystems 60, 59–83 (2001)

Carpenter, G.A., Grossberg, S.A.: Massively Parallel Architecture for a Self-Organizing Neural Pattern Recognition Machine. Computer Vision, Graphics and Image Processing 37, 54–115 (1987)

de Castro, L.N.: Fundamentals of Natural Computing: Basic Concepts, Algorithms, and Applications. CRC Press, Boca Raton (2006)

Eigen, M., Schuster, P.: The hypercycle a principle of natural self-organization. Springer, Berlin (1979)

Fraga, E.S., Wills, G., Fairweather, M., Perris, T.: "Smart Models" - a framework for adaptive multi-scale modeling. In: 16th European Symposium on Computer Aided Process Engineering and 9th International Symposium on Process Systems Engineering, Garmisch-Partenkirchen, Germany, pp. 457–462 (2006)

Guarino, N.: Review of Knowledge Representation, Logical, Philosophical and Computational Foundations. AI Magazine 22(3), 125 (2001)

Haken, H.: Synergetics; An introduction, 3rd edn. Springer Ser. Synergetics, vol. 1. Springer, Berlin (1983)

Hartmann, N.: The new ways of ontology. Greenwood Press, Westport (1952)

Heather, M., Rossiter, N.: Adjoint Typing: Is it Whitehead's Category of the Ultimate? In: 7th International Whitehead Conference, Bangalore, Karnataka, India, pp. 72–74 (2009)

Herre, H., Heller, B., Burek, P., Hoehndorf, R., Loebe, F., Michalek, H.: General Formal Ontology (GFO): A Foundational Ontology Integrating Objects and Processes. Part I: Basic Principles. Research Group Ontologies in Medicine (Onto-Med), University of Leipzig (2006)

Holland, J.H.: Hidden Order: How adaptation builds complexity. Addison-Wesley, Redwood City (1996)

Kauffman, S.: At Home in the Universe: The Search for Laws of Self-Organization and Complexity. Oxford University Press, Oxford (1995)

Kephart, J.O., Chess, D.M.: The vision of autonomic computing. IEEE Computer 36(1), 41–50 (2003)

Klir, G.J.: Architecture of Systems Problems Solving. Plenum, New York (1985)

Langton, C.G. (ed.): Artificial Life: The Proceedings of an Interdisciplinary Workshop on the Synthesis and Simulation of Living Systems. Addison-Wesley, Redwood City (1989)

Langton, C.G.: Computation at the Edge of Chaos: phase transitions and emergent computation. Physica D 42(1-3), 12–37 (1990)
MacLane, S.: Categories for the Working Mathematician. Springer, New York (1971)
Mainzer, K.: Thinking in complexity, the complex dynamics of matter, mind and mankind. Springer, Berlin (1996)
Mandelbrot, B.: The fractal geometry of nature. Freeman, San Francisco (1982)
Mann, S. (ed.): Biomimetic Materials Chemistry. VCH, New York (1995)
Maturana, H., Varela, F.: The tree of knowledge: The biological roots of human understanding. Shambala, Boston (1992)
Minai, A.A., Braha, D., Bar-Yam, Y.: Complex Engineered Systems.A New Paradigm. In: Braha, D., Bar-Yam, Y., Minai, A.A. (eds.) Complex Engineered Systems: Science Meets Technology, pp. 1–22. Springer, Heidelberg (2006)
Nicolescu, B.: Manifesto of Transdisciplinarity. SUNY, Albany (2002)
Nicolis, G., Prigogine, I.: Exploring Complexity. An Introduction. Freeman, New York (1989)
Peirce, C.S.: Collected Papers of Charles Sanders Peirce I-VIII, Weiss, P., Burks, A. (eds.). Harvard University Press, Cambridge (1931-1958)
Peirce, C.S.: Selected Writings (Values in a Universe of Chance), Wiener, P.P. (ed.). Dover Publications, New York (1966)
Peirce, C.S.: The New Elements of Mathematics, Eisele, C. (ed.), vol. I-IV. Mouton Publishers and Humanities Press, The Hague (1976)
Poli, R.: Levels. Axiomathes 1-2, 197–211 (1998)
Poli, R.: The basic problem of the theory of levels of reality. Axiomathes 12, 261–283 (2001)
Poli, R.: Three Obstructions: Forms of Causation, Chronotopoids, and Levels of Reality. Axiomathes 17, 1–18 (2007)
Prigogine, I.: From being to becoming. Time and complexity in the physical sciences. Freeman, San Francisco (1980)
Prigogine, I.: What is Entropy? Naturwissenschaften 76, 1–8 (1989)
Salthe, S.: Evolving hierarchical systems. Columbia University Press, New York (1985)
Sowa, J.F.: Knowledge Representation: Logical, Philosophical and Computational Foundations. Brooks-Cole, Pacific Grove (2000)
Thom, R.: Structural stability and morphogenesis. Benjamin, W.A. (1975)
von Foerster, H.: Observing Systems: Selected papers of Heinz von Foerster. Intersystems. Seaside (1981)
Whitehead, A.N.: Process and Reality. Corrected edn., Griffin, D.R., Sherburne, D.W. (eds.). Free Press, New York (1978)
Wolfram, S.: Cellular Automata and Complexity: Collected Papers. Addison-Wesley, Reading (1994)
Würtz, R.P. (ed.): Organic Computing: Series: Understanding Complex Systems. Springer, Heidelberg (2008)

Chapter 2
Methodological Resources

Abstract. Mathematical tools useful for PSM development as random systems, non-Archimedean analysis, and category theory are introduced at informal level.

Relations between model categorification and categories, the role of closure concepts as semantic closure or integrative closure for evolvability studies are emphasized.

The general PSM framework serving as flexible guideline for multi-level systems modeling is presented.

Tetradic architectures are endorsed by arguments from informatics, higher category, neurodynamics and semiotics.

2.1 Random Systems

One of the main features of complex systems is their randomness. Basic notions concerning "random systems", RS, and their utility for PSM will be presented in this section.

The so-called Markovian dependence characterizes the evolution of systems with memory restricted to the last step. Consequently Markovian models describe linear systems and cannot describe complex processes characterized by self-learning, hysteresis, instability to initial conditions and chaotic behaviors. As an attempt to treat such complex processes and systems, different extensions of the concept of Markovian dependence have been proposed.

The theory of "random evolutions", RE, has as objective the study of a significant class of RS. In this theory, random means not only stochastic inputs or initial conditions, but also random media and stochastic process in the equation of state (Hersh 1974, 2003).

PSM makes use of RE to describe phenomena in which several component stochastic process are connected by the control chain describing the random evolution of the environment that induces the switching from a component process to another. RE describe situation in which a process controls the development of

another processes, the other processes being described as operators (Keepler 1998).

This is the situation considered by the PSM in which the control process of conditions connects the component stochastic process associated to the operators.

The discrete control process determines the switching from a component process to another. Random evolutions are non-Markovian random systems if they need more than one step for memory. The connection between random evolutions, products of random matrices and random processes in random environments was studied by Cohen (Cohen 1979 a, b).

Resourceful for PSM development proved to be the "random systems with complete connections" RSCC (Iosifescu and Theodorescu 1969, Iosifescu and Grigorescu 1990). RSCC are systems formed by pairs of stochastic chain evolving in inter-related manner, allowing to model stochastic evolution. One of the two chains is Markov, typically with relatively complicated states and transition functions, while the other is a "chain of infinite order" with simpler states but non-Markovian. The later chain is used to infer properties of the more complicated Markov chain. The Markov chain includes specification of the system "states" while the second refers to "events". RSCC characterizes non-Markovian processes with infinite memory that is processes that have an evolution in which all previous states, from starting one, are significant for dynamics. Classical learning models introduced from the 50's have been later presented in the general frame of RSCC (Iosifescu and Theodorescu 1969, Norman 1972).

RSCC may be linked to the more recents "random iterated function systems", RIFS, (Barnsley 1993). These random systems demonstrated their importance in the study of fractals. For RIFS, an index process controls which function of the indexed family of functions will be operated. The index process is the control process from RE the event in RSCC or the conditions process for PSM. The family of functions in RIFS corresponds to operators in RE or to the component stochastic processes in PSM.

Another mathematical tool useful for PSM is that of "random dynamical systems", (Arnold 1998, Kifer 1998). PSM makes use of results for stochastic differential equations, random difference equations, dynamic systems approach for non-linear time series. It should be noted that frames similar to RSCC or to RIFS were reformulated several times in the last decades. Comparable mathematical objects have been introduced under different names some associated to particular additional properties others to notions proven to be similar or nearly equivalent. The chains with complete connections, chains of infinite order, learning models, RSCC, g-measures (Keane 1972), list-processes, RIFS, uniform martingales or random Markov processes, contractive Markov chains, stochastic processes in random environments, random product of operators, represents some of the theoretical frames and names for more or less similar problems and methods (Stenflo 2003). There exist so numerous comparable approaches since these type of random systems correspond to the first order cybernetics scheme that of adaptive learning, deeply rooted in biosystems behavior. The learning process is a feedback based adaptive modification of actions by repeated trials. The iterative step-by-step nature is an important feature of all learning processes and models.

The deciphering of the classical 1st order cybernetic schemes of learning in the existing random systems theories explains their frequent reformulation but also may suggest the innovative direction for the pursuit of investigations namely the area going beyond learning, adaptivity and 1st order cybernetics, towards emergence of novelty, towards evolvable, autonomous or creative multi-level systems.

2.2 Non-Archimedean Analysis

The non-Archimedean, NA, analysis represents an appropriate mathematical tool in the study of systems involving the concepts of multi-level hierarchy, scaling and self-similarity (Appendix 1). According to the axiom of Archimedes, for any two positive numbers a, b, with a being smaller than b, the continued addition of a, to itself, ultimately will yield number which are grater than b. Archimedes' axiom affirms the existence of an integer multiple of the smaller of two numbers which exceeds the greater. The informal meaning of Archimedes' axiom is that anything can be measured by a ruler.

The last decades has seen the beginning of a unity of methods and approaches starting from the hypothesis that in very complex systems, the axiom of Archimedes fails more exactly that there exists numbers a and b, having physical significance, that contradict this axiom. In such cases, a, is an infinitesimal while b is an infinite number. NA mathematics has a long history, going back in modern times to Leibniz.

Several NA constructions have been developed at the end of the 19th century (Ehrlich 2006). Despite the success of Cantor in constructing the continuum from arithmetical materials, a number of mathematicians of the late 19th and early 20th centuries remained opposed, in varying degrees, to the idea of explicating the continuum concept entirely in discrete terms. These include Peirce, Veronese, Poincaré, and Brouwer.

Studies of interest for multi-level modeling are the geometry of Veronese (1891) and the p-adic number theory due to Hensel (1905).

In physics, chemistry, engineering as in other domains, the real field R and the complex field C play the main roles. But there are a lot of other fields as the p-adic field, and the finite fields, their metrics being NA that is satisfying the strong triangle inequality instead of the usual triangle inequality. This modified triangle inequality causes important deviations from the classical real structure as the fail of the axiom of Archimedes. Initially, the NA valued fields have been investigated from an algebraic point of view. After 1940 with the introduction of simple topological notions in the field of p-adic numbers, the study of NA functional analysis begins. Some results of the real functional analysis have been obtained in a similar form in the NA area but notable differences are also accounted for instance in what concerns integral and differential equations, normed spaces and so on (Monna 1970, Narici et al. 1971, van Rooij 1978, Mahler 1981, Schikhof 1984).

Attempts, to apply NA methods in physics are not recent. The papers of Everett and Ulam (1966), van der Blij and Monna (1968), Beltrametti (1971) are pioneering papers. More recent works are motivated by advances in the theory of

spin glasses (Paladin et al. 1985, De Dominicis 1986, Rammal et al. 1986), quantum physics (Freund and Olson 1987, Frampton 1990), complex media (Blumen et al. 1986), turbulence, computer architecture, combinatorial optimization, parallel computers, and artificial intelligence.

Elements of NA are encountered in the singular perturbation methods (Lightstone and Robinson 1975, Kevorkian and Cole 1981), the fractal theory initiated by Mandelbrot (1982) and the automatic differentiation (Berz et al. 1996). NA features have been detected and studied in economy (Skala 1975, Blume et. al. 1991) decision theory (Fishburn and LaValle 1993), classification, optimization theory (Charnes et. al. 1992), and cryptography. Relatively independent research is the domain of “dyadic analysis” or “Boolean analysis” in information theory (Harmuth 1977, Bochmann and Posthoff 1981, Schipp et al. 1990).

It is from a theorem of Ostrowski that the NA valuations derive their significance (van Rooij 1978). According to this theorem each nontrivial valuation on the field of the rational numbers Q, is equivalent to the absolute value or to some NA valuation. The real and the NA metrics are the only possible metrics on Q to obtain a complete number field. This justifies affirmations as "the analysis is either Archimedean or non-Archimedean" and the need for closure methods to bring together these two types of analysis for practical purposes.

The NA study was long-time considered as an example of purely academic activity performed by specialized groups (Dieudonné 1978). However elements of the NA methods have seen a renewed general interest in the last decades, especially in mathematical physics (Rammal et al. 1986, Vladimirov et al. 1994, Varadarajan 2001).

Without any doubt, NA methods are promising tools for modeling and engineering of multi-level complex systems.

2.3 Categorical Frames

2.3.1 Introducing Category Theory

Elements of mathematical category theory are presented here in an informal way.

MacLane (1971) monograph is the reference for the formal approach (Appendix 2).

The benefits of category theory, CT, are rooted in the possibility to apply all its powerful constructions and methods to the specific problem if this is formulated in the categorical frame. There exist strong arguments in favor of utilizing category theory as foundation for cognitive sciences and modeling (Goguen 1991, MacNamara and Reyes 1994).

A category can be seen as a diagram that is a graph, where objects are the vertices of the graph and morphisms or arrows are the paths in the graphs. CT put emphasizes on morphisms that is on processes. CT highlights the relational point of view considering that everything can be defined as an arrow between objects and actually objects can be defined using only arrows. This is one of the main differences between the set theory and CT.Whereas the first focuses on describing

objects with inner structure that is separating them into parts and elements, the latter characterizes an object by its connections, focusing on the role of the object within the net of relationships.

It is possible to define a category in which the objects are categories and the morphisms are mappings between categories. The mappings between categories preserving the categorical structures, namely identities and composition, are called functors. A functor between two categories maps objects and morphisms of one category to objects and morphisms of the other in such a way that morphism between two objects is mapped to morphism between the mapped objects. Thus a functor appears as the transformation which maintains the framework of the involved categories.

A diagram commutes, if for all paths with equal domain and codomain the value of the diagram functors is equal. This expresses the fact that the results of compositions are equal. Commutative diagrams represent the categorical equivalent of a system of equations in set theory, but are more general in nature. Diagrammatic presentations provide a convenient tool to study the passage between designs and their implementations.

There exists a category in which the objects are functors. Natural transformations are morphisms between the two functors. They provide a way to switch from one mapping of a structure to another in a manner that is interchangeable with the two images of any morphism. The naturality allows holding functorial implementation together and the knowledge coherence.

Observe that the focused relationship is that between objects for categories, between categories for functors and between functors for natural transformations.

A change of structure can be modeled as a functor between the two categories modeling the structure. Deeper structure transformations can be performed by defining natural transformations between functors, which allows a reengineering of the model of a system.

The effectiveness of CT lies in the possibility of universal constructions as for instance limits, and colimits. The colimit is a formalization of assembly of objects and morphisms. A colimit for a diagram can be thought of as a structure that completes the diagram to a minimal commutative diagram containing it. The colimit puts everything together. The tool for describing putting together is called a cocone. It describes the gluing or fusion.

The category denoted by Set, has sets as objects and functions between sets as morphisms. The category Grp has as objects all the groups and maps all group homeomorphisms. The category Man has as objects all smooth manifolds and as arrows all smooth that is infinitely differentiable mapping between them.

In the category Set the colimit corresponds to the least set.

Limits are the dual notion to colimits, which is the one notion obtained from the other by reversing the arrows and interchanging initial and terminal for objects. Intuitively a limit extracts the abstraction part. Given a diagram, an element is called a limit if there are morphisms from that element to all vertices of the diagram, and if for any other element satisfying the same property there is a unique morphism from it to the limit. In the category Set the limit corresponds to the biggest set.

Limit can be seen as an emergent concept summing up in itself the properties of its constituents. This allows considering a hierarchy where at any level the objects are the limits of objects of the lower level. This may be correlated with the opinion that complexity is a relative notion depending on the level of observation. The tool to obtain limits is called a cone.

The coproduct and the product represent the categorical notions corresponding to disjoint union and to Cartesian product in the category Set. The coproduct is a special type of colimit and the product is a special type of limit. The pushout gives composition of objects having the same domain under two morphisms. The pushout is a universal property of two morphisms. The coproduct is a universal property of any set of objects.

The pullback gives decomposition of objects having the same image or codomain under two morphisms. A Cartesian closed category is one which is closed under all kinds of universal constructions for example limits, and colimits.

To any canonical construction from one type of structures to another, an adjunction between the associated categories, will corresponds. Adjoint functors are pairs of functors which stand in a particular relationship with one another. A functor can be left or right adjoint to another functor that maps in the opposite direction. A pair of adjoint functors typically arises from a construction defined by a universal property, and it can be seen as a more abstract and powerful view on universal properties.

2.3.2 Higher Dimensional Categories

The n-categories are high-order generalizations of the notion of category (Leinster 2004).

The n-categories algebra overcomes the linear thinking in mathematical modeling that is, the trend to limit the operations to those that can be expressed in terms of 1-dimensional strings of symbols.

The multi-level modeling is naturally rooted in the n-categories frames. It is the high complexity that imposes to develop higher dimensional modeling. The difficulty to study multi-level complexity is correlated to the lack of a higher dimensional theory.

An n-category is the algebraic structure consisting of a collection of objects, a collection of morphisms between objects, a collection of 2-morphisms between morphisms and so on up to n, with various coherent and practical ways of composing these j-morphisms, $j<n$. The 0-category is a set, while 1-category is a standard category. An n-category consists of 0-cells (objects, types), 1-cells (morphisms, processes), 2-cells (morphisms between morphisms, processes of processes) and so on, all the way up to n-cells together with composition operations.

As an informal example, we consider the description levels in multi-level systems that are naturally associated to specific observation scales and categories (Cruz et al. 2006). The representation of information at different resolution levels or scales can be approached in terms of n-categories and illustrative n-graphs.

An n-graph generalizes the notion of graph that is diagram of arrows. Instead of considering only nodes and links, states and transitions, and many information networks, we can consider a sequence of nested families of elements, called in this context cells.

Fig. 2.1 illustrates the n-graphs associated to a multiple scale information systems.

The reality level n=0 corresponds to the 0-categories, or 0-graphs. In real systems this may be associated to the objects or to areas of interest. They are called also 0-cells, or set of nodes.

The reality level n=1 corresponds to the 1-categories and 1-graphs. These are illustrated by directed graphs including the morphisms that is, relations between different objects or areas of interest. The morphisms are 1-cells. They are represented here by single arrows: "$\rightarrow$". The level n=2 corresponds to the 2-categories and 2-graphs. These are illustrated by graphs plus the so-called 2-cells between paths of same source and target. The 2-cells describe relations between relations or in other words modifications of relations.

The 2-cells are represented here by double arrows:" $\Rightarrow$". The reality level n=3 corresponds to the 3-categories. These are 2-graphs that include 3-cells that is, the cells between 2-cells.

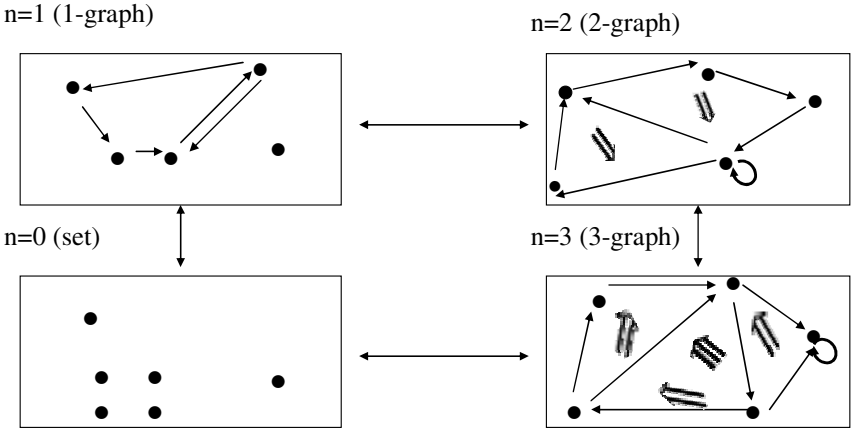

Fig. 2.1 Multiple scales networks and n-graphs

The 3-cells are represented here by triple arrows "$\Rrightarrow$". They describe 2-graphs modification or perturbation and are subjected to conditions of natural transformations. More than this level n=3, may be in theory imagined but as observed from practical case studies, just a modification of modifications for n=4 seems to not bring new information (Cruz et al. 2006, Iordache 2010).

2.3.3 Models Categorification

PSM represents an attempt to study the complex systems in which the hierarchy of conditioning levels and the stochastic self-adaptability represent the main characteristics (Iordache 1987). Concepts as multi-level hierarchy of scales and the stochastic evolution with memory, learning and adaptability, corresponding to the non-Markovian tools were naturally involved.

The PSM frame based on real field models, as developed in the monograph published in 1987, clarifies the physical mechanisms and makes possible the numerical simulation but opens, combinatorial parameter estimation and results interpretation problems. Real field detailed models are over-parameterized and in some cases it is difficult to obtain practically relevant results without extensive experiments and calculations.

New challenge has been to model the coupling of component stochastic processes not only in series but also in parallel, to describe the increasing of complexity and the learning and also the processes beyond learning as for instance the evolvability and autonomy. The interaction between multiple conditioning levels can't be appropriately studied and proven by experimental devices in which causality is restricted to a single level. For such reasons the usefulness of real field polystochastic frames appears to be limited for complex systems modeling.

To reduce the difficulties accumulated in the study of PSM, by conventional real field methods, innovative and specific methods were used in more recent works. These are recent developments of stochastic modeling methods in the setting of non-Archimedean, NA, functional analysis. Such new methods have been applied in chemical engineering and chemistry, environmental science, and system engineering (Iordache 1992). More recently, categorification methods start to be applied in PSM (Iordache 2009, 2010).

Mathematical categorification is the process of finding category-theoretic analogs of set-theoretic concepts by replacing elements with objects, sets with categories, functions with functors and equations between functions by natural isomorphisms between functors, which in turn should satisfy certain equations of their own, called coherence laws (Crane and Frenkel 1994, Baez and Dolan 1998).

The term categorification refers roughly to a process in which ordinary categories are replaced by higher categories that is n-categories. The transition in the direction of increasing n, in systems as that shown in Fig. 2.1 corresponds to categorification.

Decategorification is the reverse process of categorification. Decategorification is a systematic process by which isomorphic objects in a category are identified as equal.

The categorification methods apply to theories that add new dimensions that is new levels.

The so-called" other than real" or in other words, "non-standard" fields methods have been used as new model categorization steps for the real field models and solutions. We will consider "other than real" fields as associated to the

higher level categories going beyond real field. The use of such fields allows interpretation of the experimental data in multi-level complexity studies.

The model categorification methods were employed with a meaning inspired from mathematics and physics. Model categorification implies that the new proposed theory, for instance that for new conditioning levels, should reduce to the previous one to which it corresponds when the new theory apply in conditions for which the less general theory is known to hold. In this way, the model categorification method provides a procedure for checking the reasonability of a new theory even before new experiments are made.

A significant class of model categorizations in the considered here sense is based on infinitesimal calculus. The infinitesimals allow describing a "perturbation" or "deformation" of the existing models to attain new categorical levels (Iordache 1992).

The model categorification methods come across fundamental concepts as that of time and probability. Time is necessary to describe processes whereas probability is associated with information and entropy. Time and probabilities are related concepts since probability refers to events taking place in time.

The use of non-standard algebraic frames for time and probability represents one of the claims for effectiveness in PSM. For "other than real" modeling practice, it happens to be confronted to notions that don't have conventional real field correspondent. Also there are parts of the real field and "other than real" field models or theorems that can't be considered in model categorification so far because of the conceptual discrepancies between them. Difficulties are related to the absence of developed probability theory or measure theory on "other than real" frames, for n-category theory.

The reformulation of an infinitesimal calculus provided by NA methods does not alter the results of the conventional real calculus. The NA approaches clarifies the conceptual bases of calculus and doing so opens the way for previously unforeseeable developments, but it does not modify the results of conventional calculations. A well known example justifying the above assertion is the synthetic differential geometry, SDG.

2.3.4 Synthetic Differential Geometry

The synthetic differential geometry, SDG, valorizes the concepts of infinitesimal quantities and represents a modern validation of Leibniz thinking. As described by Leibniz, the infinitesimal is a quantity that is not necessarily equal to zero and smaller than any finite quantity.

SDG is a method of reasoning which has one of its modern roots in algebraic geometry (Grothendieck 1971) and the other in category/topos theory.

A topos is a specific kind of category with some extra properties that make it similar to the category of sets (Baez 2006). Noteworthy is the fact that the law of the excluded middle don't hold in a topos. This means, for a property P, that the

system can't be in the situation "either P or not P" as in the usual Boolean, "yes or no" logic.

Kock (2006) monograph contains a formal presentation of SDG. The monograph of Goldblatt (1979) studies categories before going on to toposes and their relation to logic (Appendix 2).

According to SDG, an infinitesimal quantity can be taken to be a straight micro segment just long enough to have a slope but too short to bend. It is an entity possessing location and direction without magnitude, intermediate in nature between a point and a Euclidean straight line. As far as time is concerned, it can be regarded as a plurality of smoothly overlapping timelets each of which may be held to represent a now and over which time is still passing. In a smooth world any interval is indecomposable in the sense that it cannot be split in any way whatsoever into two disjoint nonempty parts.

The SDG provides the conceptual background for development of a mathematically based theory of potentiality and tendency.

In conventional approaches, the life trajectory of actual items is characterized by the specific direction that it assumes at any one of its points and by the range of possibilities they have. On the other hand linelets and wavelets considered in SDG are too small to have either probabilities or directions. Instead, they have potentiality and tendency.

The aim of SDG was to describe the methodological integration that is a synthetic reasoning for differential geometry (Kock 2006, Drossos 1987).

The SDG reasoning deals with space forms in terms of their structures that are the basic geometric and conceptual constructions that can be performed on them. The SDG constructions are morphisms which constitute the base category in terms of which we work, the space forms themselves being objects of it. This category is Cartesian closed, since whenever we have two spaces A and B we can define B^A, the space of all functions from A to B.

SDG reasoning is based on a category over a natural base topos. Depending on the nature of the subject under consideration, the corresponding natural geometric form of the objects determines the natural base topos and its logic. The methodology of the analytic element wise versus the holistic structural remains the same. For example the objects of physics and chemistry have their own geometric form and corresponding logic. If the objects of the theory have a constant and crisp geometric form we may use classical logic but if the geometric form is variable and fuzzy then we have to use a non-classical more flexible logic, for example the intuitionist or in other words constructive logic.

This approach is characteristic for categorical constructivism. According to this methodology we are able to store mental representations of external objects; these internal objects do not necessarily represent the structure of the real external objects but are rather the product of the categorification and conceptualization. Therefore the own view onto the world, that is the structuring of reality via the perceived objects is primarily a categorical construct of the mind.

2.4 Closure

2.4.1 Semantic Closure

Closure concepts play a prominent role in systems theory where may be used to identify or define the whole system in correlation with its environment and to allow the autonomy of the systems.

Significant is the relation between self-adaptivity, cognitivity, intelligence and different notions of closure as encountered in systems theory: closure to efficient cause (Rosen 1991), organizational closure (Maturana and Varela 1992), catalytic closure (Kauffman S. 1993), semantic closure (Pattee 1995), and operational closure (Luhmann 1995).

These definitions refer to different facets of complexity.

For example, a system is considered catalitically closed just in case every product of the system is also a catalyst in the system (Kauffman S. 1993).

Closure does not mean that the considered system is not in contact with its environment or with other systems. Rather the term closure refers to the closed loop which connects the whole structures and the functions of individual, elementary entities or levels.

In a significant investigation of closure applicable to both real and artificial life, Pattee pointed out that the complex evolutions, requires a two-level complementary description of the material and symbolic aspects of events (Pattee 1995, 2000). Life involves a semantically closed organization between symbolic records and dynamical constraints. Symbols, as discrete functional switching-states, are seen in all evolvable systems in form of codes, and at the core of all neural systems in the form of informational mechanisms that switch behavior. Symbolic information as that contained in genotype has no intrinsic meaning outside the context of an entire symbol systems as well as the material organization that interprets the symbol for a specific function such as construction, classification control and communication. Self-reference that has evolvability potential is an autonomous closure between the dynamics-physical laws of the material aspects and the constraints-syntactic rules of the symbolic aspects of a physical organization. Pattee refers to this condition as “semantic closure” or more recently as “semiotic closure” (Rocha 2001). Semantic closure requires a separate symbolic description (genotype, design, and software) and material embodiment (phenotype, machine, and computer). The symbolic description must be capable of generating the material embodiment. Finally, the material embodiment must be capable of re-generating the symbolic description with the possibility of mutation. Cariani (1989, 2001) evaluated the semantic closure principle relation with the design of devices with emergent semantic functions. Self-modification and self-construction of own categories were recognized as important to the symbol-matter problem and as a requirement for semantically adaptive devices or evolvable ones. Temporal codes and neural pulse codes that use the time patterns of spikes to encode information appeared as potential tool for evolvable devices and for brain study.

Fig. 2.2 illustrates the concept of semantic closure for genetic systems. Two levels are considered, the genotype and the phenotype. The genotype initiates the dynamics, while the phenotype is developed by genome iterated dynamics. The environment determines the stability and reproductive activity of the genome.

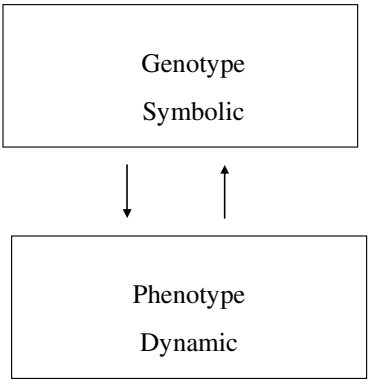

Fig. 2.2 Semantic closure

In model categorification terms, the symbolic system is at a higher level category relative to the dynamic system. The model for symbols involves "other than real", that is "non-standard" fields.

2.4.2 Two Levels Modeling

The transition from one level to multiple level modeling appears to be simple, in principle.

To describe evolution in emergent hierarchical systems, one replaces the parameters of the accepted models or theorems for "real" field systems by the "non-standard" field counterparts, and one sees at least in some cases meaningful general models, and true statements for the emergent complex systems that results.

Fig. 2.3 shows a two-levels architecture. Notice that the two levels are supposed to have different categorical organization. In some cases there appear discrepancies and this is the indication of significantly new phenomena.

In a more general context this is the general problem of closure between the experiment and theory in scientific or engineering modeling. One considers as a natural approach in science or engineering, to start from phenomena to which one may associate formal mathematical frames. Then, the predictions are tested empirically. It is a succession of theoretical and testing steps. The evolution back and forth between models and testing results, changing things on the one side and checking the effect on the other side, forms the basis of science and engineering methods. It may be a difference in language, that is in the algebraic frames for modeling and testing models and this represent one of the challenges for closure.

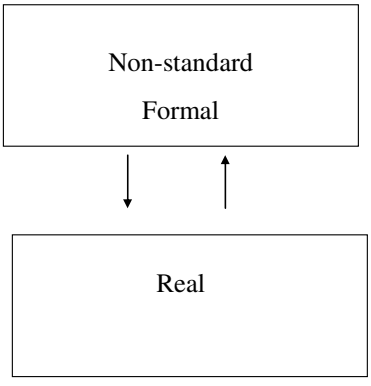

Fig. 2.3 Two-level models

The closure between experiment and theory for scientific and engineering modeling may appears as the closure of "real" field relative to "other than real" fields for models or theorems. The closure request is the need for both types of models to have a complete view for emergent complexity.

One has to make additional modifications and reinterpretations to obtain physically and mathematically adequate complete or semantically closed theories.

Required by closure methodology is an analysis involving both real-valued and "other than real" valued functions. This explains the fact that, during the PSM study, both the real valued probabilities and "other than real" that is "non-standard" probabilities continue to be associated. The attention was focused on problems not on purity of methods, surely inappropriate to the objective of study, the emergence of multi-level complexity. It should be a clear cut between mathematical frames for different categories but the natural complexity has neither pure real, nor pure "other than real" fabric. Understanding complexity should involve, real frames interacting with "other than real" ones, at different levels not privileging any one in particular.

One might ask why to support non-standard or categorification frames in the study of complexity. After all there are numerous studies of complexity that make use of real field analysis only. The involvement of non-standard and higher categories frame in PSM is not motivated by the tendency to construct unusual frames that may appears to a certain extent novel and unexpected as theories, but is imposed by the PSM objective to understand and built evolvable systems that is systems that go beyond the learning and adaptability level and may be evolvable and capable to take autonomous and creative control of their environment. The semantic advantage of making use of "other than real" frames, of higher categories in close relation with real ones is the decisive enhancement for multi-level system responsiveness, evolvability and autonomy.

2.4.3 Integrative Closure

Integrative closure appeared as the direct consequence of mutual restrictedness or exclusiveness of the new levels relative to the previous ones, and of the finite number of levels to be considered. Integrative closure approach is not looking for an identity between the philosophical and mathematical categorical viewpoints but for a structural analogy and a general methodology shared by different domains as knowledge organization, ontological problem solving or technological developments (Iordache 2010).

Significant examples of structural analogy, parallelism and recapitulation in the field of mathematics and physics have been presented by Piaget and Garcia (1989).

The starting idea for integrative closure was to reconsider the interrelated four main ontological levels in the study of nature: "material", "biological", "cognitive or psychological" and "intelligent or logical" (Hartmann 1952).

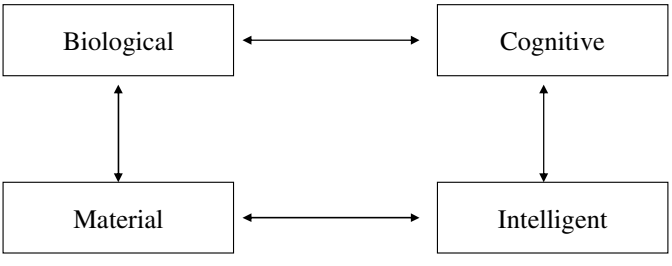

Fig. 2.4 Integrative closure network

It was acknowledged that the hierarchical structures cannot serve as general models for multi-level knowledge organization. Facing complexity the task of knowledge integration remains pertinent.

Fig. 2.4 shows an actualization of the integrative closure hypothesis as a network version of Hartmann's four levels ontological hierarchy. The traditional hierarchical structure is closed and replaced by a network.

The integrative closure aims to make ends meets, for the four levels or realms, emphasizing the hypothetical interconnection between the Hartmann's material and intelligent realms. An artificially or naturally evolvable system is supposed to cross the gap between these two levels.

Observe that a two-level modeling relation between material and intelligent realms could accomplish this closure task directly. For integrative closure the objective is not to reduce several interconnection steps to two-level interactions, as an attempt to achieve closure in the speediest manner. Contrary to these, integrative closure looks to the four interactions steps to facilitate the study and to take into account the necessary basic ingredients, as followed by the evolvable systems existing in nature.

Systems analysis may require consideration of several sub-levels for different levels of the main structure. Fig. 2.5 shows an integrative closure network with sub-levels. For this illustrative example, the biological level is described by four sub-levels: genes, cells, organisms denoted here by "org" and populations denoted by "pop".

The splitting in four sub-levels appears as natural in this illustration. It recapitulates the basic splitting of reality in four levels.

The closure aspect outlined in Fig. 2.4 or Fig. 2.5 represents a source of inspiration for emerging technologies in their transition toward evolvable and autonomous systems.

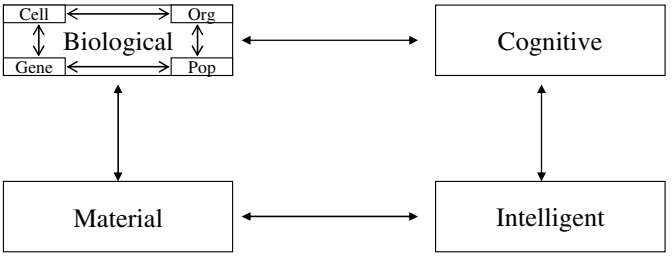

Fig. 2.5 Integrative closure network with sub-levels

Fig. 2.6 proposes an extended structural analogy that of the hypothetical integrative closure architecture including philosophical categories architectures as studied by Kant ("quantity", "quality", "relation and "modality") and Peirce ("substance", "firstness", "secondness" and "thirdeness") and to mathematical n-categories (n=0, 1, 2 and 3). We refer to such general framework as "integrative closure hypothesis" (Iordache 2010).

Fig. 2.6 emphasizes the significance of the relation of inter-dependence between the categories and also the hypothetical closure of the gap between the lowest level (n=0) and highest levels (n=3).

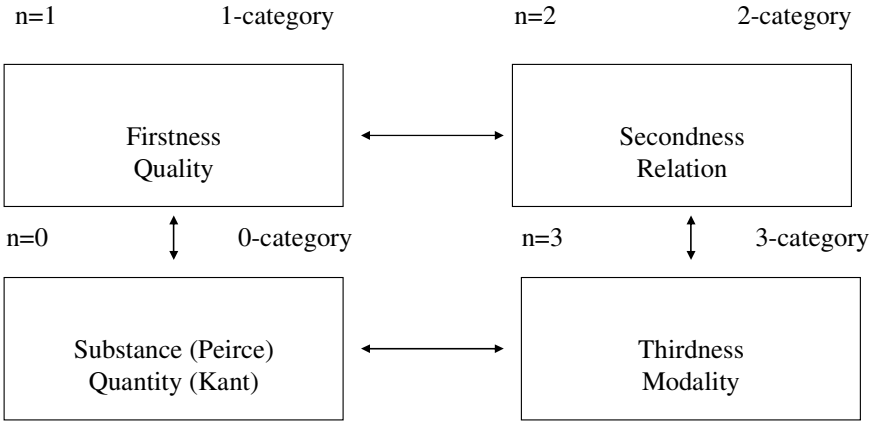

Fig. 2.6 Integrative closure for categories

Although the diagrams associated to integrative closures show four corners, they may be considered in agreement with Peirce's triadic diagrams since Peirce's objective was the architecture for metaphysics. The fact that Peirce's diagrams don't include the physics category naturally associated to 'substance" or background, explains the triadic character of such diagrams.

Adoption of the higher categorical standpoint, suggests extending the investigation to four levels or realms.

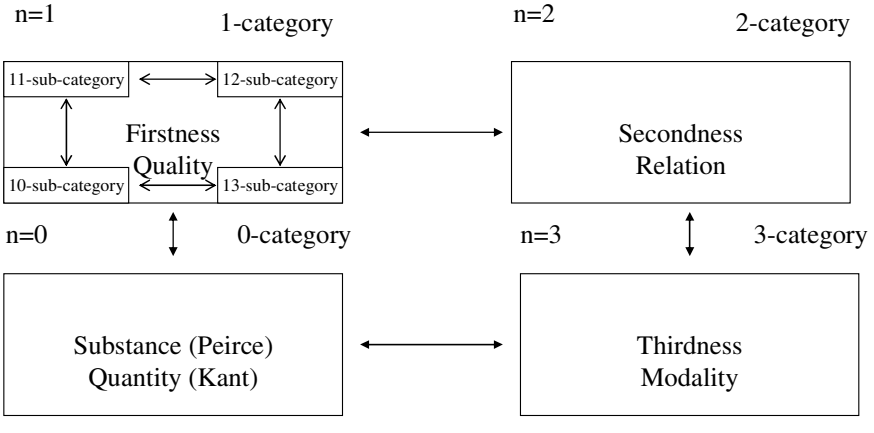

Fig. 2.7 Integrative closure for categories and sub-categories

Analysis may require taking into account of several sub-categories for each category of the main structure. For the example shown in Fig. 2.7, the 1-category reveals four sub-categories denoted here by 10, 11, 12 and 13. The splitting in four sub-categories recapitulates the basic splitting of reality in four categories.

Support for the four level architectures is offered by different domains.

A source is in data processing and neurodynamics (Cowan 2000). According to Cowan the capacity of short-term memory is limited to the number of four items to which attention can be simultaneously directed. There exists a central capacity limit of four chunks in short-term explicit memory presumably corresponding to the focus of attention. This theory assumes that attention is depending on oscillation of cortical potentials. A cortical wave of about 10 Hz is supposed to select items from a large short terms store. Other wavelets at a frequency at about 40 Hz then select one item each. Such considerations don't exclude to direct attention to more than four items or realms but the resulting processes may be transient.

As shown in Fig. 2.6 or Fig. 2.7, the four levels of reality or the four philosophical categories have been associated to the corresponding mathematical n-categories.

Implicit support for the four levels or four categories architectures in data processing is given by mathematical category theory too (Baez and Dolan 1995, Rossiter and Heather 2003). In CT, four levels are required to define morphism as unique up to isomorphism. The four levels are the objects, that is, the elements within a category, the category comparing the objects, the functors comparing categories and the natural transformation comparing the functors. These four constituents represent the categorification of the four corresponding elements in set theory namely: the elements of sets, the sets, the functions and the equations between morphisms (Appendix 2). Four levels seem to be necessary for data analysis and interoperability (Rossiter and Heather 2003). Less than four offers only local interoperability. More than four may be formally defined but yields no benefits for interoperability. The practical consequence of a framework with more levels is equivalent to alternatives of the fourth level.

Apparently complexity of n-categories rises with n dramatically. Baez and Dolan (1998) suggested the occurrence of stabilization phenomena as n increases (Appendix 2).

Limiting the study to four levels means to limit the categorical approach to 3-categories.

The four levels are associated in increasing order of complexity to 0-category that is to sets, to 1-category that is to conventional categories, to 2-categories, and then to 3-categories.

The difficulty to work with mathematical higher categories is that as the number of dimensions increases the complexity of the necessary rules to be specified increases rapidly. For 1 dimension the rules may be written down on one line, and those for 2 dimensions may be expressed in diagrams occupying a page. For 4 dimensions the diagrams are so large that they will not fit in any sensibly-sized book. The 4-category diagram techniques are as yet entirely non-existent.

The difficulty of presentation may be considered as a supplementary reason to restrict the study to 3-categories, without excluding higher categories in the long run if some other ways of approaching the theory became effective.

For the time being we focus the multi-level investigations to four levels that is, to the successive levels of complexity indexed by 0, 1, 2 or 3, and to the associated 0-categories, 1-categories, 2-categories and 3-categories (Fig. 2.6).

The "integrative closure hypothesis" may be correlated to the philosophical categorification studies. The relationships between logic and CT appear in several directions (Costa-Leite 2007):

- Logical operators can be represented in categories, since objects are propositions and morphisms are proofs
- Logics can be assumed as objects of categories where morphisms are translations
- Methods for combining logics are universal constructions in some categories where objects are logics

There are some examples of how category-theoretic concepts can replace logical concepts. However, given that logic is the tool allowing understanding concepts from philosophical areas, a natural hypothesis is that category theory can also play an important role in philosophy. CT is a tool which can be used in philosophical theories and itself has an ontological status. Philosophical categorification is the philosophical counterpart of categorification introduced in mathematics, but replacing logical concepts for categorical concepts, and also set-theoretic notions by category-theoretic notions in order to investigate philosophical concepts. According to integrative closure hypothesis illustrated by Fig. 2.6 the n-categories, n=0,1,2 and 3, may be associated in succession to the study of "quantity", "quality", "relation" and "modality" for Kant architecture or to the study of "substance", "firstness", "secondness" and "thirdness" for Peirce architecture.

Taking into account the evolution during the years of Peirce's concepts of "substance" and "being" we have considered as a first development step the tetradic categorical architectures with just four levels of reality: "substance", firstness", "secondness" and "thirdness". This means to develop the Peirce's triadic frames to tetradic ones including the "substance".

Lately, the category "being" was no longer considered by Peirce as a category but as a concept about categories a kind of "meta-category" (Ika 2002). The prefix "meta", is used to mean "information about".

This suggested to study a centered architecture with "being" as a centered category surrounded by "substance", "firstnees", "secondeness" and "thirdness".

Moreover, we may consider "substance" as the beginning and "being" as end of the categorification or we may take into consideration the reverse situation (Ika 2002). In the latter case "substance" will be taken as a centered category surrounded by "being", "firstnees", "secondeness" and "thirdness".

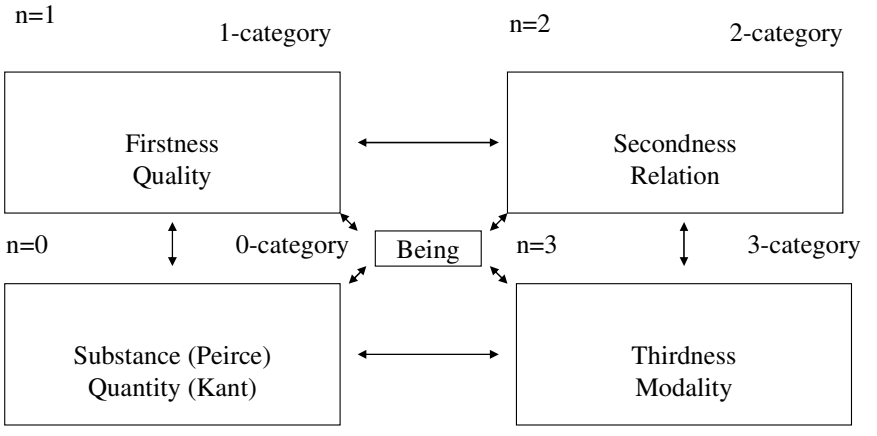

Fig. 2.8 Integrative closure for centered categories

Fig. 2.8 represents a centered variant of Fig. 2.6 in which the Peirce's fifth category of "being" centers the four levels framework.

This centered architecture suggests the possibility to repeat the initial four category analysis in a self-similar manner or to induce a fourfold analysis. This still confines the study to a four categorical or sub-categorical frame.

For applications, the center may be considered as the starting area or as the final area of investigations. The switching between the two roles may be considered too.

Traditionally philosophical categories were not studied in terms of mathematical n-CT. Consequently the significance of the hypothetical structural analogy between categorical approach in philosophy and mathematics needs more study.

However, the connection between Kant categories or Peirce categories and mathematical category theory can not be interpreted as a coincidence. Inspired by Kant, Peirce is acknowledged today as a precursor of higher-dimensional algebra and in this way to n-category study. So it would be interesting to re-evaluate Peirce's work categories, in terms of mathematical n-categories. This implicitly relates n-categories to pragmatism as formulated by Peirce. What may be called categorical pragmatism refers to Peirce's fundamental concern to discover the basic elements or principles essential in the process of inquiry, rather than to just formulate a criterion of truth by means of which the results of inquiry are to be judged for their truth value.

It should be emphasized that there exists others attempts to challenge and develop the Peirce's triadic architectures.

Brier formulated a transdisciplinary theory of information, semiotics, consciousness and cultural social communication illustrated by the four fold cybersemiotic star (Brier 2008, 2009). Fig. 2.9 shows an integrative closure presentation of the Brier's cybersemiotic star.

The four legs correspond to the four main areas of knowledge that is: material, living, cognitive and social systems. A comparison with the Hartmann's hierarchy would be of interest.

The center was associated to "knowing" by semiotic mind. It may be considered as a meta-representation of the four fold star.

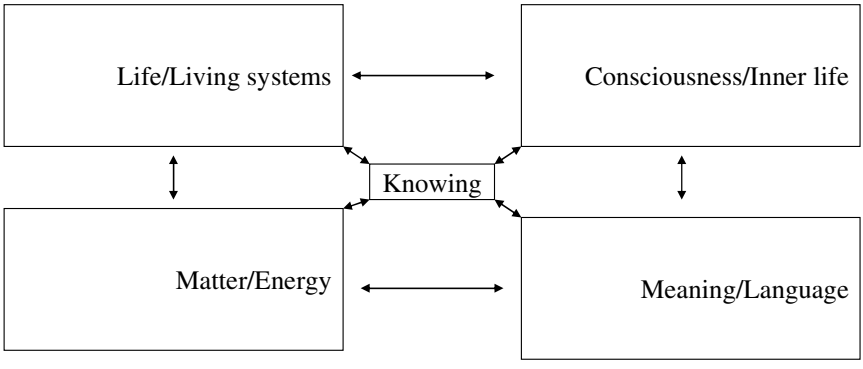

Fig. 2.9 Cybersemiotic star and integrative closure

An interesting development of triadic Peirce's approach is the so called tetradic sign in semiotics (Klinkenberg 1996).

A representation of tetradic sign is shown in Fig. 2.10.

The sign is composed of stimulus, signifier, signified and referent.

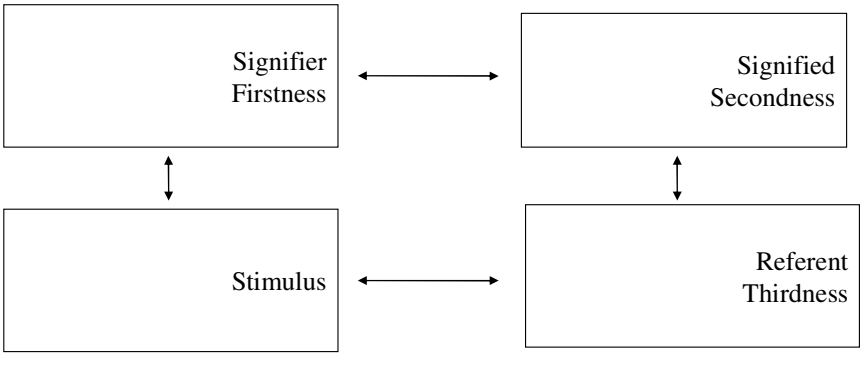

Fig. 2.10 Tetradic sign

Completing the Peirce's triadic approach, the stimulus is supposed to have a formal signification as the signifier, the signified and the referent.

The main terms that enter into the definition of the tetradic sign are the following: the stimulus (the physical signal being used), the signifier (the model, of which the stimulus is a manifestation), the signified (the meaning or content of the sign), the referent (what we are taking into account when we use a particular

sign). The relation between the stimulus and the referent is considered to be not as direct as the relation between other terms of the sign.

References

Arnold, L.: Random Dynamical Systems. Spinger, Berlin (1998)

Baez, J.: Topos theory in a nutshell (2006), http://math.ucr.edu/home/baez/topos.html

Baez, J., Dolan, J.: Higher dimensional algebra and topological quantum field theory. Jour. Math. Phy. 36, 6073–6105 (1995)

Baez, J., Dolan, J.: Categorification. In: Getzler, E., Kapranov, M. (eds.) Higher Category Theory, Contemp Math., vol. 230, pp. 1–36. Amer. Math. Soc., Providence (1998)

Barnsley, M.F.: Fractals Everywhere. Academic Press, New York (1993)

Beltrametti, E.G.: Note on the p-adic generalization of Lorentz transformations. Discret. Math. 1, 239–246 (1971)

Berz, M., Bischof, C., Griewank, A., Corliss, C. (eds.): Computational Differentiation. Techniques, Applications and Tools. SIAM, Philadelphia (1996)

Blume, A., Branderburger, A., Dekel, E.: Lexicographic probabilities and choice under uncertainity. Econometrica 59(1), 61–79 (1991)

Blumen, A., Klafter, J., Zumofen, G.: Models for reaction dynamics in glasses. In: Zschokke, I. (ed.) Optical Spectroscopy of Glasses, pp. 199–265. Reidel, Dordrecht (1986)

Bochmann, D., Posthoff, C.: Binare Dinamische Systeme. Springer, Berlin (1981)

Brier, S.: Cybersemiotics: Why information is not enough. University of Toronto Press, Toronto (2008)

Brier, S.: Cybersemiotic pragmaticism and constructivism. Constructivist Foundations 5(1), 19–39 (2009)

Cariani, P.: On the Design of Devices with Emergent Semantic Functions. Ph.D. Thesis, Binghamton University, NY (1989)

Cariani, P.: Symbols and dynamics in the brain. Biosystems 60, 59–83 (2001)

Charnes, A., Rousseau, J., Semple, J.: Non-Archimedean infinitesimals, transcendentals and categorial inputs in linear programming and data envelopment analysis. International Journal of Systems Science 23(12), 2401–2406 (1992)

Cohen, J.E.: Long-run Growth Rates of discrete multiplicative processes in Markovian environments. Journal Math. Anal. and Appl. 69, 243–251 (1979a)

Cohen, J.E.: Random evolutions in discrete and continuous time. Stochastic Proc. Applications 9, 245–251 (1979b)

Costa-Leite, A.: Interactions of metaphysical and epistemic concepts. PhD Thesis, Université de Neuchâtel - Switzerland (2007)

Cowan, N.: The magical number 4 in short-term memory: A reconsideration of mental storage capacity. Behavioral and Brain Sciences 24, 87–185 (2000)

Crane, L., Frenkel, I.: Four dimensional topological quantum field theory, Hopf categories and the canonical bases. Jour. Math. Phys. 35, 5136–5154 (1994)

Cruz, G., Lewandowicz, E., Oziewicz, Z.: Multiscale geographic information with multigraph of multigraphs. In: The 12th International Symposium on Data Handling, Univ. of Vienna, Austria (July 2006)

De Dominicis, C.: Dynamics of random levels in spin glasses. Journal of Magnetism and Magnetic Materials 54-5, 17–18 (1986)
Dieudonné, J.: Abrégé d'histoire des mathématiques. Hermann, Paris (1978)
Drossos, C.A.: Cognition, Mathematics and Synthetic reasoning. General Seminar of Mathematics, Department of Mathematics, University of Patras, Greece 13, 107–151 (1987)
Ehrlich, P.: The Rise of non-Archimedean Mathematics and the Roots of a Misconception I: the Emergence of non-Archimedean Systems of Magnitudes. Archive for History of Exact Sciences 60, 1–121 (2006)
Everett, C.J., Ulam, S.M.: On some possibilities of generalizing the Lorentz group in the special relativity theory. J. Combinatorial Theory 1, 248–270 (1966)
Fishburn, P.C., LaValle, I.H.: On Matrix Probabilities in Nonarchimedean Decision Theory. Journal of Risk and Uncertainty 7, 283–299 (1993)
Frampton, P.: Non-Archimedean geometry and application to particle physics. In: Chau, L.L., Nahm, W. (eds.) Differential Geometric Methods in Physics, pp. 399–408. Plenum Press, New York (1990)
Freund, P.G.O., Olson, M.: Non-archimedean strings. Phys. Lett., B 199, 186–190 (1987)
Goguen, J.A.: Categorical manifesto. Mathemathical Structures in Computer Science 1(1), 49–67 (1991)
Goldblatt, R.: Topoi: The Categorical Analysis of Logic. North-Holland Publishing Theory, Amsterdam (1979)
Grothendieck, A.: Éléments de géométrie algébrique, vol. 1. Springer, Berlin (1971)
Hartmann, N.: The new ways of ontology. Greenwood Press, Westport (1952)
Harmuth, H.F.: Sequency Theory, Foundations and Applications. Academic Press, New York (1977)
Hensel, K.: Uber eine neue Begrundung der Theorie der algebraischen Zahlen. Journ. Reine Angew. Math. 128, 1–32 (1905)
Hersh, R.: Random evolutions: a survey of results and problems. Rocky Mt. Math. J. 4(3), 443–477 (1974)
Hersh, R.: The Birth of Random Evolutions. The Mathematical Intelligencer 25(1), 53–60 (2003)
Ika, S.: A critical examination of the philosophy of Charles S. Peirce. A Defence of the Claim that his Pragmatism is Founded on his Theory of Categories. PhD Thesis, University of Notre Dame, Australia (2002)
Iordache, O.: Polystochastic Models in Chemical Engineering. VNU-Science Press, Utrecht (1987)
Iordache, O.: Dyadic frames for intermittency. Perturbed models. In: Bayod, J.M., De Grande De Kimpe, N., Schikhof, W.H. (eds.) Proceedings of the Conference on p-adic Functional Analysis, Laredo, Spain, May 1990. Lecture Notes in Pure and Applied Mathematics, vol. 137, pp. 89–99. Marcel Dekker, New York (1992)
Iordache, O.: Evolvable Designs of Experiments Applications for Circuits. J. Wiley VCH, Weinheim (2009)
Iordache, O.: Polystochastic Models for Complexity. Springer, Heidelberg (2010)
Iosifescu, M., Grigorescu, S.: Dependence with complete connections and applications. Cambridge Univ. Press, Cambridge (1990)
Iosifescu, M., Theodorescu, R.: Random Processes and Learning. Springer, New York (1969)

Kauffman, S.: The Origins of Order. Self-organization and selection in evolution. Oxford University Press, New York (1993)
Keane, M.: Strongly mixing g-measures. Invent. Math. 16, 309–324 (1972)
Keepler, M.: Random evolutions processes induced by discrete time Markov chains. Portugaliae Mathematica 55(4), 391–400 (1998)
Kevorkian, J., Cole, J.D.: Perturbation Methods in Applied Mathematics. Springer, New York (1975)
Kifer, Y.: Random dynamics and its applications. In: Documenta Mathematica, ICM, vol. II, pp. 809–818 (1998)
Klinkenberg, J.-M.: Le sens et sa description. In: Précis de sémiotique générale, Seuil, Paris, pp. 92–100 (1996)
Kock, A.: Synthetic Differential Geometry, 2nd edn. Cambridge University Press, New York (2006)
Leinster, T.: Higher Operads, Higher Categories. Cambridge University Press, Cambridge (2004)
Lightstone, A.H., Robinson, A.: Nonarchimedean fields and asymptotic expansions. North-Holland Publ. Co., Amsterdam (1975)
Luhmann, N.: Social Systems. Stanford University Press, Stanford (1995)
MacLane, S.: Categories for the Working Mathematician. Springer, New York (1971)
MacNamara, J., Reyes, G. (eds.): The Logical Foundation of Cognition. Oxford University Press, Oxford (1994)
Mahler, K.: P-Adic Numbers and Their Functions. Cambridge University Press, Cambridge (1981)
Mandelbrot, B.: The Fractal Geometry of Nature. Freeman, San Franciso (1982)
Monna, A.F.: Analyse Non-Archimédienne. Springer, Berlin (1970)
Narici, L., Beckenstein, E., Bachmann, G.: Functional Analysis and Valuation Theory. Marcel Dekker, New York (1971)
Norman, M.F.: Markov Processes and Learning Models. Academic Press, New York (1972)
Paladin, G., Mézard, M., De Dominicis, C.: Diffusion in an ultrametric space: a simple case. J. Physique Lett. 46, 1985–1989 (1985)
Pattee, H.H.: Evolving self-reference: matter, symbols and semantic closure. Communication and Cognition-Artificial Intelligence 12(1-2), 9–28 (1995)
Pattee, H.H.: Causation, control and the evolution of complexity. In: Anderson, P.B., et al. (eds.) Downward Causation, pp. 63–77. Aarhus University Press, Aarhus (2000)
Piaget, J., Garcia, R.: Psychogenesis and the History of Science. Columbia University Press, New York (1989)
Rammal, R., Toulouse, G., Virasoro, M.A.: Ultrametricity for physicists. Rev. Mod. Phys. 58, 765–788 (1986)
Rocha, L.M.(ed.): The Physics and Evolution of Symbols and Codes: Reflection on the work of Howard Pattee. Biosystems 60(1-3) (2001)
Rosen, R.: Life itself: A comprehensive enquiry into the nature, origin and fabrication of life. Columbia University Press, New York (1991)
Rossiter, N., Heather, M.: Four-level Architecture for Closure. In: 5th International Workshop on Engineering Federated Information Systems Interoperability, EFIS 2003, Coventry, UK, July 17-18, pp. 83–88 (2003)
Schikhof, W.H.: Ultrametric Calculus. Cambridge University Press, Cambridge (1984)

Skala, H.J.: Non-Archimedean Utility Theory. Wiley, New York (1975)
Schipp, F., Wade, W.R., Simon, P.: Walsh Series. An Introduction to Dyadic Harmonic Analysis. Adam Hilger, New York (1990)
Stenflo, O.: Uniqueness in g-measures. Nonlinearity 16, 404–410 (2003)
van der Blij, F., Monna, A.F.: Models of space and time in elementary physics. Journal of Math. Analysis and Appl. 22, 537–545 (1968)
van Rooij, A.C.M.: Non-Archimedean Functional Analysis. Marcel Dekker, New York (1978)
Varadarajan, V.S.: Non-Archimedian Models for Spacetime. Modern Physics Letters A 16(4-6), 387–395 (2001)
Veronese, G.: Fondamenti di geometria a piu dimensioni e a piu specie di unita rettilinee. Padua (1891)
Vladimirov, V.S., Volovich, I.V., Zelenov, E.I.: p-adic Analysis and Mathematical Physics. World Scientific, Singapore (1994)

Chapter 3
Conventional PSM Frames

Abstract. The polystochastic models, PSMs, are conceptual tools designed to analyze and manage multi-level complex systems.

PSMs characterize systems emerging when several stochastic processes occurring at different conditioning levels, interact with each other, resulting in qualitatively new processes and systems. The capabilities of random systems with complete connections, RSCC are outlined. The real field frame, developed to enclose multi-level modeling confronts over-parameterization problems.

Examples pertaining to the domains of chemical engineering and material science include mixing in turbulent flow and diffusion on hierarchical spaces.

The challenges of different views for the same phenomenon are pointed out.

3.1 One Conditioning Level Frame

The first objective for PSM methodology was to describe adaptive stochastic systems whose mode of evolution varies according to the rules given by a hierarchy of conditioning processes (Iordache 1987).

Consider that stochastic processes defined on the common space of "states", s, describing the possible evolutions of a particle or of a system. The system switches randomly back and forth among the collection of component processes defined on the space s. Examples of states are the particle positions or dimensions, values of properties as concentration, velocity, energy, number of particles, but also probability vectors of different positions and so on. The transition rule among different s-valued processes is given by another process defined on "conditions" space, k. The usual interpretation is that this is the process of conditions or connections in which the controlled process defined on the space of states develops. Examples of conditions are for a diffusion process in a disordered medium the randomly established scale of dimensions for pores, the scale of time for temperature or the humidity condition in which the diffusion takes place. The stochastic chaining starts with given states and conditions and applies the machinery, for instance probabilities and operators generating new states. This

basic model corresponds to the evolution at the so-called first conditioning level and has been extensively studied as learning models or RSCC. The range of applicability of such models is restricted to tasks and phenomena with sequential characteristics.

The process of states (s_n) can be described as follows. Initially the state of the s-valued process is s_0. The process followed is determined by the condition k_0 achieved with probability p (k_0| s_0). The state of the process (s_n) changes from s_0 to s_1 according to the mode of evolution indexed by k_0. In the next step the conditions process jumps to k_1 with probability p (k_1| s_1). Then, the process (s_n), describes the evolution from $s_1$to s_2 in the condition k_1. During the time interval (n, n+1) the condition is k_n and the evolution from s_n to s_{n+1} is directed by the s-valued process conditioned by k_n. The interaction between the sequences of random variables (s_n) and (k_n) is carried out by stochastic or deterministic rules. In the classical examples of RSCC it is considered that the probability of k_0 conditioned on s_0 is p (k_0| s_0) the value of s_1 is given by the rule s_1= u (s_0, k_0) where u is a deterministic operator. Moreover it is postulated that:

$$s_{n+1}=u\ (s_n, k_n) \tag{3.1}$$

The probability distribution of k_n , given s_n , k_{n-1},.., s_1, k_0, s_0, depends only on last state s_n that is:

$$P\ (k_n|\ s_n, k_{n-1}, ..., s_1, k_0, s_0)= p\ (k_n|\ s_n) \tag{3.2}$$

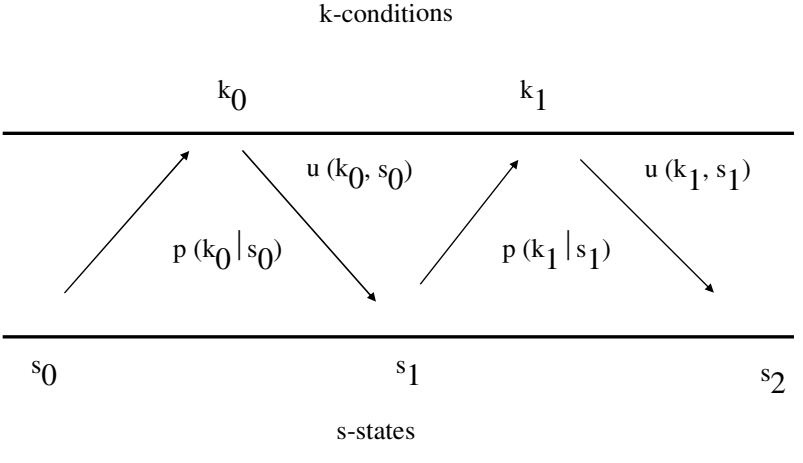

Fig. 3.1 RSCC model

Such a learning model or RSCC is shown in Fig. 3.1 where the conditions corresponding to successive steps are placed on the column while the states corresponding to the same temporal step n are indicated by lines passing through conditions.

The states are: s_0, s_1, s_2 and so on, the conditions are: k_0, k_1, k_2 and so on.

The process trajectory is from the state s_0 through condition k_0 to the state s_1, then from s_1, through condition k_1 to the state s_2, and so on.

The frame reduces to an RSCC, that is the quadruple (s, k, u, p).

$$s = \{ s_n \}; k = \{ k_n \}; u (s_n , k_n) = s_{n+1}, P (k_n | s_n, k_{n-1}, ..., s_1, k_0, s_0) = p (k_n | s_n)$$

Some variants of RSCC in which the deterministic operator u was replaced by conditional probabilities have been also considered (Iosifescu and Grigorescu 1990).

Another mathematical formulation in terms of learning models is based on RSCC with continuous time (Pruscha 1983). It was observed that in some cases, the condition k_n is not sufficient to characterize the system evolution. Consequently the conditions space k is enlarged to include an indication of the waiting time σ_n. Instead of k, the product space k x L with L = [o,∞) is used. The elements of k x L are pairs of the type (k_n, σ_n).

In this enlarged frame the operator u becomes an application from s x k x L to s and p a probability of transition from the states s to k x L.

Fig. 3.2 shows a continuous time learning model. Consider that the system starts from the state $s_0 \in s$. With probability $p ((k_0, \sigma_0) | s_0)$ the condition is k_0 and the waiting time is σ_0. Consequently the new state is:

$$s_1 = u (s_0, (k_0, \sigma_0)) \tag{3.3}$$

Then with probability $p ((k_1, \sigma_1) | s_1)$ the pair (k_1, σ_1) occurs. The new state is:

$$s_2 = u (s_1, ((k_1, \sigma_1)) \tag{3.4}$$

RSCC with continuous time are similar to the continuous time random walks useful in the study of disordered media.

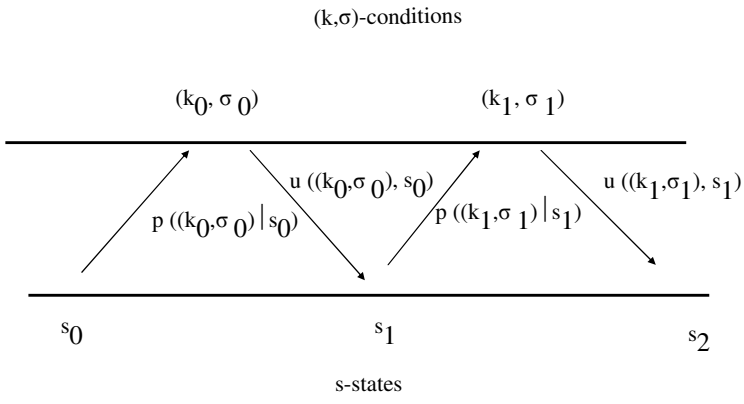

Fig. 3.2 Continuous time RSCC model

RSCC are closely related to random dynamical systems and implicitly to stochastic difference equations as resulting from the following example.

Consider the linear stochastic differential equation:

$$y'(t) = - a\, y\,(t) \tag{3.5}$$

Here a, is a random variable. This model describes a linear relaxation process as encountered in perfect mixing, with a random mean residence time 1/a. The discrete version of equation (3.5) is the random difference equation:

$$y(n+1) = k(n)\, y(n) \tag{3.6}$$

Here k(n) = 1-a(n). Denote by p (k (n)) the probability of the condition k (n). The process starts from s_0=y (0). Then, with probability p (k (0)) the condition k_0 = k (0) = 1-a (0) appears. Consequently the new state will be s_1=y (1) =k (0) y (0), given by (3.6). The next step starts from s_1=y (1). With probability p (k (1)) the condition k_1 = k (1) = 1-a (1) appears. Consequently the new state will be s_2=y (2) =k (1) s (1), given by (3.6) and so on. The associated RSCC has the elements (s, k, u, p):

$$\{s(n)\}=y;\ \{k(n)\}=k;\ u(s(n), k(n))=k(n)s(n);\ p(k(n)|\, s(n))=p(k(n)) \tag{3.7}$$

The probability p is independent on states but depends on conditions. This ensures the Markovian character of s (n).

3.2 Multiple Conditioning Levels

For one conditioning level cases we may associate the states s, to the level m=0 and the conditions, k, to the level m=1.

Suppose that instead of a single conditioning level, m=1, characterized by a process defined on the space k^1, there are more such levels. In other words, a new process defined on a new space of conditions k^2 at m=2, may control the transition from an s-valued process to another s-valued process. This relies on the fact that the condition that practically determines the evolution on s, pertains to a new set of conditions k^2. The new condition, at the level m=2, may depends on the condition established on the first level of conditions m=1.

Denote by (k_n^m) the process defined on k^m where n = 0, 1,… is the time step and m = 1, 2,… is the conditioning level. For some models (k_n^1) is a process having a self-governing evolution (k_n^2) is conditioned on (k_n^1), while (k_n^m) is conditioned on (k_n^1),…, (k_n^{m-1}). For given conditioning level m the condition that ultimately but not completely governs the s-valued process (s_n) is (k_n^m). The order in which various random conditions (k_n^m) are mutually conditioned determines the order in which different processes could appear and finally determines the hierarchy of the complex system. Observe that (k_n^m) is an m-parameter process or equivalently a process with an m-dimensional time, in the sense that at any level a dimension of time corresponds. Here, n denotes the usual time whereas m, shows how many intermediary conditioning levels occur in the achievement of a given evolution.

Consider now the more general situation when the space of states s depends on the complexity level m. Denote this space by s^m. The stochastic process of states is in this case denoted bys (s_n^m). To illustrate the random evolution consider a particle or a system starting from the state (s_0^0) that is at the moment n=0 from a state corresponding to the level m=0 were the new condition will be (k_0^1) with probability p^1. On account on the new condition of evolution, the state of the system is modified and becomes (s_1^1) at the moment n=1 and at the conditioning level m=1. To take into account the fact that the occurrence of a new condition at the level m=1, effects a change of the previous state, it is necessary to consider mappings of the type:

$$s_1^1 = u^1(s_0^0, k_0^1) \tag{3.8}$$

The new state will be s_1^1. With probability p^3, the condition k_1^3 is selected at n=1 at the level m=3. The new resulting state at the moment n=2 and at the level m=3 will be:

$$s_2^3 = u^3 (s_1^1, k_1^3) \tag{3.9}$$

Modeling as presented above requires extensive parameters estimation.

This is a difficult task and one of the open problems of this multi-level modeling method in the presented real frame. The main difficulty in utilizing such real frames was the need to introduce a large number of adjustable parameters. Unless the parameters possess a precise physical meaning the multi-level modeling becomes an exercise in curve fitting while the important qualitative feature of the phenomenon could be lost within the numerical simulation of the model. The organization of the knowledge towards the window where the phenomena are linear is inappropriate for high complexity multi-level modeling.

The condition process as shown in Fig. 3.1 and Fig. 3.2 outlined a single conditioning level. This limits the applicability of the concept to linear and sequential processes. It is physically reasonable to consider a model in which the stochastic evolution is governed not only by the k-valued process of conditions $k(n) = k_n^1$, but also by a hierarchy of conditioning processes taking place at successive conditioning levels. The condition process at the level m, k_n^m could be dependent on $k_n^{m-1}, k_n^{m-2}, \ldots, k_n^1$.

An example of systems with multiple conditioning levels will be detailed in the following.

Fig. 3.3 shows a PSM frame with multiple levels of conditions.

Consider for instance a system starting from the state s_0 at the level m=0, taking the condition k_0^1 at m=1, arriving at s_1 according to this condition in the first step. Then, at n = 1 the condition could be k_1^r at the level r, with r = 1, 2... According to k_1^r the new state of the s-valued process is $s_{2'}$ where $2'=1+2^{-r}$. It was considered that at the level r the duration of a step is 2^{-r}. In the following step the conditioning level m=1 is again reached and the process continues indefinitely.

The interaction between the sequences of random variables (s_n) and k_n^m could be either stochastic or deterministic. For instance the probability of k_0^1

conditioned on s_0 is $p(k_0^1|s_0)$, the probability of s_1 conditioned on s_0 and on k_0^1 is $p(s_1|s_0,k_0^1)$ the probability of k_1^r conditioned on s_1 is $p(k_1^r|s_1)$ and so on.

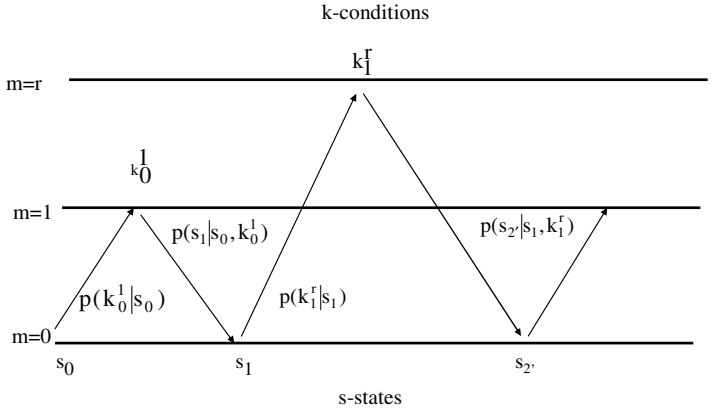

Fig. 3.3 Example of PSM frame

In the case shown in Fig. 3.3 during the first step the system goes to higher conditioning levels. Decreasing of the conditioning level can appear in some complex systems if the probabilities of transition to higher levels are null.

Observe that on different conditioning levels m, different stochastic processes develop and this justifies the term of PSM.

Examples as that shown in Fig. 3.3 clarify the component processes and their interconnections. They offer a preliminary modeling tool for experiments and numerical simulations despite the fact that the real field models are over-parameterized.

3.3 Illustrative Case Studies

3.3.1 Mixing in Turbulent Flow

Examples of phenomena and models that could be studied using the conventional real field PSM frame will be presented in the following.

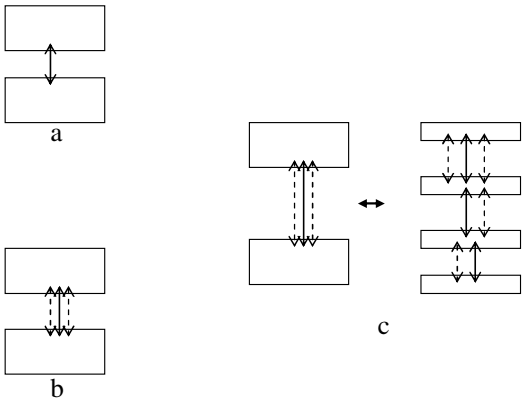

Fig. 3.4 Mixing process

Fig. 3.4 illustrates the mixing process.

The analysis of a flow system consisting of a number of connected compartments using Markov chains theory is a classical technique. It is assumed that the flow breaks into a number of connected compartments and to every compartment a state in the Markov chain is associated. The one-step probabilities of transition of the Markov chain depend on the volumes of compartments and of the interconnecting flows. The resulting Markovian process describing the time evolution of the particles is the classical stochastic model of mixing. Such a two-compartmental model of mixing is shown in Fig. 3.4 a. The probabilities of transitions from one compartment to another are supposed to be constants. If a number of different type of particles are introduced in one of the two compartments, after a certain time interval a mixing occurs and all type of particles will be found in any compartment. It is a very crude, Markovian approximation of the real mixing processes.

In a next more evolved step of modeling the turbulent flow was considered as a network of compartments with interconnecting flows that are random variables (more arrows on Fig. 3.4 b, every arrow corresponds to a possible value of the random interconnecting flow). In this case the mixing model fits to a Markov chain in random environments (at every time step the matrix of transition is changed according to stochastic rules). The condition k, established at the moment n establishes which is the Markov chain followed by particles (Krambeck et al. 1967, Cohen 1979a, b). This model is known as a controlled stochastic process in which a single level of control is accounted for. This model was correlated to products of random matrices and to random evolutions. The resulting process is more complex since the particle distributions depends of the randomly established interconnecting flows. In the above described models it is assumed that the number of compartments is constant and that the changes of flow proceed at fixed time intervals. The mixing condition is established on a single scale of time. This is restrictive since in turbulence a hierarchy of widely separated scales of motion

is exhibited. The scales corresponds to smaller and smaller compartments resulting by breaking existing ones in order to accommodate the turbulent energy. The model describing the mixing in a self-similar structured environment is still too simple as compared to the turbulent flow complexity. It would be necessary to take into account that the breaking process as well as the reverse process of coalescence of some compartments could continues during the mixing process (Fig. 3.4 c). To give an example, consider a system containing a unique compartment. The situation is formally associated to the level m = 0 of conditioning. The compartment splits into a number z of smaller compartments. This corresponds to the level m = 1 of conditioning. At the level m, z^m compartments results. In this case the condition governing the process at the time n and at the conditioning level m is denoted by k_n^m. It includes information concerning the level of compartments splitting as well as on the randomly established interconnecting flows. In this case, the number of breaking levels gives the index m. At every breaking some changes in the material and energy distribution among compartments are possible. At any level m in the hierarchy of compartments a process of diffusion or of coalescence-dispersion happens. In this case the condition gives the level m and the pair (e,k) of compartments that suffers a coalescence-dispersion process. Consequently it is considered that: $k_n^m = (m;(e,k))$. The space s^m could be represented for instance by vectors of the type $p^m(n) = (p_0^m, p_1^m, ..., p_{z^{m-1}}^m)$ where $p_i^m(n)$, is the probability that a particle is in the compartment i at the level m at the moment n. The model outlines a set of "state" processes $s^m = (p^m(n))$ and a set of "condition" processes $k^m = (k_n^m)$. The mixing process in the complex system shown in Fig. 3.4 c starts with two cells from the state characterized by the probability vector (p_0^0, p_1^0) and due to a breaking of each cell the new state is: $(p_0^1(0), p_1^1(0), p_2^1(0), p_3^1(0))$ An evolution step during n' determines a transition to the state: $(p_0^1(n'), p_1^1(n'), p_2^1(n'), p_3^1(n'))$. If a new breaking, at m = 2, happens, the state will be $(p_0^2(n'), p_1^2(n'), p_2^2(n'), ..., p_7^2(n'))$. A new evolution step at level m during n"-n' determines the transition to: $(p_0^2(n''), p_1^2(n''), p_2^2(n''), ..., p_7^2(n''))$. The time step (n"-n') could be for instance 2^{-m}. The mixing process takes place at random at a level or another. This type of situation is encountered in the case of imperfect mixing of flows.

The PSM able to describe evolution on more temporal scales should replace the time and the residence time distribution, RTD, by elements of a non-standard frame.

The shifting from breaking to coalescing processes could be formally modeled by “non-standard” frames for time, for the same generic mixing model.

3.3.2 Diffusion on a Hierarchical Space

Diffusion in homogeneous spaces is well studied in physical and in engineering sciences. The classical diffusion model describes the corresponding Markovian stochastic process. Recently much interest has centered on diffusion in non-homogeneous disordered media outlining a hierarchy of timescales. To illustrate the peculiarities of such processes, consider the stochastic dynamics of a complex system with a countable space of states, which evolves in time by fluctuation from state to state. The states are the particle positions, the possible energies, and so on. In numerous cases a hierarchy of positions or energies may happen. The transitions between states are thermally activated with probabilities determined by the free energy barriers separating the states (Ogielski and Stein 1985, Paladin et al. 1985). It is expected that such complex systems will be naturally described by PSM.

The applications of the diffusion in hierarchical spaces are numerous ranging from hydro-geology, oil industry, chromatography, membrane science, to pharmacology.

Consider that the diffusion space is the one level Cayley tree shown in Fig. 3.5. The upper ends of the branches are the possible states denoted by j=0, 1, 2,... The diffusion occurs only on the top level, m=0, but the required energy depends on the road from a state to another.The characterizing parameters of the system are the number of levels labeled here by m =0, 1, 2, and so on (in this case from the top to the bottom), the branching ratios z, on level m and the transition rates between states. Consider for simplicity that z=2 and that the transition rate p_m from a state to another depends only on the level m of the lowest node common to the states connected by the jump. The system has m-1 different transition rates p_1,..., p_m.

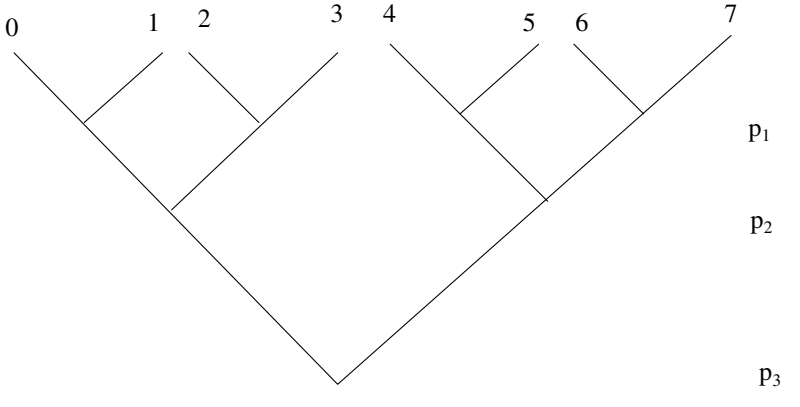

Fig. 3.5 One level of states

Denote by p_{ij} the transition probability from i to j. The transition rates on the space shown in Fig. 3.5 are for instance $p_{01}=p_1$, $p_{13}=p_2$, $p_{35}=p_3$ and so on. Suppose that: $p_1 > p_2 > p_3$ that is transitions across more levels are hardly. Observe that:

$$p_{ij} = \min_k (p_{ik}, p_{kj}) \tag{3.10}$$

This is valid for any states i, j, k of the system. Consequently the distances d_{ij}, defined by: $d_{ij}=1-p_{ij}$, satisfy the NA axiom.

$$d_{ij} = \max_k (d_{ik}, d_{kj}) \tag{3.11}$$

Fig. 3.6 shows the energy barriers between different states.

The NA tree shown in Fig. 3.5 is equivalent to the one dimensional hierarchy of energy barriers as shown in Fig. 3.6.

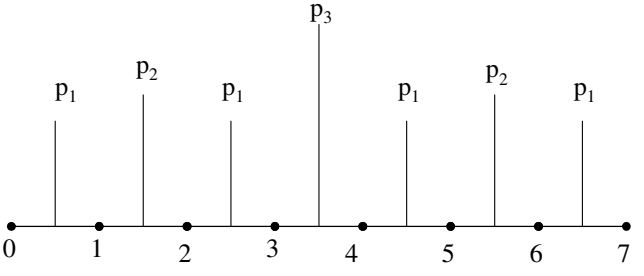

Fig. 3.6 Energy barriers

The studied case corresponds to jumps of arbitrary distance with transition rates depending only on the highest energy barrier between initial and final state. For instance $p_{12}=p_{56}=p_2$, $p_{25}=p_3$ and so on. The fact that the transition depends only on the highest barrier is a scale effect. In order to illustrate the evolution of a particle in such a space as shown in Fig. 3.5 or in Fig. 3.6 consider the processes diagram presented in Fig. 3.7.

Fig. 3.7 shows the PSM frame associated to one level of states for Cayley tree.

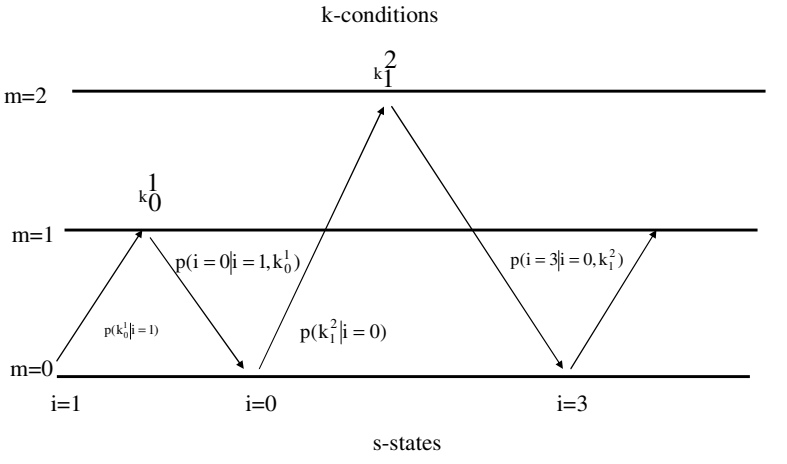

Fig. 3.7 PSM frame for one level of states

The studied particle starts from position i=1. With probability $p(k_0^1|i=1) = p_1$ the level m=1 is chosen. Then taking into account the state i=1 and the level m=1 the position i=0 appears with probability $p(i=0|i=1,k_0^1)$. Starting from state i=0, with probability $p(k_1^2|i=0) = p_2$ the new chosen level is m=2. The new position i=3 is established with probability $p(i=3|i=0,k_1^2)$. Starting from position i=3, with probability p_1 the new chosen level is m=1 and so on. Observe that the choice of a new level depends on the present position while the choice of the next position depends on previous position and level.

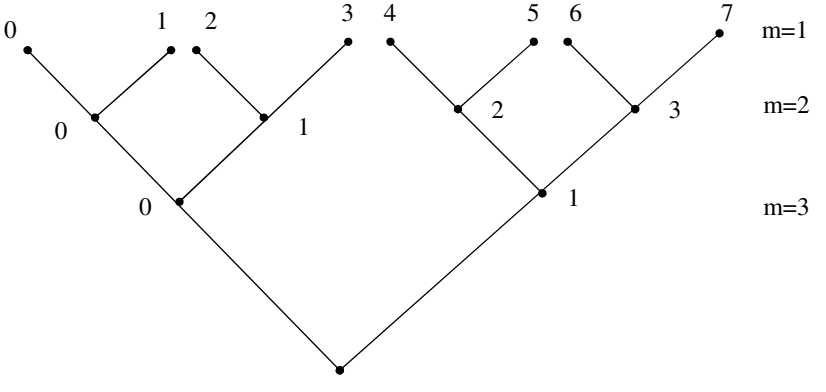

Fig. 3.8 Multi-levels of states

In this simplified case the space of states can be the position space s={i} and the space of conditions the levels k={m}.

In a more complex model it is considered that all nodes of the tree shown in Fig. 3 .5 corresponds to physical states not only those at the top level.

Fig. 3.8 shows a Cayley tree with multiple levels of states.

This is the so-called multi-level of transitions Cayley tree studied in order to describe the structure of the turbulent fluid.

To any level m, corresponds a new set of possible states. Let characterize the state of the particle by both position and levels that is by the pair (i, m) = (position, level). After a step the phase points (i, m) either stay there or are mapped upwards in the hierarchy, for instance from m to m', with probability $p_{m,m'}$.

Assume that a particle is in position i=1 at the level m=1 that is in the state: (1, 1). With probability p_{11} the next level m=1 is selected. According to this and to the previous state, the new position i=0 is selected with probability p (i=0 |(1, 1), m=1) obviously at the level m=1. The new state of the particle, in the phase space, is (0, 1).

Then with probability p_{12} the level m=2 arises and according to this and to the next state, with probability p (i=0| (0, 1), m=2) the new position is i=0 at the level m=2 that is the new state is (0, 2). Then with probability p_{21} the level m=1 is selected again. The above described evolution is shown in Fig. 3.9. Fig. 3.9 shows the PSM frame for multiple levels of states and transitions for Cayley tree.

The complex system could be studied as a PSM with a unique conditioning level if the same scale of time is envisaged at different levels. In this case the space of states is s = {(i, m)} while the space of conditions will be k = {m}.

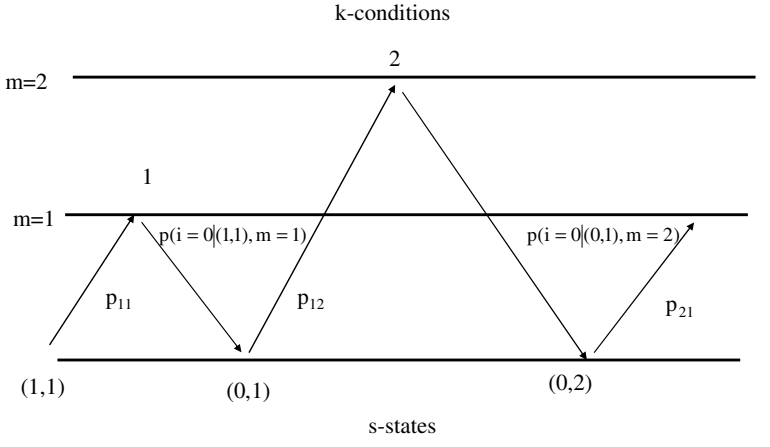

Fig. 3.9 PSM frame for multiple levels of states

The coexistence of different timescales leads to difficulties in simulating the dynamics and in reconstructing the model from experimental data.

The random walk in such trees essentially depends on the previous walk history. This means that the non-Markovian character is mandatory. Interesting problems for practice arises when the supporting tree itself has a random evolution.

3.3.3 Different Views for the Same Phenomenon

The following illustrative example allows pointing out the main differences between various views over the same phenomenon, namely, the random walk of a particle, on discrete spaces in discrete time (Iosifescu and Grigorescu 1990). The specificity of the PSM frame will be emphasized.

Fig. 3.10 shows states at different levels.

Consider the finite sets of particle positions $k^1 = (1, 2,..., i,..., r)$, $k^2 = (1, 2,..., j,..., s)$, $k^3 = (1, 2,..., k,..., t)$, corresponding to the levels m = 1, 2 and 3 respectively. The stochastic transition matrices: $p^0 = (p_{ij})$; $1 \le i,j \le r$, $p^1 = (p_{ij})$; $1 \le i,j \le s$, $p^2 = (p_{ij})$; $1 \le i,j \le t$.

They describe the particle transitions from a position to another at constant levels m = 1, 2 and 3 respectively. Using the stochastic transition matrices p^0, p^1, and p^2 it is possible to define, for given initial distributions, Markov chains on k^1, k^2 and k^3 respectively. If the particle transition from a level to another may be considered, the Markovian random walk model fails since the evolution depends not only on the last state but also on the last level.

The problem is to construct a stochastic chain describing the random walk on the entire set of conditions $k = k^1 \cup k^2 \cup k^3$. If the time step is identical at any level, it is easy to define a Markov chain on k. Difficulties and opportunities are related to the existence of various scales of time at different levels. For example it is considered in the following that a transition between two states at the level m takes place during 2^m (or during 2^{-m}) units of time while the transition from a level to another are instantaneous.

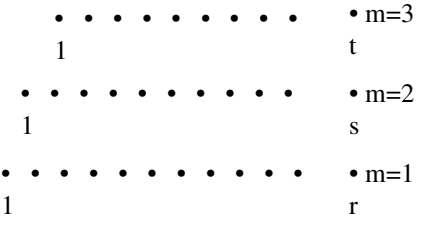

Fig. 3.10 States at different levels

The existence of timescales imposes to take different look at the single and multi-level chains.

Consider the sets:

$$s^0 = \{p^0 = (p_1^0,...,p_i^0,...,p_r^0)\},\ s^1 = \{p^1 = (p_1^1,...,p_i^1,...,p_r^1)\},\ s^2 = \{p^2 = (p_1^2,...,p_i^2,...,p_r^2)\}$$

Here the probability vectors are denoted by $p_i^0 \in s^0$, $p_i^0 = (p_{i1},...,p_{ir})$ the i-th row in the matrix p^0, $p_j^1 \in s^1$, $p_j^1 = (p_{j1},...,p_{js})$ the j-th row in the matrix p^1 and $p_k^2 \in s^2$, $p_k^2 = (p_{k1},...,p_{kt})$ the k-th row in the matrix p^2. The "states" are probability vectors represented by the rows in transition matrices p^0, p^1, p^2. Let us limit the first case study to the level m = 1 that is to the conditions, k^1 and the states s^0. In order to introduce RSCC, as a natural extension of the Markovian dependence two sequences of random variables the s^0-valued and the k^1-valued chains will be associated to the Markov chain with transition matrix p^0.

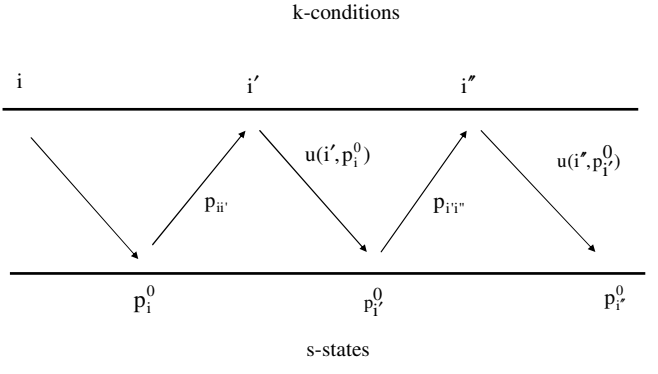

Fig. 3.11 RSCC associated to one level conditional stochastic chain

Fig. 3.11 shows the RSCC associated to one level conditional stochastic chain.

The paths of the two chains of states and of conditions are shown in Fig. 3.11.

The particle random walk starts from the position $i \in k^1$. If the particle evolving according to the k^1-valued chain is in the position i, at a given time, its next position will be chosen according to the vector $p_i^0 \in s^0$. An account of this, the probabilities of transition at one of the positions at the level m = 1, in the set of

positions k^1, will be given by $p_i^0 = (p_{i1},...,p_{ir})$. This is the i-th row of the matrix p^0 giving the one-step probabilities of transition from position i to another one at the same level m=1.

Taking into account p_i^0 the position $i' \in k^1$ was sampled with probability $p_{ii'}$ (an element of the vector p_i^0). The new s^0-valued vector is $p_{i'}^0 = (p_{i'1},...,p_{i'r})$. This is the i'-th row of the matrix p^0, giving the one-step probabilities of transition from position i' to another one at the same level m=1. According to the vector $p_{i'}^0$ the new position $i'' \in k^1$ was chosen, then according to $p_{i''}^0$, the new position $i''' \in k^1$ may be chosen and so on. The stochastic dependence is given in this case by the transition probability from s^0 to k^1 given for instance by $p(p_i^0, i') = p_{ii'}$. This is the probability to arrive in the position i' conditional on the previous state vector p_i^0. Observe that this depends on both positions i and i'. Furthermore $p(p_{i'}^0, i'') = p_{i'i''}$ and the process continues indefinitely. The operatorial dependence is in this case given by functions as: $u(p_i^0, i') = p_{i'}^0$. This outlines that the new probability vector $p_{i'}^0$ depends on the new condition i'. The transition from i to i' as well as that from p_i^0 to $p_{i'}^0$, take place with a uniform time step. The time is indexed here by n.

Let us consider the complex situations when different levels of conditions k^1, k^2 and k^3 exists. An example of such an evolution is shown in Fig.3.12.

Fig. 3.12 shows the PSM associated to multi-level conditional stochastic chain.

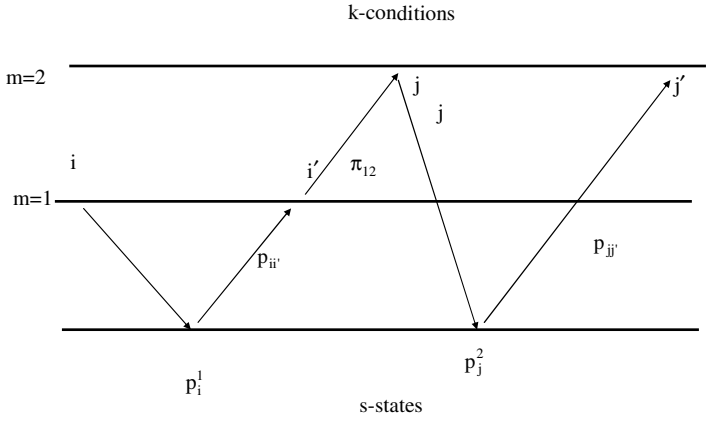

Fig. 3.12 PSM frame associated to multiple levels conditional stochastic chain

The particle starts from position i at the level m = 1. The state vector $p_i^1 = (p_{i1},..., p_{ir})$ will characterize the next transition from position i at the level m = 1. The new position is $i' \in k^1$ with probability $p_{ii'}$ (an element of p_i^1). Simultaneously, a transition from m = 1 to m = 2 takes place with probability $\pi_{l2} = 1/2$. The chosen state, at the level m = 2, is j. Consequently the new vector of particle state, will be $p_j^2 = (p_{j1},..., p_{js})$.

According to this, the position $j' \in k^2$ is selected with probability $p_{jj'}$ an element of p_j^2. The system outlines the existence of more scales of time. The process illustrated in Fig. 3.11 describes the following random walk: i→ i'→i"→ and so on while the Fig. 3.12 corresponds to the random evolution: (i) →(i', j) →(j') → and so on. At different levels we are faced with chains that differ from that associated to Fig.3.11 from the point of view of time steps.

Observe that the used method is not a simple accommodation of the classical Markov chains or RSCC to a more general situation. It corresponds to interesting practical situations having no analogue and solutions in the theory of Markov chains or the RSCC, due in this case to the time scales associated to different conditioning levels and the possibility to characterize not only sequential but also parallel evolutions.

Confronting the large number of parameters, schemes as shown in Fig.3.12, make clear the difficulties accumulated by the numerical investigation of the complex processes and support the advent of calculus based on “other than real” that is “non-standard” frames.

The conventional PSM were not developeded as formal mathematical tools but rather as constructive point of views according to which in practical situations it may be useful to look at a complex process as an emergent structure resulting by the hierarchical superposition and interaction of component processes operating at different levels and different time frames. The attention was focused firstly on the hierarchy of conditional processes allowing self-adaptive evolution. To establish the states, the scales and levels, the conditions, the probabilities and the operators relating different component processes the real field PSM methodology was useful rather constructively than conceptually. In order to improve the potentialities for applications of the real polystochastic frame this should be developed using “non-standard” field concepts and methods.

References

Cohen, J.E.: Long-run Growth Rates of discrete multiplicative processes in Markovian environments. Journal Math. Anal. and Appl. 69, 243–251 (1979a)

Cohen, J.E.: Random evolutions in discrete and continuous time. Stochastic Proc. Applications 9, 245–251 (1979b)

Iordache, O.: Polystochastic Models in Chemical Engineering. VNU-Science Press, Utrecht (1987)

Iosifescu, M., Grigorescu, S.: Dependence with complete connections and applications. Cambridge Univ. Press, Cambridge (1990)

Krambeck, F.J., Shinnar, R., Katz, S.: Interpretation of tracer experiments in systems with fluctuating throughput. Ind. Engng. Chem. Fundam. 8, 431–444 (1968)

Ogielski, A.T., Stein, D.L.: Dynamics of ultrametric spaces. Physical Review Letters 55, 1634–1637 (1985)

Paladin, G., Mézard, M., De Dominicis, C.: Diffusion in an ultrametric space: a simple case. J. Physique Lett. 46, 1985–1989 (1985)

Pruscha, H.: Learning models with continuous time parameter and multivariate point processes. J. Appl. Probab. 20, 884–890 (1983)

Chapter 4
New PSM Frames

Abstract. The hierarchy or the network, which allows modeling at several levels is deep-rooted in the higher categories frames. Models of models, that is, meta-models allowing the study of processes of processes, and so on, are presented.

Four realms general PSM frames results by integrative closure.

Innovative is the model categorification for multiple levels modeling. This imposes making use of unconventional notions of time and probabilities.

Non-Archimedean frames based on infinitesimals and on non-well-founded sets are presented.

4.1 General Frameworks for PSM

4.1.1 Basic Categorical Frameworks

The elements of PSM are quadruple of vectors {S, K, U, P} denoted also SKUP.

The notations are: S-states, K-conditions, U-operators, and P-possibilities (Iordache 2009).

Each component of the vectors corresponds to a different conditioning level and a different time scale.

The basic elements of the SKUP, will be denoted as follows:

$$S = (s^0, s^1, ..., s^m, ..., s^M) ; K = (k^0, k^1, ..., k^m, ..., k^M);$$

$$U = (u^0, u^1, ..., u^m, ..., u^M); \; P = (p^0, p^1, ..., p^m, ..., p^M).$$

Here s^m represents the particular state at the level m, and k^m represents the particular condition at the level $m \leq M$. Upper indices are reserved to levels, while lower indices are reserved to time steps. The components of U are operators such as: $u^m : k^m \times s^{m'} \rightarrow s^{m''}$

PSM should describe parallel evolutions. Moreover S and K are associated to different types of algebraic fields. Despite algebraic framework differences, S and K are interconnected. This interconnection is described by operators U and possibilities P. U characterizes the K to S transition and P characterizes the S to K transitions, that is:

$$U: K \rightarrow S \text{ and } P: S \rightarrow K.$$

Operators U should be able to describe change of conditioning level and splitting of levels.

Possibilities P, replacing and generalizing probabilities have been defined in game theory (Blume et al. 1991, Hammond 1994) in fuzzy logic (Dubois and Prade 2001, Schumann 2008) and in other domains.

The possibilities P are defined by vectors such as:

$P(K) = (p(k^0), p(k^1),\ldots, p(k^m),.., p(k^M))$. The component $p(k^m)$ is an evaluation of the condition k^m. Such components may be, eventually, conventional probabilities but in some cases this choice may complicate the calculus without benefice for understanding.

An innovative aspect for PSM concerns the differential model for K process. The elements of K are resulting as solutions of differential equations.

These may be functional as meta-models that is, generic models producing other models. The differential models proposed here are formally similar to the real valued differential models characterizing the single level systems.

The RSCC model outlined a set of states s, a set of conditions k, and transition relations between them, expressed by operators as u, and probabilities p (Fig. 4.1).

The categorical approach for PSM appears as a categorification of such transition systems for increasingly higher dimensional problems.

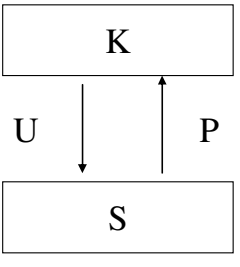

Fig. 4.1 Two levels framework

Mathematical categorification associates category-theoretic concepts to set-theoretic notions (Appendix 2).Categories are linked to the different levels of reality. The notion of level or reality which was firstly studied from an intuitive point of view was approached from a more formal point of view based on CT. The levels and sub-levels of reality are characterized and distinguished by their categories and sub-categories (Poli 2001).

A two levels framework is shown in Fig. 4.1. It shows the basic SKUP framework that contains in the categorical interpretation two categories S and K, and two functors, U and P, between these categories.

The SKUP associated to PSM represents a general architecture, shared by numerous adaptive and evolvable systems (Iordache 2009).

For PSM frameworks the conditions K represent the category describing the types of component processes. In this case, the processes types are the objects of category. Interactions among types can be modeled as morphisms.

The arrows that is, the morphisms describe the transition relations between the states of the component processes. Different algebraic frameworks for states-S (dynamical, analogical, and natural) and conditions-K (symbolic, digital, and formal) have to be considered.

Functors as U are accounting for interactions in K, and between K and S.

Functors as the possibilities P, supplements the probabilities to express potentiality, fuzziness, uncertainty, and emergence.

4.1.2 Multiple Levels

Observe that the SKUP framework from Fig. 4.1 still involves only two levels or realms, S and K. Advancements in modeling higher complexity, the evolvability request, impose to take into account multiple levels and multiple SKUPs interaction.

Any two levels SKUP may have more complicated relations to other two level SKUPs than can be functional in the multiple levels situation.

In such cases it is necessary to consider 2-categories and more general n-categories (Appendix 2). This means in fact to continue the categorification process (Appendix 2).

Horizontal and vertical composition of elementary two level SKUPs should be taken into account.

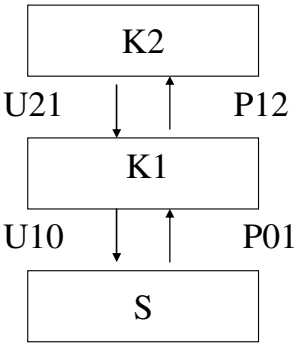

Fig. 4.2 Three levels hierarchical framework

Fig. 4.2 and Fig. 4.3 show the three categories S, K1 and K2 and their interconnections by operators Uij: Ki→Kj, and possibilities, Pij: Ki→Kj. S is considered to be the K0 level.

Fig. 4.2 shows the three levels hierarchical framework.

Fig. 4.2 shows the elements of the SKUPs, the lower cell {S, K1, U10, P01} and the upper cell denoted by {K1, K2, U21, P12}.

It is a vertical composition of SKUPs.

The upper cell appears as a second structuring for the category K mirroring and extending in a specific sense the basic SKUP structure.

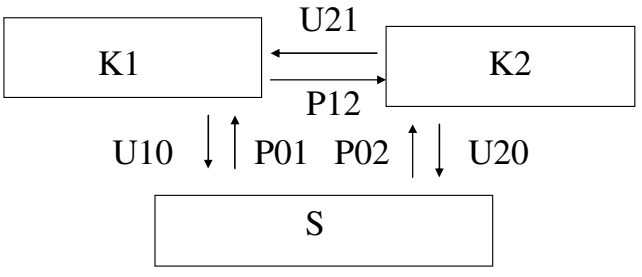

Fig. 4.3 Three realms network

Fig. 4.3 shows the three realms network.

Fig. 4.3 shows the elements of three SKUPs, the left cell {S, K1, U10, P01}, the right cell {S, K2, U20, P02} and also the SKUP cell denoted by {K1, K2, U21, P12}. It is a kind of horizontal composition of SKUPs.

Since in Fig. 4.2 and Fig. 4.3 we replaced K by two categories K1 and K2, there are two possible operations for the conditions K.

We will refer to operation in K as the tensor product,"$*$".

There are various tensor products we can consider for categories. The Cartesian product is a special case. The categorical product "$\times$" and the coproduct, "$\cup$" are other examples.

Fig. 4.2 and Fig. 4.3 outlines two possible ways in the conditions category K, for instance, the coproduct, "$\cup$", way in K1 the categorical product "$\times$" way in K2.

The switch from product "$\times$" to the coproduct, "$\cup$" and reverse is possible but the two types of categorical product cannot be observed simultaneously.

The interaction between S and K2 as shown in Fig. 4.3 allows a three-fold integrative closure hypothesis including in the loop S, K1, K2 and again S and this allows evolutionary properties of the whole system .

The Gray tensor product denoted here by" Γ", and its generalizations are of interest for 3-categorical constructions (Appendix 2). In such cases, instead of the category K we consider three categories K1, K2 and K3.The tensor product proves to play a significant role for the emergence and evolvability mechanisms.

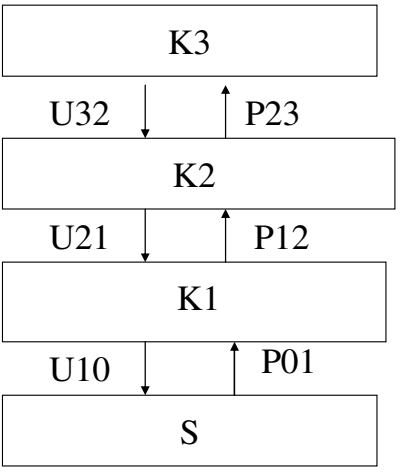

Fig. 4.4 Four levels hierarchical framework

The two levels and three levels architecture may be generalized to four levels or realms as shown in Fig. 4.4 and Fig. 4.5.

Fig. 4.4 shows the four levels hierarchical framework.

Fig. 4.4 outlines the elements of three SKUP cells. The initial cell is {S, K1, U10, P01}, the next cell {K1, K2, U21, P12} and the next cell is {K2, K3, U32, P23}. The SKUPs are composed vertically.

Fig. 4.5 shows the four realms network.

Fig. 4.5 outlines the elements of four SKUP cells. We may denote S by K0 for uniform notations. The initial cell is {S, K1, U10, P01}, the next cell {K1, K2, U21, P12} the next cell {K2, K3, U32, P23} and the closing cell is {S, K3, U30, P03). It is a cyclic composition of SKUPs.

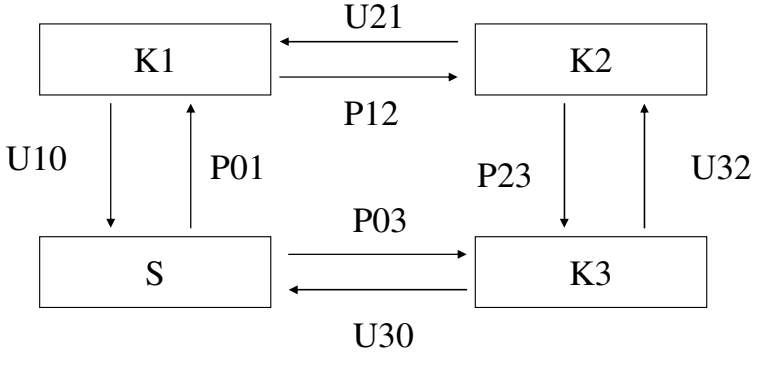

Fig. 4.5 Four realms network

The tetradic network form is shown in Fig. 4.5.

Usually the notations are: S-data, K1-models, K2-meta-models, K3-meta-meta-models.

In the illustrative case of statistical methodologies the notations are: K0 for data, denoted also by S, K1 for statistical information definitions and K2 for descriptive statistic methodologies. K3 denotes methodologies that define methodologies (Iordache 2010).

The 1st evolution step determines the K1 emergence, 2nd evolution step the K2 emergence, and so on.

The network can be used to distinguish different roles in the information system. Basically, the idea is that a role consists in using the model on a certain level in order to produce models at the lower level.

According to the order of reality levels in the diagram shown in Fig. 4.5 it results that the generic modeller or statistical methodologist U32: K3→ K2 uses a general purpose model to produce statistical methodologies. This corresponds to the 3rd order evolution step.

The statistics definer U21: K2→ K1 uses a statistical methodology to produce subject matter definitions. The statistics producer and user U10: K1→ K0 uses a subject matter definition to produce statistics to understand the reality and possibly produce actions on it. The interaction between K0-Data and K3-Methods that define methods allows and confirm the integrative closure hypothesis and make the statistical models system evolvable. This corresponds to the 4th order evolvability step.

The roles defined above are independent of the nature of the agent, the role of executor, that can be human or software artefacts. The same role can be played in principle by people or by machine. In this role-playing, the upper level model supplies specifications to the agent that interprets and applies them in order to produce the lower level model. When this behavior is enforced in practice, the system is active because the upper level model drives the agent behavior.

Fig. 4.5 suggests how software artefacts can be made active: they have to be driven by the respective upper level model. The major data processing software packages in the statistical system should be founded on the idea of active models in hierarchy or network. To process a level, the software is driven by upper level. For example, to produce a level K1-model, a set of statistical informations, software is driven by its level K2- model, expressed in a formalized subject matter language and therefore highly independent from the technical aspect of the implementation. To produce a level K2-model, the activity of subject matter experts is supported by software tools, driven by the level K3-model in use. The specificity of the statistical field is located at the level of K2. The K2-model is considered as the formal representation of a descriptive statistic methodology.

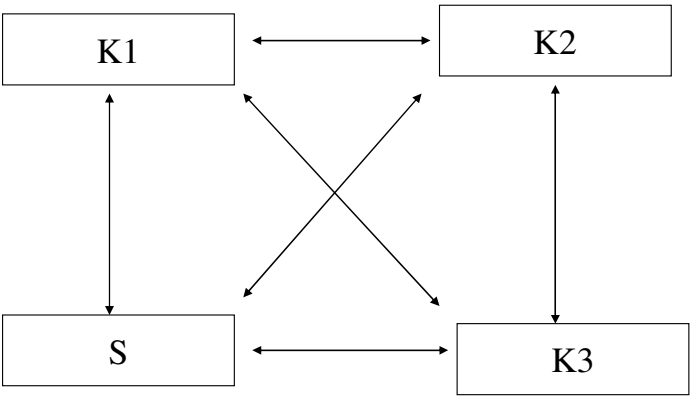

Fig. 4.6 Fully integrated four realms network

Fig. 4.6 shows a version of the four realms network with more interactions.

This may be compared to NBIC diagrams of convergent technologies (Bainbridge and Roco 2006).

Notice that we make use of K1, K2, and K3 to characterize firstness, secondness and thirdness as in Peirce's notations for categories.

The centered architectures as shown in Fig. 4.7 are also of interest for the study of evolvable and autonomous systems. In the centered architecture a model can describe elements from every meta-model below it.

Theoretically the centered structure architecture is not restrained to four realms.

Fig. 4.7 highlights centered and self-similar spiral architectures.

A similar structure is repeated to four sub-realms denoted here by k0, k1, k2 and k3.

Fig. 4.7 suggests that an integrative closure hypothesis does not have to be seen as a final stage or a balance due to equilibrium, but rather as a process that can develop self-similar patterns.

Centered structures may unify large systems. The initial frame offers a generic, four-fold, relational model whose elements are configured as a self-similar structure. This means that it can be re-scaled from the smallest to the largest or reversely without compromising its form. This has the advantage that it is a configuration that is shareable across different domains. The self-similarity allows analogous processing with similar software.

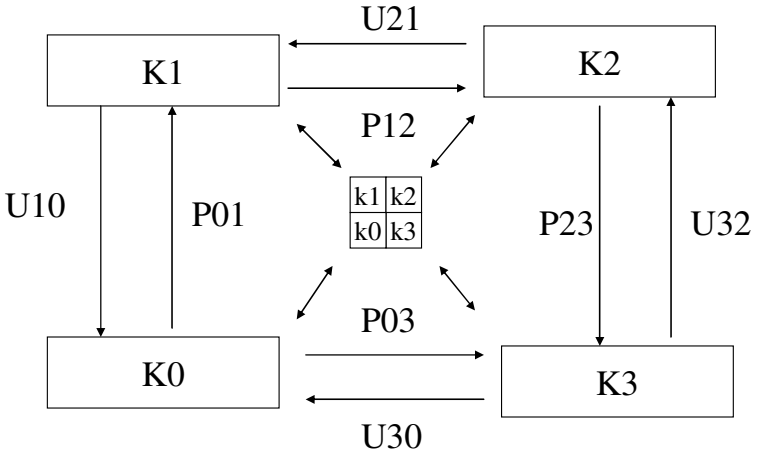

Fig. 4.7 Centered four realms network

The centered framework has a supplementary element in specific position and significance. This may be associated to Peirce's fifth category of "being".

It appears as a meta-category or a meta-representation of the four realms frame.

It offers information about the four realms frame.

The four realms frameworks are very general. In particular cases, only some of the operators, possibilities and interactions may be activated.

An interesting case study is the so called reasoning cycle of Peirce (Sowa 2002, 2004). In this case the notations are: K0-World, K1-Knowledge soup, K2-Theory and K3-Prediction. The names of interactions between categories as interpreted by Sowa (2004) are induction, abduction, deduction and action. Fig. 4.8 shows the Peirce's cycle of cognition.

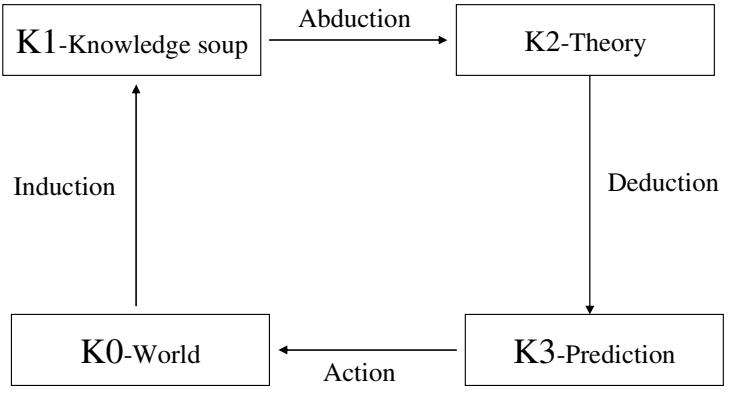

Fig. 4.8 Cycle of cognition

Induction or learning starts from observations and looks for commonalities to summarize observed data.

Abduction or guessing starts with disconnected observations and guesses (hypothesizes) a theory that relates them.

Deduction or inference starts with a theory, observe new data and is used to generate implications.

Fig. 4.8 expresses the Peirce's pragmatic method as a cycle coupling action on real systems K0, and the formal systems K1, K2 and K3. The regularity that mediates between firstness K1 and secondness K2 is the thirdness K3. These universal categories are also modes of inference from abduction to deduction, and from this to induction where induction mediates between abduction and deduction (Brier 2009).

4.2 Time Frames

4.2.1 The Problem of Time Frame

The adopted point of view for PSM developments is that the functional frame for time and for probability must agree first of all with the nature of analysis of the studied system. Unconventional concepts of time and probability are permitted and naturally implemented if the system analysis can proceed on this basis. The use of multi-dimensional, multi-scaled, dyadic, and cyclic time proves to be beneficial depending on the studied context (Iordache 2009).

Time, space, probability and information are intuitive concepts and one cannot define their properties by entirely arbitrary mathematical rules. It is necessary to put in the frame, the physical and engineering knowledge allowing a pragmatic and reasonable choice out of mathematical possibilities.

Supplementing the time based on the field of real numbers, NA frames for time offer a variety of options in modeling since NA frames are capable to describe artificial structures. The convention to use only the one-dimensional time "n" to describe all types of evolution has the starting point in the belief according to which all phenomena are linear or a superposition of linear phenomena in essence. But, in the domain of complex systems, there exists phenomena that appear very unregulated when they are studied using the real time "n" and, contrary to this, follow simple rules when they are studied using "other than real" time frames. Making use of NA time one can find regularity for process, which appear chaotic with respect to the real time. Beneficial may be the frame involving both the time step "n" and the conditioning level "m". The coexistence of processes at multiple conditioning levels leads to difficulties in simulating the resulting dynamics and in reconstructing the governing equations given experimental data. The introduction of the multidimensional time in the study of the conditioning process (k_n^m) facilitates the study of systems with variable complexity in the course of development. This development represents in fact the unceasing transformation of

the potential in the empirical and of the empirical in the potential, which characterize emergent complex systems.

The concept of multidimensional time, according to which time is to be thought of not as a real number, but as a vector, with a finite number of components play significant role in PSM. Different relations may define an order for such vectors of time. The introduction of the multidimensional time will permit to study in a natural way, the complex hierarchical systems. PSM may describe systems having an ensemble of interacting levels that is, systems composed of conditioned sets of interacting subunits. Usually the level m receives selective information from above (levels m-1, m-2,…,1) and in its turn it exercises commands on the dynamics of the lower levels. The reverse order of conditioning is of interest too.

For emergent systems the physical interactions give rise in a concomitant way to progressive differentiation, to entropy production, increasing complexity and increasing organization. The decrease of complexity and of the conditional level "m" should be considered too to ensure evolvability. One of the main characteristic features of the level "m" contrasted with the usual time "n" is that "m" may have reversible order. The index "m" gives an idea about the hierarchy of qualitative steps in the closed system evolution as distinguished from a mere increase of the index "n" by ambient evolution.

4.2.2 Frame of Infinitesimals

NA structure of time allowing the description of complex systems presenting many parallel ways of evolution with strongly different time characteristics will be the main example of "other than real" time. Consider systems in which a scale of time corresponds to every conditioning level. The present illustration is limited to the case of two time scales, a long time scale for n and a slow time scale for t.

The time is $T=n+\varepsilon t$ with $\varepsilon>0$, a positive constant. It has two components corresponding to the two scales. The set of time vectors denoted also as $T = [n, t]$ is ordered by the relation:

$$[n_1, t_1] < [n_2, t_2] \text{ if } n_1<n_2 \text{ or if } n_1=n_2 \text{ and } t_1<t_2 \tag{4.1}$$

For example, if n or t is in hours and $\varepsilon = 1/24$, then εn or εt is in days.

According to this lexicographic order when two complex systems being in the step n_1 and n_2 of evolution respectively are compared, the system whose step is the greatest of the numbers n_1 and n_2 appears as the more evolved one. If they are in the same n step that is if $n_1 = n_2$ it needs to compare the next index of time, t, in order to establish the ordering. This signifies that the evolution according to t can be considered as less significant than the evolution according to n. The time elapsed on n appears to be more important for the studied phenomenon. Very important is that reverse steps on the infinitesimal scales of time become intuitively acceptable. For instance a transition from [n, 1] towards [n+1, -1] is in the usual order for the time T since [n, 1] is anterior to [n+1, -1]. The last includes an infinitesimal negative time step.

The reverse order of importance anti-lexicographic for coordinates n and t is of practical interest too. This is:

$$[n_1, t_1] < [n_2, t_2] \text{ if } t_1<t_2 \text{ or if } t_1=t_2 \text{ and } n_1<n_2 \tag{4.2}$$

The above-defined time T is an NA frame (Neder 1941, 1943). Indeed let A and B, be two different times, A = [0, 1], B = [1, 0]. For any integer k, kA = [0, k] <B. So A is an infinitesimal time relative to B while B is an infinite time relative to A. In the real field of times, the interval of time is perceived as a distance on the real time axis. Accordingly in the NA frame proposed here, a measure of the time interval between $[n_1, t_1]$ and $[n_2, t_2]$ will be:

$$d([n_1,t_1], [n_2,t_2]) = (n_2-n_1)+\varepsilon(t_2-t_1) \tag{4.3}$$

The axiom of Archimedes is not verified in this case. Indeed d([0,0], [0,kt])= kd([0,0],[0,t])=ktε<d([0,0], [n,0])=n for any integers k and n. Failure of the axiom of Archimedes naturally follows from the fact that the time is not represented as a real number at all but instead as a lexicographically ordered vector.

An intuitive example is provided by the study of mixing. The existence of the so-called "dead spaces" characterized by very slow mixing processes impose to describe the basic mixing process on the usual scale of time n or t and the dead space process on the scale εt. The hierarchy of dead spaces can continue giving time scales as ε^2t and so on. The considered scales of time are widely different. Any scale appears as a perturbation of the preceding one. The translated structure of time T induces a similar structure of the functions of time. A real function f(n) of time n have to be replaced by the NA function $F(T) = [f^0(n), f^1(n, t)]$ of T = [n, t] where $f^0(n)$, $f^1(n, t)$ are real valued functions. Both functions depend on the time n (Neder 1941, 1943). Obviously F (T) is an element of the same NA structure as T. More generally a non-Archimedean function on K, F: K $\rightarrow$ K is defined by $F(K) = [f^0(k_0), f^1(k_0,k_1),..., f^m(k_0,k_1,\ldots,k_m),...]$ where $K = [k_0, k_1,..., k_m,...]$ and f^0, f^1,..., f^m,... are real functions Expansions as that used for time T and functions F(T) introduce extensions of the domain of the studied variable.

The vector T represents the construction of different clocks with which the variation of the function can be described in a natural fashion. T includes information concerning the existing structuring in scales. One limit of the above frame is the complete separation of the scales. By taking ε=0 the real frame would be validated.

4.3 Probabilities and Possibilities

4.3.1 Frame of Infinitesimals for Probabilities and Possibilities

Probability is the useful tool for representing uncertainty, conditioning, and information.

It was observed that the set theory and corresponding probability theory are inadequate frameworks to capture the full scope of the concept of uncertainty for multi-scale systems. Uncertainty in set theory means non-specificity and exactly the specificity is important for some complex systems. Conventional probabilities may be of interest when it is not detrimental to flat individual features while they are not adequate to account for strong individual deviations.

Conventional probabilities are also inappropriate to illustrate qualitative concepts as fuzziness, vagueness, partial truth and opportunities, all having significant role in complexity studies.

Answering to the need of probability-like concepts in the study of complex multi-scale systems, the probability construction for infinitesimal frame is considered here. The starting point is the fact that the probabilities are functions. This means that the definitions should be based on the definition of function in the NA frame.

The NA probabilities are considered as an example of possibilities. Difficulties of construction and interpretation are related to the definitions of events for an NA frame.

Denote by X the space of all elementary events. Denote by X the Borel ring of all compact subsets of X. An event is a subset of X. The elements of X are expansions of the type

$V= [k_0, k_1, k_2,\dots]$ where $k_j \in R$. The number $V=\Sigma_n k_n \varepsilon^n$ is naturally associated to the event V. Let K denotes the NA structure of infinitesimals.

Define the possibility $P: X \to K$ as follows:

If $V=[k_0, k_1, k_2,\dots]$ then $P(V) =[p^0(k_0), p^1(k_0, k_1), p^2(k_0, k_1, k_2),\dots]$

With other notations, the possibility assigned to $V=k_0+\varepsilon k_1 +\varepsilon^2 k_2,\dots$ is

$$P(V) =p^0(k_0) + \varepsilon p^1(k_0, k_1) +\varepsilon^2 p^2(k_0, k_1, k_2) +\dots. \quad (4.4)$$

Here p^0, p^1, p^2 and so on, are measures functions, the more significant being p^0, followed by p^1, this followed by p^2, and so on. The infinitesimal contributions as events may have infinitesimal contributions as probabilities.

Such ideas have been used in the study of the so-called lexicographic probabilities (Blume et al. 1991, Hammond 1994).

Obviously the possibility P(V) is positive, $P(V) \geq 0$, but this inequality should be considered in the NA frame. The NA definition of positive possibility accommodates situations as: $p^0 \geq 0$, $p^1 \leq 0$, $p^2 \leq 0$, and so on.

The probabilities p^m, $m \geq 1$ may be negative but their impact is infinitesimal. Interesting situations corresponds to systems having: $p^0 = 0$, $p^1 =p^{m-1} =0$, $p^m \geq 0$, $p^{m+1} \leq 0$,..., for increasing m. This situation ensures that P (V) is a positive number in NA frame. Observe that even if the function p^0 is 0, the condition k_0 still may have an impact since $p^m >0$ and p^m may be function of k_0.

The contact with the real field is possible by real valuations or norms as exemplified by applications and case studies. Obviously, when $\varepsilon=0$ the real frame is again recovered, as expected for model categorification method.

4.3.2 Non Well Founded Sets and Probabilities

The sets that contain themselves as members are called abnormal sets. The elimination of abnormal sets leaves us with the standard well-founded set theory.

A non-well-founded (NWF) set theory belongs to axiomatic set theories that violate the rule of well-found sets and, as an example, allow sets to contain themselves (Aczel 1988, Barwise and Moss 1996). Denying the foundation axiom in number systems implies setting an NA ordering structure.

Aczel proved that a graph will contain no cycles or loops if and only if it is well-founded. This means that a graph that contains loops or cycles is a picture of a non-well-founded set. The presence of cycles and loops would indicate that some set has itself as a member or that the concept system or definition it models is impredicative.

The antifoundation axiom which embraces non-well-founded sets is as follows: every graph cyclic or not, pictures a genuine set. Hypersets are defined as graphable sets. The well-founded and non-well founded sets are both types of hypersets.

The antifoundation axiom was explained as follows. Suppose that all initial objects are ways and the operations over those initial objects are motions on them. The foundation axiom says that there exist finite ways. In this case, we use the induction principle. According to this it is possible to achieve an aim at the shortest distance between points. The negation of the axiom of foundation causes that all ways are infinite. Then we cannot apply the induction principle since there are no shortest distances. Therefore one uses there the so-called coinduction principle. According to this it is possible to achieve an aim at the largest distance between points.

Taking into account the existence of infinitely large numbers in NA mathematics (for instance in analysis of infinitesimals or of infinite), we can state that initial objects of NA mathematics are objects obtained implicitly by denying the axiom of foundation. NA numbers may be represented only as infinite ways. These objects are NWF.

NWF or hypersets represents useful tool to make sense of the kind of complexity characteristic to evolvable systems. Chemero and Turvey (2006) showed that the hypersets provides significant models of living complex systems. Hypersets have been applied for models of complex systems like autocatalytic cyclic reactions, hypercycles, metabolic cycles and autopoietic systems.

The interest in non-well-founded phenomena is also motivated by developments in computer sciences. In this area, many objects and phenomena have non-well-founded features: self-applicative programs, self-reference, graph circularity, looping processes, transition systems, paradoxes in natural languages, and so on.

A significant class of PSM involves cyclic evolution and cyclic time concept (Iordache 2009, 2010). The probabilities associated to cyclic evolutions have been based on similarities. They represent a kind of fuzzy probabilities, or in other terms, an example of possibilities.

Another class of fuzzy probabilities has been associated to NWF sets by Schumann (2008). The conventional probability theory is built in the language of well-founded mathematics. It sets a framework of physics, taking into account that physical reality is regarded in physics as reality of stable repetitive phenomena.

Real probabilities are obtained as a result of a limiting process for rational frequencies in real topology by means of the law of large numbers. Using these probabilities we use to accept only well-founded phenomena. In NA physics and in NA probability theory it is assumed that reality is NWF. Since statistical stabilization, that is the limiting process, can be considered not only in the real topology on the field of rational numbers but also in NA topologies, it results that reality can be considered as NWF too.

According to the hypothesis that reality is NWF, experimental results should be analyzed not only in the field of real numbers but also in NA fields.

In the standard way, probabilities are defined on algebra of subsets.

Paralelling standard definitions, it is possible also to set probabilities on the algebra $F^V(X)$ of fuzzy subsets $A \subset X$ that consists of the following: (1) union, intersection, and difference of two fuzzy subsets of X; (2) Φ and X. Here V denotes an NA set.

In this case a finitely additive probability measure is a nonnegative set function P(·) defined for sets $A \in F^V(X)$ that runs the NA set V and satisfies the following properties:

1. $P(A) \geq 0$ for all $A \in F^V(X)$
2. $P(X) = 1$ and $P(\Phi) = 0$,
3. if $A \in F^V(X)$ and $B \in F^V(X)$ are disjoint, then $P(A \cup B) = P(A)+P(B)$.
4. $P(\neg A) = 1 - P(A)$ for all $A \in F^V(X)$

Here 1 is the largest member of V and 0 is the least member of V.

This probability measure is a fuzzy probability or in other terms a possibility.

The originality of fuzzy probability is that conditions 3, 4 are independent. As a result, for a probability space $\{X, F^V(X), P\}$, some Bayes' formulas do not hold in the general case (Schumann 2008).

4.4 Models Categorification Methodology

4.4.1 Frame of Infinitesimals for PSM

The SKUP frames associated to PSM represents the model categorification of the (s,k,u,p) frames associated to RSCC.

Let us consider here that a scale of time is associated to every conditioning level. To take into account the existence of different scales of time the discrete time n will be translated into the vector:

$$N = n + \varepsilon w_1 n + ... + \varepsilon^m w_m n + ... + \varepsilon^M w_M n \tag{4.5}$$

Denotes also N = [n, w_1n,..., w_mn,..., w_Mn]. Here w_m are real random variables proportional to the lifetime on the level m while ε are positive arbitrary small constants. Taking into account the definition of order on the field K containing elements as N, one observe that the evolution at the level m, performed during $w_m n \varepsilon^m$ units of time appears as infinitesimal relative to the evolution at the level m - 1 performed during $w_{m-1} n \varepsilon^{m-1}$, units of time. The structure of time N induces a similar structure of the states s(n) = s_n. The states s(n) have been translated into S(N) = [s^0(n), s^1(n),..., s^m(n),...,s^M(n)] where s^m(n) are real valued functions. Obviously S (N) ∈ K but number such as S= s^0(n)+εs^1(n) may be evaluated by their real value too.

If the expansions contain a finite number of elements the NA structures are rings (Appendix 1). Let B = [b_0, b_1], D = [d_0, d_1]. A function U of two variables is defined in the NA structure of Neder by:

$$U(B,D)=U([b_0,b_1],[d_0,d_1])=[u^0(b_0,d_0), v^1(b_0,d_0,b_1)+w^1(b_0,d_0,d_1)] \tag{4.6}$$

Here u^0, v^1, w^1 are real functions. To obtain (4.6) usual series expansions are used. Now the elements of an RSCC are translated in the NA frame. Denote the vector of time by T = [n, t] that is T = n + ε t where n and t are integers. Denote also by S(T) the state of the system at the moment T = [n, t] and by K(T) the corresponding condition. In the above described NA frame S(T) = [s^0(n), s^1(n)], K(T) = [k^0(n), k^1(n)] where s^0(n), s^1(n), k^0(n), k^1(n) are real valued functions. Notice that k^1(n) includes information concerning t.

With possibility P (K(T')| S(T)) the system arrives at the condition K(T') where T' = [n, t+ σ]. Observe that K (T') = [k^0(n), k'^1(n)] where k'^1(n) includes information concerning t+σ. To simplify notations consider that P(K(T')| S(T))=[p^0(k^0(n)), p^1(k^0(n), k'^1(n))] that is S(T) does not play. In the next step a change of state takes place, the new state being S(T") = U(S(T), K(T')) where T" = [n+1, t+ σ]. Next, a new condition K(T"')=[k^0(n+1), k'''^1(n+1)] with T"' = [n+1, t + σ + ρ] is established with possibility P(K(T"')| S(T"))=[p^0(k^0(n+1)), p^1(k^0(n+1), k'''^1(n+1))]. According to K(T"') the system arrives in S(T^{iv}) with T^{iv} = [n+2, t + σ + ρ]. Using the properties of K the model gives:

$$[s^0(n+1), s^1(n+1)] = U([s^0(n), s^1(n)], [k^0(n), k^1(n)]) =$$
$$=[u^0(s^0(n), k^0(n)), v^1(s^0(n), k^0(n), s^1(n))+w^1(s^0(n), k^0(n), k^1(n))] \tag{4.7}$$

Consequently, using the definition of equality in the NA frame it results:

$$s^0(n+1) = u^0(s^0(n), k^0(n)) \tag{4.8}$$

$$s^1(n+1) = v^1(s^0(n), k^0(n), s^1(n)) + w^1(s^0(n), k^0(n), k^1(n)) \tag{4.9}$$

The equation (4.8) corresponds to the usual operator of an RSCC while the equation (4.9) outlines the contribution of the next conditioning level. When $\varepsilon=0$ the real frame is validated, according to the model categorification method.

Instead of the elements of the RSCC denoted by (s, k, u, p) that is s(n), k(n), and s(n+1) = u(s(n), k(n)), p(k(n)| s(n)), a SKUP frame that is S(T); K(T'); U(S(T), K(T'))=S(T''), P(K(T')| S(T)) results. This represents the model categorification model translating the real field elements of an RSCC denoted by (s, k, u, p) in the more affluent set of elements SKUP with $S=(s^0, s^1,...,)$, $K=(k^0, k^1,\ldots,)$, $U=(u^0, v^1, w^1,...,)$, $P=(p^0, p^1,\ldots)$.

In the NA case T = [n, t] where t is a R-valued random variable, S (T) is an RxR=S, valued random variable, K(T) is defined on K^0 x K^1. In applications K^1 may include a specification of the waiting time or scale. U is a measurable mapping from S x K^0 x K^1 to S. Obviously u^0, v^1, and w^1 are measurable mappings.

The resulting system (4.8), (4.9) shows the class of real models being compatible with an NA model described by the model: S (T'') = U(S(T), K(T')). The proposed general theory includes and extends the case of real field theory.

4.4.2 NA Difference Equation

Consider again the example described by the equation (3.5).

The real model (3.5) may be translated into the NA stochastic difference equation:

$$\frac{Y(N) - Y(N_1)}{N - N_1} = -AY(N_1) \tag{4.10}$$

For the sake of simplicity we restrict here to m = 1, N = [n, n], Y(N) = [$y^0(n)$, $y^1(n)$].

Here N_1 = [n-1, n-1], A = [a, 0]. According to N_1 a single step is performed at any level. From (4.10) it results using the definition of the product in the NA frame:

$$y^0(n)-y^0(n-1) = -a\, y^0(n-1) \tag{4.11}$$

$$y^1(n)-y^1(n-1)=-ay^1(n-1)-a\, y^0(n-1) \tag{4.12}$$

This gives:

$$y^0(n) = k\, y^0(n-1) \tag{4.13}$$

$$y^1(n) = k\, y^1(n-1)-(1-k)\, y^0(n-1) \tag{4.14}$$

Here k = 1-a. Taking N_1 = [n-1, n-1+w] with w, a random variable the model reduces to:

$$y^0(n) = k\, y^0(n-1) \tag{4.15}$$

$$y^1(n) = k\, y^1(n-1)-(1-k)(1-w)y^0(n-1) \tag{4.16}$$

The resulting SKUP contains the elements:

$S(N) = Y(N)= [s^0(n), s^1(n)]$, $k^0(n) = k$, $k^1(n) = w$, $K(N) = [k,w]$,

$$u^0(s^0(n),k^0(n))=k^0(n)s^0(n) \tag{4.17}$$

$$v^1(s^0(n), k^0(n), s^1(n))=k^0(n)s^1(n) \tag{4.18}$$

$$w^1(s^0(n), k^0(n), k^1(n) = - (1-k^0(n))(1-k^1(n))s^0(n) \tag{4.19}$$

$$P(K(N')| S(N)) = P(K(N)) = [p^0(k^0(n)), p^1(k^0(n), k^1(n))] \tag{4.20}$$

Observe that S may be considered as: $S= s^0(n)+\varepsilon s^1(n)$.

The difference equation (4.10) is replaced by a system of m difference equations. The resulting structure seems complicated but using an NA calculus the result can be obtained directly from (4.10). Solving (4.10) one obtains by simple NA calculus solutions for systems as: (4.15), (4.16).

The proposed approach appears as a method of finding new classes of solutions supplementing known classes of solutions, at the basic level m = 0. New solutions may be of similar type, as in ordinary bifurcation theory, or they may be different, as in the Hopf bifurcation of periodic solutions from stationary solutions of ordinary partial differential equations.

The significance of the NA model can be seen first of all, in its ability to express the main qualitative behavioral features that are masked by the complicated structure of real valued detailed models, in a simpler, even if skeletal or generic form. According to the model categorification method, the predictions for the one level frame should be validated by the general multi-level theory.

References

Aczel, P.: Non-well-founded Sets, Stanford CSLI (1988)

Bainbridge, W.S., Roco, M.C. (eds.): Managing Nano-Bio Info-Cogno Innovations: Converging Technologies in Society. Springer Science and Business Media, Berlin (2006)

Barwise, J., Moss, L.: Vicious Circles, On the Mathematics of Non-Wellfounded Phenomena. CSLI Lecture Notes Number, vol. 60. CSLI Publications, Stanford (1996)

Blume, A., Branderburger, A., Dekel, E.: Lexicographic probabilities and choice under uncertainty. Econometrica 59(1), 61–79 (1991)

Brier, S.: Cybersemiotic pragmaticism and constructivism. Constructivist Foundations 5(1), 19–39 (2009)

Chemero, A., Turvey, M.T.: Complexity and "closure to efficient causation". In: Ruiz-Mirazo, K., Barandiaran, R. (eds.) Proceedings of ALifeX: Workshops on Artificial Autonomy, pp. 13–19

Dubois, D., Prade, H.: Possibility theory, probability theory and multiple valued logics: a clarification. Annals of Mathematics and Artificial Intelligence 32, 35–66 (2001)

Hammond, P.J.: Elementary Non-Archimedean Representation of Probability for Decision Theory and Games. In: Humphreys, P. (ed.) Patrick Suppes: Scientific Philosopher. Probability and Probabilistic Causality, vol. I, pp. 25–59. Kluwer Academic Publishers, Dordrecht (1994)

Iordache, O.: Evolvable Designs of Experiments Applications for Circuits. J. Wiley VCH, Weinheim (2009)

Iordache, O.: Polystochastic Models for Complexity. Springer, Heidelberg (2010)

Neder, L.: Modell einer Differentialrechnng mit aktual unendlich kleinen Grossen erster Ordnung. Math. Annalen. 118(2), 251–262 (1941)

Neder, L.: Model einer Leibnizischen Differentialrechnung mit aktual unendlich kleiner Grossen samtlicher Ordnungen. Math. Annalen. 118(5), 718–732 (1943)

Poli, R.: The basic problem of the theory of levels of reality. Axiomathes 12(3-4), 261–283 (2001)

Schumann, A.: Non-Well-Founded Probabilities and Coinductive Probability Logic. In: Proceedings of the 2008 10th International Symposium on Symbolic and Numeric Algorithms for Scientific Computing, Timisoara, Romania, pp. 54–57 (2008)

Sowa, J.F.: Representing Knowledge Soup. In: Language and Logic, Conference on Knowledge and Logic. Technische Universität Darmstadt (2002)

Sowa, J.F.: The challenge of knowledge soup. In: Proc. First International WordNet Conference, Goa, India (2004)

Chapter 5
Mixing in Chemical Reactors

Abstract. The mixing plays a fundamental role in domains as fluid dynamics, chemical engineering, environmental studies and pharmacology.

Discrete and continuous time models, based on model categorification method have been developed. The residence time distributions, RTD, for multi-scale imperfect mixing are expansions in terms of Meixner and Laguerre polynomials.

The resulting RTD are compared to different models of imperfect mixing.

Local anesthetic effects on membranes are presented in the general PSM framework.

The SDG solution for imperfect mixing is exposed.

5.1 Discrete Model of Imperfect Mixing

5.1.1 Residence Time Distribution, RTD

The problem of mixing in chemically reactive flows is of technological importance in chemical reactors, combustion and propulsion systems, environmental studies, pharmacology, biophysics and so on. The aim of the research in the domain of mixing is to obtain an understanding of the physics of mixing, of the effect of these motions on the transport properties, of the effect of chemical kinetics and to combine all these aspects in the form of a model of the process. Physical effects in chemical reactors are difficult to separate from the chemical rate processes. In trying to do so one usually distinguishes between chemical kinetics and fluid dynamics putting down the performance equation of a chemical reactor as follows:

Output = f (input, kinetics, flow pattern)

While turbulent mixing continues to be largely a very difficult subject, there exists a considerable need for the development of methods for the calculation of mean flow properties. A number of predictive methods have therefore been developed based largely on heuristic reasoning. Improvements in such methods

have arisen principally through the use of computational facilities. At present the mathematical description of the intricate process in a chemical device is usually worked out with the aid of approximate pictures of the internal structure of the flows (Fogler 2006).

Two types of ideal flow are commonly used as limits of flow patterns in process vessels; these are the "plug flow" and the "perfectly mixed" flow. The conditions for the physical realization of the plug flow are fulfilled in a piston-type flow, when it is assumed that no mixing takes place in the direction of flow. The model is employed to describe tubular apparatus with a large length-to-diameter ratio. At the other extreme, perfect mixing assumes that the vessel contents are completely homogeneous and the outlet-stream properties are identical to the vessel-fluid properties. In chemical engineering the usual tendency is to come closer to conditions of perfect mixing by fitting apparatus with special mixers, baffle plates etc. Non-idealities of flow in industrial apparatus can be traced to the following most important reasons: presence of dead spaces, channeling or by passing, recycling or cross-flow streams, developed turbulence etc. Stagnant fluid or dead spaces represent regions with extremely poor contacting. A dead space will contain fluid elements for interval of time with an order of magnitude over the mean residence time. In bypassing or channeling some of the fluids slip or pass through the vessel considerably faster than others do. Bypassing may be found in flow through poorly packed vessels, through heat exchanger in two-phase operations etc. In recycling a certain amount of fluid is recirculated or returned to the vessel inlet. This type of flow may be desirable for example in auto-thermal reactions. When constructing a flow model for a given chemical reactor one starts by knowledge of the pattern of fluid passage through the reactor. This flow behavior could be determined by finding the complete history of each fluid element. It was pointed out that, instead of this complexity of the flow pattern, it is enough to know how long the fluid elements stay in the reactor, in other words, to determine the RTD of the fluid particles in the exit stream.

The concept of RTD, has deeply contributed to chemical engineering science (Pethö and Noble 1982, Nauman 2004). It is obvious that RTD theory is not restricted to chemical engineering; it finds application in areas such as biology, pharmacology, hydrology and environmental sciences, reliability and so on (Jacquez 1985).

The residence time of a fluid element is the time that elapses from the time the element enters the vessel to the time it leaves it. The age of a fluid element at a given instant of time is the time that elapses between the element's entrance into the vessel and the given instant. It is considered that a fluid element once entered the system cannot leave and reenter it again and steady state RTD holds. The RTD, E (t), is the age distribution frequency of the fluid elements leaving the vessel. This function is normalized so that:

$$\int_0^\infty E(t)dt = 1 \tag{5.1}$$

The moments of the RTD are given by:

$$\bar{t}^{n} = \int_{0}^{\infty} t^{n} E(t)dt \tag{5.2}$$

The cumulative RTD function is:

$$F(t) = \int_{0}^{t} E(t)dt \tag{5.3}$$

It gives the fraction of material introduced after a given instant that emerges at a time t later. This is the response of the system to a step change of tracer concentration in the input. The response to an impulse of tracer to the inlet gives E (t), by normalization. In fact, some experimental techniques for getting the RTD from experiments have been proposed. In many problems, however, it is difficult to obtain an analytical expression for E (t). Naor and Shinnar (1963) introduced the intensity function Λ (t) dt or the fraction of material of age t that will leave the system in the interval (t, t+dt) to give a clear insight into stagnancy. The relations between E(t), F(t) and Λ(t) are given by:

$$E(t) = F'(t) = \Lambda(t)\exp-[\int_{o}^{t} \Lambda(t)dt] \tag{5.4}$$

$$F(t) = 1 - \exp-[\int_{o}^{t} \Lambda(t)dt] \tag{5.5}$$

$$\Lambda(t) = -\frac{d}{dt}\ln[1 - F(t)] \tag{5.6}$$

The system with stagnancy has an escape probability that decreases over some interval because in such an interval the longer a particle stays the less likely it is to leave. The intensity function shows a maximum when there is stagnancy.

Transfer functions proved to be useful in RTD studies. Denote by Y(s)=L(y(t)) and by X(s)=L(x(t)) the Laplace transforms of the exit y(t) and the entrance x(t) of a linear system. By definition G(s) = Y(s)/X(s) is the transfer function of the system. If the entrance is a Dirac pulse, x(t)= δ(t) then G(s)=Y(s).

A significant development of the chemical engineering RTD concept for pharmaceutical purposes is ADMET.

ADMET is an acronym in pharmacokinetics and pharmacology for absorption, distribution, metabolism, excretion, and toxicity and describes the distribution and the interactions of a pharmaceutical compound within an organism. The five

criteria all influence the drug levels and kinetics of drug exposure to the tissues and the performance and pharmacological activity of the drug.

The chemical reactor for RTD studies corresponds to the organism for ADMET studies.

For a compound to reach a tissue, it usually must be taken into the bloodstream - often via intestinal absorption - after being taken up by the target cells. This can be a difficult problem at some natural barriers like the blood-brain barrier, for example.

Factors such as compound solubility, transit time, chemical instability, and inability to permeate the walls or membranes, can all reduce the extent to which a drug is absorbed after administration.

Absorption significantly determines the compound's bioavailability. Drugs that absorb poorly when taken orally must be administered in some other ways, like intravenously or by inhalation.

The compound needs to be carried to its effectors site, via the bloodstream, for instance. From there, the compound may distribute into tissues and organs, usually to differing extents. After entry into the circulation, either by intravascular injection or by absorption from any of the various extracellular sites the drug is subjected to a number of process, as distribution process that tend to lower its plasma concentration.

Distribution is defined as the reversible transfer of a drug between compartments.

Factors affecting distribution include blood flow rates and the drug binding to serum proteins forming a complex.

Compounds begin to break down as soon as they enter the body. The majority of small-molecule drug metabolism is carried out in the liver by enzymes. As metabolism occurs, the initial compound is converted to new compounds, the metabolites. When metabolites are pharmacologically inert, metabolism deactivates the administered dose of parent drug and this usually reduces the effects on the body. Metabolites may also be active.

Compounds and their metabolites need to be removed from the body.

Unless the removal is complete, accumulation of foreign substances can adversely affect normal metabolism.

There are several sites where drug removal occurs. Removal of drugs by the kidney involves different mechanisms as: glomerular filtration of unbound drug, active removal of free and protein-bound drug by transport filtrate concentrated in tubules for a favourable concentration gradient so that it may be reabsorbed by passive diffusion.

Computational methods allow predicting the ADMET qualities of compounds through methods like Quantitative structure-activity relationship (QSAR).This is the process by which chemical structure is quantitatively correlated with a well defined process, such as biological activity or chemical reactivity. The route of drug administration critically influences ADMET.

5.1.2 Discrete Model for Residence Time Distributions

The RTD for discrete-time measurements in flow systems exhibiting many scales of time particularly for systems presenting a number of parallel pathways with widely different residence time is described here. Denote by x (n) the input at the moment n, by y (n) the output at the same moment and by h the RTD function, then:

$$y(n) = \sum_{\infty}^{-\infty} h(n-k)x(k) = h(n) * x(n) \tag{5.7}$$

Here " *" is the convolution mark and h(n-k) stands for the output at the moment n due to an input which is equal to unit at the moment k and is null for all the others. Several discrete-time studies have attempted to develop methods for interpreting inlet-outlet tracer tests in vessels and mixers with flow heterogeneities. The model developed in the following is based on the observation that perturbations of an RTD take place at different scales of time. Possible behavior of mixing systems could be classified using the number m of conditioning levels. Such levels correspond to a hierarchy of dead spaces in the sense that the space related to the level m appears as a dead space with respect to the space corresponding to the level m-1 but as short-circuit with respect to the space related to the level m+1. Intuitively a complex system presenting m parallel pathways with strongly different residence times should give rise to a hierarchy of m conditioning levels corresponding to m more slower motions. Obviously in this picture a scale of time is associated to each conditioning level.

Fig. 5.1 shows an imperfect mixing system. In the physical picture shown in Fig. 5.1 there exist three scales of time. The space corresponding to m=0 is active while those corresponding to m=1 and m=2 are more and more slow.

A classical quantitative approach to the non-ideality of mixing is due Cholette and Cloutier (1959) who proposed several models for a real stirred tank consisting of a "perfectly mixed" region a "dead" or "stagnant" region and a certain fraction of the feed by passing both regions. In this model three scales of time have been considered.

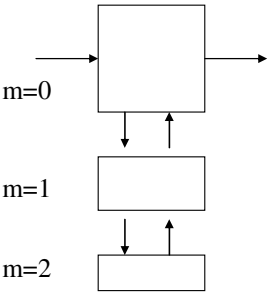

Fig. 5.1 Imperfect mixing

An NA frame for interpreting inlet-outlet tracer tests in discrete time will be proposed in the sequel.

First, one translates by model categorification the discrete time n into the expansion N:

$$N = n + \varepsilon w_1 n + ... + \varepsilon^M w_M n \tag{5.8}$$

The RTD density function h (n) is replaced by model categorification by the expansion H (N):

$$H(N) = h_0(n) + \varepsilon h_1(n) + ... + \varepsilon^M h_M(n) \tag{5.9}$$

Here M is the (finite) number of scales of mixing, ε is an arbitrary small positive constant, w_m, $0 \le m \le M$ are constants. Denote also N = [n, w_1n,...,w_Mn], H(N) = [h_0(n), h_1(n),..., h_M(n)] the expansions (5.8) or (5.9). The time N introduced here enables us to study changes at slower and slower scales of time. The evolution at the level m+1, performed during $\varepsilon^{m+1} w_{m+1} n$ units of time, appears as infinitesimal relative to the evolution at the level m, performed during $\varepsilon^m w_m n$ units of time. Replacing n by N, allows accounting for the fact that the interval elapsed between events occurs on many time scales. Consequently, the time is thought as a vector with two or more components, and no more as a scalar. The sequence w_m was introduced in order to improve the information on the inter-occurrence time. The structure of the RTD function is NA too. H (N) contains the term h_0(n) corresponding to the basic mechanism of mixing indexed by m=0 and different corrections accounting for infinitesimals of this mechanism at different scales.

Consider that the generic mechanism is the perfect mixing. The differential equation for the RTD function of a perfectly mixed vessel is:

$$\frac{dh}{dt} = -ah \tag{5.10}$$

Here h(t) dt is the probability for a fluid element to have the residence time between t and t + dt, a=v/V where v is the volumetric flow rate and V is the volume of the entire complex system. In the NA frame it is necessary to translate (5.10) by model categorification method into the NA equation with finite differences:

$$\frac{H(N) - H(N_1)}{N - N_1} = -AH(N_1) \tag{5.11}$$

Here N = [n, n..., n], N_1 = [n-1, n-1,..., n-1], A = [a, 0,...,0]. The vectors N, N_1, and A contains M+1 elements. The derivative is taken along the direction [1, 1,..., 1],

which corresponds to a physical complex system where a single step is performed at the m-th scale during $\varepsilon^m n$ units of time. Applying the operations defined in the Appendix 1 (the structure of Neder) that is equating the coefficients of different powers of ε with zero, equation (5.11) is translated by model categorification method to the following system of M+1 difference equations:

$$h_0(n) - h_0(n-1) = -ah_0(n-1) \tag{5.12}$$

$$(h_m(n) - h_m(n-1)) - (h_{m-1}(n) - h_{m-1}(n-1)) = -ah_m(n-1) \tag{5.13}$$

$$(h_M(n) - h_M(n-1)) - (h_{M-1}(n) - h_{M-1}(n-1)) = -ah_M(n-1) \tag{5.14}$$

It should be emphasized that to obtain the elements of (5.12-5.14) one considered in all steps of the proof that there exists a finite and fixed number of scales, m, $0 \le m \le M$.

Consider that a fluid particle has the same probability to enter any scale of mixing. Consequently the initial condition is:

$$h_0(0) = h_1(0) = ... = h_M(0) = 1 \tag{5.15}$$

From (5.13) and (5.15) it results the solution:

$$h_m(n) = \alpha^n M_m(n,1,\alpha)/m!, 0 \le m \le M \tag{5.16}$$

Here α = 1-a, $M_m(n,\beta,\alpha)$ are the Meixner orthogonal polynomials. The orthogonality relation is:

$$\sum_{n=0}^{\infty} \alpha^n (\beta)_n / n! M_m(n,\beta,\alpha) M_e(n,\beta,\alpha) = m!(\beta)_m \alpha^{-m} (1-\alpha)^{-\beta} \delta_{me} \tag{5.17}$$

Here: $(\beta)_n = \Gamma(\beta+n)/\Gamma(\beta)$ with Γ the Gamma function. An explicit representation is:

$$M_m(n,\beta,\alpha) = (\beta+n)_m F(-m,-n,1-\beta-m-n,\alpha^{-1}) \tag{5.18}$$

F is the hypergeometric function given by:

$$F(a,b,c,z) = 1 + a.b.z/c.1! + a(a+1)b(b+1)z^2/c(c+1)2! + ... \tag{5.19}$$

By experiments, measurements at the basic scale m=0 are obtained and the experimental RTD function is:

$$h_{exp} = [h_{exp},0,...,0] \tag{5.20}$$

Here h_{exp} denotes the measured RTD. It is a real value. The general NA solution of the equation (5.11) is:

$$H = [h_0, h_1, ..., h_M] \tag{5.21}$$

Here h_m is given in equation (5.16). In order to compare the NA function H with the real data, h_{exp} we need to use the series expansions given by equation (5.11) that is, to translate the contribution of all scales m=1, 2,..., M to the basic scale m=0. It results:

$$h = \left[\sum_{m=0}^{M} q_m h_m, 0, ..., 0 \right] = \sum_{m=0}^{M} q_m [h_m, 0, ..., 0] \tag{5.22}$$

The coefficients q_m are constants. This is in fact a representation of the RTD using the NA orthogonal basic $\{[h_m, 0, ..., 0]\}$, m=0,...,M. (Appendix 1). According to (5.16) one obtains the computed RTD:

$$h(n) = \alpha^n \sum_{m=0}^{M} q_m M_m(n, 1, \alpha)/m! \tag{5.23}$$

In this way the solution (5.21) obtained for particular N, N_1, and initial conditions represents the basis for any other solution of (5.11). The constants q_m, are related to the contribution of the m-th scale of the process. The new problem is to identify q_m in order to minimize the distance between $h_{exp}(n)$ and h(n). Following Robert (1967), an NA distances d (h,g) = ||h-g|| is defined by:

$$||h|| = p^{w(h)} \tag{5.24}$$

with 0<p<1 and

$$w(h) = \min \{m; \mu_m(h) \neq 0\} \tag{5.25}$$

Here:

$$\mu_j(h) = \sum_{n=0}^{\infty} h(n) M_j(n, 1, \alpha) \tag{5.26}$$

The NA distance d (h_{exp}, h) is minimum, namely it is zero if:

$$\mu_j(h_{exp} - h) = 0 \tag{5.27}$$

Equation (5.27) is verified when:

$$\sum_{n=0}^{\infty} (h_{exp} - \sum_{m=0}^{M} q_m h_m) M_m(n, 1, \alpha) = 0 \tag{5.28}$$

This is valid for any m≤M. Using the orthogonality property of the Meixner polynomials it results that:

$$\alpha^{-m}(1-\alpha)^{-1}q_m = \sum_{n=0}^{\infty} h_{exp}(n)\,M_m(n,l,\alpha)/m! \tag{5.29}$$

A main characteristic of the PSM model is its finitude as number of scales to be considered that is: $q_0 \neq 0$, …$q_M \neq 0$ but $q_M = 0$ if m≥M+1.This means that there exists a finite number of scales and that after the last scale the process is in no way scaled. A consequence of this fact is that the NA frame doesn't discriminates between models with different number of scales of mixing.

The practice is confronted with real field experimental data. In this case the best model will be obtained using a real objective function as for instance the sum of squares of deviations S (M):

$$S(M) = \sum_{n=0}^{\infty} (h(n) - h_{exp}(n))^2 \tag{5.30}$$

Here, $h_{exp}(n)$ represents the experimentally measured RTD whereas h(n) is calculated, for various M, using (5.23) and (5.29). This is the place where the real and "other than real" frames should be in touch. The "other than real" frame is useful to outlines the possible classes of solutions, the basic solutions corresponding to different scales. Confronting this with real data allows limiting the number of scales. After each model step, the confrontation with reality consists in establishing q_m.

Fig. 5.2 shows the discrete time scales and integrative closure for one cell.

Fig. 5.2 illustrates the situation in which we may limit the system at only four scales of time. Any new level includes the previous ones. The Meixner polynomials included at any new level are indicated as well as a hypothetical connection of the lower and top levels. It suggests that the ε^4 terms will be neglected.

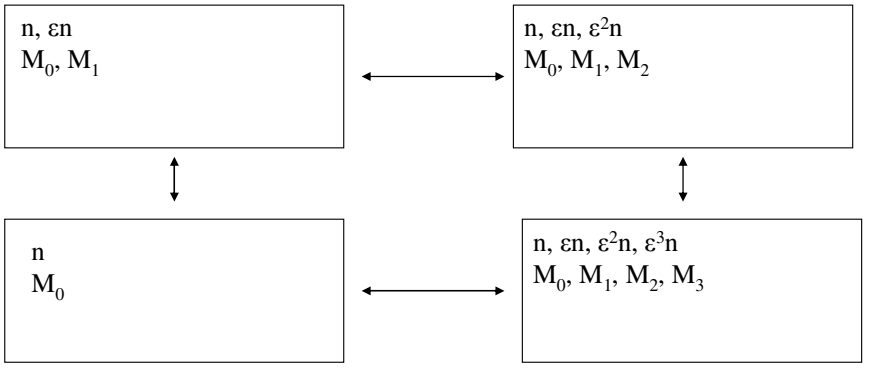

Fig. 5.2 Discrete time scales and integrative closure for one cell

5.1.3 Local Anesthetic Effects

The primary effect of chemical inactivation of the membrane functions by drugs or other chemicals consists of modifying the conformations of the active membranes components.

Anesthetics are supposed to act on the excitable membrane in a charged form inside the nerve axon (Strichartz and Ritchie 1987).

Some correlations of the exponential type have been proposed for the relaxation of the amplitude of compound action potential. An application of multi-scale models concerns some experiments describing the decrease of the action potential by procaine (Iordache and Frangopol 1988a, Iordache et al. 1988a).

Table 5.1 shows experimental data, the action potential relative amplitude of procaine 10mM as a function of time step n.

The value of α in eq. (5.23) may be correlated to the mean residence time, $\bar{n} = 1/(1-\alpha)$. Taking $\bar{n} = 6.25$ it results α= 0.84 (the time step size is 5 min).

Table 5.1 Action potential amplitude for the anesthetic effect

n	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
experiment	1	.85	.71	.58	.50	.41	.35	.28	.22	.18	.14	.10	.08	.05	.04
Eq.(5.23) M=0	.88	.74	.62	.52	.44	.37	.31	.26	.22	.18	.15	.13	.11	.09	.07
Eq.(5.23) M=1	.96	.80	.66	.54	.45	.38	.31	.25	.21	.17	.14	.12	.09	.07	.06

Table 5.2 shows the objective function S (M) for different number of scales, M. This allows selecting a model that is a truncation number M.

Table 5.2 Objective function for single compartment model

Nr of scales, M	0	1	2
S(M)	6.10^{-4}	$1.7.10^{-4}$	0.2

We conclude that M=1 provides a satisfactory picture of the studied phenomenon.

For M=1 the coefficients are q_0=0.878 and q_1=0.081.

Table 5.1 compare also the perturbed model (M=1) and the ideal model (M=0).

M=2 shows uncorrelated results.

If the statistics of flow and kinetics as well as the coefficients q_m, are known the multi-scale modeling method could represent a progress towards an a priori design of anesthetic treatments. The existence of more scales of the processes suggests that the excitation or inhibition of a given scale may be an efficient mean for drug kinetics control.

To take into account stochastic character at different scales confidence intervals of variables must be added to ensure significant conclusions.

5.1.4 Stochastic Features. Real Field Probabilities

There are systems that exhibit random responses for deterministic signals. Systems in which the fluctuations are strong enough to cause different tracer experiments to yield different results are encountered in fluidized beds in turbulent combustion, multi-jet reactors, mixing vessels etc. Firstly consider that only w_m are real random variables. This implies that the coefficient q_m is random too. Obviously, in this case the equation (5.23) is replaced by the following stochastic RTD:

$$h(n,\omega) = \alpha^n \sum_{m=0}^{M} q_m(\omega)\, M_m(n,1,\omega)/m! \tag{5.31}$$

Here $\omega \in \Omega$ a probability space. The mean of h (n,ω) is given by:

$$\bar{h}(n) = \alpha^n \sum_{m=0}^{M} \bar{q}_m\, M_m(n,1,\alpha)/m! \tag{5.32}$$

An approximation of its variance is:

$$V(h(n,\omega) = \alpha^{2n} \sum_{m=0}^{M} V(q_m(\omega)).(M_m(n,1,\alpha)/m!)^2 \tag{5.33}$$

If for instance, q_m is supposed to be discrete independent identically distributed random variable, taking the values $q_{m,j}$ ($j \in J$) with the probability p_j, then it results:

$$\bar{q}_m = \sum_j p_j q_{m,j} \tag{5.34}$$

$$V(q_m) = \sum_j p_j q_{m,j}^2 - (\bar{q}_m)^2 \tag{5.35}$$

In turbulent mixing the random behavior of the flow rate must be accounted for. In this case α is a random variable and stochastic RTD results too. The main problem is to obtain the statistics of RTD at different scales of mixing. Denote by π_j the probability that the value of α is α_j, $j \in J$. Starting from the first equation (5.12) the mean of $h_0(n)$ is obtained (Iordache and Corbu 1986):

$$\bar{h}_0(n) = \sum_j \pi_j \alpha_j \bar{h}_0(n-1) = \bar{\alpha}\bar{h}_0(n-1) \tag{5.36}$$

Here:

$$\bar{\alpha} = \sum_j \pi_j \alpha_j \tag{5.37}$$

Using also the condition (5.15) it results at the basic scale

$$\bar{h}_0(n) = (\bar{\alpha})^n \tag{5.38}$$

The second order moment is:

$$\bar{h}_0^2(n) = \sum_j \pi_j \alpha_j^2 \bar{h}_0^2(n-1) = \bar{\alpha}^2 \bar{h}_0^2(n-1) \tag{5.39}$$

$$\bar{\alpha}^2 = \sum_j \pi_j \alpha_j^2 \tag{5.40}$$

Considering, that $\bar{h}_0{}^2(0) = 1$, it results $\bar{h}_0{}^2(n) = (\bar{\alpha}^2)^n$

Denote by $V_m(n)$ the variance of $h_m(n)$. Then:

$$V_0(n) = \bar{h}_0^2(n) - (\bar{h}_0(n))^2 = (\bar{\alpha}^2)^n - (\bar{\alpha})^{2n} \tag{5.41}$$

Taking $\bar{\alpha}$ instead of α in all equations of the system (4.13) it results:

$$\bar{h}_m(n) = (\bar{\alpha})^n M_m(n,1,\bar{\alpha})/m! \tag{5.42}$$

The variance at the m-th scale is approximated by:

$$V_m(n) = \sum_{k=0}^{n-1} V_{m-1}(n-k) + V_{m-1}(n-k-1))(\bar{\alpha})^{2k} \tag{5.43}$$

Starting from $\bar{h}_m(n)$ and $V_m(n)$ for constant values of q_m, the mean of RTD results. Assuming that the scales of mixing are statistically independent the mean of RTD is obtained:

$$\bar{h}(n) = \sum_{m=0}^{M} q_m \bar{h}_m(n) \tag{5.44}$$

The variance of RTD is:

$$V(h(n) = \sum_{m=0}^{M} q_m{}^2 V_m(n) \tag{5.45}$$

Due to inherent experimental errors it is difficult to establish the number of scales of mixing. In some cases the intensity function could be useful. This is defined as:

$$\log \Lambda(n) = \frac{1}{n} \log \bar{h}(n) \tag{5.46}$$

In the case of a model without scales, that is when M = 0, it results that $\Lambda = \bar{\alpha}$. This is an immediate consequence of the model categorification method. If M ≥ 1 then log Λ(n) is varying with n and gives information about the number of time scales. From equation (5.44) it results that:

$$\log \Lambda(n) = \log \bar{\alpha} + \frac{1}{n}(\log(q_0 M_0(n,1,\bar{\alpha}) + q_1 M_1(n,1,\bar{\alpha}) + ... + q_M M_M(n,1,\bar{\alpha})) \tag{5.47}$$

Therefore $\Lambda = \bar{\alpha}$ for each solution of the equation:

$$q_0 M_0(n,1,\bar{\alpha}) + q_1 M_1(n,1,\bar{\alpha}) + ... + q_M M_M(n,1,\bar{\alpha}) = 1 \tag{5.48}$$

It is known that the zeros of $M_m(n,1,\bar{\alpha})$, lye on the positive real axis and that there are exactly m zeros of $M_m(n,1,\bar{\alpha})$. Consequently, the equation (5.48) has $m_S \leq M$ solutions, where $\Lambda = \bar{\alpha}$. The number m_S correspond to the lowest ranking level where the expansions are truncated. Each decreasing branch of the intensity function outlines the existence of a stagnant zone. It is a hierarchy of such zones.

5.1.5 PSM Frame for Discrete Model

The mixing model will be presented in the general frame of PSMs, the conditioning levels corresponding to different scales of time. Randomness of the mean residence time is also accounted for. Denote by $A_j = [a_{0j}, a_{1j}, a_{2j}, \ldots]$ the set of values of the residence time. Suppose that the stochastic process at each conditioning level has a proper scale of time that the unit of time on the m-th scale is ε^m and that the states and the conditions are elements of the NA frame. The complex system evolution starts from $H(N_0)$ where $N_0 = O = [0,0,...]$. In other words, $H(N_0) = [h_0(0), h_1(0), h_2(0),...]$ describes the initial particle distribution on different scales of mixing. With possibility $P(A_0 \mid H(N_0)) = P_0$ the condition is A_0 that is the residence time $A_0 = [a_{00}, a_{10}, a_{20}, \ldots]$ is selected for the next step evolution. This could be an NA probability for instance if $A_0 = [a_{00}, a_{10}, a_{20}, \ldots]$

then the possibility is $P(A_0) = [p_0, p_1, p_2, 0,\dots]$ with p_i probabilities associated to scales. This means that only the scales m=0, m=1 and m=2 are activated.

An evolution for a time interval from N_0=[0,0,0,...] to N_1=[1,1,1,...] takes place at this level. The resulting state is $H(N_1) = H(N_0)\text{-}A_0(N_1\text{-}N_0)H(N_0)$. Note that $H(N_1) = [h_0(1), h_1(1), h_2(1),...]$. Then with possibility $P(A_1 \mid H(N_1))=P_1$ the condition A_1 of evolution is selected. On account on this, the new state of the system is described by $H(N_2)=H(N_1)\text{-}A_1(N_2\text{-}N_1)H(N_1)$. We may have N_2=[2,2,...] and $H(N_2)=[h_0(2), h_1(2), h_2(2),...]$.

The process is continued indefinitely.

It is a SKUP for which the states are $S=(H(N)=\{[h_0(n), h_1(n), h_2(n),...]\}$, the conditions are $K=(A(N)=\{[a_{0j}, a_{1j}, a_{2j},\dots]\}$, the operators are defined by $U(H(N), K(N))=H(N')$, $N'\neq N$ where $H(N')=H(N)\text{-}A(N).(N\text{-}N')$. H(N) and the possibilities are given for instance by $P(K|H(N))=P_{ij}$ with $P_{ij} = [0, 0, \dots,0, p_i, 0,\dots,0, p_j, 0,\dots]$, if only the levels i and j are activated and the corresponding residence times are given by a_i and a_j.

5.1.6 Comparison with Theory

The described method could use, in equation (5.29), theoretical models for the RTD, h(n), to obtain q_m. It is known that the classical "perfect mixing" model $\bar{h}_0(n) = (\bar{\alpha})^n$ fails to describe accurately flow complex systems encountered in engineering applications. Cholette and Cloutier (1959) proved that a model of the type:

$$h(n) = \gamma\,\beta^n + (1\text{-}\gamma)\,\delta(n) \tag{5.49}$$

with $\beta\neq\alpha$ is better suited. Here γ denotes the flow split between the perfectly mixed part β^n and the short-circuit $\delta(n)$. $\delta(n)$ denotes the discrete Dirac delta function characterized by:

$$\sum_{n=0}^{\infty}\delta(n) = 1 \qquad \sum_{n=0}^{\infty} f(n)\delta(n) = f(0) \tag{5.50}$$

The coefficients q_m have been derived, as pointed above, with equation (5.29) resulting:

$$q_m = \gamma\frac{1-\alpha}{1-\beta}\left(\frac{\alpha-\beta}{1-\beta}\right)^m + (1-\gamma) \tag{5.51}$$

The RTD function is in this case:

$$h(n) = \gamma\alpha^n \sum_{m=0}^{M} \frac{1-\alpha}{1-\beta}\left(\frac{\alpha-\beta}{1-\beta}\right)^m M_m(n,1.\alpha)/m! + (1-\gamma)\delta(n) \qquad (5.52)$$

Observe that $\varepsilon \approx \frac{\alpha-\beta}{1-\beta}$. It can be shown that the number M of scales is a function of ε for a model (5.52) as accurate as the Cholette and Cloutier model (5.49).

Comparison of perfect mixing with Cholette-Cloutier model shows that the number of scales is a function of ε. If we take M=1 for $0 < \varepsilon \leq 0.02$, M=2 for $0.02 < \varepsilon \leq 0.05$ and M=3 for $0.02 < \varepsilon \leq 0.15$ the NA model seems to be as accurate as the Cholette-Cloutier model.

The physical meaning of this fact is that when ε is larger, that is when β is more and more different from α, the number of scales, which correct the basic model of "perfect mixing", is increasing.

5.2 Continuous Model of Imperfect Mixing

5.2.1 The Continuous Model

Cholette and Cloutier (1959) proposed several models for a real stirred having three scales of time: a perfectly mixed region a completely dead region and a fraction of the feed by passing both regions. They considered several possible cases including those where movement of fluid was allowed between the perfectly mixed region and the stagnant zone and vice-versa. The residence time for the particles of fluid from the completely dead space is infinite, while for those bypassing the system it is zero. This model represents a first approximation of the real flow. To avoid these conceptual difficulties of the Cholette and Cloutier model an NA model is investigated in the following (Iordache et al. 1988b).

An NA framework is useful in order to take into account the existence of different scales of time. The usual continuous time t is translated by model categorification method to T:

$$T = t + \varepsilon w_1 t + ... + \varepsilon^M w_M t \qquad (5.53)$$

Here M is the number of scales and wm, $0 \leq m \leq M$, are real constants. Denote also by $T = [t, w_1 t, ..., w_M t]$, the vector of time introduced by (5.53). The replacing of the usual variable of time t by the vector T in order to study changes at different scales of time is a classical technique. It is the support of the model categorification method. Vectors as T will be considered as elements of the classical NA structure of Neder. The NA structure of T induces a similar structure of the RTD function that describes the mixing in the hydrodynamic complex

system. The usual RTD function is translated by model categorification to the NA function:

$$H(T) = h_0(t) + \varepsilon h_1(t) + ... + \varepsilon^M h_M(t) \tag{5.54}$$

For the sake of simplicity, it is considered that the basic mechanism is perfect mixing that is as soon as a particle of fluid enters the system its probability to leave out is independent of the past history. A system with many scales of time should be described by a NA differential equation similar with equation (5.10):

$$\frac{dH}{dT} = -AH \tag{5.55}$$

Here the real constant was translated to the constant element of the NA structure, A = [a, 0,..., 0]. The derivative of H(T) is defined as :

$$H(T) = \lim_{T_1 \to T} \frac{H(T_1) - H(T)}{T_1 - T} \tag{5.56}$$

Here T = [t, t,..., t] and $T_1 = [t_1, t_1,..., t_1]$. The derivative is taken along the direction [1, 1,..., 1] that is a single step is performed at the m-th scale during $\varepsilon^m t$ units of time. Obviously, $H(T) = [h_0(t), h_1(t),..., h_M(t)]$, $H(T_1) = [h_0(t_1), h_1(t_1),..., h_M(t_1)]$. Because

$T_1 - T = [t_1 - t, t_1 - t,..., t_1 - t]$, it results:

$$\frac{H(T_1) - H(T)}{T_1 - T} = [\frac{h_1(t_1) - h_1(t)}{t_1 - t}, \frac{h_1(t_1) - h_1(t) - h_0(t_1) + h_0(t)}{t_1 - t}, \cdots, \tag{5.57}$$
$$\frac{h_M(t_1) - h_M(t) - h_{M-1}(t_1) + h_{M-1}(t)}{t_1 - t}]$$

Using (5.56) and (5.57) equation (5.55) becomes:

$$[h'_0(t), h'_1(t) - h'_0(t),..., h'_M(t) - h'_{M-1}(t)] = -[ah_0(t), ah_1(t),..., ah_M(t)] \tag{5.58}$$

This may be rewritten as:

$$h'_0(t) = -ah_0(t), h'_1(t) - h'_0 = -ah_1(t),..., h'_M(t) - h'_{M-1}(t) = -ah_M(t) \tag{5.59}$$

Instead of a single equation as usually encountered in the RTD analysis, in the NA frame a system of equations results. In the above computations all the expansions are truncated at the same finite level. The initial condition for (5.59) is:

$$h_0(0) = h_1(0) = ... = h_M(0) = a \tag{5.60}$$

This condition imposes the same probability for a fluid particle to enter any scale of mixing. The value a, is necessary to obtain the classical results when M = 0. It is condition imposed by the model categorification method. The solution of the problem (5.59), (5.60) is as follows:

$$h_m(t) = aL_m(at).\exp(-at), m \geq 0 \tag{5.61}$$

Here L_m denotes the Laguerre polynomial defined as:

$$L_m(at) = \frac{\exp(-x)}{m!}\frac{d^m}{dx^m}(x^m \exp(-x)) \tag{5.62}$$

The general NA solution of the equation (5.57) is:

$$H = [h_0, h_1, ..., h_M] \tag{5.63}$$

H is an NA function.

In order to compare this NA function with experimental results the series expansion given by equation (5.54) are used. It results:

$$h_{comp} = \left[\sum_{m=0}^{M} \varepsilon^m h_m, 0, ..., 0\right] \tag{5.64}$$

In h_{comp} we put the contributions of different levels in H_{comp} at the basic level since we have to compare with real values.

In a more general form one obtains:

$$h_{comp} = \left[\sum_{m=0}^{M} q_m h_m, 0, ..., 0\right] = \sum_{m=0}^{M} q_m \left[h_m, 0, ..., 0\right] \tag{5.65}$$

Here $q_m = \varepsilon^m$. The new problem is to identify q_m in order to minimize the distance between $h_{exp} = [h_{exp}, 0, ..., 0]$ and h_{comp}. An NA distance should be defined using a NA semi-norm. Restricting the analysis to our case the NA norm (Robert 1967) is:

$$\|h\| = p^{\omega(h)} \tag{5.66}$$

with $0 < p < 1$ and

$$\omega(h)=m \text{ if } \mu_j=0 , j<m\leq M : \omega(h)=\infty \text{ if } \mu_j=0, j\leq M \tag{5.67}$$

Here:

$$\mu_j(h) = \int_0^{\infty} h(t)\, L_j(at)dt \tag{5.68}$$

The solution of the equation (5.55) can be written as:

$$H(T) = \sum_{m=0}^{M} V^m [h_m, 0..., 0] \tag{5.69}$$

Here h_m are given by the equation (5.57) and V = [0,1,0,...,0]. The distance between two RTD functions h and g is defined by :

$$d(h,g) = \|h\text{-}g\| \tag{5.70}$$

The distance between h_{exp} and h_{comp}, $d(h_{exp},h_{comp})$ is minimum namely it is zero, if $\mu_m(h_{exp}\text{-}h_{comp})=0$ for any $m \leq M$, that is when :

$$\int_0^{\infty} (h_{exp} - \sum_{m=0}^{M} q_m h_m) L_m(at)dt = 0 \tag{5.71}$$

for any $m \leq M$. In this case, $\omega (h_{exp}\text{-}h_{comp}) \rightarrow \infty$ and $\|h_{exp}\text{-}h_{comp}\|=0$. Using the orthogonality property of the Laguerre polynomials it results that:

$$q_m = \int_0^{\infty} h_{exp} L_m(at)dt = 0 \tag{5.72}$$

The mathematical problem is to use the set $\{[h_m,0,...,0]\}$, m=0,..., M as an NA orthogonal basis able to represent (uniquely) different RTD functions H(T) as given by (5.69).

Observe that $[h_m, 0,..., 0]$ forms a NA orthogonal basis of X if:

$\|\Sigma_i q_i[h_i,0,..., 0]\|=\max_i \|q_i [h_i ,0,..., 0]\|$ with $q_i \in K$ and $[h_i,0,..., 0] \in X$. Here X is the set of all finite linear combinations of elements of the type $[h_m (t),0,..., 0]$ and K is the valuated structure. General results concerning the use of a NA orthogonal basis to obtain solutions for NA differential equations as (5.55) are due to Gruson and van der Put (1974) and Monna (1970). Their results allow considering more general initial conditions and definitions of the derivative.

It should point out that q_m , m=0, 1..., M, computed by (5.72) minimize the above defined NA distance. Using different values of M, the number of scales, different models have been obtained.

This is the place where the real and "other than real" frames are in relation. The "other than real" frame is useful to outline the possible classes of solutions, the solutions corresponding to different scales. Confronting this, with real data allows limiting the number of scales.

After each model step, the confrontation with reality consists in establishing q_m.

The NA frame cannot discriminate between them, because in all cases the norm of the deviation between the model and the experiment is zero. The sum of squares of deviations or other real norms, are useful to choose one of some models being equivalent in the NA frame.

Each of the frame, "other than real" and real one has its utility.

Observe that the one level model is the conventional one-cell perfect mixing model.

This is a general condition for model categorification method.

5.2.2 PSM Frame for Continuous Model

The continuous time mixing model will be presented in the general frame of PSMs, the conditioning levels corresponding to different scales of time. Randomness of the mean residence time a, is accounted for. Denote by $\{a_j\}$ the set of values of the residence time. Suppose that the stochastic process at each conditioning level has a proper scale of time that the unit of time on the m scale is ε^m and that the states and the conditions are elements of the NA frame K. The complex system evolution starts from H (O) where O= [0, 0,...]. H(O)=[$h_0(0)$, $h_1(0)$, $h_2(0)$,...] describes the initial tracer particle distribution on different scales of mixing. With possibility P(K(O) | H(O))=P_0 ,the condition is K(O) that is the level m=0 and the residence time a_0 is selected for the next step evolution. It results that K(O)=[a_0, 0, 0,...]. One can consider that P_0 = [1,0,…].

An evolution for a time interval from O=[0,0,...] to T_1=[Δt, 0,...] takes place at this level. It is a unitary step at the basic level m=0. The resulting state is $H(T_1)=H(O)-K(O).H(O)(T_1-O)$. Observe that $H(T_1)=[h_0(\Delta t), h_1(0), h_2(0),...]$. Here $h_0(\Delta t)-h_0(0)= -a_0h_0(0)$. Then with possibility $P(K(T_1)| H(T_1))=P_1$ the condition $K(T_1)$ of evolution that is the level m=1 and the residence time a_1 is selected at this level. For instance P_1 = [0,1,…], $K(T_1)$=[0, a_1,0,...]. On account on this, the new state of the complex system is described by $H(T_2)=H(T_1)-K(T_1).H(T_1).(T_2-T_1)$. Here T_2=[Δt, Δt,0,...] and $H(T_2)=[h_o(\Delta t), h_1(\Delta t), h_1(0),...]$. Moreover:$(h_1(\Delta t)-h_1(0))-(h_o(\Delta t)-h_o(0)) = -a_1h_1(0)$. The process is continued indefinitely. We are in this case faced with a SKUP in which the states are S=(H(T))={$[h_o(t), h_1(t), h_2(t),...]$}, the conditions are K=(K(T)))={$[a_o(t), a_1(t), a_2(t),...]$}, the operators are U(H(T), K(T))=H(T'),

where H(T')=H(T)-K(T).H(T).(T'-T) and the possibility are $P(K(T)|H(T))=P_i$ if the activated levels are i and j and the residence times are a_i. Specific to such frames is the significant effect of changing the number of levels.

5.2.3 Comparison with Theory

The RTD of the Cholette and Cloutier model is:

$$h(\theta) = \gamma^2\alpha \exp(-\gamma\alpha\theta) + (1-\gamma)\,\delta(\theta) \tag{5.73}$$

Here $\theta = \frac{t}{\bar{t}}$ The two parameters are the flow split $\gamma = \frac{V_R}{v}$ and the volume ratio $\alpha = \frac{V}{V_R}$ Here v is the volumetric flow rate V is the volume of the system and the index R refers to the perfectly mixed part. With h(θ) given by (5.73) it results :

$$q_m = \gamma(1-\frac{1}{\alpha\gamma})^m + (1-\gamma) \tag{5.74}$$

For the sake of simplicity the analysis is restricted to systems without by pass. However it should be emphasized that by-pass can be important especially at low levels of agitation. In this case the RTD function is:

$$h(\theta) = \exp(-\theta)\sum_{m=0}^{M}(1-\frac{V_R}{V})^m L_m(\theta) \tag{5.75}$$

The truncation number M cannot be identified in the NA semi-norm and could be determined through the least squares method resulting the values $1 > V_R/V \geq 0.98$ if M = 1, $0.98 > V_R/V \geq 0.67$ if M = 5. Consider for instance the case V_R/V = 0.90. The sum of squares of deviations of the NA model with respect to the Cholette and Cloutier model is a function of M; when M increases from 0 to 3 the above sum decreases sharply, while for values of M larger than 3 it remains constant being practically zero.

This result should be correlated with the suggestion to limit the number of levels of investigation to just four.

Fig. 5.3 shows the continuous time scales and integrative closure for one cell.

Fig. 5.3 illustrates the situation in which we may limit the system at only four scales of time. This corresponds to integrative closure hypothesis. Any new level includes the previous ones. The Laguerre polynomials included at any new level are indicated as well as a hypothetical connection of the lower and top levels.

It suggests that the ε^4 terms may be neglected.

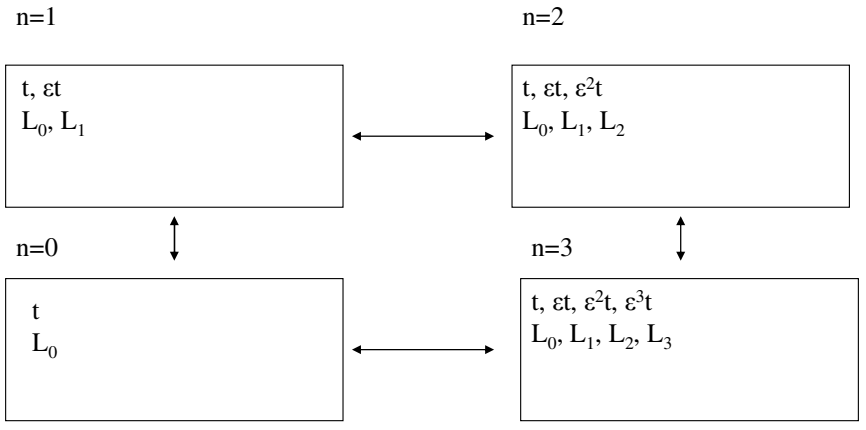

Fig. 5.3 Continuous time scales and integrative closure for one cell

The number of scales of time increases when completely dead region increases, that is when V_R/V decreases. As a measure of concordance between the Cholette and Cloutier model and the NA one the following index is defined:

$$I = \left(\int_0^\infty (h_{CC}(t) - h_{NA}(t))^2 dt\right)^{0.5} / \int_0^\infty (h_{CC}(t))^2 dt)^{0.5} \qquad (5.76)$$

This is practically zero (less than 10^{-6}). Here h_{CC} is given by the Cholette and Cloutier model whereas h_{NA} (t) is the NA model. A similar index computed for the Cholette-Cloutier model and the "perfectly mixed" one has values, for $0.67 \leq V_R/V \leq 1$, up to 0.26. The NA model predicts the same mean residence time as the Cholette-Cloutier model that is V_R/v, which is different from the mean residence time predicted by the perfectly mixed one, that is, V/v. B, the exit reactant concentration. For an irreversible first order reaction A→ B, the exit reactant concentration has been computed, as predicted by different models, and the results are listed in Table 5.3.

Table 5.3 contains the RTD functions predicted by different models.
Here c_f denotes the feeding concentration, k the kinetic constant, c_{NA} the concentration given by the NA model. For values of k V/v between 10^{-3} and 10^{+3} the ratio between the predictions of the NA model and those of the Cholette and Cloutier model varies between 0.99 and 1.

The ratio between the predictions of the "perfectly mixed" model and those of Cholette-Cloutier model varies between 0.66 and 1. These investigations show a fair agreement between the NA model and the Cholette-Cloutier model. The analysis has been restricted to the case $V_R/V \geq 0.67$ because values of $V_R/V < 0.67$ are considered irrelevant for a system with nearly perfect mixing.

Table 5.3 RTD functions predicted by different models

Model	Dimensional form	Dimensionless form	Exit concentration for reaction A→B
Perfectly mixed	$h(t)=\frac{v}{V}\exp(-\frac{tv}{V})$	$h(\theta)=\exp(-\theta)$	$c=\frac{c_f}{1+\frac{kV}{v}}$
Cholette-Cloutier	$h(t)=\frac{v}{V_R}\exp(-\frac{tv}{V_R})$	$h(\theta)=\frac{v}{V_R}\exp(-\frac{\theta v}{V_R})$	$c=\frac{c_f}{1+\frac{kV_R}{v}}$
Non-Archimedean	$h(t)=\frac{v}{V}\exp(-\frac{tv}{V})$ $\sum_{m=0}^{M}(1-\frac{V_R}{V})^m L_m(\frac{tv}{V})$	$h(\theta)=\exp(-\theta)$ $\sum_{m=0}^{M}(1-\frac{V_R}{V})^m L_m(\theta)$	c_{NA}

$$c_{NA}=c_f\left\{1-\frac{(1-\frac{V_R}{V})(\frac{kV}{v})}{(1+\frac{kV}{v})^{M+1}}\right\}\frac{1}{1+\frac{kV_R}{v}}$$

Moments of the RTD could be obtained starting from h (t) given by (5.65). Denote by $\bar{t}_m^c$ the computed moment of order m of the residence time. It results:

$$\bar{t}_c=\frac{q_0-q_1}{a},\qquad \bar{t}_c^2=\frac{2q_0-4q_1+2q_2}{a^2} \tag{5.77}$$

$$\bar{t}_c^m=\frac{m!}{a^m}\sum_{i=0}^{m}(-1)^i\binom{m}{i}q_i \tag{5.78}$$

Taking into account the properties of the orthogonal polynomials it results that $\bar{t}_c^m$ contains q_m. Consequently it is possible to interpret q_m as usual in statistics in terms of means, coefficients of variation skewness, flatness and so on. But such interpretations are useful only for careful experiments. Otherwise it is hard to obtain physical insight into them.

Suppose that applying the method presented here one obtains the RTD:

$$h(\theta)=\exp(-\theta)(q_0+q_1(1-\theta)) \tag{5.79}$$

Let us observe that for $\theta > (q_0+q_1)/q_1$ the RTD becomes negative. On account on the fact that in normalized cases, $q_0=1$ and q_1 is low, for instance $q_1=0.1$, it results that this unphysical result characterizes only the very long time behavior. Negative probabilities are due to infinitesimal contributions. Notice that h (θ) dθ is Events with the probability of a residence time in the interval (θ, θ+dθ). negative probability and decreasing cumulative RTD is to be considered despite the fact that they appear as practically negligible. Experimentally measured decreasing cumulative RTD may correspond to de-mixing processes. In this way the developed theory allows to accommodate phenomena unexplained by more conventional approaches.

5.2.4 SDG Solution for Imperfect Mixing

The SDG frame allows s rigorous study of differential equations (5.55) characterizing the imperfect mixing (Kock and Reyes 2006, 2008).

Consider a linear vector field on a microlinear and Euclidean *R*-module V (Moerdijk and Reyes 1991).

Denote by $D = \{d \in R \mid d^2 = 0\}$ the first order infinitesimals and by $D_\infty = \{d \in R \mid (\exists k \in N) d^{k+1} = 0\}$ the nilpotent infinitesimals.

D_∞ is the set of all infinitesimal elements of the number line.

For any *R*-module V, we define the map $V \times V \to V^D$ given by $(a, b) \to [d \to a+d.b]$. To say that V is Euclidean is to say that this map is a bijection; in other words, every tangent vector $\tau: D \to V$ is uniquely of the form $d \to a+d.b$. The element b, is called the principal part of the tangent vector τ and a, the base point of τ.

To say that the vector field is linear is to say that its principal part formation $V \to V$ is a linear map, denoted here by Γ.

Kock and Reyes (2006) established the following proposition:

Let a linear vector field on a microlinear Euclidean *R*-module V be given by the linear map $\Gamma: V \to V$. Then the unique formal solution H(T) of the corresponding differential equation:

$$\frac{dH}{dT} = \Gamma(H(T) \tag{5.80}$$

with the initial position v is the map $D_\infty \times V \to V$ given by:

$$(T, v) \to e^{T\Gamma}(v) \tag{5.81}$$

Here the right hand side means the sum of the following series which has only a finitely many non-vanishing terms, since T is assumed nilpotent.

$$H = v + T\Gamma(v) + \left(T^2/2!\right)\Gamma^2(v) + \left(T^3/3!\right)\Gamma^3(v) + \ldots \tag{5.82}$$

Here $\Gamma^2(v) = \Gamma(\Gamma(v))$ and so on.

The solution (5.82) confirms that obtained by model categorification method.

References

Cholette, A., Cloutier, L.: Mixing efficiency determinations for continuous flow systems. Canad. J. Chem. Engng. 37, 105–111 (1959)

Fogler, H.S.: Elements of Chemical Reaction Engineering. Pearson Education Inc., Upper Saddle River (2006)

Gruson, L., van der Put, M.: Banach spaces. Bull. Soc. Math. France 39-40, 55–100 (1974)

Iordache, O., Corbu, S.: Random residence time distribution. Chem. Engng. Sci. 41, 2099–2102 (1986)

Iordache, O., Frangopol, P.T.: Polystochastic features of compartmental biosystems. In: Frangopol, P.T., Morariu, V.V. (eds.) Seminars in Biophysics, vol. 5, pp. 143–150. CIP Press, Bucharest (1988a)

Iordache, O., Apostol, M., Frangopol, P.T.: Non-exponential relaxation of drug-membrane interaction. Effects of cross-linking aldekydes and procaine. Rev. Roum. Biochim. 25, 275–281 (1988a)

Iordache, O., Isopescu, R., Isopescu, A., Iacobini, A., Jinescu, G.: Non-Archimedean models of mixing I, Residence time distribution for systems with imperfect mixing. Chem. Engng. Sci. 43, 693–697 (1988b)

Jacquez, J.A.: Compartmental Analysis in Biology and Medicine. The University of Michigan Press, Ann Arbor (1985)

Kock, A., Reyes, G.E.: Ordinary differential equations and their exponentials. Central European Journ. of Mathematics 4(1), 64–81 (2006)

Kock, A., Reyes, G.E.: Some differential equations in SDG. arXiv:math.CT/0104164 (2008)

Moerdijk, I., Reyes, G.E.: Models for Smooth Infinitesimal Analysis. Springer, New York (1991)

Monna, A.F.: Analyse Non-Archimédienne. Springer, Berlin (1970)

Naor, P., Shinnar, R.: Representation and evaluation of residence time distributions. Ind. Engng. Chem. Fundam. 2, 278–286 (1963)

Nauman, E.B.: Residence Time Distributions. In: Handbook of Industrial Mixing: Science and Practice, pp. 1–17. Wiley Interscience, Hoboken (2004)

Nauman, E.B., Buffham, B.A.: Mixing in Continuous Flow Systems. J. Wiley, New York (1983)

Pethö, A., Noble, R.D. (eds.): Residence Time Distribution Theory in Chemical Engineering: Proceedings of a Summer School Held at Bad Honnef, August 15-25. Verlag Chemie, Weinheim (1982)

Robert, P.: On some non-Archimedean normed linear spaces 1-IV. Compositio Math. 19, 1–77 (1967)

Strichartz, G.R., Ritchie, J.M.: The action of local anesthetics on ion channels of excitable tissues. In: Strichartz, G.R. (ed.) Handbook of Experimental Pharmacology, Local Anesthetics, vol. 81, pp. 21–52. Springer, Heidelberg (1987)

Chapter 6
Compartmental Systems

Abstract. Several hydrodynamic systems can be viewed as consisting of interconnected flow regions with various types of flow in and between regions called compartments.

The mixing in multi-scale compartmental systems is analyzed. Discrete and continuous time models are developed using model categorification method.

RTD for tracer experiments in hydrological systems is described in terms of Laguerre polynomials.

Local anesthetic effects on multi-compartmental membranes are studied.

6.1 Compartmental Models

With the motion of real flows, it may happen that none of the ideal hydrodynamic models permits a sufficiently accurate reproduction of the properties of the flow involved. Many flow system lies probably between perfect mixing and plug flow. For instance ideal flows are not adequate to provide a representative model for stirred tanks, fluidized beds and so on. In practice such processes can be viewed as consisting of interconnected flow regions with various types of flow in and between the regions (the so called combined or compartmental models) (Jacquez 1985, Nauman 2004).

Combined models may consist, for instance, of individual perfect mixing cells or plug flow and a stagnation zone, the cells being interconnected by cross, recirculating and by passing flows. The sizes of the various regions and the flow rates between and around the regions represent the parameters of the model. The parameters are determined on the basis of the experimental residence-time distributions functions. The large number of parameters used in compartmental models allows great flexibility in matching the response curve of these models to that for the real flow systems. So many possible compartmental models have been considered in practice that it is difficult to organize them. Table 6.1 presents compartmental models significant for chemical engineering studies.

Table 6.1 represents an outline of the problem (Aris 1982, Nauman 2004)). Of the combined models most commonly used in analyzing mass-transfer processes performed in columns (towers) a cellular model with back-mixing between cells finds application.

Table 6.1 Compartmental models

Type	References
Sequence of stirred tanks	(Seinfeld and Lapidus 1974)
With bypass	(Naor and Shinnar 1963)
In parallel	(Wen and Fan 1975)
With cross flow	(Seinfeld and Lapidus 1974)
With back-mixing	(Seinfeld and Lapidus 1974)
With stagnant region	(Cholette and Cloutier 1959)
With transport delay	(Nauman and Buffham 1983)
Arrays of stirred tanks	(Wen and Fan 1975)
General networks	(van de Vusse 1962)
Stochastic flows	(Krambeck et al. 1967)
Recycle systems	(Nauman and Buffham 1983)
Plug flow with diffusion	(Levenspiel and Bischoff 1963)
Combined stirred tanks and plug flow	(Wolf and Resnick 1963)

One complete mixing vessel and a plug flow reactor are the extremes cases. Intermediary flows between these two cases are approximated by n vessels in series. Vessels in series with a smaller number correspond to a flow reactor with a high mixing intensity. Therefore the performance of the reactor may be estimated by replacing it with that of n complete mixing vessels in series of equal volume. Consider for instance the cellular model of mass transfer on plates.

The plate is divided in the direction of the liquid flow into a number of cells, assuming that complete mixing takes place in each of the cells and there is no mixing between them. It is also assumed that:

i) The liquid and vapor rates are constant for each cell
ii) At the inlet of each cell the vapor has one and the same composition
iii) The number of perfect mixing cells depends on the liquid path, on the liquid viscosity, on the vapor velocity, on plate construction.

Compartmental models find wide application in analyzing the flow liquid in agitated vessels. Recirculation flows appear in agitated vessels, therefore a separate class of models has been created, the so-called class of recirculation models. One of the advantages of recirculation models is that they consist of single type elements, that is, perfect mixing cells. A main parameter is the degree of recirculation q/Q, which is equal to the ratio of flow created by the impeller (the pumping capacity of the impeller is q) to the main flow entering apparatus Q. The

experimental and theoretical investigations conducted to correlation between pumping capacity and the geometry of the mixers.

An illustrative example is the formula suggested by van de Vusse (1962) for flat-blade paddles and impellers:

$$q = K\, w\, d^2\, b \tag{6.1}$$

Here b is the blade with, w the impeller speed, d the impeller diameter, K a proportionality factor depending on the kind of impeller, number and arrangement of blades. A simple recirculation model is a cellular model with recycles. The entire volume of the apparatus is divided into two zones: a perfect mixing zone around the impeller and the zone around one mixing cell (the remaining volume of the apparatus). The two zones are linked with a recirculation loop. However, single-loop models do not fully reflect the actual hydrodynamic processes occurring in agitated vessels. Some well-know compartmental models will be presented in the following.

6.2 Discrete Models for a Series of Imperfectly Mixed Vessels

The approach proposed here is to use a cascade of storage elements as shown in Fig. 6.1 as a general conceptual model describing the mixing process where each of the storage elements in the cascade is assumed to be uniformly mixed.

Fig. 6.1 shows a cellular model

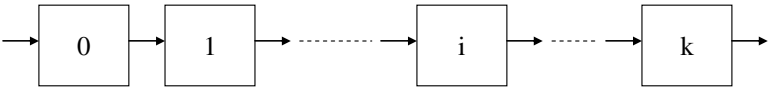

Fig. 6.1 Cellular model

A system consisting of k+1 mixing cells connected in series each cells having equal volumes is considered now. The sum of the compartmental volumes is equal to the volume of the apparatus and the volumetric flow rate is constant. The system is described by the system of equations:

$$\frac{dh^{(i)}}{dt} = -ah^{(i)} + ah^{(i-1)}; 1 \le i \le k \tag{6.2}$$

Here $h^{(i)}(t)$ denotes the RTD function of the i-th cell. Here a = v/V where v is the steady flow rate and V the volume of each cell. Imperfect mixing signifies that more scales of time should be accounted for (Fig. 6.2).

Fig. 6.2 shows cellular models with imperfect mixing.

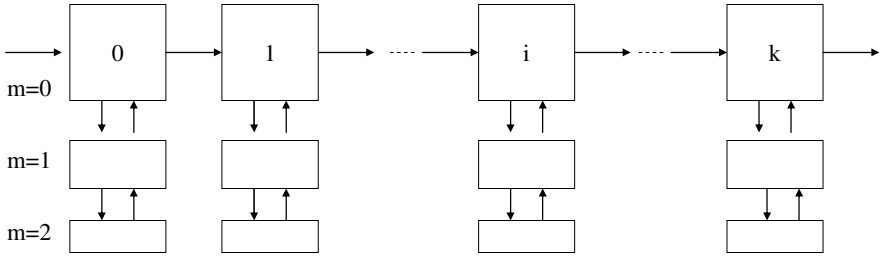

Fig. 6.2 Cellular models with imperfect mixing

For the model shown in Fig. 6.2 there are three scales of time. The space corresponding to m=0 is active while those corresponding to m=1 and m=2 are more and more slow. Moreover it is considered that the cells are identical.

Denote by $H^{(i)}(N)=\left[h_0^{(i)}(n),...,h_M^{(i)}(n)\right]$ the discrete NA RTD function of the i-th cell. The model categorification model is:

$$\frac{H^{(i)}(N)-H^{i}(N_1)}{N-N_1}=-AH^{(i)}(N_1)+AH^{(i-1)}(N_1):1\le i\le k \tag{6.3}$$

The function $H^{(0)}(N)$ refers to all mixing scales of the first cell. The following system of difference equations results:

$$(h_m^{(i)}(n)-h_m^{(i)}(n-1))-(h_{m-1}^{(i)}(n)-h_{m-1}^{(i)}(n-1)=-ah_m^{(i)}(n-1)+ah_m^{(i-1)}(n-1) \tag{6.4}$$

This is valid for $0\le i\le k,0\le m\le M$.

Consider the initial conditions:

$$h_0^{(0)}(0)=h_1^{(0)}(0)=...=h_M^{(0)}(0)=1 \tag{6.5}$$

$$h_0^{(i)}(0)=h_1^{(i)}(0)=...=h_M^{(i)}(0)=0\quad 1\le i\le k \tag{6.6}$$

Thus in the i-th cell, 1≤ i≤k, no initial stratification of the fluid in scales of mixing is needed. The obtained solutions are:

$$h_m^{(i)}(n)=(\overset{n}{i})(1-\alpha)^{i}\alpha^{n-i}M_m(n-i,i+1,\alpha)/m! \tag{6.7}$$

α= 1-a. The general solution of Here α the NA model is:

$$h^{(i)}(n) = \binom{n}{i}(1-\alpha)^i \alpha^{n-i} \sum_{m=0}^{M} q_m^{(i)} M_m(n-i, i+1, \alpha) \Big/ m! \tag{6.8}$$

The NA model used to select the best model is:

$$\|h\| = p^{w(h)} \tag{6.9}$$

with $0 < p < 1$ and

$$w(h)=\min \{m; \mu_m(h) \neq 0\} \tag{6.10}$$

where:

$$\mu_j(h) = \sum_{0}^{\infty} h^{(i)}(n) M_j(n-1, i+1, \alpha) \tag{6.11}$$

Calculus should be performed for i-th cell.

Using the orthogonality relations for Meixner polynomials and the NA norm it results:

$$\binom{m+i}{i}(1-\alpha)^i \alpha^{-m} q_m^{(i)} = \sum_{m=0}^{M} h^{(i)}(n) M_m(n-i, i+1, \alpha) \Big/ m!, 0 \leq m \leq M \tag{6.12}$$

Here $h^{(i)}(n)$ is the experimental or theoretical RTD for the i-th cell.

6.3 Continuous Time Model

6.3.1 Residence Time Distributions

In real hydrological systems the mixing processes occurring during the flow make the whole process rather too complex for a mathematical formulation on the base of ideal models. Some aquifer systems can be considered as consisting of various component volume elements interconnected with each other. The physical model of the so-called multi-cell model consists in that the flow breaks up into a number of compartments connected in series. Such models seems to be advantageous in studies concerned with the use of environmental isotopes as tracer in regional hydrological investigations as they enable the study of average properties of the system on a time scale and do not require a detailed description of the parameters and the processes. The design of a given multi-cell model is determined by "a priori" knowledge of the flow system or by calibration procedure. If the multi-cell approach is applied to interpret the input-output time relations-ship of a given

system and if the prior knowledge is limited or lacking an arbitrary number of fitting parameters results. The multi-cell approach was used to model the transport of radiotracer in a large shallow aquifer (Zuber 1974, 1986, Berne and Thereska 2004).

The approach was used to model large and deep aquifers. On the basis of prior physical knowledge and determinations in samples taken from different sites and depths a three-dimensional network of cells was arranged. The calibration yielded the flow through boundaries the flows between the cells and the mean residence times. The multi-cell model was modified by introduction of "dead cells" which took into account a possible effect of diffusion into zones with no net flow. A corrective term should be introduced to transit time through each cell to account for a possible delay of tracer when the multi-cell approach is used to a complex system of fissured rocks with a porous matrix. In general it seems that the multi-cell models are gaining a wide acceptance due to their easy use. When they are used to correlate tracer data distributed in space, their use justified through the assumption of good mixing in cells is questionable. The NA model developed in the following is valuable when the flow could be separated into zones with appreciable but finite scales of time. In many hydrological systems there exists "stagnant water" and short-circuiting. The zone corresponding to a given mixing scale appears as stagnant relative to the portion of flow that travels much more rapidly from entrance to exit and as a short-circuit with respect to the portion of flow that moves more slowly.

It is assumed that the "imperfect mixing" takes place in each of cells and that there is no mixing between the cells (Iordache et al. 1988a, Iordache and Frangopol 1990, Iordache et al. 1991). The number of ideal cells k is a parameter characterizing the real flow. If the cells are of the same volume, the sum of the volumes is equal to the volume of the apparatus and the volumetric flow rate is constant, the multi-cell model is described by the system of equations:

$$\frac{dh^{(i)}}{dt} = -ah^{(i)} + ah^{(i-1)}; 1 \le i \le k \tag{6.13}$$

Here $h^{(i)}(t)$ denotes the RTD function in the i-th cell and a=v/V where v is the steady flow rate through the system and V is the volume of each cell. By model categorification method, one replaces the time t by the expansion:

$$T = t + \varepsilon w_1 t + ... + \varepsilon^M w_M t \tag{6.14}$$

that is $T = [t, w_1 t,..., w_M t]$, and the RTD function $h^{(i)}(t)$ by the expansion:

$$H(T) = h_0^{(i)}(t) + \varepsilon h_1^{(i)}(t) + ... + \varepsilon^M h_M^i(t) \tag{6.15}$$

$$H^{(i)}(T) = \left[h_0^{(i)}(t), h_1^{(i)}(t),..., h_M^{(i)}(t) \right] \tag{6.16}$$

A system with many scales of time will be described by model categorification by the system of NA differential equations:

$$\frac{dH^{(i)}}{dT} = -AH^{(i)} + AH^{(i-1)}, 1 \le i \le k \tag{6.17}$$

The mode results by the model categorification method.

Here a is translated to the constant vector A = [a, 0,..., 0]. Taking T = [t, t,..., t] and T1 = [t-Δt, t-Δt,..., t-Δt] in the i-th equation of the system written:

$$H^{(i)}(T) - H^{(i)}(T_1) = -AH^{(i)}(T_1)(T - T_1) + AH^{(i-1)}(T_1)(T - T_1) \tag{6.18}$$

Using the rule of product of the NA structure K of Neder (Appendix 1), letting $\Delta t \to 0$, the system (5.3.6) is translated into:

$$(h_1^{(i)})' - (h_0^{(i)})' = -ah_1^{(i)} + ah_1^{(i-1)} \tag{6.19}$$

……..

$$(h_m^{(i)})' - (h_{m-1}^{(i)})' = -ah_m^{(i)} + ah_m^{(i-1)} \quad , \ 2 \le i \le k \tag{6.20}$$

It is considered that in the i-th cell, $i \ge 2$, no initial stratification of the fluid in scales of mixing appears. Thus the initial conditions are:

$$h_0^{(0)}(0) = h_1^{(0)}(0) = ... = h_M^{(0)}(0) = a \tag{6.21}$$

$$h_0^{(i)}(0) = h_1^{(i)}(0) = ... = h_M^{(i)}(0) = 0 \quad , \ 2 \le i \le k \tag{6.22}$$

The solution is:

$$h_m^{(i)}(t) = a\frac{(at)^i}{i!}\exp(-at)L_m^{(i)}(at) : 0 \le m \le M \tag{6.23}$$

Here $L_m^{(i)}(at)$ denotes the Laguerre polynomials $L_m^{(0)}(at) = L_m(at)$. Taking i = 0 but $M \to \infty$ the solution obtained for imperfect mixing in a single cell results.

Contrary, taking M = 0, $i \to \infty$ the solution for a series of cells with perfect mixing is obtained.

The vectors:

$$\left\{h_m^{(i)}(t)_m\right\}, 0 \le i \le n; h_m^{(i)}(t) = \left[h_m^{(i)}(t), 0, ...0\right] \tag{6.24}$$

represents a NA orthogonal basis of RTD functions. Denote by X the NA normed valued space of RTD functions. Any RTD is represented uniquely using the elements of

$$\left\{h_m^{(i)}\right\} = \left\{\left[h_m^{(i)}, 0, \ldots 0\right]\right\} \tag{6.25}$$

The coefficients are from the valuated structure K. Observe that $H \in X$ the solution of (6.3.5) could be represented uniquely as:

$$H^{(i)} = \sum_{m=0}^{M} q_m^{(i)} V^m h_m^{(i)} \tag{6.26}$$

Here V = [0,1,0...,0].

In experiments we are faced with measurements at the basic level that is with RDT of the type:

$$h_{exp} = [h_{exp}, 0, \ldots, 0] \tag{6.27}$$

Here h_{exp} denotes the measured RTD.

The most general form of an RTD function is in this case:

$$h_{comp} = \sum_{m=0}^{M} q_m^{(i)} h_m^{(i)} = \left[\sum_{m=0}^{M} q_m^{(i)} h_m^{(i)}, 0, \ldots 0\right] \tag{6.28}$$

An equivalent form is:

$$h_{comp}(\theta) = \frac{\theta^i}{i!} \exp(-\theta) \sum_{m=0}^{M} q_m^{(i)} L_m^{(i)}(\theta); 0 \le m \le M \tag{6.29}$$

Here $\theta = at$. The new problem is to determine the coefficient q_m to ensures the minimum of the distance between h_{exp} and h_{comp}. It is necessary to define a norm on the space X of RTD functions. Let:

$$\|h\| = p^{w(h)} \tag{6.30}$$

with $0 < p < 1$ and:

$$w(h) = \min \{m; \mu_m(h) \neq 0\} \tag{6.31}$$

Here:

$$\mu_j(h) = \int_0^{\infty} h^{(i)}(\theta) L^{(i)}{}_m(\theta) d\theta \tag{6.32}$$

Calculus should be performed for i-th cell.

The associated distance is defined by:

$$d(h,g) = \|h-g\| \tag{6.33}$$

Here h, g∈ X. Therefore:

$$\mu_m(h_{exp}-h_{comp})=0 \tag{6.34}$$

Using the orthogonality property of the Laguerre polynomials it results that:

$$\binom{m+i}{i} q_m^{(i)} = \int_0^{\infty} h_{exp}(\theta) L_m^{(i)}(\theta) d\theta \tag{6.35}$$

Due to the fact that the distance (6.33) is null the best model that is, a truncation number M is selected using the sum of squares of deviations between theory and experiment.

Fig. 6.3 highlights the time scales and integrative closure concept for multiple cells.

Fig. 6.3 illustrates the situation in which we may limit the system at only four scales of time. This corresponds to integrative closure hypothesis. Any new level includes the previous ones. The Laguerre polynomials included at any new level are indicated as well as a hypothetical connection of the lower and top levels. It suggests that the ε^4 terms will be neglected.

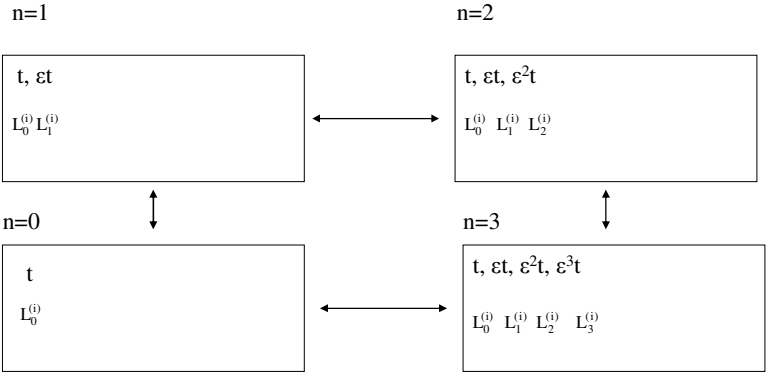

Fig. 6.3 Time scales and integrative closure for multiple cells

6.3.2 Interaction of Chemical Compound with Membranes

Stochastic compartmental models are widely used in modeling processes such as drug kinetics (Jacquez 1985, Yu and Wehrly 2004).

In many biochemical experiments one observes the decay of some ligands populations due to capture by appropriate systems of compartments.

Important examples appear in the study of drug membrane interactions. Some classes of drugs as the protein-linking aldehydes and the local anesthetics have well known relaxation effects on the functions of membrane ionic channels and pumps.

The multi-compartment case is studied herein. It should be emphasized that a compartment may be defined as indicating not only the location but also the change of state of a material object. The transport of such an object includes changes of position and change of its nature.

Table 6.2 Relative height of the compound action potential

Time min	0	10	20	30	40	50	60	70	80	90	100	110	120	130	140
experiment	1	0.99	.97	.95	.81	.72	.62	.53	.45	.37	.25	.19	.10	.04	.02
Eq.(6.29) M=0	-	.97	.83	.79	.69	.59	.50	.42	.35	.29	.24	.20	.16	.13	.11
Eq.(6.29) M=3	-	1	.98	.93	.84	.74	.62	.51	.41	.32	.25	.18	.13	.10	.07

The prediction of the model are discussed with respect to the effect of a cross-linking aldehydes, glutaraldehyde, GA, 0.25% on the amplitude of the compound action potential of frog sciatic nerve (Iordache et al. 1988a).

Table 6.2 shows the experimental results, that is the relative height of the compound action potential as a function of time.

Table 6.3 shows the objective function S(M) for multi-compartmental models.

Table 6.3 Objective function for multi-compartments model

M	0	1	2	3	4	5	6
S(M)	.27	.21	.05	.03	.03	.025	.02

In this case the relaxation rate a, is obtained taking $a = (k+1)/\bar{\tau}$ with $\bar{\tau}$ the mean relaxation time of the studied system and k+1 compartments. In this case $\bar{\tau}$ =70.275 min.

It has been found that two compartments and four scales (M=3) provide a satisfactory picture of the relaxation process as the objective function S(M) stays practically unchanged for M≥3. It resulted q_0=0.98, q_1=-0.055, q_2=-0.226, q_3=-0.133.

The purely exponential decay corresponding to M=0 compare badly with the experimental data especially for long times.

The above results could be interpreted in the form of a "label" of a specific interaction where the coefficients q_m, depends on the contribution of the m-th scale of the relaxation process. It is possible to interpret the two compartments obtained in this correlation in terms of the so-called "two-membrane theory that considers the skin as consisting of two functional membranes in series, the apical membrane and the latero-basal membrane.

An interesting feature is that the spectrum q_m, is similar for various cross-linking aldehydes and this similarity supports the assumption of a unique physical mechanism of their interactions with the membrane.

The theory may be applied to a broad class of biophenomena. Possible applications include different types of inactivation of membrane functions, the bacteria killing by disinfectants, the ion-channel kinetics and so on.

References

Aris, R.: The Scope of the RTD Theory. In: Pethö, A., Noble, R.D. (eds.) Residence Time Distribution Theory in Chemical Engineering, Proceedings of a Summer School Held at Bad Honnef, August 15-25, pp. 1–21. Verlag Chemie, Weinheim (1982)

Berne, P., Thereska, J.: Simulation of a radiotracer experiment by flow and detection-chain modelling: a first step towards better interpretation. Appl. Rad. Isotopes 60, 855–861 (2004)

Iordache, O., Apostol, M., Frangopol, P.T.: Non-exponential relaxation of drug-membrane interaction. Effects of cross-linking aldekydes and procaine. Rev. Roum. Biochim. 25, 275–281 (1988a)

Iordache, O., Frangopol, P.T.: Nonarchimedean modeling for biosystems evolving on many time scales. In: Rivail, P. (ed.) Proceedings of the 44th International Meeting of Physical Chemistry, Nancy, 1989 (1990)

Iordache, O., Isopescu, R., Gaspar, E., Isopescu, A.: Interpretation of tracer experiments in hydrological systems. Theoretical and Applied Speleology 4, 87–96 (1991)

Jacquez, J.A.: Compartmental Analysis in Biology and Medicine. The University of Michigan Press, Ann Arbor (1985)

Krambeck, F.J., Shinnar, R., Katz, S.: Interpretation of tracer experiments in systems with fluctuating throughput. Ind. Engng. Chem. Fundam. 8, 431–444 (1968)

Levenspiel, O., Bischoff, K.B.: Patterns of flow in chemical process vessels. Advances in Chem. Eng. 4, 95–198 (1963)

Nauman, E.B.: Residence Time Distributions. In: Handbook of Industrial Mixing: Science and Practice, pp. 1–17. Wiley Interscience, Hoboken (2004)

Seinfeld, I.H., Lapidus, L.: Mathematical Methods in Chemical Engineering, vol. 3. Prentice-Hall, New York (1974)

van de Vusse, J.A.: A new model for the stirred tank reactor. Chem. Engng. Sci. 17, 507–513 (1962)

Wen, C.Y., Fan, L.T.: Models for Flow Systems and Chemical Reactors. Dekker, New York (1975)

Wolf, D., Resnick, W.: Residence time distributions in real systems. Ind. Engng. Chem. Fundam. 2, 287–293 (1963)

Yu, J., Wehrly, T.E.: An approach to the residence time distribution for stochastic multi-compartment models. Math. Biosci. 191, 185–205 (2004)

Zuber, A.: Theoretical possibilities of the two-wall-pulse method. In: Isotope Techniques in Groundwater Hydrology, vol. 11, pp. 277–299. IAEA, Vienna (1974)

Zuber, A.: Review of existing mathematical models for interpretation of tracer data in hydrology. In: Mathematical Models for Interpretation of Tracer Data in Groundwater Hydrology, pp. 69–116. IAEA, Vienna (1986)

Chapter 7
Turbulent Mixing

Abstract. Knowledge of turbulent dispersion plays a significant part in various problems of chemical engineering, pharmacology and hydrology investigations related to protection of the environment.

Turbulent mixing, in multi-scale systems is studied here.

Wavelets based on Hermite polynomials are the solutions obtained by model categorification.

The SDG solution for dispersion and the dispersion effects associated to convective flows is presented.

The energy intermittency by vortex line stretching characteristic to turbulent flow shows in multi-scale situations new regimes of instability.

7.1 Dispersion

7.1.1 The Dispersion Equation

Hydrodynamic dispersion is a classical topic of statistical physics and serves as a useful tool to improve the understanding of various phenomena such as mixing, oil recovery, pollutant transport and generally speaking, the spreading of a tracer in a medium of complex and disordered structure. The axial dispersion model is a popular feature of chemical engineering analysis. It has been used in a variety of dispersion problems, in analysis of tubular chemical reactors in numerous applications of continuous separation processes, in describing the flow though porous media (Dullien 1992). Knowledge of dispersion has been increasing in practical importance since it plays a decisive part in various problems of groundwater investigations related to protection of the environment (McGuire and McDonnell 2006). This applies particularly to investigations of pollutants entering groundwater from refuse tips, safety problems of nuclear power stations, intrusion of salt water into drinking water galleries and so on. The main attractiveness of the

axial dispersion model is its power to amend the predictions of the plug flow model without loss of the later simplicity. The conditions for the physical realization of the dispersion model are met in a piston-like flow if there is a mixing in the direction of flow, described by equations similar to the equation of molecular diffusion, but with modified coefficients.

A general mathematical expression of the dispersion is:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} + D_r\left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r}\frac{\partial c}{\partial r}\right) + P \tag{7.1}$$

Here c is the concentration, D is termed the axial dispersion coefficient and D_r the radial dispersion coefficient, v is the mean velocity, and P is the source term. The coefficients are assumed to be independent of concentration and position. The dispersion equation is used very frequently for turbulent flow of fluids in pipes, flow through packed beds, flow of liquids through fluidized beds etc. The equation has been applied to many other homogeneous and heterogeneous systems in which axial symmetry can be assumed and in which the flow behavior is not too far from that of plug flow. When the flow behavior deviates considerably from plug-flow such as in a stirred tank, in a bubbling fluidized bed, and in the two-phase flow of gas-liquid systems the behavior can not always be represented by this model. However the dispersion model can be used in each phase when two phases are involved. When radial dispersion can be neglected in comparison with axial dispersion equation (7.1) is reduced to:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} + P \tag{7.2}$$

Such a model can be used, for instance, when the ratio of column diameter to length is very small and the flow is in turbulent regime. There are a number of solutions of equation (7.2) for different initial and boundary conditions. Sometimes it may be difficult to decide which conditions are best for a given experimental situation.

The dispersion model has been successfully applied to single-phase flow of fluids through an empty tube or pipe. Taylor (1953) showed for laminar flow in round empty tubes that a process of mass transfer described by molecular diffusion accompanied by radial-velocity variations may be equally well described by flow with a flat velocity profile equal to the actual mean velocity $\bar{v}$ and with an effective axial-dispersion coefficient, $D = \frac{R^2\bar{v}^2}{48}D_m$ where R is the tube radius; D_m is the molecular diffusion coefficient. Later it was shown that we have:

$$D = D_m + \frac{R^2\bar{v}^2}{48}D_m \tag{7.3}$$

Experimental data confirm the accuracy of this equation. Unlike liquids, dispersion of gases in fixed or packed beds is affected by the molecular diffusion. If molecular diffusion is the only operating mechanism, the axial dispersion coefficient D under extremely low flow rate is related to the molecular diffusivity D_m by the equation $D = \gamma D_m$ where γ known as the tortuosity factor, ranges from 0.4 to 0.9 depending on shapes of particles. To obtain this expression for D, it is considered that the interstitial channels created by the packing hinder the diffusion. At the other extreme where the Reynolds number is very high: $D=0.5 \varphi v d_P$ whereφ is the void fraction of the bed and d_P a diameter. If the mechanism of axial dispersion can be considered to be composed of molecular diffusion and turbulent mixing, and if it is assumed that the effects of these mechanisms are additive, then the dispersion coefficient may be approximated by:

$$D = \gamma D_m + 0.5 \varphi v d_P \tag{7.4}$$

Compared with the plug flow model the dispersion model meets to greater extent the conditions existing in real, apparatus used in chemical engineering in which mixing is based on the principle of displacement. The defect of this model consists in the intricacy involved in stating boundary conditions and in the necessity of estimating preliminarily the coefficients of axial and radial dispersion.

7.1.2 The Frame of Infinitesimals

For present needs the one-dimensional form of the dispersion equation is of interest that is:

$$\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \tag{7.5}$$

Here c is the tracer concentration t the time, x the space, v the interstitial flow velocity and D the dispersion coefficient. This coefficient is in general a tensor but in the one-dimensional approximation is treated as a scalar. The coordinate system is selected in such a way that the x-axis is parallel to the velocity vectors. In groundwater experiments for instance, the concentration is usually measured in wells, caves or sources, at a given distance x as a function of time. Let us define the dimensionless variable:

$$\eta = \frac{x - vt}{(2Dt)^{0.5}} \tag{7.6}$$

The model (7.5) reduces to the differential equation:

$$w' + \eta w = 0 \tag{7.7}$$

Here:

$$w(\eta) = c'(\eta); c(\eta) = \int_{-\infty}^{\eta} w(\eta) d\eta \tag{7.8}$$

In the NA frame the parameter η is translated by model categorification into:

$$H = \eta + \varepsilon\omega_1 + ... + \varepsilon^M \omega_M \tag{7.9}$$

Here ω_m are random variables.

The concentration c is translated by model categorification method into:

$$C(H) = c_0(\eta) + \varepsilon c_1(\eta) + ... + \varepsilon^M c_M(\eta) \tag{7.10}$$

Instead of w (η) one takes by model categorification W (H) = [w_0 (h), w_1(h),...,w_M(h)]

that is:

$$W(H) = w_0(\eta) + \varepsilon w_1(\eta) + ... + \varepsilon^M w_M(\eta) \tag{7.11}$$

Here c_m(η) and w_m(η) are real functions on η. In the NA frame the equation (7.7) is translated into:

$$\frac{dW}{dH} + HW = 0 \tag{7.12}$$

It is the result of the model categorification method.

The formal solution of the equation (7.12) is:

$$W(H) = C\exp(-\frac{H^2}{2}) \tag{7.13}$$

C is an NA constant. For identical initial conditions w_m (0) =1 the constant is C= [1, 1,..., 1]. Taking: H=[η, η,...,η] that is: ω_1=ω_2=....=ω_M= 1 and applying the operations in the NA structure it results from (7.13) the expression of W(H)= [w_0(η), w_1(η),..., w_M(η)] with:

$$w_m(\eta) = c_m \exp(-\frac{\eta^2}{2}) \tag{7.14}$$

Here c_m denotes coefficients depending on η via Hermite polynomials. Moreover:

$$c_0(\eta)=1;\ c_1(\eta)= -H_2(\eta);\ c_2(\eta)=(1/2)(H_4(\eta)+H_2(\eta));c_3(h)=-(1/6)(H_6(\eta)+3H_4(\eta));$$

$$c_4(\eta)=(1/24)(H_8(\eta)+6H_6(\eta)+3H_4(\eta))) \tag{7.15}$$

Taking H=[η, η,..., η] , in the formal solution (7.13) is equivalent to perform a multi-scale derivative in which a unit step is accounted for at any level (scale) of the process. The computed solution is:

$$C_c(\eta)=\frac{1}{(2\pi)^{0.5}}\int_{-\infty}^{\eta}\sum_{m=0}^{M}q_{2m}H_{2m}(\eta)\exp(-\eta^2/2)d\eta \tag{7.16}$$

The coefficients q_{2m} include different values of c_m and ε. If M=0 the equation (7.16) reduces to the well known solution describing the infinite bed when both injection and detection of tracer are measured in resident fluid (Kreft and Zuber, 1978).

Taking into account the orthogonality relations and (7.16) it results that:

$$\int_{-\infty}^{+\infty}H_{2m}(\eta)\exp(-\frac{\eta^2}{2})dC_c(\eta)=q_{2m}(2m)! \tag{7.17}$$

The coefficients q_{2m} given by equation (7.17) ensure the minimum distance between the experimental values u(η) and the model (in the NA norm ‖ ‖*.Define

$$\|w\|^*=p^{j(w)} \tag{7.18}$$

Here p is a constant, p < 1 and:

$$j(w) = \min\{m,\ \mu_{2m}(w)\neq 0\} \tag{7.19}$$

with:

$$\mu_{2m}(w)=\int_{-\infty}^{\infty}H_{2m}(\eta)w(\eta)d\eta \tag{7.20}$$

One takes $w(\eta)\,d\eta = d\,C_c(\eta)$. One observes that

$$\mu_{2m}(w) = (2m)!q_{2m} \tag{7.21}$$

where q_{2m} is given by equation (7.17). The NA orthogonal basis is in this case.

$$\{w_{2m}\}=\exp(-\eta^2)H_{2m}(\eta):\|w_{2m}\|^*=p^{2m} \tag{7.22}$$

The coefficient q_{2m} ensure the minimum of the distance:

$$\left\| w(\eta) - \sum_{m=0}^{M} q_{2m} w_{2m}(\eta) \right\|^{*} \tag{7.23}$$

At the minimum:

$$\mu_{2m}\left(w(\eta) - \sum_{m=0}^{M} q_{2m} w_{2m}(\eta)\right) = 0 \tag{7.24}$$

This means that (7.17) is verified. The coefficients q_0, q_2,..., q_{2M} resulting by numerical integration are then used to obtain the computed solution. The computed response $C_c(\eta)$ is compared with the experimentally founded response of the system $c(\eta)$. The truncation number M ensures the minimum of the objective function. The computed response $C_c(\eta)$ should be compared here with the experimentally founded response of the system $c(\eta)$. One retains the truncation number M that ensures the minimum of the objective function S (M):

$$S(M) = \int_{-\infty}^{\infty} (c(\eta) - C_c(\eta))^2 d\eta \tag{7.25}$$

The NA model differs from expansions of the probability distribution for instance that of Gram-Charlier or Wiener-Hermite (Kraichnan 1980, Saffman 1969). In principle such expansions contains Hermite polynomials of practically all order. In Gram-Charlier method the dimensionless variable η is defined using the mean and the variance resulting directly from experiments; the accuracy increases as the number of terms in expansion increases. In fact the used coefficient of dispersion does not have a physical interpretation being a fitting parameter for an invalid model situation. In the NA method starting from a given number of scales the expansion diverges and this could be interpreted as a limit in scaling. The aim is not the best fitting but the labeling of the mixing process according to its organization in scales.

Fractal concepts may be applied to the dispersion process (Mandelbrot 1982). Basically this signifies that the dispersion is related by a fractal dimension to the time. Using a fractal dispersion coefficient an infinity of time-dependent coefficients q_{2m} results with (7.22). It is difficult to justify the idealized physical picture associated to the self-similar fractal-type dispersion process of the tracer traveling at the same velocity in many non-interacting streams tubes of different lengths in parallel connection. It is more reasonable to assume that the tracer moves through pores of different permeability at different velocities that is using a reduced number of scales of the process.

The NA approach has some common features with dispersion theories developed by Gill (Gill and Sankarasubramanian 1970, Iordache et al. 1987, Iordache et al. 1988c, Iordache et al. 1992). Gill considered an infinite order dispersion equation for the average value of the transported property.

As in NA approach the first term in the concentration expansion satisfies the standard form of the dispersion equation. The Gill method is a perturbation one but the scaling is spatial. Consequently their correction coefficients depend on time.

7.1.3 Hydrological Experiments

The studied natural systems posses complex internal flow fields resulting from large-scale flow heterogeneities. In field experiments there appear heterogeneous medium with more or less continuous stratifications of permeability, with the presence of pores having stagnant water or coat films, with trapping effects etc. Water flow through a karstic system is far from ideal (Gaspar and Simon 1986, McGuire and McDonnell 2006). RTD theory and the concept of residence time may be applied only in association with a flow pattern. The generally valid flow patterns cannot be defined as each karst boasts its own salient features and it is impossible to estimate all the parameters responsible for the behavior of the respective karsts. These patterns are intended for understanding or simulation of the operation of the system. The lack of concordance between the results of observations and the pattern employed may be a consequence of an erroneous definition of the system, or of an estimation of the input and output functions. If the flow pattern is appropriate selected then the experimental curves will more or less superpose the theoretical curves. In this situation, a series of important characteristics, such as static and dynamic reserve, the dispersivity of the aquifer, and, consequently, the vulnerability of the karst could be determined and, what is highly important, the behavior of the karst in various hydrological conditions and its evolution are predicted.

Several mathematical models have been applied in the interpretation of environmental isotope data obtained in systems with flow heterogeneities. All these models differ by assumed shape of the transit-time distribution of flow. The dispersion equation is one of the best mathematical formulations available for the description of macroscopic effects in the tracer transport in porous and densely fissured media, hydro-karstic structure, rivers, channels and other natural or artificial systems. But in complex practical hydrological systems there exists notable discrepancy between the experimental and theoretical curves.

The purely dispersion model is improved by the use of an NA perturbed model which more adequately describes natural flow systems. The applicability of the perturbed model is illustrated by the reinterpretation of known case studies and by comparison of the results obtained with those obtained by the use of purely dispersion models. The new models will also be used for interpretation of tracer experiments (tracers and environmental isotope data) performed in karstic zones. The axial dispersion is assumed to be the basic mechanism which ensures the tracer transfer in groundwater system. The flow across large fissures, the transfer

in porous matrix etc. takes place at other characteristic scales of the turbulent mixing process and could be interpreted as small perturbations of the basic dispersion mechanism. For instance it is well known that in systems with bound water in solid matrix the movement of the tracer is delayed with respect to the movement of the water flux. In other cases, in fractured media or in hydro-karstic systems certain fractions of the feed tracer travel rapidly and bypass the main flow.

The use of the (step) response of a groundwater system to determine a solution like equation (7.13) is presented in the following. The input data for the calculations are the experimental concentration of the tracer and some parameters as t = x/v, D/v, and the number of Péclet. Here D is the coefficient of dispersion and v the velocity. Empirical data can be represented by a diagram of concentration c(t) for fixed x: (Zuber 1986, McGuire and McDonnell 2006). In this case c(t) is the output relative concentration corresponding to a step input. The dispersion coefficient depends mainly on heterogeneities of the porous formation, presence of fissures, on the existence of double porosity and so on. This makes an exact prediction of the dispersion coefficient very difficult. Usually dispersion coefficients are estimated using correlations or diagrams from literature. It is known, for instance that for granular media of fluvial or glacial origin the dispersion constant D/v may range from a few centimeters to a few meters whereas for fissured rocks the quoted values range from 2 to 200 meters or even more. Obviously under field conditions the stochastic features of hydraulic conductivity of particular zones should be considered. The experimental results obtained by Gaspar and Simion (1986) in the Cerna-Valley have been analyzed in the NA frame (Iordache et al.1987). In this case D = 7.10^5 m^2/day ; x=13550 m, v=953 m/day. It contains the dimensionless response C/C_0 as a function of the dimensionless variable η. A model with two scales is selected. It results $q_0 = 1$, $q_2 = 0.14$. In this case the distances S as defined by (7.25) are: 0.05; 0.04, and 1.4 at M=0, 1and 2 respectively. The q_2 positive is correlated with the presence of dead-spaces. In both cases it is assumed that the curves of the best fitting give the best NA model but a caution is necessary as a field measurement is always of a limited accuracy.

Taking into account the properties of the orthogonal polynomials it results that the moment of order 2m contains q_{2m}. Consequently it is possible to interpret q_{2m} in terms of means, coefficients of variation and other statistics. Denote by V_M the variance resulting when M+1scales are taken into account. One obtains using (7.21) that:

$$\frac{V_M}{V_0} = \frac{q_0 + 2q_2}{q_0} \tag{7.26}$$

Observe that the resulting coefficient outlines a unique correction no matter the number of scales and that the ratio depends on q_2. V_M corresponds to hypothetical

dispersion coefficient as calculated if the model is restricted to a purely dispersion model (the centered second moments of the recorded curves).

The flatness factor F is given by:

$$F = \frac{3q_0 + 12q_2 + 24q_4}{3(q_0 + 2q_2)^2} \tag{7.27}$$

It depends on q_2 and q_4.

Finally observe that the approach proposed here always remain closely linked with experiment for final parameter evaluation. The open problem is to relate the spectrum q_{2m} with dispersion in non-ideal porous media characterized by high heterogeneity, stratification, poor connectivity and anisotropy, with the dynamics of the invasion of a non-wetting fluid, and so on.

The multi-scale analysis of dispersion may be considered from the point of view of the integrative closure concept (Fig. 7.1).

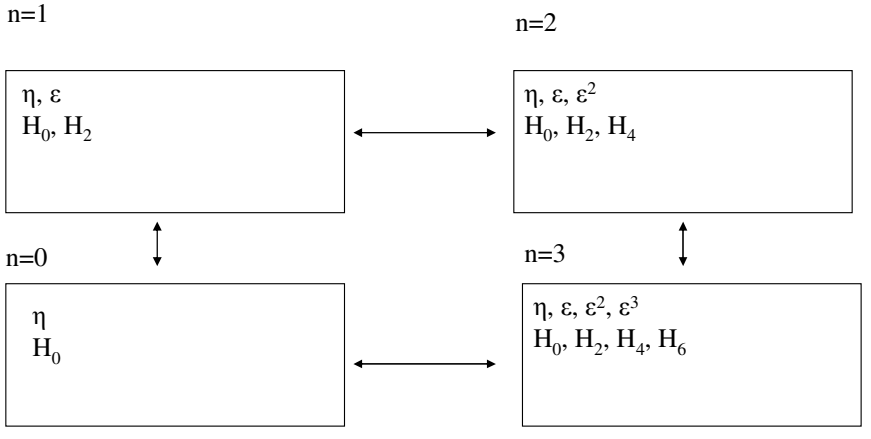

Fig. 7.1 Scales and integrative closure

Fig. 7.1 illustrates the situation in which we may limit the system at only four scales of perturbation.

The Hermite polynomials included at any new level are indicated as well as the hypothetical connection between low and top levels of perturbations.

7.1.4 SDG Solution for Dispersion

A rigorous study of differential equations as (7.5) makes use of SDG concepts (Kock and Reyes 2006, 2008).

We will consider solutions for the vector field on the Euclidean vector space D'(R), whose principal part is given by Γ: D'(R) → D'(R). Denote by $R_{\geq 0}$ the non-negative numbers.

Summarizing SDG results, we have a smooth function W: $R_{\geq 0} \rightarrow$D'(R), satisfying the dispersion equation (7.5). This may be written as (7.28).

$$\frac{\partial W}{\partial T} = \Gamma(W(T) \tag{7.28}$$

We may ask for the values of W for nilpotent T.

The answer can be deduced from the Taylor series at 0 for the function W.

We get for T assumed nilpotent.

$$W(T) = \delta(0) + T\Gamma(\delta(0)) + \left(T^2/2!\right)\Gamma^2(\delta(0)) + \left(T^3/3!\right)\Gamma^3(\delta(0)) + \ldots \tag{7.29}$$

Here Γ^2 (δ (0)) = Γ (Γ (δ (0))) and so on.

The series is a finite sum, since T is nilpotent.

In particular for d with d^2=0, we have:

$$W(d) = \delta(0) + d\,\delta(0)'' \tag{7.30}$$

In some cases the motivation for the study of the dispersion equation was to see to see how δ (0) evolves in nilpotent lapse T of time and specially when for T=d with d^2=0.

The answer is offered by (7.30) or more generally by (7.21).

Being an extensive quantity, a distribution like (7.30) should be drawable. It can be exhibited as a finite linear combination of Dirac distributions δ (a).

Let us consider for instance that h^4=0.

Then:

$$h^2 = \delta(0)'' = \delta(-h) - 2\delta(0) + \delta(h) \tag{7.31}$$

To make a drawing of W (d) where d^2=0, assume that d= h^3 for some h with h^4 =0.

Then:

$$W(d) = \delta(0) + d\,\delta(0)'' = \delta(0) + h((\delta(-h) - 2\delta(0) + \delta(h)) \tag{7.32}$$

The drawing of δ (x) is a column of height 1 at x.

The distribution above then comes by removing 2h units from the unit column at 0, and placing the small columns of height h at –h and h. This is the beginning of the dispersion of a Dirac distribution.

Applications of the new solutions of dispersion equations have been found in the study of anomalous diffusion (Schreckenberg 1985, Metzler and Klafter 2000).

Another domain of applications of multi-scale dispersion may be the neurophysiology of sensing for visual systems (Petitot 2003).

The receptive field of a visual neuron is defined as the domain of retina to which it is connected through neural connections of the retino-geniculo-cortical pathways and whose stimulation outlines a spike response. It is a classical result of neurophysiology that the receptive fields of the retinal ganglion cells are second order spatial derivatives of Gaussians.

7.1.5 Convection Model

Turbulent dispersion effects may result by superposition of several convective processes.

The Taylor dispersion is a phenomenon of this type (Taylor 1953). The velocities are different due to the laminar flow.

The dispersion is due to transitions between different component processes, between slow and active spaces. Such transitions represent change of velocities and this corresponds to the physical mechanism of dispersion phenomena relative to a mean velocity.

For numerous transport processes the basic material balance may be restricted to a first order wave equation.

The model (7.33) shows that the variation of concentration in time is due to a convective process with velocity V, and to a kinetic process of interaction, Q(C).

$$\frac{\partial C}{\partial T} + V\frac{\partial C}{\partial x} + Q(C) = 0 \tag{7.33}$$

Here C (T, x) denote a concentration, variable in T-time and x-space, V denotes the velocity, and Q(C) denotes a separation rate.

The model (7.33) known also under the name of Euler's equation describes the incompressible fluid flow and many other phenomena of physical and technological interest (Rhee et. al. 1989). Significant examples are the plug-flow model of chemical reactors, separation in columns and so on.

Suppose that there are two scales of time for different variables and parameters as concentration C, time T, velocity V and separation rate Q.

This may be written:

$$C = c_0 + \varepsilon c_1 \quad T = t + \varepsilon t \quad V = v_0 + \varepsilon v_1 \quad Q = q_0 + \varepsilon q_1 \tag{7.34}$$

Replacing (7.34) in (7.33) and making use of the calculus rules in NA frame we obtain two equations:

$$\frac{\partial c_0}{\partial t} + v_0\frac{\partial c_0}{\partial x} + q_0 c_0 = 0 \tag{7.35}$$

$$\frac{\partial c_1}{\partial t} + v_0 \frac{\partial c_1}{\partial x} + v_1 \frac{\partial c_0}{\partial x} + q_0 c_1 + q_1 c_0 = 0 \tag{7.36}$$

Eliminating one of the two variables we obtain a model containing the second derivative of the concentration and multiplied by coefficients as: v_0^2 / q_0 .

This confirms the occurrence of dispersive effects resulting by superposition of purely convective processes.

An SDG solution of the transport equation (7.33) is due to Kock and Reyes (2006).

Suppose that the initial condition is:

$$C(0, x)=f(x) \tag{7.37}$$

The general solution of (7.33) is:

$$C(T,x)=G(T, f(F(-T, x)) \tag{7.38}$$

Here F and G are solutions of:

$$\frac{\partial F}{\partial T} = V; \frac{\partial G}{\partial T} = -Q \tag{7.39}$$

7.2 Intermittency by Vortex Line Stretching

7.2.1 Conventional Frame

In turbulent flow the energy associated with small-scale structures is distributed very unevenly in space being confined in a smaller and smaller fraction of the available space as the eddy size decrease. This spottiness of the small scales is called intermittency. The two basic features to be considered here in the study of intermittency are the stochastic character of flow and the multiplicity of the time scales. The vorticity is relevant in understanding intermittency gives a configurationally space interpretation of the energy transfer to small-scale motions in three dimensional turbulences. In effect in the absence of viscosity the vorticity w = rot v (v denotes velocity) satisfies the equation (7.40) resulting from Navier-Stokes equations:

$$\frac{\partial w}{\partial t} + (v.\nabla)w = (w.\nabla)v \tag{7.40}$$

The equation (7.40) reveals an intimate connection between the energy transfer and the distortion by velocity gradients of a small line element carried by the fluid flow. The question of the stretching of a line element by a random velocity field

has been studied in literature (Rose and Sulem 1978). The main result is that a line element which, is initially statistically independent of the velocity field, is in the mean, stretched, but the lax of stretching is not known. Vortex line stretching is considered to be the dynamical mechanism behind the intermittency, as suggested from the following argument. Consider a point within a large scale structure which at the initial time has the largest vorticity amplitude |w|. This point is also likely to shave a large velocity gradient $|\nabla| \sim w$. Consequently, the straining action of the velocity gradient on the vorticity may be described by a simplified form of the vorticity equation (7.40) that is by:

$$\frac{dw}{dt} = bw(w-1) \tag{7.41}$$

Here b is a parameter closely related to the time scale of the process. Here it is expected that vorticity downstream of the point will rise to large values in a time of the order of the large eddy turnover time. Associated with this local vorticity is a local increasing of the vortex line stretching in the volume originally occupied by the vorticity overload.

Its volume remains constant because of the incompressibility constraint and the self-amplifying feature of vorticity will cause the shearing of the volume to be non-uniform with the strongest concentration of vorticity found in a small sub-volume. So, small-scale structure may be generated in a localized fashion.

A discrete version of (7.41) obtained by replacing w'(t) by w_{n+1}-w_n and w^2 by $w_n w_{n+1}$ gives:

$$w_{n+1} = \frac{w_n}{(w_n + c(1-w_n))} \tag{7.42}$$

Here w_n is the vorticity at the moment n, c=1/(1-b). To take into account the fact that the vortex stretching is stochastic the parameter c is assumed to be a random variable. Denote also by c_n the value of c at the moment n. Random difference equation as (7.42) can be studied as a RSCC In this case:

$$S=\{w_n\}=[0,1],\ K=\{c_n\},\ P(c_n|w_n)=p(c_n),\ w_{n+1}=u(w_n,c_n) \tag{7.43}$$

Here the operator u is given by (7.42).

Fig. 7.2 illustrates the intermittency by vortex line stretching.

The RSCC starts with vorticity w_0. Then with probability $P(c|w_0) = p_c$ the condition c is selected. Consequently the new vorticity $w1 = w_0/(w_0 + c\ (1-w_0))$ results. In the next temporal step the condition d is established with probability $P(d|w_1) = p_d$ and the next vorticity will be: $w_2 = w_1 / (w_1 + c\ (1-w_1))$ (Fig. 7.2).

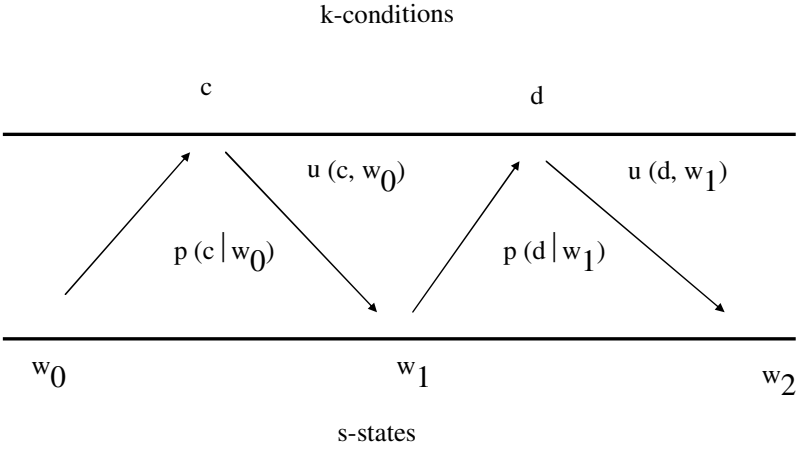

Fig. 7.2 Intermittency by vortex line stretching

7.2.2 Multi-level Frame

The above model corresponds to a single conditioning level of evolution. However in turbulent flow there are more scales of time that is more conditioning levels. We limit in the sequel the study to only two such scales.

Fig. 7.3 illustrates the two time scales intermittency.

The model categorification method is applied. The time n is replaced by the vector N = [n, γ] (that is by n + εγ), the vorticity w_n by the vector $W(N) = [w_n^0, w_n^1]$ and the parameter c_n by the vector $C(N) = [c_n^0, c_n^1]$ Consider that the condition C (N) at $N = [n, \gamma]$ is

$C(N) = c_n^0(1 + \varepsilon\gamma_n)$ where c_0^n and γ_n are random variables. Observe that in this case we have $c_n^1 = c_n^0\gamma_n$ and that the effect of the evolution at the second conditioning level is a small perturbation of the condition c_n^0. The general evolution model is in this case:

$$W(N') = \frac{W(N)}{(W(N) + C(N)(1 - W(N))} \tag{7.44}$$

Restrict the study to the occurrence of only two conditions at any level that is $c_n^0 \in \{c, d\}$ and $\gamma_n \in \{\gamma, \delta\}$. Denote also by p_c, p_d , π_γ and π_δ the probabilities of c, d, γ , or δ respectively. The diagram shown in Fig. 7.3 describes a system starting from W[0,0]. With possibility $P(c \mid W[0,0]) = p_c$ the condition

c is selected and with probability $P(\gamma \mid c) = \pi_\gamma$ the small perturbation γ of c appears. The new vorticity is at [1,γ]:

$$W([1,\gamma]) = \frac{W([0,0])}{(W([0,0]) + c(1+\varepsilon\gamma)(1-W([0,0])} \tag{7.45}$$

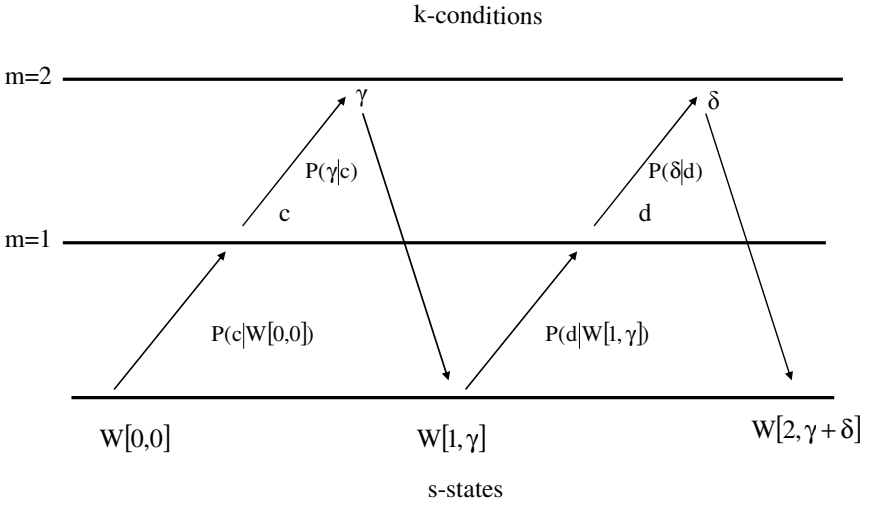

Fig. 7.3 Two time scales intermittency

Then with possibility $P(d \mid W[1,\gamma]) = p_d$ the new selected condition is d and the new perturbation denoted by d, appears with probability $P(\delta \mid d) = \pi_\delta$. The resulting vorticity is:

$$W([2,\gamma+\delta]) = \frac{W([1,\gamma])}{(W([1,\gamma]) + d(1+\varepsilon\delta)(1-W([1,\gamma])} \tag{7.46}$$

By successive iterations we obtain:

$$W([n,\gamma]) = \frac{W([0,0])}{(W([0,0]) + c^m d^{n-m}(1+\varepsilon\gamma)^\mu (1+\varepsilon\delta)^{\tau-\mu}(1-W([0,0]))} \tag{7.47}$$

if in the first n trials there are m occurrences of the condition c and n-m occurrences of the condition d. Moreover at the second level there are μ occurrences of the perturbation (1+εγ) and τ-μ ,occurrences of the perturbation (1+εδ)

Denote:

$$c^m d^{n-m}(1+\varepsilon\gamma)^{\mu}(1+\varepsilon\delta)^{\tau-\mu} = (\bar{c})^n(1+\varepsilon\bar{\gamma})^{\tau} \tag{7.48}$$

Let us approximate expressions as $(1+\varepsilon\gamma)^{\mu}$ by $1+\varepsilon\gamma\mu$ and then separate the infinitesimal part. It results:

$$c^m d^{n-m} = (\bar{c})^n \tag{7.49}$$

$$\mu\gamma + (\tau-\mu)\delta = \tau\bar{\gamma} \tag{7.50}$$

Observe that:

$$\log\bar{c} = \frac{m}{n}\log c + \frac{n-m}{n}\log d \tag{7.51}$$

$$\bar{\gamma} = \frac{\mu}{\tau}\gamma + \frac{\tau-\mu}{\tau}\delta \tag{7.52}$$

When n $\to\infty$, then $m/n \to p_c$,$(n-m)/n \to p_d$, $\mu/\tau \to \pi_\gamma$ and $(\tau-\mu)/\tau \to \pi_\delta$

It results that:

$$\log\bar{c} = p_c \log c + p_d \log d \tag{7.53}$$

$$\bar{\gamma} = \pi_\gamma\gamma + \pi_\delta\delta \tag{7.54}$$

In order to characterize the stability of the iteration process it is necessary to compare with unity the coefficient r:

$$r = \bar{c}(1+\varepsilon\tau\bar{\gamma})^{1/n} \tag{7.55}$$

If r > 1, then W [n, γ] tends to zero. On the contrary if r < 1 then W[n,γ] tends to unity when n and τ tends to ∞. If r = 1 then W[n,γ] oscillates between 0 and 1.

Interesting situations appear when $\bar{c}$ < 1 but r ≥1. In such cases a stabilizing effect at the basic level of evolution with a short relaxation time is coupled with a non-stabilizing effect with a long relaxation time. This competition may explain the random intermittences or bursts.

References

Dullien, F.A.L.: Porous Media. Fluid Transport and Pore Structure. Academic Press, New York (1992)

Gaspar, E., Simion, G.: Tracer research on the dynamics of underground waters in the Cerna Valley. Theoretical and Applied Karstology 2, 183–197 (1986)

Gill, W.N., Sankarsasubramanian, R.: Exact analysis of unsteady convective diffusion. Proc. Roy. Soc. London A 197 A 316, 341–350 (1970)

Iordache, O., Isopescu, R., Gaspar, E.: Interpretation of tracer dispersion in karst groundwater experiments. Theoretical and Applied Karstology 3, 223–227 (1987)

Iordache, O., Isopescu, R., Isopescu, A., Iacobini, A., Jinescu, G.: Non-Archimedean models of mixing II, A nearly dispersional model for packed bed thermal storage systems. Chem. Engng. Sci. 43, 698–701 (1988c)

Iordache, O., Corriou, J.P., Tondeur, D.: Nonarchimedean Models for Dispersion in Disordered Media. In: AICh E Annual Meeting, Miami Beach, FL (1992)

Kock, A., Reyes, G.E.: Ordinary differential equations and their exponentials. Central European Journ. of Mathematics 4(1), 64–81 (2006)

Kock, A., Reyes, G.E.: Some differential equations in SDG. arXiv:math.CT/0104164 (2008)

Kraichnan, H.: Relizability inequalities and closes moment equations. Ann. New York Acad. Sci. 316, 37–47 (1980)

Kreft, A., Zuber, A.: On the physical meaning of the dispersion equation and its solutions for different initial and boundary conditions. Chem. Engng. Sci. 33, 1471–1480 (1978)

Mandelbrot, B.: The Fractal Geometry of Nature. Freeman, New York (1982)

McGuire, K.J., McDonnell, J.J.: A review and evaluation of catchment transit time modeling. Journal of Hydrology 330, 543–563 (2006)

Metzler, R., Klafter, J.: The random walk's guide to anomalous diffusion: a fractional dynamics approach. Physics Reports 339, 1–77 (2000)

Petitot, J.: The neurogeometry of pinwheels as a sub-Riemannian contact structure. Journal of Physiology-Paris 97, 265–309 (2003)

Rhee, H.K., Aris, R., Amundson, N.R.: First Order Partial Differential Equations II. In: Theory and Applications of Hyperbolic Systems of Quasilinear Equations. Prentice-Hall, Englewood Cliffs (1989)

Rose, H.A., Sulem, P.H.: Fully developed turbulence and statistical mechanics. J. Physique. 39(5), 441–484 (1978)

Saffman, P.G.: Application of the Wiener-Hermite expansion to the diffusion of a passive scalar in a homogeneous turbulent flow. Phys. Fluids. 12, 1786–1798 (1969)

Schreckenberg, M.: Long range diffusion in ultrametric spaces. Z Phys B-Comndensed Matter 60, 483–488 (1985)

Taylor, G.I.: Dispersion of soluble matter in solvent flowing slowly through a tube. Proc. Roy. Soc. London A 219, 186–203 (1953)

Zuber, A.: Theoretical possibilities of the two-wall-pulse method. In: Isotope Techniques in Groundwater Hydrology, vol. 11, pp. 277–299. IAEA, Vienna (1974)

Zuber, A.: Review of existing mathematical models for interpretation of tracer data in hydrology. In: Mathematical Models for Interpretation of Tracer Data in Groundwater Hydrology, pp. 69–116. IAEA, Vienna (1986)

Chapter 8
Entropy

Abstract. Entropy and entropy production for multi-scale and multi-level systems are studied here with reference to physical and informational aspects.

Entropy balance, entropy increase and entropy production principles are formulated in new frames based on model categorification.
Case studies pertain to biosystems and ecosystems.

For the general PSM framework, new entropic criteria are proposed based on the study of different types of causation.

Evolvability maximization role for integrative closure is emphasized.

8.1 Background

Entropy is a significant concept in the study of irreversible transformations. The entropy concept is related to time, probabilities and information. Boltzmann emphasized the probabilistic meaning of the classical entropy in thermodynamics, realizing that the entropy of a physical system can be considered as a measure of the disorder in the system.

A fundamental law of nature concerning entropy in macroscopic systems is the law of entropy increase. For all real transformations of isolated systems, no change of heat with the external world being assumed, entropy must increase, or ideally, in reversible cases, remains constant with time. Thus:

$$\Delta s \geq 0 \tag{8.1}$$

Here s denotes the entropy.

Some basic aspects correlating entropy and evolution of complex systems will be reviewed in the following (Prigogine 1980, 1989).

Typical for complex systems is their irreversibility. According to this, if there is evolution, past and future have to be different.

Isolated systems might be considered as an artificial situation in real systems. Consequently, entropy production that is entropy variation, for any given system

splits into two additive terms, the one accounting for entropy exchanges with the environment, and the other for internal entropy production, this latter being always positive for systems presenting irreversible processes. If a system has the entropy s, then any elementary transformation induces a change in his entropy, which always will be broken down into two terms:

$$ds = ds_i + ds_e \tag{8.2}$$

The term ds_i represents the internal production of entropy and is always positive or null.

This term is the entropy production due to irreversible processes inside the system such as diffusion, chemical reaction, heat conduction and so on.

The second term ds_e represents the entropy exchanged with the external surroundings.

As a result, when there is no entropy flow, as in the case of isolated systems, $ds_e=0$ and the entropy may only grow and will reach a maximum.

The entropy production is closely related to irreversible processes being a mechanism for producing order. At equilibrium the internal rate of entropy production is zero. In systems for which the equilibrium state cannot be reached because external constraints do not lead the system to reach it, the rate of production of entropy takes the minimum value compatible with the constraints. This is the so-called principle of minimum entropy production due to Prigogine (Prigogine 1980, 1989). It refers to linear thermodynamics that is to linear relation between thermodynamic forces and fluxes.

A typical feature of complexity is the randomness meaning that concerning the future states it is possible to formulate only stochastic statements. In a physical system having many degrees of freedom, the number measuring the disorder of the system measures also the uncertainty concerning the states of the individual particles. This fact is expressed by the Boltzmann equation:

$$s=k \log W \tag{8.3}$$

Here k is the Boltzmann's constant and W is the number of different ways the macroscopic properties of the system could be reproduced, by giving distinct values to its internal that is microscopic degrees of freedom. The stochastic and chaotic aspect was clarified and developed when one comes to study of non-linear complex systems and bifurcations. Far from equilibrium, systems enter into the nonlinear range and display a multiplicity of solutions to the equations describing their evolution. At bifurcation points, the role of fluctuations is decisive in that it is impossible to predict on the basis only of the deterministic equations which branch the behavior of the system will follow.

Another entropy related aspect of complexity refers to the necessity of some coherence mechanism in order to account for an evolvable system in which new, organized phenomena arise. Coherence implies for instance that millions of molecules follow each other. This appears as unexpected, because for classical physics the order is associated with equilibrium, as in the case of crystals, while

disorder is associated with non-equilibrium, as in the case of turbulence, embryogenesis and so on.

8.2 Informational Entropy

There is a significant connection between the notion of entropy in thermodynamics and the notion of information and uncertainty. In 1948, based on the classical Boltzmann's work, Shannon proposed a quantitative measure of the amount of information or uncertainty supplied by a probabilistic experiment. Consider an experiment in which the event i, results with probability p_i. It is described by the finite probability distribution:

$$p_i \geq 0,\ i=1,...,\ n;\ \sum_i p_i = 1 \tag{8.4}$$

The informational Shannon entropy associated to this experiment is:

$$h_n(p_1, p_2, ..., p_n) = -\sum_i p_i \ln p_i \tag{8.5}$$

This function has properties, which give a reasonable measure of uncertainty in a probabilistic experiment. For instance:

i. $h_n(p_1, p_2, ..., p_n) \geq 0$

ii. $h_n(p_1, p_2, ..., p_n) = 0$ if $p_i = 1$ for some i and $p_j = 0$ for i # j. This means that if only a result is possible the uncertainty is null.

iii. $h_{n+1}(p_1, p_2, ..., p_n, 0) = h_n(p_1, p_2, ..., p_n)$. This means that adding the impossible event to the possible results of a given experiment does not change its uncertainty.

iv. $h_n(p_1, p_2, ..., p_n) \leq h_n(1/n, 1/n, ..., 1/n) = h_{max}$.

This shows that the greatest uncertainty corresponds to equally likely outcomes.

There exist random events whose probabilities cannot be directly evaluated. For instance the results of the measurements made on a microscopic scale on microscopic systems are such mean values of some random variables. There exist many random distributions compatible with a given mean value. The problem is how to select the best one. The principle of maximum entropy can be considered as such a criterion. According to this principle systems choose the random distribution that maximizes the entropy or the conditional entropy subject to some set of restraints.

Information entropy may be considered as the primary concept and use the probability distribution that maximizes the entropy subject to certain constraints for the statistical inference of the evolution (Jaynes 1957). This principle appears to have a subjective character. As long as entropy is accepted as being the most suitable measure of uncertainty the system select that particular random distribution which contains the largest amount of uncertainty compatible to the

given restraints. The success of the principle of maximum information in classical and quantum mechanics suggests extending its range of application. In making inferences on the basis of partial information, it is necessary to use that probability distribution which has maximum entropy, as a measure of uncertainty, subject to whatever is known (Dewar 2003).

A significant result in the study of entropy is the Boltzmann's H-theorem that states the increase of the entropy as a measure of uncertainty. For a large class of stochastic evolutions of the Markovian type the H-theorem holds.

We dente by $p_{t,t+1}(w', w)$the probability of transition from the state w, at the moment t to the state w', at the moment t+1.

Observes that $p_{t,t+1}(w', w) \geq 0$ and that:

$$\sum_{w'} p_{t,t+1}(w', w) = 1 \tag{8.6}$$

The Markovian evolution is described by the following equation:

$$p_{t+1}(w') = \sum_{w} p_t(w)\, p_{t,t+1}(w', w) \tag{8.7}$$

At every moment the entropy is given by:

$$h_t = -\sum_{w} p_t(w) \ln p_t(w) \tag{8.8}$$

The H-theorem establishes that: if the transition stochastic matrix $p_{t,t+1}(w', w)$ is bistochastic, that is if for any w and w':

$$\sum_{w} p_{t,t+1}(w', w) = \sum_{w'} p_{t,t+1}(w', w) = 1 \tag{8.9}$$

then:

$$h_t \leq h_{t+1} \tag{8.10}$$

The NA counterpart of the principle of maximum information say that the systems choose the random distribution, which maximizes, in the NA frame, the informational entropy or the conditional informational entropy subject to some set of restraints. But maximums are not unique in NA frames. Consequently a variety of acceptable distributions will result and other choice criteria should be selected to ensure uniqueness. Specific real norms would be used to choose one of them (Appendix 1).

The NA categorification of the Boltzmann H-theorem is discussed in what follows.

Consider for instance two NA times T = [n, t], T' = [n', t'] and the corresponding NA entropies: H(T) = [h_0(n), h_1(n)], H(T') = [h_0(n'), h_1(n')]. The NA counterpart of the H-theorem would establishes that the NA entropy, H(T) always increases in time but the relation of order is a new one in NA frame. For instance

if T < T' in the NA order, by model categorification, the NA valid H-theorem implies that:

$$H(T) < H(T') \tag{8.11}$$

The above inequality should be considered with the same NA order as for the time T. This NA inequality shows that it suffices that the entropy increases at the level m=0, that is $h_0(n) < h_0(n')$ for n<n', to assure the increasing of NA entropy despite the entropy decreasing of other levels contribution. Therefore it is possible that $h_1(n)>h_1(n')$ that is on higher levels the level associated entropy could decrease. Restricting the analysis to a single level m=1, may show results apparently in contradicting the principle of increasing entropy but they are clarified in the multi-level frame. The multi-level entropy increases, while allowing self organization at the focused level m=1.

8.3 Entropy Production for Biosystems

Whether biosystems or ecosystems augment or diminish the rate of entropy production is a highly intriguing question of practical and theoretical interest. According to the principle of minimum entropy production, systems constrained to remain slightly away from thermodynamic equilibrium will take on the configuration of forces and flows that minimizes the rate of entropy production (Prigogine 1980, 1989). This theorem has received the status of a principle of organization for living systems that in some conditions grow toward a state of minimum metabolism per unit mass. The validity of the principles seems to be broken in embryogenesis where an initial increase of the heat production is observed. Then the entropy production decreases during adult life, but there still are notable exceptions as for instance tissue regeneration of malignant growth. Similar behavior has been observed in the case studies of prebiotic polymer formation. There have already been several attempts to solve this apparent contradiction. Hiernaux and Babloyantz (1976) proposed nonlinear biochemical models for embryogenesis in order to obtain models that outline a time of maximum production of entropy. Lurie and Wagensberg (1979) considered that linear thermodynamics provides an appropriate framework for the description of the development of biosystems but abandoned the usual approximation that the specific heat-dissipation is the negative of the specific entropy production during the evolution. Assuming the correctness of a linear relation between metabolic fluxes and metabolic forces within biochemical machinery the phenomenological coefficient of coupling can be determined.

The starting point of the approach presented here resides in assuming that due to nonlinear interactions characteristic to the embryogenesis, such far from equilibrium systems are structured in a finite number of different timescales of evolution (Iordache and Frangopol 1988b, 1988c, 1989). The existence of more than one scales of evolution is a well known feature of complex biophenomena as for instance membrane transport, mitosis, prebiotic evolution etc. A variety of timescales is displayed by the ionic pumps considered as channels whose energy

barrier profile is transiently modified by the cycle of phosphorylation-dephosphorylation.

The entropy balance could be formulated in the NA formalism resulting in a significant enlargement of the validity domain of this balance. The entropy production p(s) is:

$$p(s) = \frac{\partial s}{\partial t} + f(s) \geq 0 \tag{8.12}$$

Here s is the entropy and f(s) denotes the entropy flow through the surface of the system.

The formalism of infinitesimals and an application of the model categorification method are presented in the following. The existence of more than one scales of time is considered by translating the time t and the entropy s(t) by expansions as:

$$T = t + \varepsilon w_1 t + ... + \varepsilon^M w_M t \tag{8.13}$$

$$S(T) = s_0(t) + \varepsilon s_1(t) + ... + \varepsilon^M s_M(t) \tag{8.14}$$

Here M+1 is the number of timescales, ε is the expansion parameter w_m, m=1,..., M are constants, $s_m(t)$ are functions. Denote also the time T = [t,w_1t,..., w_Mt], and entropy S(T) = [s_0(t), s_1(t),..., s_M(t)]. The generalized time T and the generalized entropy S(T) are viewed here as elements of an NA frame. The model categorification method consists in replacing the real equation by an NA equation of the same form but with a different signification. In the NA frame of infinitesimals the balance of entropy (8.12) is translated by model categorification into the NA differential equation:

$$P(S) = \frac{\partial S}{\partial T} + F(S) \geq O \tag{8.15}$$

Here O = [0,...,0] is the null element of the NA structure, f(s) is replaced by F(S) and the entropy production p(s) by P(S):

$$F(S) = [f_0, f_1, ..., f_M], P(S) = [p_0, p_1, ..., p_M] \tag{8.16}$$

The functions f_m and p_m represents the contribution of entropy flow and entropy production at different scales.

The NA form of the entropy balance expresses an NA form of the second law of thermodynamics:

$$P(S) \geq O \tag{8.17}$$

This accommodates situations as: $p_0 \geq 0$ but $p_1 < 0$ .. , $p_{m-1} < 0$, $p_M < 0$.

The additional equations in the hierarchy of scales cannot reverse the existing results concerning the real entropy but are compatible with them and represents an extension of the classical point of view. The restriction of observations to infinitesimal scales, allows detecting evolutions that apparently contradict the second law.

Interesting situations corresponds to systems having: $p_0 = 0$, $p_1 = p_{m-1} = 0$, $p_m \geq 0$, $p_{m+1} < 0$,..., and so on for increasing m.

Suppose that the zero-th order contribution in S(T) that is s_0 corresponds to the thermodynamic equilibrium while the following terms, s_1,..., s_M, are corrections due to non-equilibrium conditions. The number of timescales, M+1, depends on the studied system, the greater M is, the more departing the system is from equilibrium. Consequently, one needs more and more timescales to correct the basic equilibrium model corresponding to M=0. This follows the model categorification method.

To avoid insignificant calculations consider $w_m = 1$, that is the derivative is taken along the direction [1, 1,...,1]. Thus the derivative in (8.12) is translated into:

$$S'(T) = \left[s_0^{'}, s_1^{'} - s_0^{'}, ..., s_M^{'} - s_{M-1}^{'} \right] \tag{8.18}$$

Taking into account the significance of equality in the NA structure it results:

$$p_0 = s_0^{'} + f_0 \geq 0 \tag{8.19}$$

$$p_1 = s_1^{'} - s_0^{'} + f_1 \tag{8.20}$$

$$p_2 = s_2^{'} - s_1^{'} + f_2 \tag{8.21}$$

$$p_3 = s_3^{'} - s_2^{'} + f_3 \tag{8.22}$$

$$p_M = s_M^{'} - s_{M-1}^{'} + f_M \tag{8.23}$$

A system of balance equations is obtained in the NA formalism instead of a single real balance equation. They refer to different scales of the process and to neighboring ones. Taking into account the fact that both the flows of the irreversible process and the corresponding forces vanish at equilibrium, Glansdorff and Prigogine (1971) assumed that the entropy production is a quantity of second order with respect to the deviations from equilibrium. More exactly, $p_0 = 0$, $p_1 = 0$, $\varepsilon^2 p_2 = p(s)$ that is P(S) = [0, 0, p_2, p_3,..., p_M]. The second law of thermodynamics asserts that $p(s) \geq 0$. The equality applies only to reversible processes. The postulated positive value of P(S) signifies, in the NA formalism, that the first non-null element of this expansion is positive.

Glansdorff and Prigogine (1971) considered that the first non-null element in the expansion of F(S) is of the first order in the deviation from equilibrium that is $f_0=0$, $f_1\neq 0$ and F(S) = [0, f_1, f_2,..., f_M]. Here f_1 corresponds to the equilibrium flux. When inertial effects or velocity fluctuations are taken into account such specifications are no longer valid.

At equilibrium, due to the fact that $p_0=0$, $f_0=0$ the classical condition is obtained:

$$s_0^{'} = 0 \tag{8.24}$$

Obviously the equilibrium entropy is time independent quantity. Equation (8.20) becomes in this case:

$$s_1^{'} + f_1 = 0 \tag{8.25}$$

This is an equilibrium condition according to which an infinitesimal change of the entropy s'_1 has to be compensated by an infinitesimal entropy flow f_1 through the surface of the system. Further, equation (8.21) now becomes:

$$p_2 = s_2^{'} + f_1 + f_2 \geq 0 \tag{8.26}$$

Consider (8.26) under the boundary condition $f_1+f_2 = 0$, for instance if the heat flow and diffusion flow vanish through the boundary surface. In this case the condition (8.26) reduces to:

$$s_2^{'} = p_2 \geq 0 \tag{8.27}$$

Inequality (8.27) gives an evolution criterion for near-equilibrium states. In the stability analysis of Glansdorff and Prigogine the expansion of entropy around its equilibrium value is given by:

$$s=s_0+(\delta s)_0+ (1/2)\ (\delta^2 s)_0 \tag{8.28}$$

In the used here notation it is possibly to identify:

$$s_0=s_0;\ (\delta s)_0=\varepsilon s_1;\ (1/2)(\delta^2 s)_0 = \varepsilon^2 s_2 \tag{8.29}$$

Obviously using a generalized form of the expansion (8.29) it results:

$$(1/M!)(\delta^M s)_0 = \varepsilon^M s_M \tag{8.30}$$

At different degrees of thermodynamic non-equilibrium the entropy production can no longer be considered as a second order quantity. Condition (8.27) could be of no help in studying biosystems with high rates of dissipation, where the nonlinear effects are considerable. Numerical evaluations show an initial increase

of the entropy production p(s) in the case of biopolymer synthesis on a template with an auto-catalytic effect (Nicolis and Prigogine 1989). Such a behavior is easily explained if two timescales are assumed for the reacting system. A fast reaction pathway and a high rate of dissipation are followed by a decrease of rates and affinities for the template and catalytic processes owing to the fact that the inverse steps begin to build up along the reaction sequence. In some reacting systems of biochemical interest one step of the reaction becomes very rapid as compared to the others and the resulting chemical instability induces an increase of the entropy production. If after a certain period of time this fast step becomes extinguished or attains a rate comparable to the others, one might expect the entropy production to decrease. During the synthesis of some key substances necessary for process continuation that is after an increase in dissipation the above-described systems tend to adjust their entropy production.

Consider that the first period of the process is characterized by $p_1 \geq 0$. The condition (8.25) is replaced by:

$$p_1 = s_1^{'} + f_1 \geq 0 \tag{8.31}$$

If M = 3 it is possible that the entropy production is a third order quantity with respect to the deviations from equilibrium that is $p_1 = p_2 = 0$ but necessarily $p_3 \geq 0$. In this case the condition (8.26) reduces to:

$$s_2^{'} + f_1 + f_2 = 0 \tag{8.32}$$

New stability condition in the hierarchy should be considered.

From (8.26) it results that:

$$p_3 = s_3^{'} + f_1 + f_2 + f_3 \geq 0 \tag{8.33}$$

As m increases, conditions of the type $p_0 = ... = p_{m-1} = 0$, $p_m \geq 0$ with $p_{m'} < 0$ for $m' \geq M+1$ become possible. The transition from m scale to m+1 scale signifies that the system gains a quite different more complex structure. Observe that for this type of conditions, the first non-null component of P(S) has properties similar to the thermodynamic potential which take the minimum at the steady state. This point of view represents an extension of that based on principle of minimum entropy production. In the case of fixed external entropy flux F(S) the time variation of the production of entropy is given by S'(T).

Fig. 8.1 illustrates the entropy production for multi-scale systems as a function of time.

According to (8.18):

$$S^{'}(T) = s_0^{'} + \varepsilon(s_1^{'} - s_0^{'}) + ... + \varepsilon^M(s_M^{'} - s_{M-1}^{'}) \tag{8.34}$$

At M=1 due to the fact that $s'_0 = 0$ it results that $S'(T) = \varepsilon s'_1$. If $p_1 \geq 0$ it results that $s'_1 \geq 0$ and a domain of increasing s_1 is outlined in this case (domain a). Then, during evolution, the system outlines a new scale of time that is M = 2. In this domain

$$S'(T) = \varepsilon s'_1 + \varepsilon^2 (s'_2 - s'_1) \tag{8.35}$$

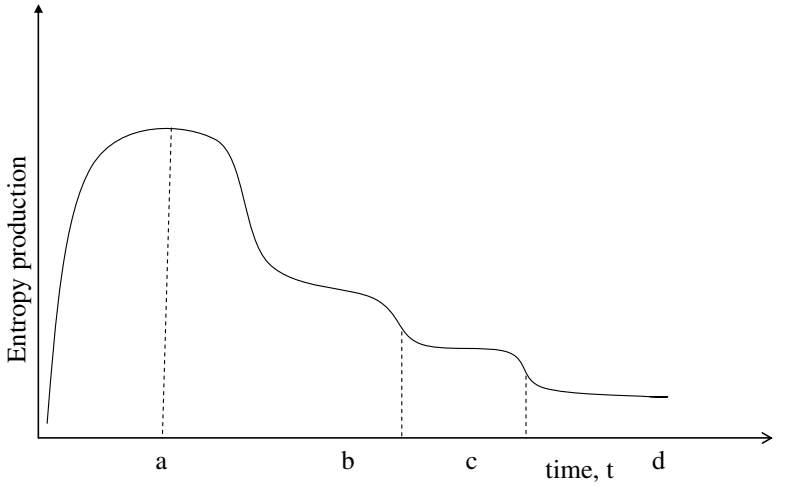

Fig. 8.1 Entropy production for multi-scale systems

Following Neder (1941, 1943) consider as a first approximation $s_2 \sim s'_1$, $s_3 \sim s'_2$,..., $s_M \sim s'_{M-1}$. At M=2 if $p_1 = 0$, $p_2 \geq 0$ then $s'_1 = 0$, $s''_1 > 0$. This corresponds to the domain of validity of the theorem of minimum production of entropy (domain b). At M=3 it happens that $p_1 = p_2 = 0$ but $p_3 \geq 0$. Consequently, $s_1 = 0$, $s'_2 = 0$, $s'_3 = 0$ or $s'_1 = 0$, $s''_1 = 0$, $s'''_1 > 0$. This corresponds to the third domain in the diagram S'(T) versus time (domain c).

At M > 3 the system will be characterized by $s'_1 = 0$, $s'_2 = 0$,..., $s'_{M-1} = 0$, $s'_M \geq 0$ and the time dependence is similar to that encountered in the domain with M ≥ 2.

Fig. 8.1 shows the time variation of S'(T) according to the above proposed mechanism. The domains are:

a: $p_1 \geq 0$; b: $p_1 = 0$, $p_2 \geq 0$; c: $p_1 = 0$, $p_2 = 0$, $p_3 \geq 0$; d: $p_1 = 0$, $p_2 = 0$, $p_3 = 0$, $p_4 \geq 0$.

A discussion of oscillations in the entropy production can be found in Desvilletes and Villani (2005).

Similar dependences have been observed for the rate of heat production at different stages of development in embryogenesis. According to the above theory, there exist different levels of quasi-stationarity of the rate of entropy production. For every state different but near enough to equilibrium, the ecosystem remains at the nearest possible value to the zero entropy production. As the level increases the production of entropy has a variation near the extreme that is more closely, as m increases, to the horizontal. A hierarchy of domains of quasi-stationary entropy production appears. Each decrease in the entropy production diagram defines a zone of local stability with a local minimum (non-vanishing) of the flux of entropy. The decreases may trap the system in a steady state of some sort, at different complexity levels. This is one of the ways in which nonlinear steady state systems like biological organisms can get their relative stability by increasing complexity.

Entropy production in biosystems system consists of multi-stages with time, early increasing, later decreasing and possible with intermediate stages (Aoki 1995). According to Aoki the entropy production in plants leaves oscillates during the period of one day paralleling the daily solar absorbed by leaves. For this case of environment studies the cyclic character of time is obvious. Multi-scale structure of cyclic time may be due to day-night cycle coupled to tidal cycles or other environmental cycles.

Salthe evaluated the possibility that the periods of increasing entropy production (immature stage), are followed by periods of constant entropy production (mature stage), and by that of decreasing entropy production (senescence stage) (Salthe 2003).

Dissipative structures continually incorporate new informational constraints also the rate of incorporation eventually slow down in levels or scales (Fig. 8.1).

This kind of entropy production behavior may be easily explained in the presented here framework starting from the fact that the living systems are not isolated and not nearly equilibrium.

8.4 Entropy and Integrative Closure

The evolution at different time scales may be examined in the conceptual framework of integrative closure. Fig. 8.2 highlights the integrative closure hypothesis for entropy production.

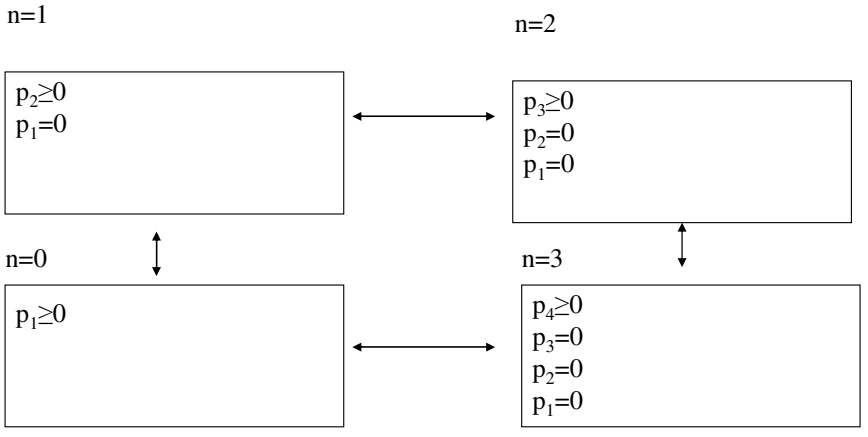

Fig. 8.2 Integrative closure for multi-scale entropy production

Any new level implies positive values for entropy production, at longer time scales.

A study correlating the Peirce's triadic framework of semiosis and the maximum entropy principle is due to Herrmann-Pillath (2010 a, b). It paves the way for a semiotic view of thermodynamics which is built on the idea that Peircean interpretants are systems of physical inference devices evolving under natural selection. In this view the principles of maximum entropy, maximum power and maximum entropy production work together to drive the emergence of information carrying structures, which at the same time maximize information capacity as well as the gradients of energy flows such that ultimately, the evolutionary process is seen to be a physical expression of the second law of thermodynamics.

The tetradic conceptual framework may also be correlated with the entropy variability considerations.

The starting point is that the tetradic structure involves the conjunction of four different kinds of causality: material, formal, efficient and final.

These causalities relate the different levels or realms of the tetradic framework (Fig. 8.3).

Fig. 8.3 correlates the integrative closure hypothesis to different entropy principles.

The observation that at successive levels successive derivatives of entropy became null suggests to associate, the principles of maximum entropy to mechanical causation, ME, and the principle of maximum production of entropy MEP, to the formal causation.

Material causation, extensively used in chemistry and biology is related in part, to what Peirce describes as firstness.

Formal causation is well described in 2nd order cybernetics.

Efficient causation manifests when the regularities and thirdness becomes significant for interactions through stable patterns.

Efficient causation is related in part, to what Peirce describes as secondness.

As the efficient causation we are looking for a principle of maximum production of entropy production, MPEP. This would be correlated to a third derivative of the entropy.

MPEP may be compared to Kauffman's tentative fourth law of thermodynamics (Kauffman S. 2000).

Kauffman proposed a tentative fourth law of thermodynamics, in which the workspace of the biosphere expands, on average, as fast as it can in this co constructing biosphere.

By as fast as it can, Kauffman means something like the edge of chaos. Faster than that, it cannot sustain itself. Slower, is not advantageous since if there is the possibility of going faster, the faster ones become selected.

The MPEP may be also be related to the maximization of the mutual information as studied by Sporns and Lungarella (2006).

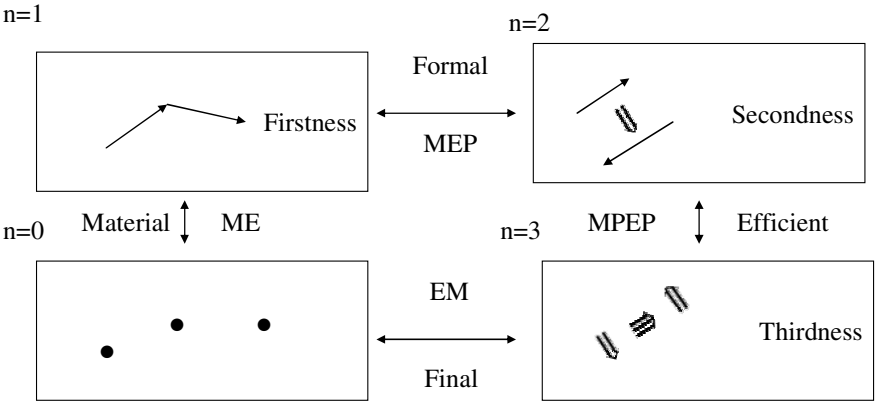

Fig. 8.3 Integrative closure and entropy principles

Sporns and Lungarella (2006) demonstrated how the maximization of the information structure of the sensory states experienced by embodied and situated agents might lead to the development of useful behavioral skills.

This suggests using informational distance, a kind of mutual information, to run MPEP calculus.

The final causation is the critical step for integrative closure.

A generic approach to derive fundamental candidates for systemic drives from properties of the integrative closure emphasizes the system as an entity that is able to select its actions (Klyubin et al. 2005, Polani 2009). It considers the informational channel capacity between the system's action at a given time and the sensory inputs at later time. Intuitively this is a measure to which extent the system's actions could potentially influence its system, in such a way that the

intensity of this influence can later be detected again by the system. This quantity, empowerment, measures the system's power to change the environment and to be aware that it did so. This can be formalized by measuring the maximal mutual information that can possibly be introduced into the environment by a suitable distribution of actions (Klyubin et al. 2005).

Capdepuy et al. (2007) demonstrated how a wide range of coordinated collective behaviors can be developed by having a population of agents situated in the same environment which adapt by maximizing their empowerment-an utility function that measures the information transfer between the action produced by an agent and the sensory states later experienced by the agent itself. The term empowerment refers to the fact that this measure encodes the perceived amount of influence or control that the agent has over its environment.

Such studies suggested to formulate an evolvability maximization, EM, criterion for n=3 step and integrative closure.

From Fig. 8.3 it can be observed that the level n=0 refers to states and for these, ME principle ensures entropy increasing.

The level n=1 refers to processes and for these MEP principle is a statement about possible trajectories and looks to the most typical trajectory. The 1-arrows associated to 1-categories are trajectories or paths.

The level n=2 refers to processes of processes. MPEP would govern the interaction between trajectories. The 2-arrows associated to 2-categories are ways of sweeping from one trajectory to the other.

The 3-arrows associated to 3-categories are defined between pairs of 2-arrows and consist of ways of interpolating between these sweepings from one trajectory to the other.

EM principle is related to final causation.

The final causation refers to the goal to be achieved by the system. This is the level where the goals are influencing the results. Embodiment and empowerment are necessary marks. Evolvability essentially measures the informational efficiency of the integrative closure.

Evolvability maximization, EM, principle can be interpreted in the following way: any evolvable system should poise itself in such a way as to be able to react in a most effective way to possible perturbations of its preferential state. The higher evolvability, the better is the possibility of the system to control perturbations. This corresponds to a kind of intelligent behavior, to self-organisatiom in integrative closure and creates systems with an interest to preserves their own organization. EM criteria goes beyond informational entropy.

The open problem is that one needs to identify beforehand the variables whose stabilization is necessary for the particular system.

8.5 Cooperative Model for Nerve Excitation

The entropy production for a non-equilibrium system originally initiated by biophysical and biochemical problems will be considered as a detailed example of model categorification.

To account for the selectivity of membrane transport one has developed the model concept of a membrane pore as a transport channel for different types of ions or molecules. The pore is a one-dimensional array of k stable sites for these kinds of ions or molecules. The state of a particle is determined, at time n, by means of a row vector $p(n)=(p_1(n),..., p_k(n))$ where $p_i(n)$ is the probability that the particle will be in the i-th stable site after n transitions. Denote by p_{ij} the one-step probability of transition from i to j, and by $P= (p_{ij})$, $1 \le i, j \le k$ the corresponding matrix of transition. The stochastic model of the process is:

$$p(n+1) = p(n)P \tag{8.36}$$

This model has applications in a variety of areas such as drug kinetics, pharmacology, intra-cellular transport, studies of metabolic systems, analysis of ecosystems, etc. A two-state model is the so-called Adam's cooperative model for nerve excitation (Schnakenberg 1977). In this model it is assumed that the axon membrane contains an irregular lattice of active centers. Each of the active centers is supposed to bind either the mono-valent K^+ ions (excited state 1) or a bivalent Ca^{2+} ion (ground state 2). Denote by $p_1(n)$ the probability for an active center to be in the excited state and by $p_2(n)=1-p_1(n)$ the probability of the ground state. In this case from (8.36) a difference equation results:

$$p_1(n+1) - p_1(n) = -p_{12}p_1(n) + p_{21}\, p_2(n) \tag{8.37}$$

To take into account the existence of different scales of time it is necessary to translate by model categorification the discrete time n to the expansion N:

$$N = n + \varepsilon w_1 n + ... + \varepsilon^M w_M n \tag{8.38}$$

with w_m, m=1,..., M, constants. The probabilities $p_i(n)$, i=1, 2 are translated to:

$$P_i(N) = p_i^0 + \varepsilon p_i^1(n) + ... + \varepsilon^M p_i^M(n) \tag{8.39}$$

The transition probabilities p_{ij} are translated by model categorification to:

$$P_{ij}(N) = p_{ij}^0 + \varepsilon p_{ij}^1(n) + ... + \varepsilon^M p_{ij}^M(n) \tag{8.40}$$

The difference equation (8.37) becomes by model categorification method the NA difference equation:

$$\frac{P_1(N) - P_1(N_1)}{(N - N_1)} = -P_{12}(N_1)P_1(N_1) + P_{21}(N_1)P_2(N_1) \tag{8.41}$$

Here $N \neq N_1$. It is considered that:

$$N = n + \varepsilon n + ... + \varepsilon^M n \ , \ N1 = (n-1) + \varepsilon(n-1) + ... + \varepsilon^M (n-1) \tag{8.42}$$

In the study of ion transport, nerve excitation, adhenosine triphosphate, ATP synthesis or other far from equilibrium phenomena the linearity may appear unrealistic and the transition probabilities, p_{ij} depends on $p_i(n)$, $1 \leq i \leq k$. Obviously the corresponding stochastic chain is in this case non-Markovian. In the cooperative model for nerve excitation, it was considered that the transition probabilities, or the rate constants, are functions of the concentrations of Ca^{2+} and of K^+ on both sides of the membrane. The cooperative mechanism is brought into play by the assumption that the transition probabilities for a certain active center to change from the ground to the excited state or inversely, depend on the states of the neighboring active centers at the time of the transition. The $Ca^{2+}(K^+)$ ion bound to a certain center in the ground (excited) state receives an additional binding energy for each neighboring center that is in the ground (excited) state. According to this it is supposed that:

$$p_{12}(n)=k_1(1-k_2p_1(n)); \qquad p_{21}(n)=k_3(1-k_4p_2(n)) \tag{8.43}$$

Here $0 < k_i < 1$, $i = 1, 2, 3, 4$ are constants. In the NA frame, the transition probabilities p_{ij} result by translating $p_i(n)$ to $P_i(N)$ that is:

$$P_{12}(N) = k_1(1 - k_2P_1(N)) \tag{8.44}$$

$$P_{21}(N) = k_3(1 - k_4P_2(N)) \tag{8.45}$$

The informational entropy associated to a stochastic model as (8.36) is:

$$S(N) = -\sum_i P_i(N) \ln P_i(N) \tag{8.46}$$

By model categorification the NA discrete entropy is defined by:
S(N) is the expansion:

$$S(N) = s_0(n) + \varepsilon s_1 n + ... + \varepsilon^M s_M(n) \tag{8.47}$$

In the case of a two-state model as the Adam's cooperative model of nerve excitation and of two timescales it results from (8.46) by equating the coefficients of different ε:powers of

$$s_0(n) = -(p_1^0 \ln p_1^0 + p_2^0 \ln p_2^0) \tag{8.48}$$

$$s_1(n) = -(p_1^1 \ln p_1^1 + p_2^1 \ln p_2^1) - (p_1^1 + p_2^1) \tag{8.49}$$

It results:

$$p_1^0(n) = p_1^0(n-1) - k_1(1 - k_2 p_1^0(n-1))p_1^0(n-1) + k_3(1 - k_4 p_2^0(n-1))p_2^0(n-1) \tag{8.50}$$

$$\begin{aligned} p_1^1(n) &= p_1^1(n-1) - k_1 k_2 p_1^1(n-1)p_1^0(n-1) - \\ &- k_3 k_4 p_2^1(n-1)p_2^0(n-1) + k_1(1 - k_2 p_1^0(n-1))(p_1^1(n-1) + p_1^0(n-1)) + \\ &+ k_3(1 - k_4 p_2^0(n-1))(p_2^1(n-1) + p_2^0(n+1)) \end{aligned} \tag{8.51}$$

The variation of the NA entropy S(N) in NA time is:

$$\frac{S(N) - S(N_1)}{(N - N_1)} = \left[s_0(n) - s_0(n-1), \ldots, (s_M(n) - s_M(n-1) - (s_{M-1}(n) - s_{M-1}(n-1))\right] \tag{8.52}$$

N and N_1 are given by (8.42). In the particular example considered, the zero-th order level M=0, is not of necessity the equilibrium one. Different numerical simulations outlined that after a certain period of time the variation of $s_0(n)$ becomes extinguished.

References

Aoki, I.: Entropy production in living systems: from organisms to ecosystems. Thermochimica Acta. 250, 359–370 (1995)

Capdepuy, P., Polani, D., Nehaniv, C.: Maximization of potential information flow as a universal utility for collective behavior. In: Proceeding of the 2007 IEEE Symposium on Artificial Life (CI-ALife 2007), pp. 207–213. IEEE Press, Piscataway (2007)

Desvillettes, L., Villani, C.: On the trend to global equilibrium for spatially inhomogeneous kinetic systems: the Boltzmann equation. Invent. Math. 159(2), 245–316 (2005)

Dewar, R.C.: Informational theory explanation of the fluctuation theorem, maximum entropy production, and self-organized criticality in non-equilibrium stationary states. J. Phys. A 36, 631–641 (2003)

Glansdorff, P., Prigogine, I.: Structure Stabilité et Fluctuation. Masson et Cie, Paris (1971)

Herrmann-Pillath, C.: Entropy, Function and Evolution: Naturalizing Peirceian Semiosis. Entropy 12, 197–242 (2010)

Herrmann-Pillath, C.: Rethinking Evolution, Entropy and Economics: A triadic conceptual framework for the Maximum Entropy Principle as applied on the growth of knowledge. In: Aussschuβ fur Evolutorische Okonomik, Linz, Austria (2010)

Hiernaux, J., Babloyantz, A.: Dissipation in Embryogenesis. J. Non-Equilib.Thermodyn. 1, 33–37 (1976)

Iordache, O., Frangopol, P.T.: Relaxations in biophysical systems. Rev. Roum. Phys. 33, 1159–1162 (1988b)

Iordache, O., Frangopol, P.T.: The production of entropy and the stability of biosystems with many timescales. Rev. Roum. Biochim. 25, 325–328 (1988c)

Iordache, O., Frangopol, P.T.: Nonarchimedean formalism for entropy balance in biosystems. Rev. Roum. Phys. 34, 217–227 (1989)

Jaynes, E.T.: Information Theory and Statistical Mechanics. Phys. Rev. 106, 620–630 (1957)

Kauffman, S.: Investigations. Oxford University Press, Oxford (2000)

Klyubin, A.S., Polani, D., Nehaniv, C.L.: Empowerment: A universal agent-centric measure of control. In: Proc. IEEE Congress of Evolutionary Computation (CEC 2005), Edinburgh, UK, pp. 128–135 (2005)

Lurie, D., Wagensberg, J.: Entropy balance in biological development and heat dissipation in embryogenesis. J. Non-Equilib. Thermodyn. 4, 127–130 (1979)

Neder, L.: Modell einer Differentialrechnng mit aktual unendlich kleinen Grossen erster Ordnung. Math. Annalen. 118(2), 251–262 (1941)

Neder, L.: Model einer Leibnizischen Differentialrechnung mit aktual unendlich kleiner Grossen samtlicher Ordnungen. Math. Annalen. 118(5), 718–732 (1943)

Nicolis, G., Prigogine, I.: Exploring Complexity. An Introduction. Freeman, New York (1989)

Polani, D.: Information: currency of life? HFSP Journal 3(5), 307–316 (2009)

Prigogine, I.: From being to becoming. Time and complexity in the physical sciences. Freeman, San Francisco (1980)

Prigogine, I.: What is Entropy. Naturwissenschaften 76, 1–8 (1989)

Salthe, S.: Infodynamics, a developmental framework for ecology/economics. Conservation Ecology (2003)

Schnakenberg, L.: Thermodynamic Network Analysis of Biological Systems. Springer, Berlin (1977)

Sporns, O., Lungarella, M.: Evolving coordinated behavior by maximizing information structure. In: Rocha, L.M., Yaeger, L.S., Bedau, M.A., Floreano, D., Goldstone, R.L., Vespignani, A. (eds.) Artificial life X, Proccedings of the Tenth International Conference on the simulation and Synthesis of Living Systems, pp. 323–329. MIT Press, Cambridge (2006)

Chapter 9
Formal Concept Analysis

Abstract. Formal concept analysis identifies conceptual structures among data sets. Multi-level modeling potentialities in formal concept analysis are highlighted.

Triadic formal concept analysis is related to Peirce's categories.

Rough sets approximations and hierarchical class analysis are applied for separation schemes. A tetradic formal concept analysis is presented as general PSM framework.

Case studies refer to separation lattices flow-sheets, drugs mixtures formulation, security for information technology, reliability management systems and failure analysis for printed circuits.

9.1 Galois Lattices

The formal concept analysis, FCA, is a theory of data analysis which identifies conceptual structures among data sets (Ganter and Wille 1999).

The main goal of FCA has been the support of rational communication and the representation and processing of knowledge based on the so called restructuring program (Wille 1996a). The program of restructuring has a philosophical background which goes back to the pragmatism of Peirce. Lattice theory is reworked in order to integrate and rationalize origins, connections to and interpretations in the real world. The potential connection between restructuring goals and integrative closure is significant.

A strong feature of FCA is its capability of producing graphical visualizations of the inherent structures among data.

The FCA plays a prominent role in conceptual modeling by combining the ease of handling data base object that are defined via a list of properties to a mathematical model rooted in a formalization of logic by which reasoning is based on communicative rationality in the sense of pragmatism.

In FCA the concept understanding is considered as the basic unit of thought. A particular concept has both an extension and an intension.

FCA supposes that some relation between objects and properties is already established in the form of a context F= (G, M, I) where G is the set of objects, M is the set of properties or attributes and I $\subseteq$ G x M is the incidence relation between objects and properties (Ganter and Wille 1999).

A formal context F can best be represented by a table specifying which objects fall under which properties. This suggests that a context may be associated to classification purposes.

For a set of objects A$\subseteq$ G, we can define all the properties shared by all objects, provided a context F is given:

$A' = \{m \in M \mid \forall\, g \in A: (g, m) \in I\}$

These are the common properties of A

Similarly the dual operation can be defined provided a property set B $\subseteq$ M is given:

$B' = \{g \in G \mid \forall\, m \in B: (g, m) \in I\}$

These are the common objects of B.

Assume a context F= (G, M, I) is given. A formal concept of F is defined as a pair (A, B) where A$\subseteq$ G (called extent) and B$\subseteq$ M (called intent), A′=B and B′=A.

Given a context F = (G, M, I) the collection of all formal concepts $\mathcal{B}$(G, M, I) forms a complete Galois lattice, GL, where the partial order $\leq$ is defined by (A1, B1) $\leq$ (A2, B2) iff A1$\subseteq$A2 (which is equivalent to B1 $\supseteq$B2). The supremum and the infimum are defined as follows:

$$\bigvee_{t \in T} (A_t, B_t) = ((\bigcup_{t \in T} A_t)'', \bigcap_{t \in T} B_t)$$

$$\bigwedge_{t \in T} (A_t, B_t) = (\bigcap_{t \in T} A_t), (\bigcup_{t \in T} B_t)'')$$

From an abstract point of view the complete lattice $\mathcal{B}$ (G, M, I) may be interpreted as a category. The operation denoted by: " can be interpreted as a closure operator on both sides the object level, G and the attribute level, M.

The closure operation induces a complete lattice and the concept lattice corresponds to a Galois-connection between two closure operators.

A concept lattice $\mathcal{B}$(G, M, I) determines a hierarchy of formal concepts.
This hierarchy can be used to perform inferences with respect to properties of concepts or with respect to extensions of concepts.

9.2 Separation Lattice

Classification methods have been applied in chemical engineering for separation flow-sheet generation. Similarity based clustering method and informational criteria allow generating flow-sheets on the bases of properties allowing separation (Iordache et al. 1993a, Iordache et al. 1993b). Obviously, GL methodology can be applied for the same problems.

The GL allows outlining the chemical compound separation schemes and also the properties related to the separation devices.

Studies correlating FCA and classifications are numerous.

A comparison between similarity-based clustering and GL methods is done by Valtchev and Missaoui (2000).

Two interesting adaptations of FCA that allow the systematic analysis of drugs structure-activity and structure-selectivity relationship have been studied by Lounkine and Bajorath (2010). Fragment FCA assesses the distribution of molecular fragment combinations among ligands with closely related biological targets. Molecular FCA was introduced for the systematic comparison of the selectivity of a compound against multiple targets and the extraction of compounds with complex selectivity profiles from biologically annotated databases.

Our starting point for GL applications are tables as Table 9.1 that contain objects-in our case chemical compound and properties (Iordache et al. 1993 a, Iordache et al. 1993 b).

Table 9.1 shows the isomers properties volatility, magnetic dipole, freezing point, and diameter for different compounds.

Table 9.2 contains the same information as Table 9.1 in normalized form. We use "1" for high values and "0" for low values relative to the mean value in any column.

Typically network data take the form of a rectangular table, in this case component by property, a kind of binary adjacency matrix.

A cell entry is 1 if and only if the there exists a relation between that component and the property.

The set of objects G consists of the components 1, 2, 3 and 4 whereas the set of properties M consists of volatility, magnetic dipole, freezing point, and diameter.

Table 9.1 Input information-isomers properties

Data	Name	Volatility	Dipole, D	Freezing Point, K	Maximum Diam., Å
1	m-xylene	1.6	0.4	225.4	8.33
2	o-xylene	1	0.6	248.1	7.8
3	p-xylene	1.63	0.0	286.6	8.67
4	ethyl benzene	1.73	0.58	178.4	9.00

D-Debye, K-Kelvin degrees, Å-Angstrom

Table 9.2 Formal context: components and properties

Component	Volatility	Dipole	Freezing Point	Diameter
1	1	1	0	0
2	0	1	1	0
3	1	0	1	1
4	1	1	0	1

For Table 9.2, “1” denotes the high values, while “0” denotes the low values of the property.

To such tables a G L may be associated Ganter and Wille (1999).

Table 9.3 shows an example of formal context with the set of objects G= {1, 2,…,6} and the set of properties M={a, b, …,d}. In this case the objects are chemical compounds. The properties shows high,”1” or low “0” values of the corresponding properties.

To any property a separation apparatus is associated. If the property a, is the volatility the a-separation device is a distillation column, if the property b, is a solubility difference due to magnetic dipole, then b-separation device may be an absorber. If the property c, is a freezing point, then the c-separation may be done by a crystallizer.

Table 9.3 Formal context for separations-four properties

Components	a	b	c	d
1	1	0	1	1
2	1	0	0	1
3	1	0	0	0
4	0	1	1	1
5	0	1	0	0
6	0	1	0	1

Fig. 9.1 shows the GL for separation based on four properties.

Fig. 9.1 shows the GL associated to data presented in Table 9.3.

At the bottom is the union of all components. The null symbol Φ indicates that no property was activated to induce separations.

Each marked points in GL is labeled with both the components and the properties that define it.

Above and to the right of the diagram we can see that the compound 4 resulted in the light phase from the separating devices corresponding to b, d, and c.

To the left of the diagram we see that the compound 1 was separated by the separating devices corresponding to a, d and c.

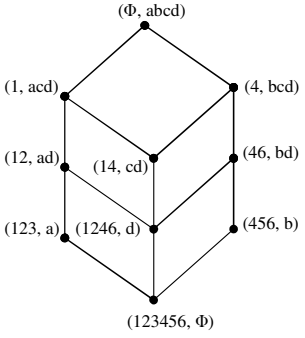

Fig. 9.1 Galois lattice for separation-four properties

As we move up, on a trajectory, we encounter smaller collections of compounds and larger collection of properties that is of separating devices.

At the top of the diagram we see that there are no compounds having all the properties.

Fig. 9.1 shows that there exists a path from the entire mixture to the component "4" making use of the sequence of properties first b, then d and then c and there exists a path from the entire mixture to the component "1" making use of the sequence of properties first a, then d and then c.

In practice it may be easier to make use of a lattice in which the labeling is reduced.

Each point is labeled only with the names of components for which it is the least element containing those components. Similarly each point gets the name of any properties for which it is the greatest element containing those properties. Points not being in these situations remain unlabelled.

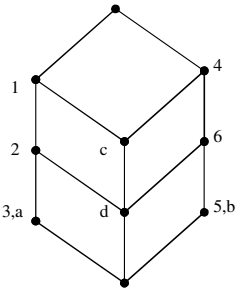

Fig. 9.2 Galois lattice for separation-reduced labeling

Fig. 9.2 shows reduced labeling for GL. This figure helps to visualize the points were every component may be collected.

9.3 Drugs Mixture

For a mixture of drugs it is possible to visualize by FCA the relation between properties and components of the mixture.

Mixtures of anesthetics will be the considered example.

The properties for anesthetics refer to their composition. The lipophilic portion, denoted by Li, the hydrophilic portion, denoted by Hy, the intermediate chain, denoted by Ch, and the number of nitrogen, N atoms, denoted by Nn are the properties considered here.

The associated vector is abbreviated as: <Li, Hy, Ch, Nn>

The procaine was selected as the reference drug.

Fig. 9.3 shows the structural formula of procaine.

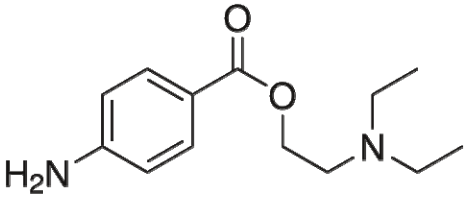

Fig. 9.3 Procaine

For procaine, the lipophilic portion is a phenyl radical, the hydrophilic portion is an amine, the intermediate chain is an ester, and there are two N atoms. The vector associated to procaine will be: <1111>.

Table 9.4 contains the vector associated to four anesthetics.

Table 9.4 Properties of drugs

	Drug	Li	Hy	Ch	Nn	Vector
1	Benzocaine	1	0	1	0	<1010>
2	Lidocaine	1	1	0	1	<1101>
3	Butamben	1	0	1	0	<1010>
4	Dimethisoquin	0	1	0	1	<0101>

Fig. 9.4 shows the GL for composed drugs associated to Table 9.4.

It offers a visualization of the step by step involvement of different properties.

This corresponds to the trajectories followed by the mixture of drugs in the GL. The trajectories or the paths correspond to the 1-categories level.

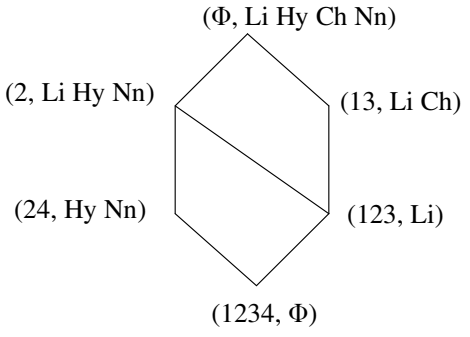

Fig. 9.4 Galois lattice for composed drugs

Suppose that the compound drug (1234) encounter a barrier were the lipophilic character of the phenyl is necessary. This step will select the mixture (123) of components 1, 2 and 3 that are benzocaine lidocaine and butamben. If in the next step a condition concerning the chain, Ch is imposed only the mixture (13) will be able to pass and so on.

If a condition of hydrophilic portion and number of nitrogen agents is imposed only the component 2 that is lidocaine would be able to meet the requirements.

For another trajectory we suppose that the compound drug encounter a barrier were the hydrophilic character of the amine and the number of nitrogen atoms is imposed. This step will select the components 2 and 4, that is, lidocaine and dimethisoquin. Then if the lipophilic character is imposed, only the component 2 is capable to fill the request.

Observe that the GL may be interpreted as a traveler for different drugs of the mixture.

In different stages some properties are necessary to allow drug transition to the next step.

This traveler should be correlated to pharmakinetic studies and this represents a significant advantage of the FCA method. Fig. 9.4 shows the possibility of transition from a trajectory to another. The associated 2-categories describe ways of sweeping from one trajectory to the other.

9.4 Failure Analysis

Failure analysis, diagnosis represents another domain of application for GL.

The electroplating voids for printed circuits fabrication is the considered example (Iordache 2009).

Plating voids is the term used to define discontinuities in electroplated through hole for copper or other metals. Table 9.5 shows the voiding failure mode and the processing steps that may be responsible for that type of voiding.

The printed circuit board processing steps that may be the source of electroplating voiding are:

p1-Mechanical
p2-Deburring-Desmear
p3-Ellectroless
p4-Dry Film
p5-Electroplating and Etching

The probable void types are established by cross-sections since to different source of voiding correspond specific patterns. Notice that several steps as failure roots may corresponds to any type of voids.

We use “1” for high probability and “0” for low probability of step process involvement. These probabilities may be based on case based knowledge.

Fig. 9.5 shows the GL associated to failure analysis from Table 9.5.

Table 9.5 associating plating voids type to different processing steps is base on failure analysis expertise.

In this case the objects are the void types denoted here by: PH, DR, WE, EL, RE, GL, TA, RM, FP, FL, EP, EO, and RG.

The attributes are the step processes: p1, p2, p3, p4 and p5.

Table 9.5 Plating voids type for different processing steps

Void type	Notation	p1	p2	p3	p4	p5
Plug Hole	PH	1	0	0	0	0
Drill	DR	0	0	0	0	0
Wedge	WE	1	1	1	0	0
Electroless	EL	1	1	0	0	0
Resin	RE	1	1	1	0	0
Glass	GL	0	1	1	0	0
Taper	TA	0	0	1	0	0
Rim	RM	0	0	0	1	0
DF plug	FP	0	0	0	1	1
DF lock-in	FL	0	0	0	1	1
Electroplating	EP	0	0	0	1	1
Etch out	EO	0	1	1	0	0
Ring	RG	0	0	0	0	1

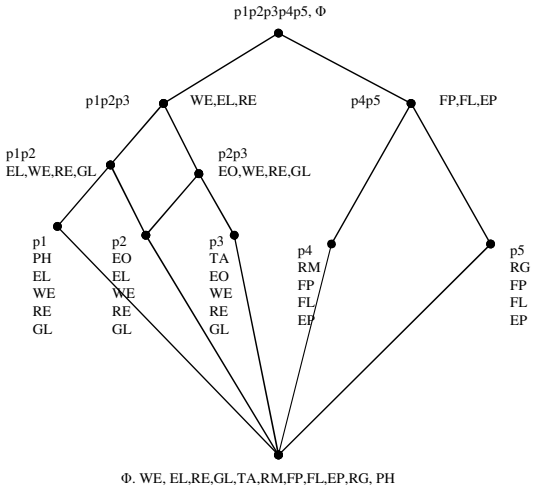

Fig. 9.5 Galois lattice for failure analysis

At the bottom of the lattice is the union of all type of voids.

At the top is the union of all processing steps.

Each marked points in GL is labeled with both the void types and the process step that define it.

The GL outlines the two main classes of processes contributing to voids (p1, p2, p3) and (p4, p5).

As we move up in the GL, we encounter smaller collections of voids types and larger collection of process steps as potential contributors.

9.5 Triadic Context Analysis

The FCA methods have been extended to complex types of knowledge representations.

One of these extensions is that for multiple contexts (Wille 1995, Wille 1996b).

Inspired by the pragmatism of Peirce with its three universal categories, firstness, secondeness and thirdness, Lehmann and Willie (1995) initiated research on concept trillatice and their visualization in triadic diagrams.

A triadic concept is defined as a quadruple (G, M, B, Y) were G, M and B are sets and Y is a ternary relation between G, M and B that is $Y \subseteq GxMxB$. The elements of G, M and B are called formal objects, attributes and conditions. An element $(g, m, b) \in Y$ is read as follows: the object $g \in G$, has the attribute $m \in M$ under the condition $b \in B$.

Formal objects, attributes and conditions, in the triadic context are in the role of the corresponding Peircean categories.

For theoretical developments and comparison with categorical approach it is convenient to use notations K1, K2, and K3 instead of G, M, and B. These alternative symbols indicate that the elements of Ki, i=1, 2 or 3, are seen in the role of the Peirce's i-th category, that is firsteness, secondeness, and thirdeness.

Obviously the elements of the single GL may be associated to that of general PSM framework.

We may identify the objects or components as K1, that is G=K1, and the properties or attributes as K2, that is M=K2.

To every pair (k1, k2), k1∈ K1 and k2∈ K2 one associates a number {0, 1}.

The operator U21: K2→ K1, maps attributes into objects.

The possibilities P12: K1→ K2, maps objects into attributes.

U21 and P12 are adjoint functors.

Lehmann and Wille (1995) elaborated a visualization of the concept trillatice in triadic diagrams. Stumme (2005) discuss how traditional line diagrams of dyadic concept lattices can be used for exploring triadic data. A data cube may be of use to present triadic contexts a (K1, K2, K3, Y).

There exist several applications of the triadic contexts but only little visualization of rather small concept trillatice. This is probably due to the complex structure of existing diagrams.

Table 9.6 shows an elementary type of triadic context, the so-called triadic power set contexts (Lehmann and Wille 1995).

In this case K1 = K2 = K3 = {1, 2, 3}.

Table 9.6 Triadic power set context

K3	1			2			3		
K1\K2	1	2	3	1	2	3	1	2	3
1		x	x	x	x	x	x	x	x
2	x	x	x	x		x	x	x	x
3	x	x	x	x	x	x	x	x	

In this table rows represents objects, K1, the columns represent attributes K2 and the sub tables represents the conditions K3.

The triadic diagram is shown in Fig.9.5. To outline the notation principle the positions are indicated here. The value 3 for K3, the value 1 for K2 and the value 2 for K1 correspond to the point 312.

Fig. 9.6 shows the power set trillatice for triadic power set context.

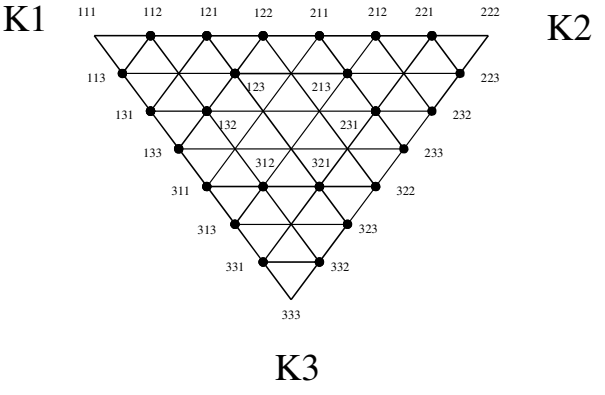

Fig. 9.6 Trillatice for triadic power set context

Fig. 9.6 shows as points the elements of the so-called Sierpinski gasket.

This result may be correlated to Galois field logical diagrams (Popel and Dani 2002).

Triadic lattices as shown in Fig. 9.6 are considered as basic elements of formal context analysis.

The modal understanding of necessity and possibility occurs naturally in triadic contexts (Dau and Wille 2001).

Modal points of views are involved in the study of rough set approximations and hierarchy class analysis (Pawlak 1982, Chen and Yao 2005).

9.6 Rough Set Approximations

The modal understanding of propositions has been correlated to the notion of possible worlds. The basic idea of modal semantics is that a proposition is necessarily true if it is true in all accessible possible worlds and possibly true if it is true in some accessible possible world.

Dau and Wille (2001) considered particular triadic concepts in which K1 represents the objects, K2 the attributes or properties while K3 represents a modus. They considered two types of contexts: the □-context corresponding to necessity and ◊-context corresponding to possibility.

FCA and rough set theory provide two related methods for data analysis (Yao 2004).

They study and model the notion of concepts from different perspectives.

Their correlation and contribution for data understanding will be illustrated by another example of GL for separation.

Let us consider the data from Table 9.7. This shows the formal context for separations-five properties. The properties indexed by {a, b, c, d, e} may be significant or not for the components 1 to 6.

Table 9.7 Formal context for separations-five properties

Component	a	b	c	d	e
1	1	0	1	1	1
2	1	0	1	0	0
3	0	1	0	0	1
4	0	1	0	0	1
5	1	0	0	0	0
6	1	1	0	0	1

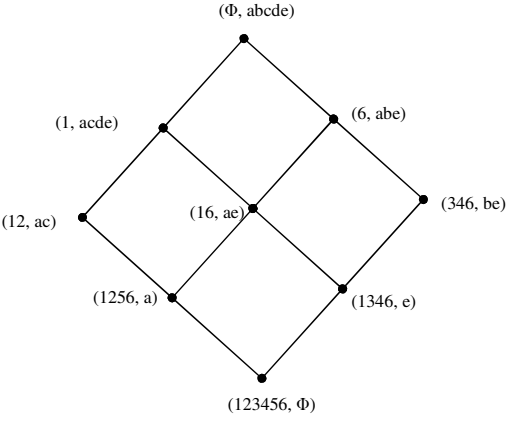

Fig. 9.7 Galois lattice for separation-five properties

The associated GL is shown in Fig. 9.7. It corresponds to separation based on five properties.

Supplementary information about the separation methods associated FCA may be obtained on the basis of approximation operators.

For a formal context (U, V, R), for a pair of elements $x \in U$ and $y \in V$ if $(x, y) \in R$ also written as xRy, we say that x has the property y or equivalently the property y is possessed by the object x. The binary relation can be equivalently expressed in two forms An object $x \in U$ has the set of properties:

$$xR = \{y \in V \mid xRy\} \subseteq V$$

A property y is possessed by the set of objects:

$$Ry = \{x \in U \mid xRy\} \subseteq U$$

Yao (2004) defined the approximation operators:

$$X^{\square} = \{y \in V \mid Ry \subseteq X\} \quad , X^{\Diamond} = \cup_{x \in X} xR \quad , Y^{\square} = \{x \in U \mid xR \subseteq Y\} \quad , Y^{\Diamond} = \cup_{y \in Y} Ry$$

Yao considered object oriented GL, OOGL, property oriented GL, POGL, and complement oriented GL, COGL.

A pair (X, Y), $X \subseteq U, Y \subseteq V$ is called an object oriented formal concept if $X= Y^{\Diamond}$ and $Y= X^{\square}$. If an object has a property in Y then the object belongs to X. Furthermore, only objects in X have properties in Y. This characterizes OOGL.

A pair (X, Y), $X \subseteq U, Y \subseteq V$ is called a property oriented formal concept if $X= Y^{\square}$ and $Y= X^{\Diamond}$. If a property is possessed by an object in X then the property must be in Y. Furthermore, only properties Y are possessed by objects in X. This characterizes POGL. Fig. 9.8 shows the oriented context lattice OOGL and property oriented lattice POGL associated to the data from Table 9.7. The COGL is the GL to the complement of Table 9.7. The complement is obtained replacing "0" by "1" and inversely "1" by "0" in the Table 9.7.

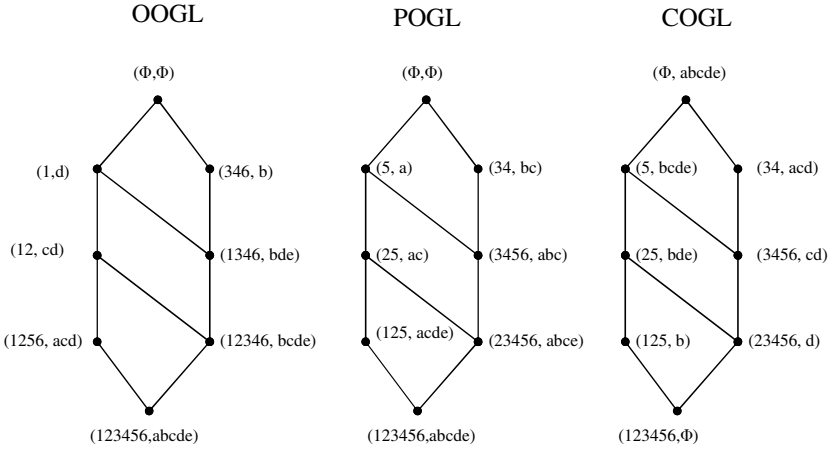

Fig. 9.8 Oriented formal contexts

An important difference between the oriented concepts and formal concepts of FCA is that the first use disjunction that is parallel ways, in forming a condition while the last one uses conjunction that is series ways.

Each of them captures a particular aspect of knowledge embedded in a formal concept.

The oriented formal contexts offer separation scheme in which supplementary conditions should be verified. POGL corresponds to a modern request in formulations were the query refers to properties rather than the traditional query for composition.

The COGL scheme describes separations as that described by the standard schemes but instead of light phase the heavy phase is of interest.

9.7 Hierarchical Class Analysis

Practical methods to analyze triadic contexts may be based on hierarchical class analysis, HCA coupled to FCA (Chen and Yao, 2005, Hwang and Kang, 2007).

HCA is a set of theoretical cluster analysis technique.

To illustrate HCA we consider the dyadic formal context shown in Table 9.8.

Table 9.8 Dyadic formal context

K1\K2	a	b	c	d	e
1	0	1	1	1	0
2	1	1	1	1	0
3	1	1	1	1	0
4	1	0	0	1	0
5	0	1	1	1	1
6	0	0	0	1	1
7	1	1	1	1	1

Table 9.8 corresponds to the objects K1 = {1, 2,...,7} the properties K2 = {a, b, c, d, e} and some relations I between them. For the set $G \subseteq K1$ of objects and a set $M \subseteq K2$ of properties, two derivation operators, intent and extent are given by: Int (G) and Ext (M).

Intuitively, Int (G) is the set of properties common to all objects in $G \subseteq K1$.

Dually, Ext (M) is the set of objects that have all the attributes from $M \subseteq K2$

For example Int ({1, 2, 3})={b,c,d} and Ext ({b,c,d})={1, 2,3,5,7}.Given two objects 1, 2∈ K1, 1 and 2 are equivalent if Int ({1}) = Int ({2}). Correspondingly an equivalence relation may be established in K2 considering the definition: a and b are equivalent if Ext ({a}) = Ext ({b}). The hierarchical structures of the classes from Table 9.8 are shown in Fig. 9.9. Fig. 9.9 highlights the hierarchical structure of classes for dyadic context.

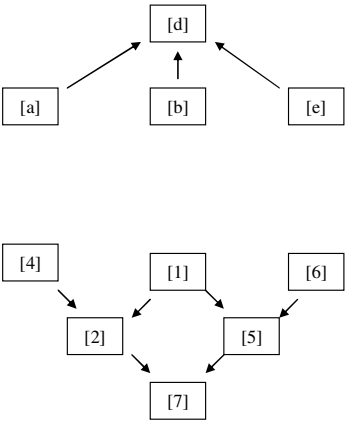

Fig. 9.9 Hierarchical structure of classes for dyadic context

The open problem is to visualize the triadic context situations.
We may consider the data from Table 9.9, as an example of triadic context.
In this case K1 = {1, 2,..,7}, K2 = {a, b, c,d,e}, and K3 = {A, B, C}.
The new considered level corresponds to conditions.

Table 9.9 Triadic context

K3	A					B					C				
K1\K2	a	b	c	d	e	a	b	c	d	e	a	b	c	d	e
1	0	1	1	1	0	0	1	1	1	0	0	1	1	1	0
2	0	1	1	1	0	1	1	1	1	0	1	1	1	1	0
3	0	1	1	1	0	1	1	1	1	0	1	1	1	1	0
4	0	0	0	0	0	1	0	0	1	0	1	0	0	1	0
5	0	1	1	1	1	0	1	1	1	1	0	1	1	1	0
6	0	0	0	1	1	0	0	0	1	1	0	0	0	0	0
7	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

In a separation study A, B, C may correspond to ambient conditions as changed during the day. Variations in K3 may change the properties values and the ranking of component for different properties.

Fig. 9.10 shows how the K1 object hierarchical classification is related to K2 properties hierarchy.

The connection is mediated by K3.

Fig. 9.10 outlines the triadic class hierarchy.

Fig. 9.10 shows that there exists a path from component class [2] to properties class [a] via the conditions [B], [C]. K3 intermediates between K1 and K2 allowing the closure between K1, K2 and K3.

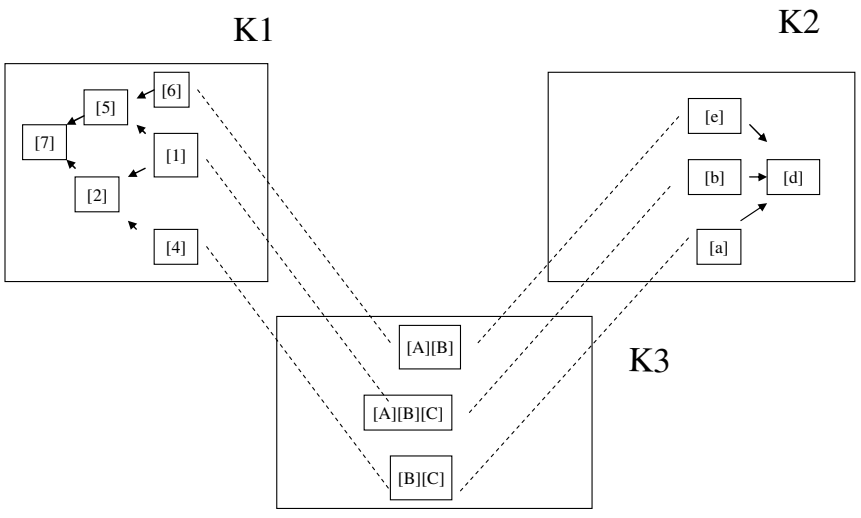

Fig. 9.10 Triadic classes hierarchy study

9.8 Tetradic Context Analysis

Observe that previously discussed FCA studies refer to formal contexts only. This means that K1, K2 and K3 are formal domains.

As shown in Chapter 4, the integrative closure hypothesis requires that the formal contexts are completed with the natural or real context denoted by S or K0.

Completing the Peirce's triadic approach, S is supposed to have a formal signification as that associated to K1, K2 and K3.

For integrative closure hypothesis, to any general PSM framework containing S, K1, K2 and K3 we may associate a tetradic context (S, K1, K2, K3, Y) denoted also by (K0, K1, K2, K3, Y).

A tetradic concept is the quintuple (S, K1, K2, K3, Y) where S, K1, K2 and K3 are sets and Y is a quaternary relation between S, K1, K2 and K3 that is $Y \subseteq S \times K1 \times K2 \times K3$. The elements of S, K1, K2 and K3 are called real states, formal objects, attributes and conditions. An element $(s, k1, k2, k3) \in Y$ is read: for the real state $s=k0 \in K0$, the object $k1 \in K1$, has the attribute $k2 \in K2$ under the condition $k3 \in K3$.

Recall that a concept is a pair of sets: a set of elements (extent) and a set of properties (intent) as (k1, k2) for example. We may define the hierarchy of context considering k1 as an extent relative to k2 and k2 as an intent relative to k1. In the same way k3 appear as intent relative to k2.

The time variations may be useful to visualize tetradic contexts (S, K1, K2, K3, Y) and integrative closure hypothesis.

Table 9.10 shows a segment of an elementary type of tetradic context, the so-called tetradic power set contexts. In this case K0 = K1 = K2 = K3 = {0, 1, 2, 3}.

In this table rows represents real objects, K0, the columns represent formal objects K1 the sub tables represents the formal attributes K2 and the tables represents the formal conditions K3. Only the value "0" of K3 was figured.

Fig. 9.11 illustrates the power set tetralattice for tetradic power set context.

Table 9.10 Tetradic power set context (partial data)

K3	0															
K2	0				1				2				3			
K0\K1	0	1	2	3	0	1	2	3	0	1	2	3	0	1	2	3
0		x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
1	x	x	x	x	x		x	x	x	x	x	x	x	x	x	x
2	x	x	x	x	x	x	x	x	x	x		x	x	x	x	x
3	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	

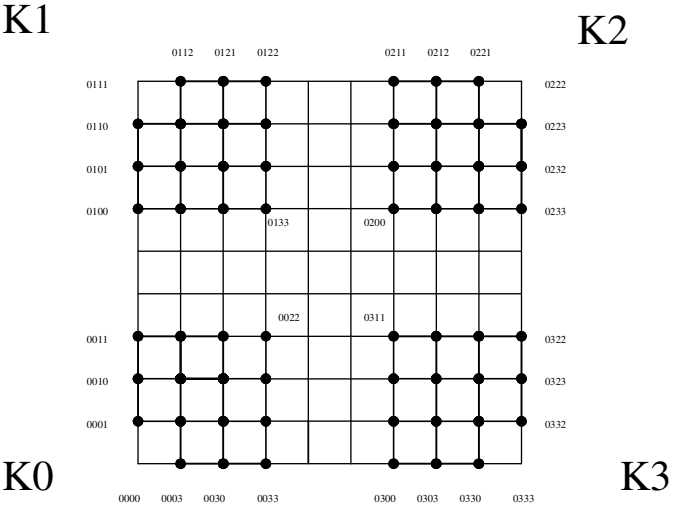

Fig. 9.11 Tetralattice for tetradic power set context

Fig. 9.11 shows as points the elements of one type of Sierpinski carpet. The complete Sierpinski carpet would correspond to a completed Table 9.10.

Visualizations for tetradic GL are complex.

A possibility is to decompose the tetradic lattices in triadic lattices.

Fig. 9.12 clarifies the integrative closure features for tetradic lattice.

Fig. 9.12 outlines the different concept contexts and the integrative closure hypothesis.

The associated Peirce's categories are indicated.

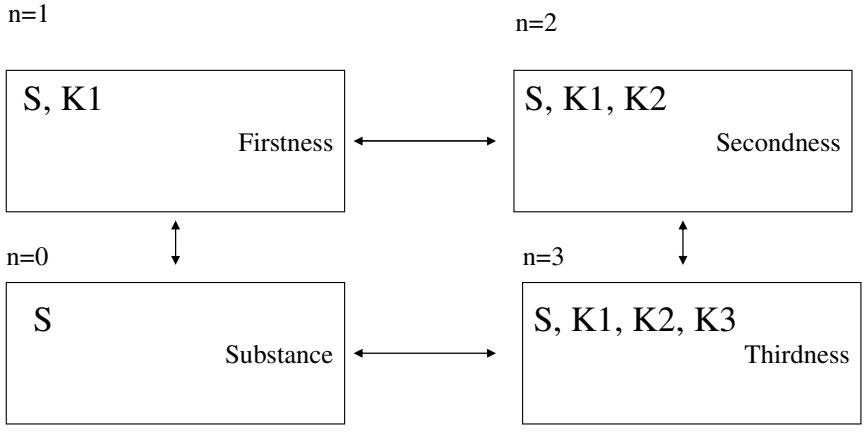

Fig. 9.12 Integrative closure for tetradic lattice

It is considered that each new module depends and embeds the previous ones as happens in the general categorification process.

9.9 Security Management Architectures

A four-level categorical approach for security of distribution information systems was presented by Sisiaridis et al. (2008).

Fig. 9.13 shows a four realms network for security of information systems.

The four levels correspond to Data, Schema, Construct and Concept (Fig. 9.13).

The improvement is representing by the integrative closure hypothesis allowing the emergence and autonomous testing of new concepts.

Restricting the levels interactions to the operators U10, U21, U32 leave the choice of control to the users and are appropriate for low-level security risks. The bottom-up approach, emphasizing the possibilities P01, P12 and P23 allows risk analysis and are more suited to high level security risks.

The signification of the functors U and possibilities P is explicit from Fig. 9.13.

U10, U21, U32 and U30 corresponds to implementation operations.

Observe that: U10: K1-Schema→S-Data, U21:K2-Constructs→K1-Schema,

U32: K3-Concepts→K2-Constructs, and U30: K3-Concepts→S- Data.

P01, P12, P23 and P03 are synthesis steps.

P01: S-Data→K1- Schema, P12: K1-Schema→K2-Constructs, P23: K2-Constructs→ K3-Concepts, and P03: S-Data→K3-Concepts

Fig. 9.13 emphasizes the role of integrative closure hypothesis via U30 and P03. This interconnection may make the system quite evolvable and autonomous.

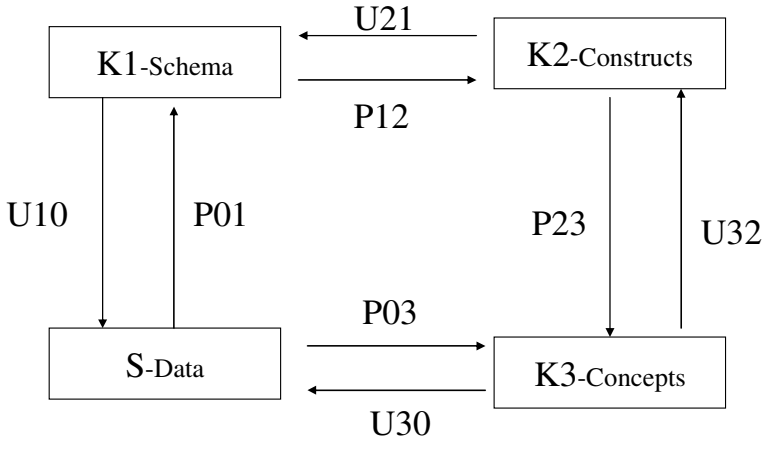

Fig. 9.13 Four realms network for security of information systems

The link via U30 and P03 may be established by implementing organic computing. In a case of failure analysis and self-healing, as sensors are installed on a device, the information can be automatically captured during preventive maintenance. It may be possible to broaden the range of environmental and device information captured and transmitted automatically. Organic computing methods may facilitate information capture and failure analysis tasks.

Another example of evolved failure analysis making use of the four-level architectures is shown in Fig. 9.14. Fig. 9.14 illustrates a four realms network for failure diagnosis (Rayudu et al. 2000).

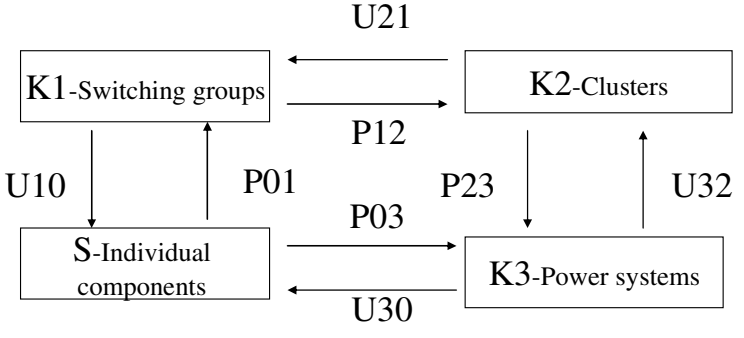

Fig. 9.14 Four realms network for failure diagnosis

The first reality level represents behavior of individual components and their present status. The second level, characterizes the switching groups and this refers for instance to isolators, protective relays, circuits breakers, and so forth.

The representation of entities bounded by a set of switching groups called clusters make the third level. The cluster level incorporates behavior knowledge concerning connected switching groups and the operational equipment between them.

The fourth level represents the whole network in terms of clusters. This level encompasses the strategic problem solving knowledge related to the complete power network. It is an integrative closure hypothesis for failure diagnosis, allowing system evolvability, self-repairing and autonomy. The operators U and P describe the testing procedures and the action in case of failure. The possibilities P describe the testing procedures and the information transfer between levels.

A triadic context model for security management of information technology was discussed by Dau and Wille (2001). In the triadic context formalizing the data the formal objects associated to K1 are the treats, the formal attributes associated to K2 are the safeguards and the formal conditions associated to K3 are the information technology units. A tetradic context model should include the real data associated to K0 (Fig. 9.15).

Fig. 9.15 shows a four realms network for security management.

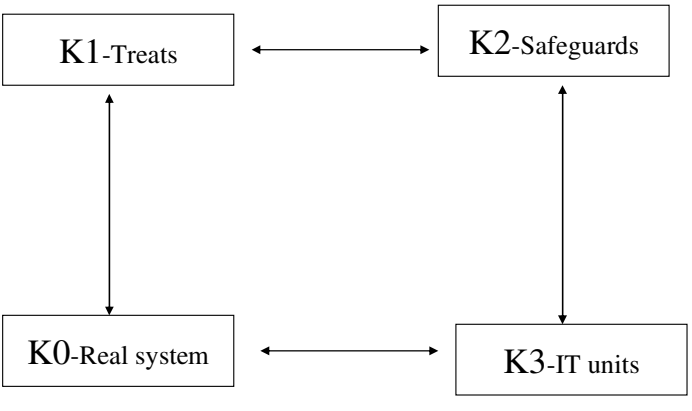

Fig. 9.15 Four realms network for security management

References

Chen, Y.H., Yao, Y.Y.: Formal concept analysis based on hierarchical class analysis. In: Proceedings of the 4th IEEE International Conference on Cognitive Informatics, ICCI 2005, pp. 285–292 (2005)

Dau, F., Wille, R.: On the Modal Understanding of Triadic Contexts. In: Decker, R., Gaul, W. (eds.) Classification and Information Processing at the Turn of the Milenium, Proc. Gesellschaft für Klassifikation (2001)

Ganter, B., Wille, R.: Formal Concept Analysis. Mathematical Foundations. Springer, Berlin (1999)

Hwang, S.-H., Kang, Y.-K.: Applying Hierachical Classes Analysis to Triadic context for Folksonomy Mining. In: International Conference on Convergence Information Technology, ICCIT 2006, pp. 103–109 (2007)

Iordache, O.: Evolvable Designs of Experiments Applications for Circuits. J. Wiley VCH, Weinheim (2009)

Iordache, O., Corriou, J.P., Garrido-Sanchez, L., Fonteix, C., Tondeur, D.: Neural network frames applied for biochemical kinetic diagnosis. Comp. Chem. Engng. 17, 1101–1113 (1993a)

Iordache, O., Corriou, J.P., Tondeur, D.: Separation Sequencing. Use of Information Distance., Canad. Journ. of Chem. Engng. 71(12), 955–966 (1993b)

Lehmann, F., Wille, R.: A triadic approach to formal concepts analysis. In: Ellis, G., Rich, W., Levinson, R., Sowa, J.F. (eds.) ICCS 1995. LNCS, vol. 954. Springer, Heidelberg (1995)

Lounkine, E., Bajorath, J.: Adaptation of formal concept analysis for the systematic exploration of structure-activity and structure-selectivity relationships. Journal of Cheminformatics 2(suppl. 1), 21 (2010)

Pawlak, Z.: Rough sets. Int. Journ. of Information and Computer Science 11, 341–356 (1982)

Popel, D.V., Dani, A.: Sierpinski Gaskets for Logic Functions Representation. In: Proc. IEEE International Symposium on Multiple-Valued Logic, pp. 39–45 (2002)

Rayudu, R.K., Samarasinghe, S., Maharaj, A.: A co-operative hybrid algorithm for fault diagnosis in power transmission. IEEE Journal of power Systems Engineering, 1939–1944 (2000)

Sisiaridis, D., Rossiter, N., Heather, M.A.: Holistic Security Architecture for Distributed Information Systems-A Categorical Approach. In: European Meeting on Cybernetics and Systems Research, Symposium Mathematical Methods in Cybernetics and Systems Theory, University Vienna, pp. 52–57 (2008)

Stumme, G.: A finite state model for on-line analytical processing in triadic contexts. In: Ganter, B., Godin, R. (eds.) ICFCA 2005. LNCS (LNAI), vol. 3403, pp. 315–328. Springer, Heidelberg (2005)

Valtchev, P., Missaoui, R.: Similarity-based Clustering versus Galois lattice building: Strengths and Weaknesses, ECOOP 2000 Workshop on Objects and Classification: a Natural Convergence, Sophia-Antipolis, France (June 2000)

Wille, R.: The basic theorem of triadic concept analysis. Order 12, 149–158 (1995)

Wille, R.: Restructuring mathematical logic: an approach based on Peirce's pragmatism. In: Ursini, A., Agliano, P. (eds.) Logic and Algebra, pp. 267–281. Marcel Dekker, New York (1996a)

Wille, R.: Conceptual structures of multicontexts. In: Eklund, P.W., Ellis, G., Mann, G. (eds.) ICCS 1996. LNCS, vol. 1115, pp. 23–39. Springer, Heidelberg (1996b)

Yao, Y.Y.: Concept lattices in rough set theory. In: Proccedings of the 23rd International Meeting of the Nort American Fuzzy Fuzzy Information Processing Society, pp. 796–801 (2004)

Chapter 10
Existential Graphs

Abstract. Diagrammatic methods as existential graphs and category theory diagrams are useful for multi-level problem solving.

Taking inspiration from systems sciences, this chapter highlights multi-level modeling potentialities for Peirce's existential graphs.

The relation with pragmatic philosophy and studies of continuity is emphasized.

High categories frames for Alpha, Beta and Gamma systems are discussed.

Case studies refer to separation flow-sheets.

10.1 Systems of Existential Graphs

Diagrammatic reasoning concerns the understanding of concepts and ideas, visualized with the use of diagrams and imagery instead by purely algebraic or linguistic means.

Peirce developed the diagrammatic calculus of existential graphs, EG, to express logical formulae and inferences (Peirce 1976, Roberts 1973, Dau 2003).

The Peirce's graphical approach to logic could be regarded as a forerunner of today's familiar "gedankenexperiment". An extension of the Venn diagram of probability theory, graphical reasoning was regarded by Peirce as the only really fertile reasoning, from which not only logic but every science could benefit. As in a "gedankenexperiment", Peirce regarded the use of such diagrams in logic as analogous to the use of experiments in chemistry.

Related to EG, the conceptual graphs can be considered as a synthesis of formal and graphical languages. Due to the graphical representation of knowledge, the conceptual graphs allow the construction of computer user interfaces. Recent developments of conceptual graphs are flexible modular frameworks that can be tailored to an open-ended variety of architectures for intelligent informational systems (Sowa 2000).

For multi-level systems modeling, it is of interest to examinee the EG applicability, the fit of EG and Peirce's concept of continuum and its place in Peirce's categories architecture.

The EG, have been developed in three stages of logical complexity: Alpha, Beta and Gamma systems. These systems are supposed to build upon each other.

Alpha graphs are geometrical representations of propositional assertions, that is, Boolean combinations of propositional variables.

To assert some statement in EG, the symbolization A of that statement is put on a sheet of paper, the so-called sheet of assertions, SA or blank. Drawing the symbolizations of two statements A and B is a juxtaposition that corresponds to conjunction of A and B. The negation of some statement is indicated by drawing a cut, called also "sep" from separation. This is a rectangle or any other enclosing figure, around the symbolization of that statement. Fig. 10.1 illustrates the concept of "sep". It is interpreted as A is false or in other words, A is separated.

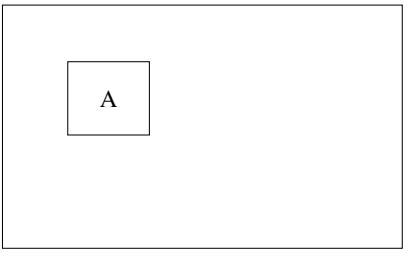

Fig. 10.1 Sep: A is false or separated

The sep without any contents is called an empty sep. Any empty sep expresses a contradiction.

Using letters or numbers for simple statements, juxtaposition for conjunction, and seps for negation any compound truth-functional statement may be symbolized in EG.

Alpha system has four inference rules: two rules of inference, insertion and erasure, and two rules of equivalence, double seps and iteration/deiteration.

To understand these inference rules, it is necessary to clarify concepts as subgraph and nested level.

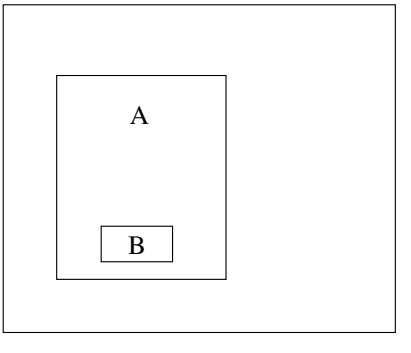

Fig. 10.2 Subgraphs

A subgraph is any part of the graph, as long as seps keep all of their contents.

Fig 10.2 illustrates the definition of subgraphs. The graph from fig. 10.2 shows five subgraphs: A, B, rectangle B (denoted also by [B]), the subgraph A and [B], and the subgraph [A, [B]].

The graph from Fig 10.2 expresses the implication relation: if A then B, or in other words A scrolls B. We may denote this implication by: A→ B. The reverse implication may be considered too.

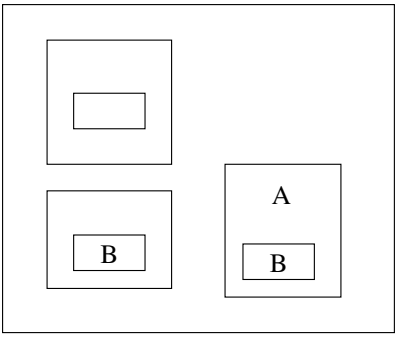

Fig. 10.3 Double seps

A double sep is any pair of seps where one is inside the other and where is only the empty graph in between. Fig. 10.3 illustrates double seps.

The left side of Fig. 10.3 shows double seps that may be denoted [[ ]] and [[B]]. The right side figure [A [B]] is not a double sep.

The level of any subgraph is the number of seps around it. The Fig 10.2 shows A, [B], the system A and [B] as the nested level 1 of subgraphs. B is a subgraph at the nested level 2. The graph itself [A, [B]] is a subgraph at the nested level 0.

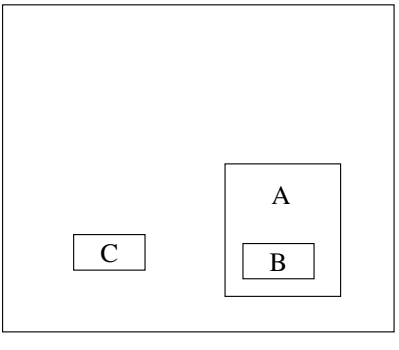

Fig. 10.4 Nested levels of subgraphs

A subgraph is said to exist at a nested level in relation to some other subgraph if and only if one can go from one graph to another by going inside zero or more seps, and without going outside of any seps. Fig. 10.4 shows nested levels of subgraphs.

In Fig. 10.4, B exists at a nested level in relation to A but not in relation to C. Also A and [B] exist at a nested level in relation to each other.

The double seps rule of equivalence allows drawing or erasing a double seps around any subgraph (Fig. 10.5).

Fig. 10.5 illustrates the double seps rule of equivalence.

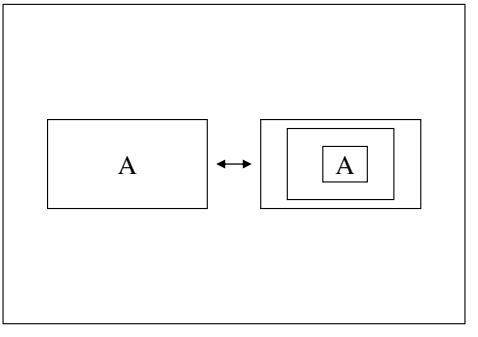

Fig. 10.5 Double seps rule of equivalence

The physical interpretation of double seps rule may be that two successive operations of separations are equivalent to the absence of separation. This is the case of an absorption followed by desorption due to a supplementary separation for instance.

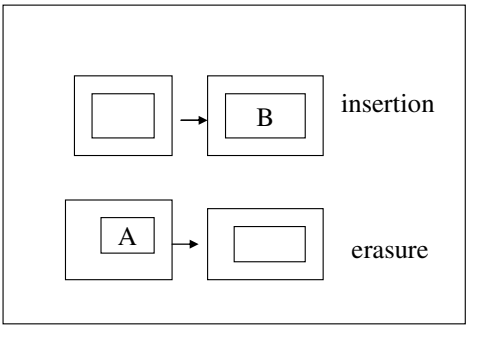

Fig. 10.6 Insertion and erasure

Fig. 10.6 illustrates the rule of insertion and erasure.

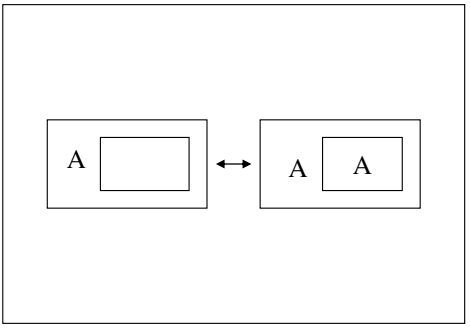

Fig. 10.7 Iteration/Deiteration

Fig. 10.7 illustrates the rule of iteration/deiteration.

A formal proof in EG consists in the successive application of inference rules to transform one graph into another.

A higher step in developing the Alpha EG systems are the Beta graphs, which represent geometrically first-order relational expressions.

A new symbol, the line of identity, LI, denoted by "—" was introduced for Beta systems. Lines of identity may designate both the existence of objects and the identity between objects.

The Beta part of EG corresponds to predicate logic, and it is an extension of Alpha system.

To define Beta graphs we need to define, how to symbolize objects, individuals constants, identity, predicates, and quantifiers.

To express that an object has a certain property P, we may write the predicate symbol next to the object: — P. To express a relationship R between two or more objects, we write the predicate symbol between the objects: — R —.

Instead of only considering predicates names of arity 0, in Beta system the predicate names of arbitrary arity may be used.

Essentially, the rules for Beta system are extensions of the five rules for Alpha system such that the Beta system rules cover the properties of the lines of identity.

The Beta system rules are: erasure, insertion, iteration, deiteration and double seps.

A higher step in developing the Beta graphs are the Gamma graphs.

Gamma graphs are related to higher order and modal logic, temporal logic and the possibility to express self-reference.

Peirce formulated some tentative rules for Gamma graphs: deletion and insertion, iteration and deiteration, and double seps.

A new graphical tool of Gamma system is the broken-sep shown in Fig 10.8.

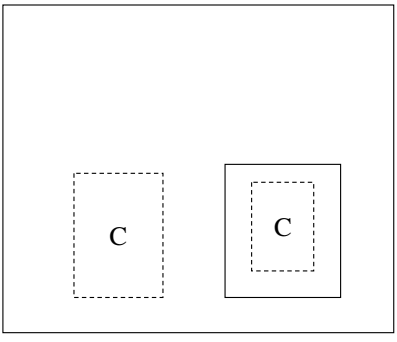

Fig. 10.8 Broken seps

Fig. 10.8 illustrates the broken seps.

For the graphs from Fig 10.8 we may use readings like: "it is possible that not C" and "it must be that C"

An important aspect of Gamma systems is the possibility to express meta-level propositions that is propositions about propositions. Graphs which have been used to describe objects so far can now in Gamma system to be treated like objects themselves such that other graphs speak about them. The graph of graphs represents a new level of abstraction for graphs. It may be considered as a graph rewriting method.

Developing Gamma system Peirce proposed to use colors or tinctures to distinguish different kind of contexts. Tinctures have not been considered logical operators but meta-level operators which can be used to describe how logic applies to the universe of discourse.

The fact that a graphic methodology of continuous gluing can be formalized in order to capture both a calculus of quantification, along joins and extensions of lines of identity, and several calculations of modalities, along completions of broken seps, is a significant result.

As a development of Gamma systems, Zalamea (2001) proposed to use a thicker identity line "▬" an existential quantifier in a second order logic.

10.2 Continuum and Existential Graphs

Peirce's understanding of EG was strongly related to his study of the continuum, and this understanding is different from the real set of Cantor.

Peirce rejected Cantor's model of continuity, and developed over a generic synthetic ground–smooth or plastic, different concepts of continuum based on NA frames (Ehrlich 2006). He outlined that the cohesiveness of a continuum rules out the possibility of it being a mere collection of discrete individuals, or points, in the usual sense.

Peirce maintained that if enough points were to be crowded together by carrying insertion of new points between old to its ultimate limit they would—through

a logical transformation of quantity into quality, lose their individual identity and become fused into a so-called "true continuum".

Peirce's continuum is notable for the presence in it of an abundance of potential infinitesimals. He supported the retention of the infinitesimal concept in the foundations of the calculus, both because of what he saw as the efficiency of infinitesimal methods, and because he regarded infinitesimals as constituting the glue causing points on a continuous line to lose their individual identity. Infinitesimals form the glue that holds the points of the line together. These kinds of intuitions were at the core of Peirce's conception of infinitesimals identified with the consciousness of the immediate moment. By taking the stance that there can be no movement in an instant, Peirce argues that the present, infinitesimal moment cannot be an instant. He has been aware that a faithful account of the continuum will involve questioning the law of excluded middle. The relation with toposes and SDG frame is obvious (Havenel 2008).

The logic of continuity represents a unifying program to coherently combine the EG and elements of Peirce continuum concept in order to advance a better understanding of geometric logic.

The correlation between the concept of EG, the continuum and categories is of practical interest since this may offer a basis for multi-level cognitive systems construction (Rosa 1993, Kauffman H.L. 2001, Zalamea 2003, 2007).

A promising way to relate EG systems to Peirces' concept of continuum was proposed by Zalamea (Zalamea 2001, 2007). Zalamea suggested a complex variable interpretation of EG. Following this approach we will consider a positive number as ε that is not zero and nevertheless smaller than any positive number. Its reciprocal 1/ε would be a number larger that any number, an infinite number. Adding ε or 1/ε to the finite numbers is an operation analogous to extending the number system to include the imaginary i, or 1/i that is to create the complex numbers.

In both cases unconventional numbers as infinitesimal "ε" or imaginary "i" are introduced for their potential usefulness.

We observe an analogy between well known results in complex analysis and results in infinitesimal analysis. Operations we are doing with numbers as B +εA are in some sense, analogous to the operations we are doing with complex numbers as B+iA.

For the example of mixing the infinitesimal part is associated to the slow space while the standard part corresponds to the active space. For a separation process the slow space and the active space are the separated species.

The graph from Fig. 10.2 shows that the event A scrolls B. This implication may be denoted by the number B+ εA. Reversing the implication, to B scrolls A, means reversing the number B+ εA to 1/ (B+ εA). Physically this means to interchange the roles of the active and the slow spaces.

Paralleling the suggestions of Zalamea (2007) we may associates the numbers containing 1/ε to residues calculus and to Alpha systems in EG. Analogously the analytic continuation for complex systems is associated to Beta system and the analogous to Riemann surfaces to Gamma systems.

Similar conclusions should be valid when complex variables are replaced by infinitesimals. In this way Peirce's EG theory may be of help in understanding the logic of infinitesimal variables.

According to integrative closure hypothesis the 1, 2 and 3-categories may be associated to Peirce's firstness, secondness and thirdness categories.

According to this hypothesis, the EG growing in complexity steps from Alpha to Beta and Gamma systems is analogous to the steps of mathematical n-categorification.

The thirdness was frequently associated by Peirce to his concept of "true continuum". It corresponds to a kind of complete gluing of entities. The gluing is ensured by infinitesimals at different scales. The "true continuum" may be that associated to 3-categories.

Brady and Trimble (2000a, 2000b) proposed categorical models for classical Alpha systems (1-categories) and Beta systems (2-categories). Their results suggest to hypothesize that Gamma graphs would be associated to 3-category.

Fig. 10.9 clarifies the integrative closure features for EG.

Fig. 10.9 shows the categories associated to EG and to continuum in the integrative closure hypothesis frame.

The level 0 for categories corresponds in this illustration to the real data or info. This level corresponds to the "substance" in the Peirce's initial list of categories.

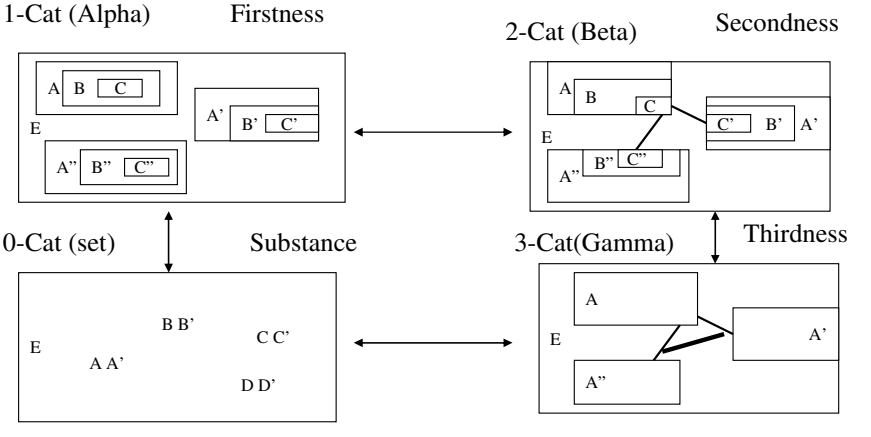

Fig. 10.9 Integrative closure for existential graphs

The level 1 corresponds also to Alpha systems and 1-categories, the level 2 to Beta systems and 2-categories, the level 3 to Gamma systems and 3-categories. For Alpha systems the implications are indicated by inclusion or by arrows, "→". The line of identity, LI, denoted "—" may be considered as 2-arrows, "⇒". The thick lines of identity "▬"may be considered as 3-arrow "⟹".

The presentation from Fig. 10.9 outlines the hypothetical way correlating the substance (level 0) with the thirdness (level 3). The Alpha systems define trajectories or sequences. The Beta system allows an identification of C with C' and C with C'' based on lines of identity,"—". These relate the trajectories.

The Gamma system allows a supplementary identification of the previous identified trajectories, by a second-order thick line of identity "▬".

It should be noted the contact of the above approach with Whitehead's process philosophy (Whitehead, 1978). In this case the four levels correspond to existence, explanation, obligation and ultimate category. As for Peirce, Whitehead theories were developed too early to see the fulfillment of their frameworks as formal n-categories but they may be a source of ideas for categorists.

10.3 Separation Flow Sheets

There exists a significant relationship between the categorification and coherence studies in CT, the possible sequences of separation for mixtures and the existential graphs, EG.

The connection between separation schemes and n-category properties aims to shows what kind of separation systems correspond to categorical properties.

As shown in the periodic table (Appendix 2) the categorification implies the succession of monoidal, braided, sylleptic, involutory and symmetry properties.

The signification of these properties for separation flow-sheets and EG will be presented in the following.

Recall that a monoid is an algebraic structure with a single associative binary operation and an identity element.

Consider that the axiom to be imposed to the separation sequence is the associativity. This means that, within a sequence of elements containing two or more of the same sequencing operations in a row, the order that the operations are performed does not matter as long as the sequence to be operated is not changed. Rearranging the parentheses in a sequence will not change sequencing general task.

The resulting associahedron are studied in CT as coherence conditions.

Suppose that there are four components and that the order of sequencing is imposed from start, by a heuristic as for instance - sequence the splits in the order of adsorbability. Denote the four components according to that order as A, B, C and D. The MacLane pentagon condition is shown in Fig. 10.10. It outlines monoidal flow-sheets.

Fig. 10.10 may be interpreted in terms of Alpha system for EG, also.

The transition from a configuration to another is pictured as a shift of rectangles or boxes.

Brady and Trimble (2000a) inserted the EG in the context of monoidal categories and have showed that every Alpha graph give rise to an algebraic operation.

Alpha graphs have been studied in the frame of the star-autonomous categories (Barr 1979).

Fig. 10.10 shows that for tensor product of four objects there are five ways to parenthesize it. The association allows us to build two isomorphisms from the sequence [[AB] C] D to A [B [CD]].

The isomorphism is interpreted in the sense that the so-called direct sequence A [B [CD]] is made equivalent to the reverse sequence [[AB] C] D, if one retains the heavy phase instead of the light phase during the separation process.

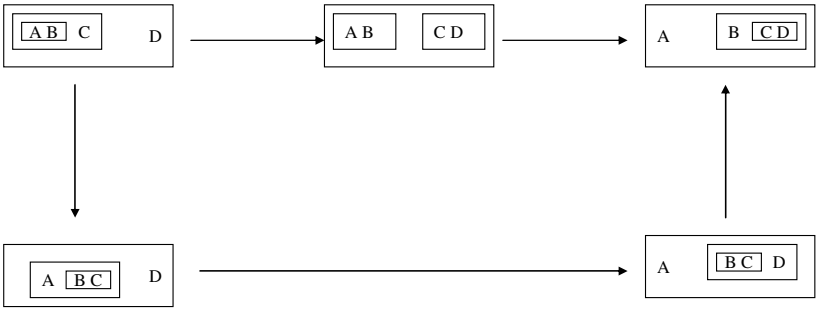

Fig. 10.10 Monoidal flow-sheets

Fig. 10.11 expresses the relations from Fig. 10.10 in a tree-like form. It shows monoidal flow-sheets in a tree like form.

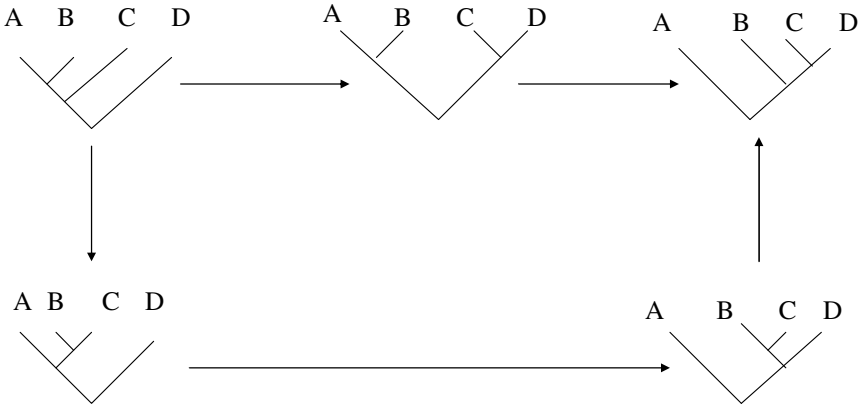

Fig. 10.11 Monoidal flow-sheets: tree like form

The next level of schemes and EGs will include braiding.

A braided monoidal category consists of a monoidal category with an extra structure of a natural isomorphism called braiding with some properties called hexagon equations (Appendix 2).

For separation processes there are processes that let us switch two systems by moving them around each other.

This switching corresponds to braiding, that is to relations as AB=BA.

Consider the case of 3 components denoted by A, B and C. The hexagon conditions shown in Fig. 10.12 ensure the coherence for braiding conditions.

Fig. 10.12 shows braided flow-sheets.

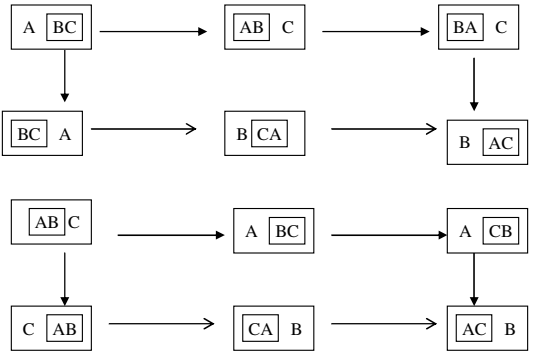

Fig. 10.12 Braided flow-sheets

The first hexagon equation says the switching the component A past BC, all at once, is the same as switching it past B and then past C.

The second hexagon is similar. It says that switching AB past C all at once, is the same as doing it in two steps. It may be a shift of the in

This kind of braiding may be interpreted as a situation in which there is a switch in the separation order. For instance, in a scheme working with adsorbability it may be a thermal swing adsorption by varying the temperature (Yang 1987). It is known that adsorbability depends significantly on temperature.

The hexagons outline all the possible separation schemes allowing associativity and braiding and their interconnection.

Fig. 10.12 may be interpreted in terms of Beta system for EG.

The transition from a configuration to another is pictured as a switching between rectangles that is boxes and individual components. There exist also shifts of boxes corresponding to the previous categorical level that is to monoids.

There are several types of operations governing the transitions between two successive states. It may be a shift of the internal box and a braiding or switch of component inside the internal box and a switch between components of the large box and that of the internal box.

Brady and Trimble (2000b) have indicated how to represent Beta graphs by means of a category theoretic relational calculus. Beta graphs represent a 2-category structure (Joyal and Street 1991).

The next level in categorification corresponds to sylleptic structures.

A sylleptic monoidal category is a braided monoidal category with extra structure (Crans 2000, McCrudden 2000).

Fig. 10.13 shows flow-sheets that results by parity cube relations (Appendix 2).

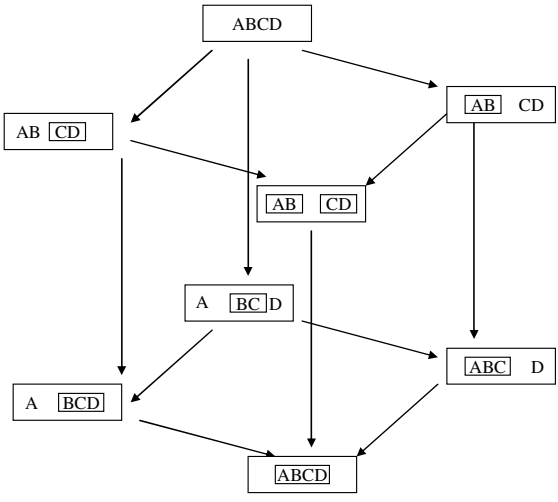

Fig. 10.13 Parity cube flow-sheets

For coherence the edges of the MacLane pentagon from Fig. 10.10 become five sides of a cube shown in Fig. 10.13. This is the so-called parity 3-cube. This cube shows what happens when an axiom as associativity is complemented by significantly more restrictive ones as required by Gray tensor product "Γ", definition and tricategorical frame (Appendix 2).

Representation for a tricategory is fundamentally different from the one and two dimensional case of categories and bicategories. The integrative closure hypothesis suggests to associates this categorization step to Gamma systems.

References

Barr, M.: *-Autonomous Categories. Lecture Notes in Mathematics, vol. 752. Springer, Berlin (1979)

Brady, G., Trimble, T.: A categorical interpretation of C.S. Peirce's propositional logic Alpha. Journal of Pure and Applied Algebra 149, 213–239 (2000a)

Brady, G., Trimble, T.: A string diagram calculus for predicate logic and C.S. Peirce's system Beta (2000b) (Preprint)

Crans, S.: On braidings, syllepses ans symmetries. Cahiers Topologie Geom. Differentielle Categ. 41(1), 2–74 (2000)

Dau, F.: The Logic System of Concept Graphs with Negation and its Relationship with Predicate Logic. LNCS (LNAI), vol. 2892. Springer, Heidelberg (2003)

Ehrlich, P.: The Rise of non-Archimedean Mathematics and the Roots of a Misconception I: the Emergence of non-Archimedean Systems of Magnitudes. Archive for History of Exact Sciences 60, 1–121 (2006)

Havenel, J.: Peirce's Clarifications on Continuity. Transactions of the Charles S. Peirce Society 44(1), 86–133 (2008)

Joyal, A., Street, R.: The geometry of tensor calculus I. Adv. Math. 88, 55–112 (2001)

Kauffman, H.L.: The mathematics of Charles Sanders Peirce. Cybernetics and Human Knowing 8(1-2), 79–110 (2001)

McCrudden, P.: Balanced coalgebroids. Theory and Applications of categories 7(6), 71–147 (2000)

Peirce, C.S.: The New Elements of Mathematics, Eisele, C. (ed.), vol. I-IV. Mouton Publishers and Humanities Press (1976)

Roberts, D.: The Existential Graphs of Charles S. Peirce. Mouton, Hague (1973)

Rosa, M.A.: Le Concept de Continuité chez C.S Peirce. These de doctorat E.H.E.S.S., Paris (1993)

Sowa, J.F.: Knowledge Representation: Logical, Philosophical and Computational Foundations. Brooks-Cole, Pacific Grove (2000)

Whitehead, A.N.: Process and Reality. Corrected edn., Griffin, D.R., Sherburne, D.W. (eds.). Free Press, New York (1978)

Yang, R.T.: Gas Separation by Adsorption Processes. Butherworths, Boston (1987)

Zalamea, F.: Peirce's Continuum. A Methodological and Mathematical Approach. University of Bogota (2001)

Zalamea, F.: Peirce's logic of continuity: Existential graphs and non-Cantorian continuum. The Review of Modern Logic 9, 115–162 (2003)

Zalamea, F.: Towards a complex variable interpretation of Peirce's Existential Graphs. In: Proceedings of Applying Peirce Conference, Helsinki (2007)

Chapter 11
Evolvable Designs of Experiments

Abstract. The multi-level modeling potentialities for evolvable designs of experiments are highlighted.

The general PSM framework based on integrative closure serves as a flexible guideline for a large variety of design of experiments.

Case studies refer to pharmaceutical pipeline, drugs discovery and development, reliability management systems, test coupons design and failure analysis for printed circuits.

New informational entropy criteria find applications.

11.1 Pharmaceutical Pipeline

Designing, building and controlling complex systems became a central challenge for scientists and engineers in the coming years. A new approach to problem solving for complexity is represented by the evolvable designs of experiments, EDOE (Iordache 2009). It is based on the constructivist thesis that knowledge can not be a passive reflection of reality, or a passive application of a formal problem solving model, but has to be more of an active and interactive construction. EDOE is a modern way to cross industrial and technological complexity frontiers by replacing pre-programmed and fixed designs and problem solving methods by evolvable ones.

The EDOE methodology may find applications for complex problems as the so-called pharmaceutical pipeline.

This refers to the new product, to research and development in pharmaceutical industry.

The typical sequence for new product implementation contains the following main steps:

Resources →Discovery→ Development→ Launching

A more detailed version of the pharmaceutical pipeline is shown in Fig. 11.1

Biological, chemical and other resources allow the discovery of drug lead.

The development step includes tests, preclinical, P0, followed by three phases of tests, PI, PII, and PIII.

The product launching starts with NDA, New Drug Application, and FDA, Food and Drug Administration, submissions and reviews, and continues with production and marketing steps.

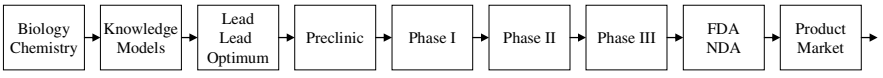

Fig. 11.1 Pharmaceutical pipeline

Some areas of pharmaceutical industry are facing a productivity crisis (Woodcock and Woosly 2008). Despite rising investment in pharmaceutical research and development, successful development of new drugs is slowing. The high costs of new drugs development may discourage investment in more innovative, risky approaches in therapeutics.

The FDA, with its dual role of promoting and protecting health is charged with implementing policies that ensures that the benefits of the new products will surpass their risks, while simultaneous promoting innovations that can improve health.

It was observed that chemical and biological systems may have huge behavior spaces and laboratory experiments and models cover only tiny aspects of a system's behavior.

The models often ignore the essential temporal and conceptual space organization of the research and implementation components. Moreover, models and methodologies lack flexibility to adapt and to faster represent more areas of the behavior space.

They neglect synergies – beneficial, nonlinear interactions between systems that cannot be inferred from existing resources and may be missed.

The architecture of the models should be in correspondence with that of the studied system within physically, biologically or cognitive recognizable spaces.

This will require combining multiple level modeling methods in innovative ways, multiple levels of organization activated both in parallel as in series.

It is a need for new modeling and simulation methods, sufficiently flexible, adaptable and evolvable that is able to explore larger portions of the behavior space, a strong request for cognitive architecture reflecting the essential temporal and spatial organization of the real substrates and allowing autonomy of the new product development system.

PSM and more specifically EDOE, are promising cognitive architectures proposed as new methodologies for multi-level problem solving in pharmacology.

The PSM general framework is based on four modules and their integrative closure.

Fig. 11.2 suggests a transition from the pharmaceutical pipelines to pipecycles.

The module K0 corresponds to substrate and resources, the module K1 to discovery step, K2 to developments and tests and K3 to product implementation and launching.

The first module involves resource mining. Resources are material, biological and of knowledge type.

The second module K1, is that of discovery and involves in this case drug-like molecules discovery, lead discovery and optimization. It may be a DOE.

The third module K2 is that of drug testing and development. It is a meta-design and for this reason may be denoted by 2-DOE since refers to processing DOE.

The fourth module K3 includes application and approval processes, manufacturing, marketing and monitoring of the product.

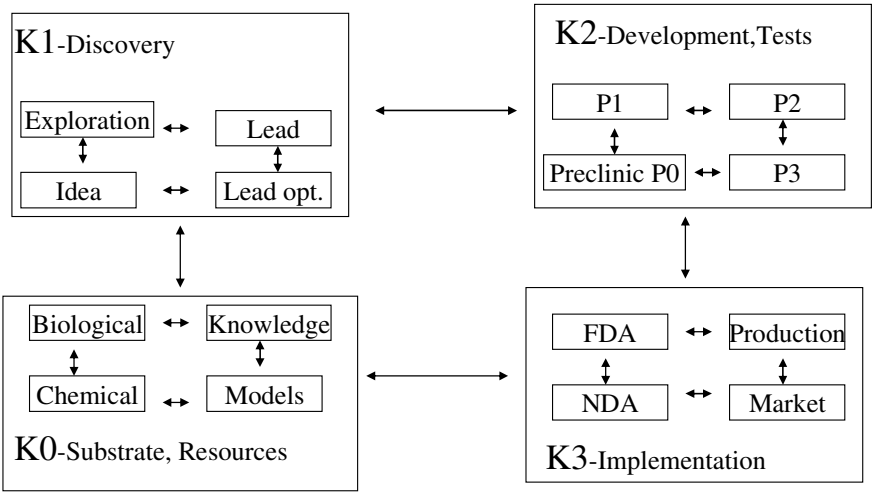

Fig. 11.2 Pharmaceutical pipecycles

Each module may involve several sub-modules organized as epicycles.

For instance in the module K2 there exists a natural cycle P0, P1, P2, P3.

For the module K3 the NDA step is followed by FDA step this by production and this by product marketing.

The transition from pipeline to pipecycles proposes a methodology that closes the loop in iterated experimentation in a high dimensional space. The cycling refers to large cycles for the whole process of four modules or just to one module or sub-module and the corresponding epicycles.

Some cycles may be fully automated if autonomous experimentation methods are used to conduct high-throughput experiments.

Modeling of matrix designs and use of informational criteria accelerate the development of new drugs.

11.2 Designs of Experiments for Drug Discovery

Drug-likeness is a qualitative concept used in drug design to outline how a substance is with respect to factors like bioavailability. It is estimated from the molecular structure before the substance is even synthesized and tested. A drug-like molecule has properties like, high solubility to both water and fat, sufficient water-solubility, low molecular weight, pharmacological properties.

A traditional method to evaluate drug-likeness is to check compliance to different rules which covers the numbers of hydrophilic groups, molecular weight, hydrophobicity and so on. The drug-likeness study should be completed with lead-likeness study (Hann and Oprea 2004).

Drug-likeness indexes are inherently limited tools since they do not evaluate the actual specific effect that the drug achieves that is, the biological activity.

In pharmacology, bioavailability is a measurement of the extent to which a drug reaches the systemic circulation. First-pass metabolism, which is bio-chemically selective, can obliterate the pharmacological activity of a compound despite good drug-likeness. Toxicity should also be taken into account.

We may address the problem of designing experiments for the exploration of high-dimensional experimental spaces using EDOE method.

We will consider that the activity of new drug discovery can be divided in four basic modules or steps.

The first module K0 corresponds to resources and research step.

The second module K1 should be based on designs of experiments, DOE.

The third module K2 is a meta-design and for this reason was denoted by 2-DOE.

The fourth module K3 is a meta-meta-design and for this reason may be denoted by 3-DOE.The general method is illustrated in Fig. 11.3.

Fig. 11.3 highlights the EDOE basic framework.

The four modules of variation, K0, K1, K2 and K3 are denoted also by S, 1-DOE, 2-DOE, and 3-DOE.

To start the EDOE, we examine experimental space of properties.

After a number of iterations at this level we may make predictions of drug-likeness too.

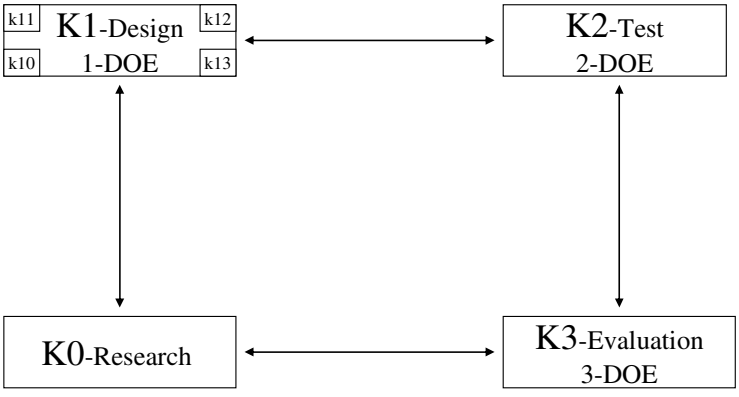

Fig. 11.3 EDOE basic framework

As a starting point we will select drug candidates according to existing rules (Lipinski et al. 1997, Ghose et al. 1999).

Lipinski's rule says that, in general, an orally active drug has no more than one violation of the following criteria:

- Not more than 5 hydrogen bond donors (nitrogen or oxygen atoms with one or more hydrogen atoms)
- Not more than 10 hydrogen bond acceptors (nitrogen or oxygen atoms)
- A molecular weight under 500 Daltons
- An octanol-water partition coefficient log *P* of less than 5

Note that all numbers are multiples of five, which is the origin of the rule's name.

Based on such rules we may select a DOE. For DOE matrix we use "1" if the rule is verified and "0" otherwise.

The DOE may be associated to a set of molecules or an embedded design if a genomic analysis is possible. The four-fold framework may be applied to just one of the levels as seen in Fig. 11.3.

In such cases the focused level is divided in four sub-levels.

Let us restrict here to the discovery stage associated to K1 as a first example.

A method of designing chemical substances is presented (Wood and Rose 1999).

The method allows sampling combinatorial chemistry space for synthesis based on DOE with Latin squares or more general with orthogonal arrays.

Libraries with four sites of variation for molecules may be designed using Greco-Latin squares.

Consider four sites of variation, k10, k11, k12 and k13 for substitute groups. They correspond to sub-levels of the level K1.

Then only four different substitutes are selected for each substitute or pendant group, k10, k11, k12 and k13.

The substitute group k10 consist of four candidates, denoted 0, 1, 2 and 3, the substitute k11 from four candidates denoted a, b ,c ,d the substitute k12 of four

candidates denoted A, B, C, D and substitute k13 of four candidates denoted α, β, γ, and δ.

Recall that a wave equation is able to generates Latin squares as solutions (Iordache 2009, 2010).

Superposition of such solutions of the wave equation gives Greco-Latin squares as shown in Table 11.1. This superposition represents a specific categorical product.

Table 11.1 shows the matrix of a Greco-Latin design.

For this table the sub-levels of the level K1 are: k10 = {1, 2, 3, 4}, k11 = {a, b, c, d}, k12 = {A, B, C, D}, and k13 = {α, β, γ, δ}.

Table 11.1 Greco-Latin square design

k10\k11	a	b	c	d
1	Aα	Bβ	Cγ	Dδ
2	Bδ	Aγ	Dβ	Cα
3	Cβ	Dα	Aδ	Bγ
4	Dγ	Cδ	Bα	Aβ

With 16 experiments only we may obtain significant info.

Running the experiment we may select the critical substituents.

EDOE framework should be seen as a general pattern rather then a predetermined fixed plan. This means that we may have partial Greco-Latins as micro-arrays.

The complete EDOE frame implies to continue the cycle from DOE matrix that is from K1 level, to tests that is K2 level, evaluation and implementation that is K3 level as shown in Fig. 11.3.

11.3 Drugs Development

11.3.1 General PSM Framework for Discovery and Development

A significant source of complexity in pharmacology is the multi-level characteristic of the involved systems. Evolvability is the proposed method to face different aspects of complexity (Iordache 2009). Applying the general PSM framework highlight the ways of implementing evolvability for drug design development and delivery systems.

Following PSM methodology the pharmaceutical discovery and development activity can be divided in four main modules or levels (Fig. 11.4).

Fig. 11.4 shows a framework for drug discovery and development.

The first module, K0 is represented by resources, data bases and involves resource mining. The next module, K1 is that of discovery and involves drug-like or lead discovery and improvement. This module may include designs of experiments, DOE. In our case study this module will refer to establishing a "reference" set or a "core" set of significant compounds (Wang et al. 2009).

The next module, K2 is that of new drugs testing and development. It may include the proof of concept by multiple trials. In this case study this consists in evaluating similarity of new drugs relative to the reference set. The next module, K3 includes decision about the new drug application and also monitoring of the product.

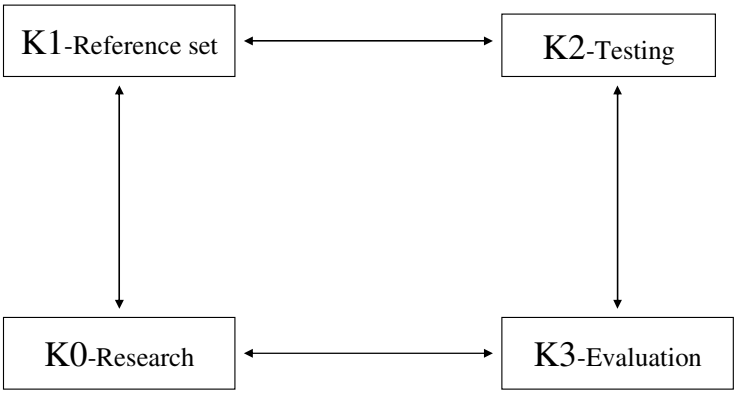

Fig. 11.4 Framework for drug discovery and development

11.3.2 Informational Tools

The initial step in quantifying the concept of similarity for chemical species in a mixture is to list the most important structural elements or properties of such species. To every species can be associated a vector the components of which take only two values "1" or "0" where "1" means the presence of a given structural element or property whereas "0" means its absence. For instance, "1" may correspond to a high value of the property, as the hydrophilic character, whereas "0" corresponds to a low value (Iordache et al. 1993b). Binary bit string representations of molecular structure and properties often called fingerprints are standard tools to analyze chemical similarity (Willett 1998).

Vectors associated to the chemicals are denoted by: $i = \langle i_1, i_2, ..., i_k, ... \rangle$ where i_k are either "1" or "0". Binary characterization according to the presence ("1") or to the absence ("0") of a given property was used initially. The use of multi-valued

digits or of the real properties instead of Boolean ones has been tested also. A hierarchy of the structural elements or properties is required. For instance, it is considered that the property indexed by i_1 is more significant that the property indexed by i_2, this more significant that i_3, and so on in the order of the coordinates in the associated vectors.

To any set of chemicals a similarity matrices is associated and to this an informational entropy. On this basis the components of the mixture may be selected.

A similarity index r_{ij}, between two different species $i= <i_1, i_2,..., i_k,...>$ and $j= <j_1, j_2,..., j_k,...>$ is defined as:

$$r_{ij} = \Sigma_k t_k \ (a_k)^k \ ; \ k=1,2,.... \tag{11.1}$$

Here: $0 \leq a_k \leq 1$ and $t_k=1$ if $i_k = j_k$, $t_k=0$ if $i_k \neq j_k$ for all k. The entire system is characterized by the matrix $R=[r_{ij}]$. The similarity index should possess the natural properties of reflexivity ($r_{ii} = 1$) and of symmetry ($r_{ij}=r_{ji}$). This definition assigns a coefficient of weight a_k to any property involved in the description of the species i and j provided that the Boolean values $i_k$and j_k are the same for these two chemicals.

The fact that the relation described by r_{ij} is reflexive and symmetric allows a partition of the set of components in classes that are not necessarily disjoint. A class consists of a number of similar chemical species gathered together. To limit here the study to partition into disjoint classes the defined similarity must be transitive that is: $\min_k (r_{ik}, r_{kj}) \leq r_{ij}$. The procedure to ensure transitivity is that the classification algorithm starts from the "stable" matrix of similarity. To obtain such a stable matrix, the sequence R, R(2),..., R(k),...with R(2)=RoR and R(k)=R(k-1)oR is calculated. The composition rule "o" is given by:

$$(RoW)_{ij} = \max_k [\min (r_{ik}, w_{kj})] \tag{11.2}$$

Here $R=[r_{ij}]$, $W=[w_{ij}]$ are two arbitrary matrices of the same type. The composition equation calculates the (i,j)-th element of the matrix RoW. It consists in taking the smallest of the two elements r_{ik} and w_{kj}, for a given row i of R and a column j of W, then repeat the procedure for all k, and select the largest of all such resulting elements. There exists an integer n such that from n on, the matrix is stable to the composition rule "o" so that R(n)=R(n+1) and so on. The elements of the stable similarity matrix R(n) verify symmetry, reflexivity and transitivity.

Denote by r_{ij} (n) the elements of the stable matrix R(n). The partition is established on the base of the "degree of classification" T with $0 \leq T \leq 1$. The classification rule is the following: two species i and j, are assigned to the same class if r_{ij} (n)$\geq$ T. Applying the rule, the set of classes at the degree of classification T is obtained. For T=0, a unique class results including all species, whereas for T=1 each class includes only one species. When T varies from 0 to 1, different sets of classes arise. Actually a new set of classes arises every time T

crosses the value of one similarity index r_{ij} of the matrix R. In this way a general tree of classes is built, which is nothing but the expected flow-sheet. The class of i, noted î, is the set of species j which satisfies the rule: $r_{ij} \geq T$. The similarity matrix of classes $\hat{R}$ is constructed as follows:

$$\hat{R}_{\hat{i}\hat{j}} = \max (r_{wt}); \; w \in \hat{i}, \; t \in \hat{j} \tag{11.3}$$

Here w designates any index of species belonging to the class of i and similarly t any index referring to the class of j.

To any similarity matrix R the informational entropy H(R) is associated:

$$H(R) = - \Sigma \, r_{ij} \ln r_{ij} - \Sigma \, (1 - r_{ij}) \ln(1 - r_{ij}) \tag{11.4}$$

This expresses the quantity of information associated to the matrix of design.

The defined entropy is a measure of the imprecision in classifying the experiments.

To compare two similarity matrices $R = [r_{ij}]$ and $W = [w_{ij}]$ a distance DD was introduced:

$$DD(R, W) = -\Sigma \, r_{ij} \ln (r_{ij} / w_{ij}) - \Sigma (1 - r_{ij}) \ln ((1 - r_{ij})/(1 - w_{ij}))$$

The distance measure the discrepancy between two similarity matrices and associated classifications.

11.3.3 Anesthetics Mixtures

Informational algorithms based on relation between chemical structures of anesthetics and their pharmacological properties may be of help in anesthetics discovery, development and delivery (Iordache et al. 1989, Torrens and Castellano 2006).

The starting point of the informational analysis consists in associating to different anesthetics digital vectors describing their composition and properties.

The relation vs. structure activity suggests using of this informational description of anesthetics for new anesthetics discovery.

Test calculations on different compound data sets, associated vectors, and screening data bases revealed the capability of the method to detect new formulations.

Significant clinical properties of local anesthetics as potency, onset and duration of action depend on the physicochemical properties of the various fragments of anesthetic compounds. Most local anesthetics are classified into the ester and amide type, by the difference in the chain that binds the hydrophobic group and the hydrophilic group in a molecule (Verderame 1986).

For anesthetics we considered associated vectors as:

x= <lipofilic, hydrophilic, intermediate chain, nr of N atoms, nr of O atoms>

The choice of this set of characteristics and of their hierarchy should be based on tests. It introduces an important subjective character into the analysis where precisely the expertise of the analyst should play an essential part.

Procaine was selected as a reference anesthetic.

For procaine the lipophilic portion is a phenyl radical, the hydrophilic portion is an amine, the intermediate chain is an ester, and there are two nitrogen atoms and two oxygen atoms. The vector associated to procaine is <11111>. The vector <10101> is associated to benzocaine since the hydrophilic portion is not an amine and there is only one nitrogen atom in this molecule.

A natural trend is to formulate mixtures of anesthetics as an attempt to answer to complex pharmacological requirements (Kaweski 2008, Kravitz 2007, Lee 2003).

Table 11.2 shows some topical anesthetics mixtures that may be considered as developments of the mixture lidocaine/tetracaine, LT. The mixtures of three anesthetics are denoted here by PFG, LET, TLP, and BLT.

LT is considered as a reference set.

This choice corresponds to the K1-module in the general PSM framework.

If possible, the reference set should be selected to offer maximum entropy, ME.

ME is the criterion to build K1 module.

Applying the informational algorithm we may calculate the informational entropy H associated to LT mixture (Table 11.3).

By adding a third compound to this LT reference mixture the entropy H varies.

There is only a small change of entropy, if the vector of the test compound is similar to the reference set and this supplementary compound is thought to have similar properties (Wang et al. 2009).

Table 11.2 Topical anesthetics

Topical Anesthetics Mixtures	Anesthetics	Vector
LT	Lidocaine	<11010>
	Tetracaine	<11111>
PFG	Prilocaine	<11010>
	Lidocaine	<11010>
	Tetracaine	<11111>
LET	Epinephrine	<11000>
	Lidocaine	<11010>
	Tetracaine	<11111>
TLP	Phenylephrine	<11001>
	Lidocaine	<11010>
	Tetracaine	<11111>
BLT	Benzocaine	<10101>
	Lidocaine	<11010>
	Tetracaine	<11111>

If a data base anesthetic shares similar bit patterns with reference set molecules, adding a similar compound will induce a change targeting the minimum entropy production.

By contrast, inclusion of a compound having dissimilar vector leads to a higher entropy production, targeting the maximum entropy production.

In this way data base compounds may be screened to identify compound that cause lower or higher changes relative to the reference set informational entropy.

Table 11.3 refers to informational entropies and distances for different mixtures. ΔH denotes the entropy production that is the difference between the entropy corresponding to the ternary mixture and that corresponding to the binary reference set, LT. It appears that supplementing the LT mixture by prilocaine as for PFG, epinephrine as for LET, or phenylephrine as for TLP, has comparable small effect.

Only benzocaine as for BLT, by its dissimilarity induces higher entropy production ΔH.

The maximum entropy production, MEP, may be the criterion to build the K2 module.

The testing of different mixture corresponds to the K2 step in the general PSM framework.

The informational distance DD is a supplementary tool in evaluating new mixture of anesthetics. The distance between the similarity matrix associated to LT and to other mixtures is shown in Table 11.3.

Table 11.3 Informational entropies for mixtures

Mixture	LT	PFG	TLP	LET	BLT
H	0.9651	2.2084	2.6838	2.5525	3.5391
ΔH	0	1.2523	1.7187	1.5874	2.5740
DD	0	0.1778	0.3810	0.4495	-1.8775

Table 11.3 shows a dramatic variation of the distance DD for BLT.

This corresponds to a significantly different partition in classes of the elements of the BLT mixture, compared to the other ternary mixtures.

Taking into account ΔH and DD it seems that PFG mixture corresponds to the conservative choice while BLT mixture to the innovative one.

Observe that both entropy production ΔH and distance DD are useful criteria.

DD criterion may be considered as an informational counterpart of a criterion for maximum production of entropy production, MPEP. According to this interpretatyion of MPEP proportional to DD criterion, the BLT mixture should be selected.

Obviously it is not in the scope of the informational method to replace clinical tests of drugs but it can be useful as a general guideline allowing asserting priorities and accelerating drug discovery and development.

The calculation should be followed by practical evaluation following the K3 step in the general PSM framework. This means to confront and overpass another level of complexity. At this level the target is to be considered.

To ensure integrative closure, the K3 module should be connectable to the reality and resources S.

If the global target is to select similar drugs the minimal entropy production may be a useful criterion. It corresponds to a conservative screening. Low ΔH and DD correspond to compounds that pertain to similar classes of drugs.

Contrary, in a new drug discovery mode the maximum entropy production criterion may be of interest. It corresponds to an innovative, higher risk, screening. Higher ΔH and DD corresponds to differences allowing multiple, different classes and potential versatility.

To illustrate the selection criterion at this level we take into account that the organisms varies and show circadian and other rhythms (Bruguerolle and Prat 1988). Rhytms are associated to metabolic closure. For different regimes for organism the delivery of different anesthetic mixtures may be beneficial, and ensure the evolvability maximization, EM. EM will be evaluated by comparing the DD values. Periodic functioning implies the swing of the organisms or organs from minimal entropy production to maximal entropy production regime. The functioning of most organisms or organs is periodic or transient according to the ambient conditions.

The high entropy production of the drug may be of interest for the period maximum entropy production of the organism. Then since the functioning is cyclic, in the relaxation functioning regime the minimum entropy production may be of interest for both drugs and organs interacting with the drugs. The evolvability maximization, EM criteria suggests using PFG mixture for minimum activity periods and BLT mixture for maximum activity. This follows the fact that EM ≈ ΔDD=DD (BLT)-DD (PFG) shows a maximum difference supposing that a ternary mixture is to be applied.

A supplementary measuring tool may be programmed to run the clinical evaluation experiment and adapt to different goals. This supplementary control device allows connecting the K3 level to resources S in the PSM scheme associated. High-throughput methods and laboratory automation technology have the potential to deliver the necessary data for drug design and development. To harvest this potential, experimental design has to become fully evolvable.

According to the presented framework, the system may ensure evolvability maximization, EM, if the level K3 is connected to the resources S. This challenging integrative closure supposes an iterated screening of drugs and drug evolution by interaction with the organism, resources and environment.

The perspective is the autonomous experimentation by systems being computationally capable of autonomous investigation of large experimental parameter space.

This may represents a first step towards, personalized drug delivery.

11.3.4 Acylthiocarbamates Library Design

Some acylthiocarbamates ATC can act as elastase inhibitors and exhibit anti-inflammatory and anti-arthritic effects. Ramise et al. (2008) investigated the anti HIV activity of ATC.

HIV, human immunodeficiency virus, is the causative agent of acquired immune deficiency syndrome AIDS.

Applicability of EDOE methodology for ATC library design is described here.

Fig. 11.5 shows the ATC structure. Different radicals are denoted by Ar1, Ar2, G-CO group and R (see Table 4.1 Ramise et al. 2008).

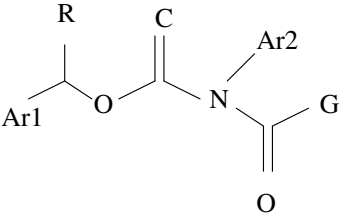

Fig. 11.5 Acylthiocarbamates structure

For ATC we considered associated vectors as: x= <Ar1, Ar2, G-CO, R>

The choice of this set of characteristics and of their hierarchy should be based on drug physiological mechanism.

Table 11.4 shows the radicals pertaining to different ATC.

Table 11.5 contains the same information as Table 11.4 in normalized form.

We use "1" for the same radical and "0" for a different one.

The cytoprotection data is EC_{50} (μM). This is the compound concentration required to reduce the viability of some cells by 50%.

The ATC denoted 19c was selected as a reference.

For 19c the Ar 1 is phenoxymethil, Ar2 is C_6H_5, the G-CO group is a benzoyl and the radical R is CH_3.

The vector associated to 19c is <1111>.

Table 11.4 Reference set for acylthiocarbamates-radicals

	Ar1	Ar2	G-CO	R	EC_{50}
19c	Phenoxymethyl	C_6H_5	Benzoyl	CH_3	1.3
17q	Phenoxymethyl	C_6H_5	2-furoyl	H	8.4
16c	Phenoxymethyl	C_6H_{11}	Benzoyl	H	200
20r	Phenoxymethyl	3-Cl- C_6H_4	2-thenoyl	CH_3	11

Table 11.5 Reference set for acylthiocarbamates-matrix

	Ar1	Ar2	G-CO	R
19c	1	1	1	1
17q	1	1	0	0
16c	1	0	1	0
20r	1	0	0	1

The compounds of the reference set have been selected to ensure a Walsh-Hadamard matrix for DOE. This offers the necessary variability for all types of drug substrate interaction.

By adding new compound to this reference mixture the entropy H varies.

There is only a small change of entropy, HΔ if the vector of the test compound is similar to the reference set and this supplementary compound is thought to have similar properties.

If a data base acylthiocarbamates shares similar bit patterns with reference set molecules, adding a similar compound will induce a change targeting the minimum entropy production.

By contrast, inclusion of an ATC compound having dissimilar vector leads to a higher entropy production, targeting the maximum entropy production.

In this way data base compounds may be screened to identify compound that cause low or high changes of the reference set informational entropy and detect other promising drug according to the established goal.

The component 17c= <1110> was tested since 17c was considered as lead compound. Other tested vectors are 24w =<0101>, 14c== <0110>, 37r== <0000>.

The results are shown in Table 11.6

Table 11.6 Informational entropies for Acylthiocarbamates

Mixture	Reference	Reference 17c	Reference 24w	Reference 37r	Reference 14c
H	7.5418	11.2615	12.8343	12.8343	13.0243
ΔH	0	3.7197	5.2925	5.2925	5.4825
DD	0	0.6348	0	0	0

It appears that supplementing the reference mixture by 17c, 24w, 37r or 14c has comparable small effect.

The compound 17c may be preferred for a conservative search based on similarity and 14c for an innovative one based on dissimilarity.

High ΔH and DD corresponds to differences allowing multiple, different classes and potential versatility.

To illustrate the selection criterion at this level we take into account that the organisms varies and show biorhythms (Beilharz et al., 2004). For different regimes for organism the delivery of different ATC mixtures may be beneficial, and ensure the evolvability maximization, EM that may be evaluated by comparing DD values.

The DD criteria suggest using reference, +17c for maximum activity periods and any other compound for minimum activity periods.

EM criteria may be correlated with the methods to monitor the biomarkers of the periodic functioning of organism. (Coventry et al. 2009) Researchers have

discovered that the body's immune system can destroy some cells within a window occurring every 12 to 14 days. By giving low-dose treatment at exactly the right time, they succeeded in halting the spread of advanced disease. Also they found the body has an immune cycle during which it switches "on" and "off". When the immune system turns off, it releases inhibitory cells which prevent it fighting disease. Treating organisms at the right time may maximize their evolvability. The timed drug delivery supposes an iterated screening of drugs and drug delivery by interaction with the organism, resources and environment.

11.4 Reliability Management System

The architecture of the reliability management system, RMS, for printed circuits is based on EDOE methodology (Iordache 2009).

The RMS includes the software allowing the reliability predictions, the reliability test mini-coupon design, the software for failure mode identification by classification, and the tests correlation software. For new product, it is necessary to addresses the problem of reliability evaluation and failure mode database grounding from the point of view of anomaly detection and the autonomous failure mode generation. Important questions are as follows. How DOE detects the newness of an unforeseen situation, which was not explicitly taken into account within design? How the control system detects a behavior anomaly? The EDOE frame emphasizes a continuous distinction between model-driven expectations and the reality based on accelerated tests. EDOE should have a scanning function that includes recognition of the familiar events and a strategy for un-programmed events. Large differences between expectation and reality indicate that a new reliability assessment possibly including new failure mode and supplementary analysis is required. It is expected that the modified EDOE will correspond more accurately to the recorded data.

The RMS architecture may be based on accelerated tests, IST (Iordache 2009).

Based on general PSM framework, it can be divided in four main modules or steps (Fig. 11.6). Fig. 11.6 shows a framework for reliability management system.

The first module K0 is represented by resources and involves resource mining. Resources are of material and of knowledge type. This module includes products to be tested, preliminary information about design tools, materials, processes, testing and application. This may include reliability prediction software.

The second module K1 is that of creation of a test coupon design. It is a step in which the basic parameter of the product are included. It should be based on designs of experiments, DOE. This DOE is embedded in a test coupon.

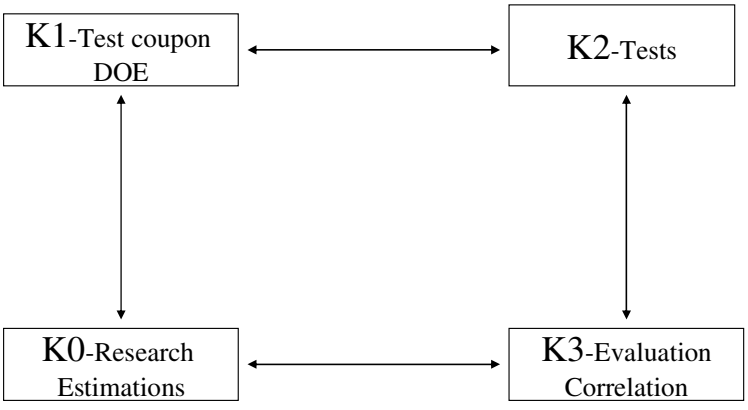

Fig. 11.6 Framework for reliability management system

An example of test coupon frame is shown in Table 11.7. Here A, B, C, D refers to hole diameters. Table 11.7 shows the matrix of a Latin square design.

Other parameters as pads diameters are selected according to recommended design ratios (Iordache 2009). The mini-coupons are embedded on the frame of production panels.

Table 11.7 Latin square design

A	B	C	D
B	A	D	C
C	D	A	B
D	C	B	A

The third module, K2, is that of reliability testing and development. It includes the proof of concept in accelerated and usual tests. A typical reject criterion is at 10 % of the initial electrical resistance. The number of thermal cycles to failure and the electrical resistance are recorded. The correlation model offers a domain for acceptable number of test cycles for different types of applications.

The anomalies, such as the inner layer, I/L, separation, called also post-separation, barrel or corner cracks should be recognized on the basis of resistance recording. The resistance versus nr of cycles is coded as 8-digit vectors (Iordache 2009). Each vector corresponds to a specific electrical resistance versus number of cycles diagram and this in turn to a tested sample. Here "1" denotes the presence and "0" the absence of resistance record in the focused rectangle of the diagram resistance as a function of number of cycles. Matrices of similarity, algorithms and grids of classification have been established.

To distinguish between conventional and non-conventional failures the algorithm must ensure that the comparison between sets of patterns is carried out in the intended way. There are several distances between database and new tested patterns to be tested. It is necessary to learn the appropriate distance, the acceptable degrees of similarity, and so forth. The classification table 11.8 shows an example. This table shows the resistance patterns in digital form for a reference set of tests and for tests to be classified.

The classification algorithm is: two patterns are assigned to the same class at the grouping degree T, 0<T<1, if their similarity in the stable matrix is larger than T.

The italicized vectors from {1} to {4}, corresponds to the examples retained for classification. This is a reference or training set.

It is a matrix with four rows and eight columns. The vectors {5}, {7}, {X} represent the samples to be classified. The Ni/Au plated samples as well as the soldered samples are classified in the same class as the barrel cracks. Both samples should show after micro sectioning, barrel cracks. The unknown sample denoted by X pertains to the same class as the vectors {3} and {4}. The cross-section outlined I/L separation.

Table 11.8 Resistance patterns. Classification table

#	Table	Failure	T =0.8	T =0.9	T =0.95
{1}	*1 0 0 0 1 0 0 0*	BC	{1,5,7}	{1,5,7}	{1}
{2}	*0 0 0 0 1 1 0 0*	CC	{2}	{2}	{2}
{3}	*1 1 0 0 0 1 0 0*	BC, CC, PS	{3,4,X}	{3,4,X}	{3,4,X}
{4}	*1 1 0 0 1 1 0 0*	CC, PS	{3,4,X}	{3,4,X}	{3,4,X}
{5}	1 0 0 0 0 1 1 1	Ni/Au	{1,5,7}	{1,5,7}	{5,7}
{7}	1 0 0 0 0 1 1 0	Soldered	{1,5,7}	{1,5,7}	{5,7}
{X}	1 1 0 0 0 1 1 0	BC, CC, PS	{3,4,X}	{3,4,X}	{3,4,X}

BC-barrel crack, CC-corner crack, PS-post-separation (I/L separation)

Table 11.8 shows evidence for two types of memory in classification tables.

Here T denotes the similarity degree. The first four digitalized patterns {1}, {2}, {3} and {4} pertain to long-term memory while the following patterns, {5}, {7} and {X} correspond to short-term memory. After coding the pattern vector enter in the short-term memory. Some information is lost by forgetting, but that which is retained is transferred to the long-term memory, where is organized in memory structures as classification tables. The knowledge database manages both static and dynamic information. Systems with permanent memory have been developed also. Recognition processes may be considered as a kind of memory; all that the task implies is the ability to advertise that what is perceived has been met before. Simply including the pattern produced by the classification algorithm within the database doesn't solve the problem. The resolution of sensors can be arbitrarily increased, so that they do not just determine whether some resistance dependence is a yes/no pattern but also detect fine differences between a “no” or “yes” class for the product. Perceptive frame should also include the evaluation of

reliability that is the system action. This is important because a change in pattern does not necessarily indicate problems unless it is coupled with an important change in external behavior. The classification soft may be supplemented with a set of corrective actions. For instance, if the I/L, inner layer-separation is detected the set of corrective actions is described according to the failure severity. It is possible to extend the frame to include other software components, as decision making once a failure mode is detected. In particular those components, which the observed anomaly-detection relies on, should have priority. The RMS needs to be periodically checked and up-dated. The method of software monitoring may involve the checking of expected signatures for failures with actual patterns and concentrates on monitoring of anomaly-detection. Modification in the control software may result in an anomalous behavior, but it may still continue to maintain the functioning level as required. It is necessary to establish what is important for survival. For some electronic devices, maintaining minimal reliability is the critical requirement.

It can be observed that different case studies may be processed by the same general EDOE framework.

Fig. 11.7 summarizes the different frameworks used in EDOE and outlines the integrative closure hypothesis.

The associated Peirce's categories are indicated also.

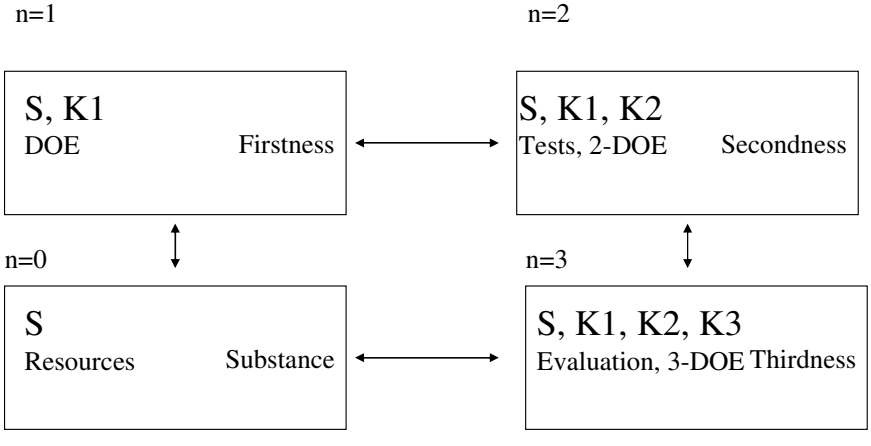

Fig. 11.7 Integrative closure for EDOE

References

Beilharz, M.W., Sammels, L.M., Paun, A., Shaw, K., van Eeden, P., Watson, M.W., Ashdown, M.L.: Timed ablation of regulatory CD4 $^{+}$ T cells can prevent murine AIDS progression. J. Immunol. 172, 4917–4925 (2004)

Bruguerolle, B., Prat, M.: Circadian phase-dependent pharmacokinetics and acute toxicity of mepivacaine. J. Pharm. Pharmacol. 40, 592–594 (1988)

Coventry, B.J., Ashdown, M.L., Quinn, M.A., Markovic, S.N., Yatomi-Clarke, S.L., Robinson, A.P.: CRP identifies homeostatic immune oscillations in cancer patients: a potential treatment targeting tool? Journal of Translational Medicine 7(102), 1–8 (2009)

Ghose, A.K., Viswanadhan, V.N., Wendoloski, J.J.: A Knowledge-Based Approach in Designing Combinatorial or Medicinal Chemistry Libraries for Drug Discovery. J. Combin. Chem. 1, 55–68 (1999)

Hann, M.H., Oprea, T.I.: Pursuing the leadlikeness concept in pharmaceutical research. Current Opinion in Chemical Biology 8, 255–263 (2004)

Iordache, O.: Evolvable Designs of Experiments Applications for Circuits. J. Wiley VCH, Weinheim (2009)

Iordache, O.: Polystochastic Models for Complexity. Springer, Heidelberg (2010)

Iordache, O., Isopescu, R., Isopescu, A., Morariu, V.V.: Structure activity relationship for local anesthetic agents based on the similarity with procaine. Rev. Roum. Biochim. 26, 321–324 (1989)

Iordache, O., Corriou, J.P., Garrido-Sanchez, L., Fonteix, C., Tondeur, D.: Neural network frames applied for biochemical kinetic diagnosis. Comp. Chem. Engng. 17, 1101–1113 (1993a)

Iordache, O., Corriou, J.P., Tondeur, D.: Separation Sequencing. Use of Information Distance. Canad. Journ. of Chem. Engng. 71(12), 955–966 (1993b)

Kaweski, S.: Topical Anesthetic Creams. Plast Reconstr. Surg. 121(6), 2161–2165 (2008)

Kravitz, N.D.: The use of compound topical anesthetics. A review, J. Am. Dent. Assoc. 138, 1333–1339 (2007)

Lee, C.M.W.: Topical Triple-Anesthetic Gel Compared with 3 topical anesthetics. Cosmetic Dermatology 16(4), 35–38 (2003)

Lipinski, C.A., Lombardo, F., Dominy, B.W., Feeney, P.J.: Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings. Adv. Drug Del. Rev. 23, 3–25 (1997)

Ramise, A., Spallarosa, A., Cesarini, S.: A successful application of parallel synthesis to computer-assisted structural optimization of new leads targeting human immunodeficiency virus-1 reverse transcriptase. The case of acylthiocarbamates and thiocarbamates. In: Kshirsagar, T. (ed.) High-Throughput Lead Optimization in Drug Discovery, pp. 117–150. CRC Press, Boca Raton (2008)

Torrens, F., Castellano, G.: Periodic Classification of Local Anaestetics (Procaine Analogues). Int. J. Mol. Sci. 7, 12–34 (2006)

Verderame, M.: Handbook of CNS Agents and Local Anesthetics. CRC Press, Boca Raton (1986)

Wang, Y., Geppert, H., Bajorath, J.: Shannon entropy-based fingerprint similarity search strategy. J. Chem. Inf. Model 49(7), 1687–1691 (2009)

Willett, P.: Chemical similarity searching. J. Chem. Inf. Comput. Sci. 38, 983–996 (1989)

Wood, J., Rose, V.S.: Method of designing chemical substances. PCT WO 99/26901 (1999)

Woodcock, J., Woosley, R.: The FDA critical path initiative and its influence on new drug development. Annu. Rev. Med. 59, 1–12 (2008)

Chapter 12
Autonomous Systems Perspective

Abstract. Complexity advent determined the drive change from learning and adaptability to evolvability and autonomy for technologies, devices and problem solving methods.

The connection of the presented multi-level modeling methods with some promising research directions for autonomous systems is outlined. This helps in understanding where future multi-level complexity studies will be heading.

Centered, four realms general PSM frameworks, resulting by integrative closure are presented here as the general architecture shared by numerous autonomous systems.

Autonomous experimentation, multi-agents systems, multi-level informational systems, organic or autonomic computing systems, and viable systems are presented as promising domains for applications.

12.1 Autonomous Experimentation

Quantitative, predictive understanding of complex systems requires comprehensive information. High-throughput methods and laboratory automation technology have the potential to deliver the necessary data. To harvest this potential, experimental design has to become evolvable and autonomous.

Autonomous experimentation systems are computational systems capable of autonomously investigating large experimental parameter space (Matsumaru et. al. 2004, Lovel and Zauner 2009).

Such systems should develop hypotheses, plan experiments and perform experiments in a closed loop manner without human interaction.

Fig. 12.1 illustrates the autonomous experimentation architecture principle.

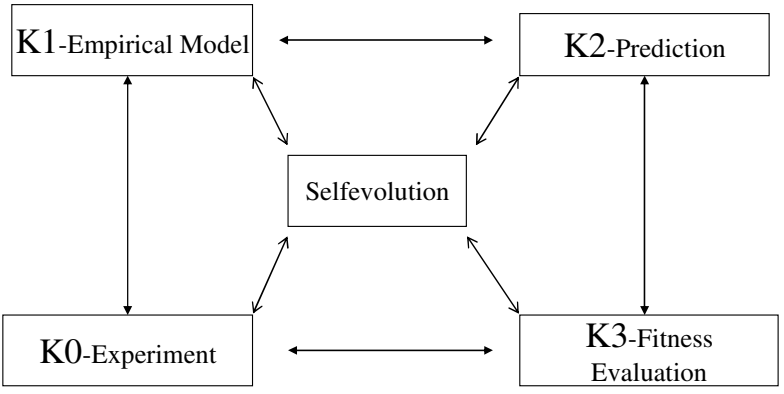

Fig. 12.1 Architecture for autonomous experimentation

It is an integrative closure technique.

The levels may be identified as follows: K0-Experiment, K1-empirical model, K2-Prediction, K3-Evaluation. To these the central level of selfevolution linked to the previous levels is joined. The center is considered either as the starting area or as the final area of one cycle of investigations. The periodic switching between the two roles may be considered too.

In this new approach, artificial intelligence techniques are employed to carry out the entire cycle of cognition including the elaboration of hypothesis to explain observations, the design of experiments to test these hypotheses and the physical implementation of the experiments using laboratory automats to falsify hypotheses.

In the coming decades a confluence of wireless networks and lab-on-chip sensor technology with application in health monitoring is expected. In such lab-on chip network each sensor node is endowed with a limited supply of chemicals. The network will collectively or via the selfevolution level decide how the drug resources will be spent.

Environmental monitoring and improving, new drugs and new material discoveries may be performed by similar autonomous experimentation architectures.

12.2 Case Based Reasoning Systems

Conventional cases based reasoning, CBR, is a problem solving paradigm that solves the new problem by remembering a previous similar situation and by reusing information and knowledge of that situation (Aamodt and Plaza 1994, Aha et al. 2001). More specifically, CBR builds and uses a database of problems to resolve new problems. The database can be built through the knowledge engineering process or it can be collected from previous cases.

In a problem-solving system, each case would describe a problem and a solution to that problem. The reasoning engine solves new problems by adapting relevant cases from the library. Moreover, CBR should learn from previous experiences. When a problem is solved, the CBR engine can add the problem

description and the solution to the case library. The new case that in general represented as a pair <problem, solution> is made available and can be considered as a new piece of knowledge.

The CBR process can be represented by a schematic cycle, as shown in Fig. 12.2.

Fig. 12.2 shows the CBR basic framework. Aamodt and Plaza (1994) have described CBR typically as cyclical process comprising the four steps: recall, reuse, revise and retain.

During the recall step, the CBR engine searches the database to find the most approximate case to the current situation.

The reuse step process includes utilizing the retrieved case and adapting it to the new situation. At the end of this process, the user might propose a new solution.

Since the proposed solution could be inadequate, the revise process can correct the first proposed solution.

The retain process enables CBR to learn and create a new solution and a new case that should be added to the case base.

The recall process in CBR is different from the process in a database. If we want to query data, the database only retrieves some data using an exact matching while a CBR can retrieve data using an approximate matching. A similarity measure should be defined.

As shown in Fig. 12.2, the CBR cycle starts with the description of a new problem, which can be solved by recalling previous cases and reusing solved cases, if possible, revising the solution and giving a suggested solution, retaining the restored case and incorporating it into the case base.

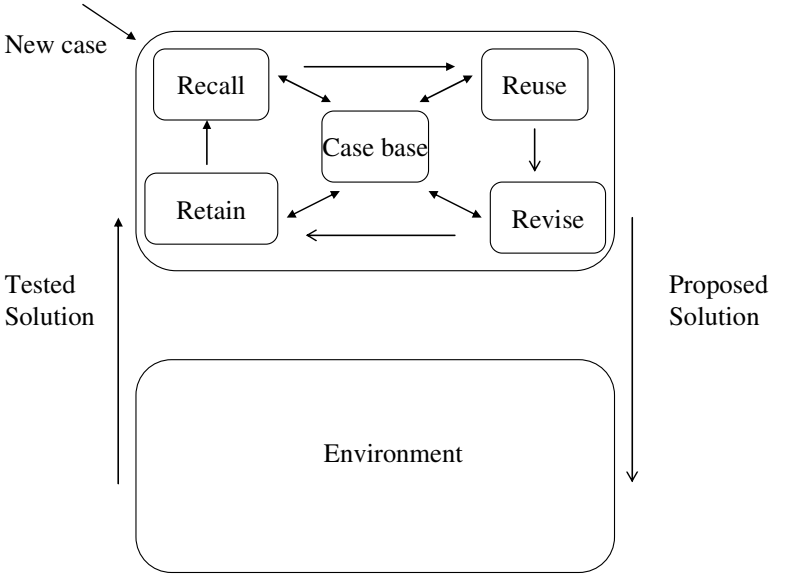

Fig. 12.2 CBR basic framework

This cycle rarely occurs without human intervention that is usually involved in the retain step. Many application systems and tools act as a case retrieval system, such as help desk systems and customer support systems.

The CBR provides support for applications if the input data tend to repeat similar patterns from time to time. When the factors recur, the studied system is likely to display regularly repetitive patterns. This repetitiveness explains why it is reasonably to apply CBR in complex problem solving situations.

Conventional CBR have limited potential. For example in standard versions, CBR involves just one user and don't answer in real-time to explosive amount of user data, to the unexpected cases, or to non-linear interacting cases and questions.

It is a need to implement CBR frameworks in which answers to multiple questions are gathered from multiple information sources, in real time.

For continuously addressing multiple-goals, multiple arrays of CBR cells systems are needed. For such arrays it is difficult to arrange the architecture or scheme of problem-solving, to schedule, to elaborate and to run rules, to adjust them to continuous changing environment.

Problem solving methodologies as case-based reasoning CBR are confronted with high complexity situation due to chaotic or random character of data, and to severe time restrictions. The method to confront the high complexity is that of evolvability and autonomy. This implies developing the conventional passive CBR, to an evolvable one, ECBR. ECBR should be active and autonomous, able to take control of its environment, able of responding to random unexpected problems and to large amounts of knowledge in real-time.

Applications of CBR methodology for autonomous service failure diagnosis have been proposed (Montani and Anglano, 2006). This kind of CBR approach allows self-healing in software systems. Pharmacological and medical applications have been considered too.

Fig. 12.3 shows a four realms categorical framework for CBR. The four realms are K0-Retain-T, K1-Recall-C, K2-Reuse-U and K3-Revise-V.

K0 reflects the environment response.

The architecture shown in Fig. 12.3 outlines the integrative closure hypothesis including the critical link between K0 and K3 and assisting evolvability and autonomy.

This link may be established by implementing autonomic computing paradigm.

This paradigm studies methods for increasing environment-awareness and automatic responsiveness. Autonomic or organic computing methods promise to facilitate CBR tasks and facilitate information capture (Montani and Anglano 2006).

Formal concept analysis, FCA, may support evolvable CBR designers in the task of discovering patterns, regularities and exceptions among the cases (Diaz-Agudo and Gonzales-Calero 2001).

Fig. 12.3 shows centered and self-similar CBR architectures.

A similar structure is repeated starting from the whole central system that may be built by four sub-realms denoted here by k0, k1, k2 and k3. This appears as a meta-representation of the four-fold architecture and is associated to knowledge.

The center may be considered as the starting as the final area of one problem solving cycle. The periodic switching between the two roles may be taken into account too.

For pharmacological and medical applications this switching may be correlated to biorhytms.

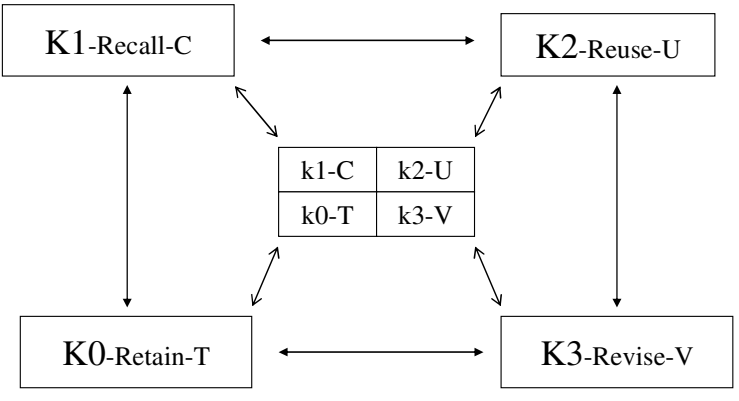

Fig. 12.3 Centered frameworks for evolvable CBR

Comparison of Fig. 12.2 with Fig. 12.3 suggests that the centering is a method similar to development of a case base. This implies long memory capability.

The interest in multi-modal approaches involving CBR is recently increasing through different application areas ranging from diagnosis to medical support (Schmidt et al. 2001). The goal was to demonstrate the advantage of relying different technologies, by coupling them, or by switching between one to other, when the aim is to provide a system with autonomic diagnosis and remediation capabilities.

12.3 Belief Desire Intention Agents

The belief desire intentions, BDI, agent introduced a formal meta-language to express agent rationality in an explicit way. BDI architecture is one of numerous architectures that enact deliberative agents. The BDI agent architecture is an attempt to encapsulate the hidden complexity of the inner functioning of an individual agent.

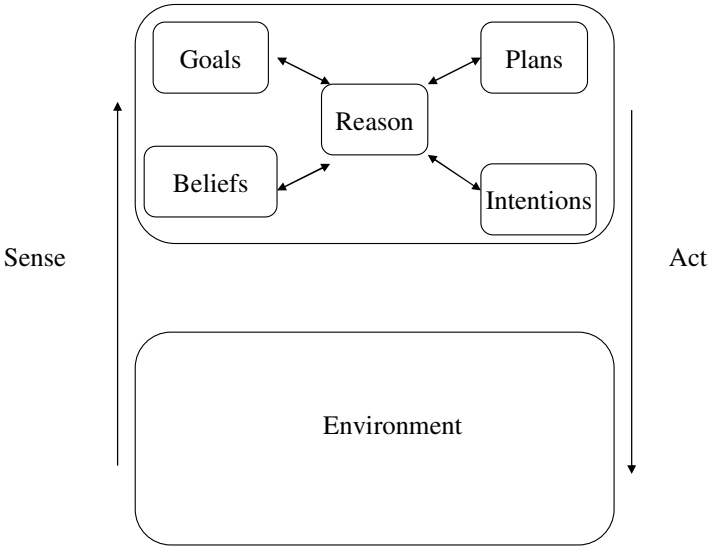

Fig. 12.4 Structure of BDI agents

Fig. 12.4 shows the structure of BDI agents.

The agent shown in Fig. 12.4 is structured in four elements: beliefs, goals, plans and intentions (Rao and Georgeff 1991).

To relate events, E to the agents who form plans and execute them, three determining factors should be distinguished: beliefs, B desires, D and intentions, I. All these elements are essential and that none of them can be reduced to the others (Bratman 1987).

Accordinf to Sowa (2003) the desire is close to Peirce's firstness, K1. Belief is a kind of secondness, K2, that relates a proposition to a situation and intention is a kind of thirdness, K3 that relates an agent, a situation, and the agent's plan for action in the situation.

Fig. 12.5 shows a categorical presentation for evolvable architecture.

In this presentation the four modules are: K0-Events, E, K1-Desire, D, K2-Beliefs, B, K3-Intentions, I.It is an EDBI frame.

The architecture shown in Fig. 12.5 outlines the possibility of integrative closure allowed by the link between K0 and K3 smoothing the road for evolvability and autonomy.

Fig. 12.5 outlines the centered and self-similar architectures

A similar structure is repeated starting from the whole central system built by four sub-realms denoted here by k0, k1, k2 and k3. This is a meta-representation of the four-fold architecture.

The center, or in other words, the "Self", may be considered as the starting and the final area of one cycle of investigations. The switching between the two roles may be considered too.

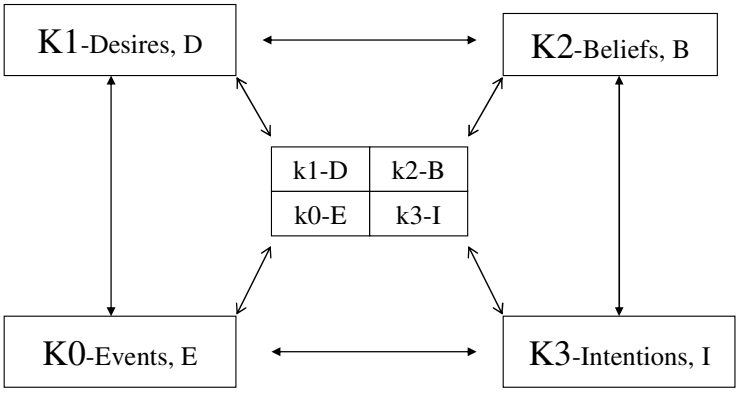

Fig. 12.5 Centered frameworks for evolvable BDI architecture

Innovative multiple-scale BDI agent architectures have been proposed by Goschnick (Goschnick 2003).

Based on analytical psychology Goschnick developed a Digital-Self cognitive architecture. This implies:

- Decomposition of a user's multiplicity of roles into a hierarchy of sub-agency
- Relaxing of the autonomy of the sub-agents under control of an autonomous central agent-the so called "Self" agent.
- Wrapping of the external services and agencies including the web services and utilizing them as if they were internal sub-agents
- Ability to apply ontology at the localized level

The proposed cognitive architecture proves that the user interface of a workstation connected continuously to a network would be most effective with an advanced agent architecture embedded deep in the workstation system software.

12.4 Autonomic and Organic Computing

Over the past years technical systems as vehicles, airplanes, telecommunication networks, manufacturing installations became more and more complex. This is the result of the embedding of hardware and software into these systems. With respect to the future evolution new advanced management principles have to be developed. A feasible principle is an autonomic behavior of the system which is addressed by two research directions, namely autonomic and organic computing. Autonomy with its reference to a self (autos) refers to an independence from external influences of different sort.

Biologically inspired autonomic and organic computing systems are essentially concerned with creating self-directed and self-managing systems based on suggestions from nature and the human body, such as autonomic nervous system.

Autonomic computing (Kephart and Chess 2003) is a computing initiative that draw analogies from the autonomic nervous system where all reactions occur without explicit override by the human brain-so to say autonomous. By embedding this behavior into technical systems, the complexity can be left to the systems themselves. One refers to this autonomy as self-x properties. This means self-configuration (configuration and reconfiguration according to policies), self-optimization (permanent improvement of performance and efficiency), self-healing (reactive and proactive detection, diagnostics and reparation of localized problems) and self-protection (defense of the system as a whole). Furthermore autonomic computing systems would be self-aware, context sensitive, anticipative and adaptive.

Organic computing system instead draw analogies from living systems and try to use perceptions about the functionality of living systems for the development and management of artificial and technical systems. In addition to the properties of autonomic computing systems they are defined as being self-organizing. This is a critical step to ensure autonomy.

It should be noted that similar architectures are of interest for both autonomic and organic computing (Trumler et al. 2004, IBM 2005, Bauer and Kasinger 2006).

The logical structure of an autonomic element is similar to that of evolvable BDI agents.

For autonomic computing, the agent structure is replaced by the so-called MAPE loop whose elements are M-Monitor, A-Analyze, P-Plans, and E-Execute.

Autonomic computing systems are composed of four levels that may be identified as K0 or S-Managed Resources, K1-Touchpoints, K2- Touchpoints Autonomic Managers, K3-Orchestred Autonomic Managers. To this a central Manual Manager is to be considered. The closed loop in which K3 is replaced by an automatic device was presented by IBM (2005).

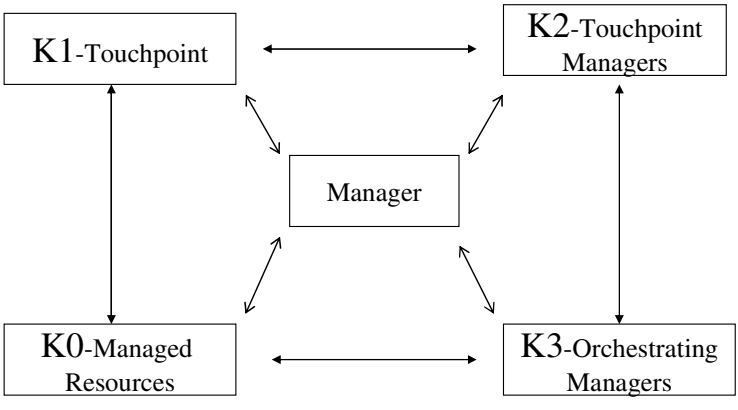

Fig. 12.6 Automatic computing architecture

Fig. 12.6 shows the automatic computing architecture.

For the organic computing middleware architecture, the levels may be identified as: K0 or S as the Network, K1-Transport Interface, K2-Event Dispatcher, K3-Service Interface and Proxy (Trumler et al. 2004). To these an Organic Manager is joined.

In the middleware architecture the organic manager is linked to the previous levels and ensures a meta-representation of them.This is critical for self-organization.

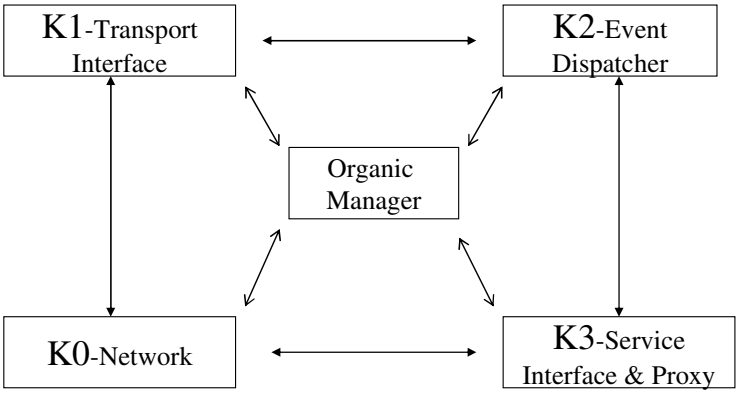

Fig. 12.7 Organic computing architecture

Fig. 12.7 shows the automatic computing architecture.

Successes of autonomic and organic computing have been reported in the fields of drug discovery, data communications, computer animation, control and command, exploration systems for space, undersea and harsh environments and there exists much promise for future progress.

12.5 Autonomous Animats

Autonomous animats should evolve in non-cooperative even hostile outdoor environments. Reaction to disturbance is a first step towards autonomy.

A more demanding definition of autonomy includes the ability to change the interaction modes with the environment. An autonomous organization has to internalize external constraints, which means the ability to integrate knowledge of its own dynamics and representation of the exterior. Such ability is closely connected to the awareness of a frontier between the inside and outside of the system, which means operational closure (Maturana and Varela 1992). Arkin (1998) presented a general overview of control architectures for animats.

Fig. 12.8 shows the autonomous animats architecture (Luzeaux 2000).

For this autonomous animats architecture, the levels may be identified as: K0 or S as the Perception, K1-Attention Manager, K2-Behavior Selection, and

K3-Action. To these the central meta-representation linked to the previous levels is joined.

The center may be considered as the final target of one cycle of environment investigations.

Sensors yield data to perception algorithms which create representations of the environment. These perception processes are activated or inhibited by the attention manager and receive also information on the current executed behavior. This information is used to check the consistency of the representation. The attention manager periodically updates representations. The action selection module chooses the animats behavior depending on the predefined goals, the current action, the representations and their reliability.

Finally the behaviors control the animats actuators in closed loop with the associated perception processes.

This modular architecture allows developing independently the various processes belonging to each of the four basic entities, integrating them together.

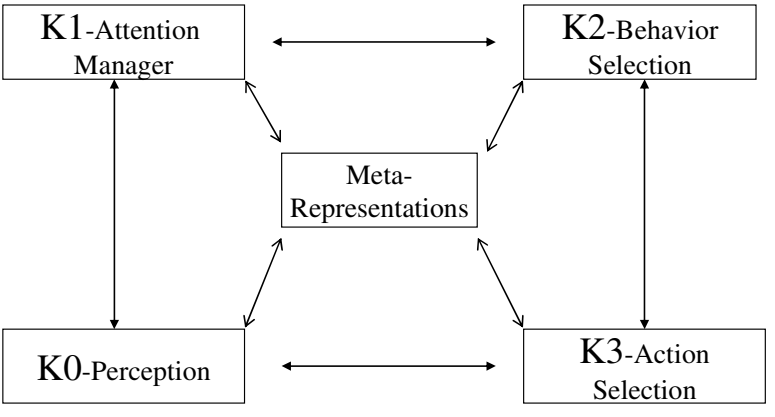

Fig. 12.8 Architecture for autonomous animats

Current developments focus on the extension of architecture to multiple animats. A major issue is to determine how the representation of every animate can be shared and how individual behavior selection can take the other animats' selected behavior into account, allowing group missions such as scouting.

12.6 Viable Systems Models

Viable system theory was a particular interest of Beer (1985) that recognized the practical utility of concepts as multi-levels and meta-system and used these as ways of exploring the viability of complex social systems through processes of self-regulation, self-organization and control. Knowledge cybernetics is an

approach principally concerned with the development of agents like autonomous social collectives that survive through knowledge and knowledge processes (Yolles 2006).

Fig. 12.9 shows an example of viable system architecture.

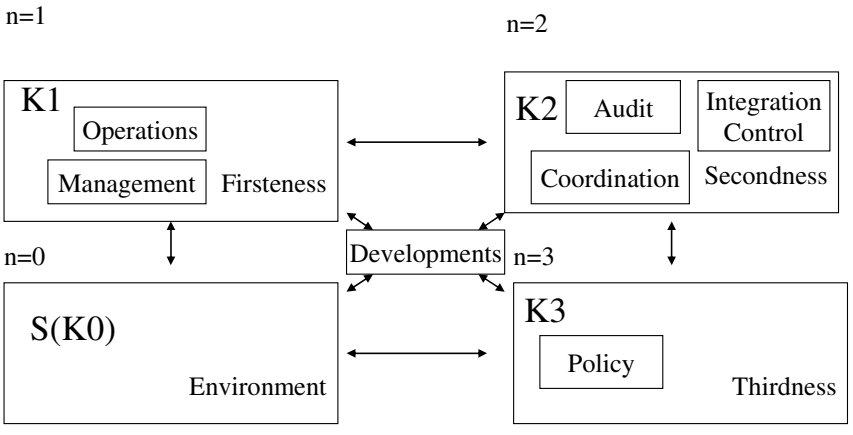

Fig. 12.9 Architecture for viable systems

For this architecture, the levels may be identified as: K0 or S as the Environment, K1-Management, K2-Control and Coordination and K3-Policy. The Developments module, linking the previous levels, is critical for viability.

The center is considered as the starting area of one life cycle of the system.

The frame of viable systems modeling architecture has demonstrated a great deal of potential in creating ways of analysing complex situations and demonstrated a possibility to be used to diagnose complex situations and to be used as a mean by which improvement can be engineered.

12.7 Meta-modeling Architectures

Since the complex systems are structured in levels of realms, associated to multiple scales it is expected that the modeling methods will adopt a similar hierarchical or network architecture.

The four level structures were proposed by the object management group OMG to describe informational systems. OMG is an organisation for the standardization in the object oriented field of the software development in which many of the leading software production companies participate

For OMG the first layer refers to data, the second layer to subject matter models that is models of data, the third layer to statistical methodologies that is to meta-models and the fourth layer to methodologies that define methodologies that is to meta-meta-models. Additionally a lower level layer representing physical reality joins the OMG architecture.

The four levels will be denoted here by K3, K2, K1, and K0, respectively. K3 is the fourth level, the so-called meta-meta-models level. One model at level K3 is necessary to define all the K2 level models. The OMG standard for the K3 model, also called Meta Object Facility, MOF, is able to define itself (Crawley et al. 1997). MOF is a common framework that is used to define other modeling frameworks within the OMG. K3-model is the language used by MOF to build meta-models, called also K2-models. Examples of the third level, K2-models are the Universal-Modeling Language, UML, model and the relational models. UML has been accepted as a standard notation for modeling object-oriented software systems. Correspondently, at the second level, K1, there are UML models and relational models relevant to a specific subject. K1 is based on user concepts. First level, K0, contains user runtime data or objects. It may be used to describe the real world.

Different meta-meta-model architectures have been considered as for instance that shown in Fig. 12.10. In this case the linear or hierarchical architecture was developed in cyclic or self-similar architectures (Alvarez et al. 2001).The top and bottom levels in architectures are different. In the hierarchical meta-meta-model architecture every element should be an instance of exactly one element of a model in the immediate next level.

For example, the level K3 could describe elements from the UML meta-model K2 but not elements from the user models K1.More flexibility is allowed by the centered architectures shown in Fig. 12.10. Fig. 12.10 shows centered meta-meta-model frameworks. In the centered architecture a model can describe elements from every meta-model below it. This is a significant feature since it means that if a tool implements the K3 meta-meta-model than it can be used to define languages such as UML but user models and objects as well. The centered Meta-Modeling Language, MML, architecture shown in Fig. 12.10 outlines the possibility of integrative closure hypothesis including the critical link between K0 and K3 and allowing evolvability and autonomy.

The centered structure architecture should be not restrained to four realms.

Fig. 12.10 shows centered and self-similar spiral architectures

A similar structure is repeated to four sub-realms denoted here by k0, k1, k2 and k3.

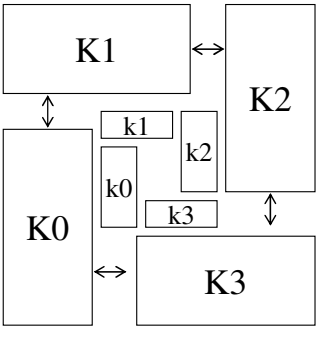

Fig. 12.10 Centered meta-meta-modeling frameworks

Fig. 12.10 suggests that an integrative closure hypothesis does not have to be seen as a final stage or a balance due to equilibrium, but rather as a process that can develop self-similar patterns. Centered structures may unify large systems. The initial frame offers a generic, four-fold, relational model whose elements are configured as a self-similar structure. This means that it can be re-scaled from the smallest to the largest or reversely without compromising its form.

This has the advantage that it is a configuration that is shareable across different domains. The self-similarity allows analogous processing with similar software. In this centered architecture, the transformation between the representation of any model at one meta-level and its representation in the meta-level below can be described by information preserving one-to-one mapping.

The mapping provides the basis for a powerful area of functionality that any potential meta-modeling tool should look to exploit.

References

Aamodt, A., Plaza, E.: Case-based reasoning: Foundational issues, methodological variations, and system approaches. AI Communications 7(1), 39–59 (1994)

Aha, D.W., Breslow, L.A., Munoz-Avilla, H.: Conversational case-based reasoning. Applied Intelligence 14(1), 9–32 (2001)

Alvarez, J., Evans, A., Sammut, P.: MML and the meta-model architecture. In: Workshop on Transformations in UML (WTUML 2001), Genoa (2001)

Arkin, R.: Behaviour-based robotics. Bradford Book, MIT Press (1998)

Bauer, B., Kasinger, H.: AOSE and organic computing-how can they benefits from each other. Position paper. AOSE III. Springer, Heidelberg (2006)

Beer, S.: Diagnosing the System. J. Wiley, Chichester (1985)

Bratman, M.E.: Intentions, Plans, and Practical Reason. Harvard University Press, Cambridge (1987)

Crawley, S., Davis, S., Indulska, J., McBride, S., Raymond, K.: Meta-meta is better-better. In: International Working Conference on Distributed Applications and Interoperable Systems, DAIS 1997, Cottbus, Germany (1997)

Diaz-Agudo, B., Gonzalez-Calero, P.A.: Formal concept analysis as a suport technique for CBR. Knowledge Based Systems 14, 163–171 (2001)

Goschnick, S.B.: Enacting an Agent-Based Digital Self in a 24x7 Web Services World. In: Zhong, N., Raś, Z.W., Tsumoto, S., Suzuki, E. (eds.) ISMIS 2003. LNCS (LNAI), vol. 2871, pp. 187–196. Springer, Heidelberg (2003)

IBM : An architectural blueprint for automatic computing (2005)

Kephart, J.O., Chess, D.M.: The vision of autonomic computing. IEEE Computer 36(1), 41–50 (2003)

Lovel, C.J., Zauner, K.-P.: Towards algorithms for autonomous experimentation. In: Naef, F., Galliot, B., Nehaniv, C. (eds.) Proceedings of the 8th International Conference on Information Processing in Cells and Tissues (IPCAT 2009), pp. 150–152 (2009)

Luzeaux, D.: Autonomous small robots for military applications. In: Proc. SPIE, vol. 4024, p. 23 (2000)

Matsumaru, N., Centler, F., Zauner, K.P., Dittrich, P.: Self-adaptive scouting—autonomous experimentation for systems biology. In: Raidl, G.R., Cagnoni, S., Branke, J., Corne, D.W., Drechsler, R., Jin, Y., Johnson, C.G., Machado, P., Marchiori, E., Rothlauf, F., Smith, G.D., Squillero, G. (eds.) EvoWorkshops 2004. LNCS, vol. 3005, pp. 52–62. Springer, Heidelberg (2004)

Maturana, H., Varela, F.: The tree of knowledge: The biological roots of human understanding. Shambala, Boston (1992)

Montani, S., Anglano, C.: Case-Based Reasoning for Autonomous Service Failure Diagnosis and Remediation in Software Systems. In: Roth-Berghofer, T.R., Göker, M.H., Güvenir, H.A. (eds.) ECCBR 2006. LNCS (LNAI), vol. 4106, pp. 489–503. Springer, Heidelberg (2006)

Rao, A., Georgeff, M.: Modelling rational agents with a BDI architecture. In: Allen, J., Fikes, R., Sandewall, E. (eds.) Proceedings of Knowledge Representation and Reasoning. Morgan Kaufman Publishers, San Mateo (1991)

Schmidt, R., Montani, S., Belazzi, R., Portinale, S., Gierl, L.: Case-based reasoning for medical knowledge-based systems. International Journal of Medical Informatics 64(2-3), 355–367 (2001)

Sowa, J.F.: Laws, facts, and contexts: Foundations for multimodal reasoning. In: Hendricks, V.F., Jørgensen, K.F., Pedersen, A. (eds.) Knowledge Contributors, pp. 145–184. Kluwer Academic Publishers, Dordrecht (2003)

Trumler, W., Bagci, F., Petzold, J., Ungerer, T.: Towards an organic middleware for the smart dooplate project. GI Jahrestagung 2004(2), 626–630 (2004)

Yolles, M.I.: Organisations as Complex Systems: An Introduction to Knowledge Cybernetics. Information Age Publishing, Inc., Greenwich (2006)

Appendices

Appendix 1
Non-Archimedean Analysis

Abstract. Non-Archimedean analysis is an appropriate modeling tool for hierarchical multi-level systems.

Notions as, valued fields, normed linear spaces, and orthogonality are introduced and compared to corresponding real analysis notions.

A1.1 Valued Fields

An NA field K is a field such that there exists a, b $\in$ K such that for any integer n, na < b. Define a mapping $|\ |: K \rightarrow R$ such that for all a, b $\in$ K:

i) $|a| \geq 0$ and $|a| = 0$ iff $a = 0$
ii) $|ab| = |a|\,|b|$
iii) $|a+b| \leq \max(|a|, |b|)$

This mapping is an NA valuation on K.

The modified triangle inequality causes important deviations from the standard (real or complex field) analysis.

The trivial valuation on K is resulting if $|a| = 1$ if $a \neq 0$ and $|0| = 0$.

Let $G = \{|a|, a \in K, a \neq 0\}$. The valuation is discrete if G is a cyclic group. Otherwise the valuation is dense.

Some examples of valuations and valued fields follow.

i) The p-adic valuation on Q (Q denotes the rational numbers).

Let p be a prime number. Any a $\in$ Q is of the form $a = \frac{m}{n} p^k$, with k, m, n $\in$ Z, and m, n not divisible by p. The p-adic valuation is defined by: $|a|_p = p^{-k}$.

ii) The field K, of Neder (Neder 1941, 1943, Lightstone and Robinson 1975). The elements of this field are of the form:

$K = \{a_0 + a_1\varepsilon + a_2\varepsilon^2 + ... + a_m\varepsilon^m + ...\}$ where $a_k \in R$, $m \in N$. Let A, B $\in$ K

$A = [a_0,a_1,...,a_m,...]$, $B = [b_0,b_1,...,b_m,...]$. A=B if $a_k=b_k$ for all k. The order on K is given by the relation A < B if $a_k=b_k$ if k < j and $a_j < b_j$ for some $j \le m$. Define $A+B=[a_0+b_0, a_1+b_1,..., a_m+b_m,...]$. The null element is $O=[0,0,...,0,...]$.Define $A.B=[a_0b_0, a_0b_1+a_1b_0, a_0b_2+a_1b_1+a_2b_0,...]$. The unit element is $I = [1,0,...,0,...]$. K is closed under this definition of addition and multiplication. Define also $kA = [ka_0,ka_1,...,ka_m,...]$ with k real. K is NA Indeed let $A =[0,1,0,...,0]$ and $B = [1,0,...,0]$. For any integer k, $kA = [0,k,0,...,0] < B$. So A is infinitesimal.

Moreover any $A = [0,..., 0, a_j,...,a_m]$ is infinitesimal for j < m.

Let the two-component vectors $A = [a_0, a_1]$, $B = [b_0, b_1]$.

Then $A/B = [a_0/b_0, (a_1b_0-a_0b_1)/b_0^2]$ if $b_0 \neq 0$ and $A/B = [a_1/b_1,0]$ if $a_0=b_0=0, b_1 \neq 0$.

The ratio A/B=C is obtained solving the equation A=B.C with $C = [c_0, c_1,..., c_m]$.

Let $A = [a_0, a_1,..., a_m,...]$. A non trivial NA valuation on K is defined by:

$|A| = r^{-k}$ with r > 1 if $a_0,..., a_{k-1} = 0$ but $a_k \neq 0$. An NA function $F : K \rightarrow K$ is defined by $F(A) = [f_0(a_0), f_1(a_0),..., f_m(a_0),...]$ where $A = [a_0, a_1,..., a_m,...]$ and $f_0, f_1,..., f_m$ are real functions.

If the expansions will be limited to a fixed m the resulting structure is a ring, the Neder ring, K. For fixed or variable m, we will refer to K as the Neder NA structure.

iii) For any integer $n \in \{2, 3,...\}$ let Z_n be the set of all sequences....a_m ....a_1a_0 where a_m is one of the elements 0, 1,..., n-1. The elements of Z_n are the n-adic integers. Let p be a prime and let ...$a_2a_1a_0$ be an element of Z_p.

The order of... $a_2a_1a_0$ is the smallest m for which $a_m=0$ that is: $ord_p(...a_2a_1a_0)= \infty$ if $a_i=0$ for all i or, $ord_p(...a_2a_1a_0)=\min\{s, a_s \neq 0\}$ otherwise.

Define also $|...a_2a_1a_0|_p = 0$ if $a_i=0$ for all i and $|...a_2a_1a_0|_p = p^{-ord_p(...a_2a_1a_0)}$ otherwise. The function $|\,.\,|_p$ is the p-adic valuation on Z_p.

A1.2 Normed Linear Spaces and Orthogonality

Let E be a linear space over K, an NA valued field. Define the mapping $\|\ \|$: $E \rightarrow R$ such that for any $x, y \in E$ and any scalar $a \in K$:

i) $\|x\| \ge o$ and $\|x\| = 0$ iff x=0
ii) $\|ax\| = |a|\,\|x\|$
iii) $\|x+y\| \le \max\{\|x\|, \|y\|\}$

This will be called NA norm over K. E will be called an NA normed space.

Observe that $\|x+y\| = \|x\|$ if $\|y\| < \|x\|$. In terms of geometry this means that all triangles are isosceles.

Define an NA metric $d : E \times E \rightarrow R$ by $d(x,y) = \|x-y\|$. Obviously:

i) $d(x,y) \geq 0$ and $d(x,y) = 0$
ii) $d(x,y) = d(y,x)$
iii) $d(x,z) \leq \max\{d(x,y), d(y,z)\}$

A sphere $\{x \mid d(y,x) \leq r\}$ is the set of all points such that the distance to the center y is less or equal to r. All points of the sphere can be taken as the center of the sphere.

A sphere may have infinitely many radii. The topology of an NA space has a base consisting of closed and open sets, a zero-dimensional topology. The distance between two non-empty subsets A and B is: $d(A, B) = \inf\{d(x,y); x \in A, y \in B\}$.

Let X, Y, $a \in Y$. Then b, is a best approximation of a in Y if:

$$d(a,b)=d(a,Y)=\inf\{d(x,y); x \in A, y \in B\}$$

Contrary to the Archimedean case in NA case a best approximation is, with trivial exceptions, never unique.

The orthogonality in normed linear spaces is presented in what follows.

The definition of an inner (scalar) product in a vector space over R or C makes uses of the ordering in R. The strong triangle inequality implies among other things that the NA frames is totally disconnected and cannot be made into a totally ordered field.

However it is possible to introduce orthogonality, using the concept of "best approximation" (Monna 1970).

Let E be a normed NA space on K. The family $\{(x_i), i \in I\}$, $x_i \in E$, $x_i \neq 0$ is called orthogonal if: for any $a_i \in K$ and $S \in I$

$$\| \Sigma_{i \in S} a_i x_i \| = \max_{i \in S} \|a_i x_i\| \qquad \text{(A1.1)}$$

An equivalent definition is the following: x and y are orthogonal that is, $x \perp y$, if:

$$\inf_a \|x-ay\| = \|x\| \qquad \text{(A1.2)}$$

From $x \perp y$ and $x \perp z$ it doesn't follow that $x \perp (y+z)$ as in real analysis. A basic property in NA analysis is that $x \perp y$ implies always $y \perp x$.

The family (x_i), $i \in I$ is an orthogonal base if any element $x \in E$ can be represented uniquely as a convergent series:

$$x = \| \Sigma_i a_i x_i \| \qquad \text{(A1.3)}$$

This represents the expansion of x. In the NA case such a series is convergent if and only if $\lim_i a_i x_i = 0$. Note also that $\|x\| = \sup_i \|a_i x_i\|$. An NA normed space E is said to be discretely normed if zero is the only limit point of $\{\|x\|, x \in E\}$. Every

discretely normed Banach space is orthogonalisable. All orthogonal basis of E have the same cardinality but the base is not uniquely determined.

An interesting example is the so called van der Put base (van der Put 1968).

Denote by Q_p the completion of Q relative to the metric induced by the p-adic valuation. Q_p is the field of p-adic numbers. The set $\{a \in Q_p : |a|_p \leq 1\}$ is denoted by Z_p.

Its elements are the p-adic integers. Let C (Z_p) be the space of continuous functions $F : Z_p \; Q \rightarrow_p$. Let χ_n be the characteristic function of the set U_n where:

U_0: $\{x : |x| < 1\}$,..., $U_n = \{x : |x-n| < 1/n\}$. The χ_n form an orthogonal base for C (Z_p). For every $F \in C(Z_p)$ there exists a unique sequence $a_i \in K = Q_p$ such that: $F= \Sigma_i \; a_i\chi_i$

The family (x_i) $i \in I$ is α-orthogonal if:

$$\| \Sigma \; a_i x_i \sup \|a_i\| \geq \alpha_i x_i \|, \quad 0 < \alpha \leq 1 \tag{A1.4}$$

The family (x_i) $i \in I$ is an α-base if any element $x \in E$ can be represented uniquely as a convergent series:

$$x=\Sigma_i \; a_i x_i \tag{A1.5}$$

An NA Banach space is of countable type if it contains a dense sub-space of finite or numerable dimension. If E is a Banach space of countable type then for any $\alpha < \alpha \leq 1$, E has an α - orthogonal basis. If the valuation of K is discrete then for every $0 < \alpha \leq 1$, E has an α - orthogonal base (van der Put 1968).

Examples of interest are the so-called moment spaces (Robert 1967).

Let $\{f_m(t)\}$, m = 0,1,... be a set of real functions defined on [a,b] such that:

$$\mu_m (1)= \int_a^b f_m(t)dt \tag{A1.6}$$

exist and are finite.

Let E = {x(t)} be the linear space of all real functions defined on [a,b] such that:

$$\mu_m(x)= \int_a^b x(t)f_m(t)dt \tag{A1.7}$$

exists and are finite. Note that $\mu_m (x)$ is the m-th moment of x relative to $\{f_m(t)\}$.

Let $w(x) = \inf \{m, \mu_m (x) \neq 0\}$ that is w(x) is the first non-null moment of x.

Define $\|x\| = r^{w(x)}$ for some fixed r, $0 < r < 1$. Observe that $\| \|$ defines an NA norm on E. The valuation of K is trivial. E admits an orthogonal base.

Let x_m be such that $\mu_i(x_m) = \delta_{mi}$ for $i \leq m$. The set $\{x_m\}$ form an orthogonal base on E. The completion of E, that is, the set of formal expansions in terms of $\{x_m\}$ is called a "moment space" (Robert 1967).

If $a = 0, b = \infty, f_m(t) = L_m(t)$ (Laguerre polynomials) then: $\{x_m\} = \{\exp(-t) L_m(t)\}$.

If $a = -\infty, b = \infty, f_m(t) = H_m(t)$ (Hermite polynomials) then: $\{x_m\} = \{\exp(-t^2/2) H_m(t)\}$.

References

Lightstone, A.H., Robinson, A.: Nonarchimedean fields and asymptotic expansions. North-Holland Publ. Co., Amsterdam (1975)

Monna, A.F.: Analyse Non-Archimédienne. Springer, Berlin (1970)

Neder, L.: Modell einer Differentialrechnng mit aktual unendlich kleinen Grossen erster Ordnung. Math. Annalen. 118(2), 251–262 (1941)

Neder, L.: Model einer Leibnizischen Differentialrechnung mit aktual unendlich kleiner Grossen samtlicher Ordnungen. Math. Annalen. 118(5), 718–732 (1943)

Robert, P.: On some non-Archimedean normed linear spaces 1-IV. Compositio Math. 19, 1–77 (1967)

van der Put, M.: Algebres de fonctions continues p-adiques. Indag. Math. 30, 401–420 (1968)

Appendix 2
Category Theory

Abstract. Higher categories, that is, n-categories represent promising tools for multi-level complexity studies. Specific notions as, n-categories, periodic table, monoidal, braided, sylleptic, and symmetric categories, categorification and coherence are introduced.

Elements of synthetic differential geometry, SDG, and toposes are outlined.

A2.1 Category Theory

A category C contains a class of objects ob(C) and a class of arrows hom (C) between objects (MacLane 1971). To a morphism f, in a category, we assign an object A=dom (f) in that category, which is called the domain of f, and an object B=cod (f), which is called the codomain of f.

Usually the morphism with domain A and codomain B is denoted: f: A→B.

For any two arrows f: f: A→B and g: B→C such that dom (g) =cod (f), the composite morphism gof: A→C is defined.

An identity morphism for an object X is a morphism 1_X: X→X such that for every morphism f: f: A→B we have $1_B$of=f=fo$1_{A.}$

A category *C* consists of a class of objects ob(*C*), a class of morphisms hom (*C*) between objects and a binary operation of composition "o" such that to every arrow in *C* we can assign a domain and a codomain, the composition is associative, that is, (hog)of=ho(gof) and for every object X of *C* there exists an identity morphism 1_X:X→X.

The class of sets together with the usual functions between them forms a category, Set.

A subcategory *D* of *C* is a category such that ob (*D*) $\subset$ ob (*C*) and hom (D) $\subset$ hom (C).

Examples of objects are sets, processes, structures, partial orders, concepts, and so forth.

MacLane monograph define formally the basic notions of category, functors, natural transformation, universal properties, limits and colimits, products and

coproducts, equalizers and coequalizers, pullbacks and pushouts, exponentiation, Cartesian closed categories, and subobject classifiers (MacLane 1971).

A2.2 The n-Categories

One category frame is not enough to describe the complexity of multi-level systems. For this reason, n-categories, multi-categories, operads and other higher dimensional categorical concepts should be involved (Leinster 2004).

The n-categories are high-order generalizations of the notion of category.

Roughly, an n-category is the algebraic structure consisting of a collection of objects, a collection of morphisms between objects, a collection of 2-morphisms between morphisms and so on up to n, with various rational and practical ways of composing theses j-morphisms, j<n (Baez 1997).

An n-category consists of 0-cells (objects, types), 1-cells (morphisms), 2-cells (morphisms between morphisms) and so on, all the way up to n-cells together with composition operations.

There are numerous studies dedicated to n-categories and even to ∞-categories, called also ω-categories.

As n increases, the construction of n-categories step by step may be difficult to conceive and need analysis on how higher categories are effectively working.

Consider for example the case of 2-categories of which the category of categories denoted by Cat is the standard example (MacLane 1971). In Cat, the 0-cells are categories, the 1-cells are functors, and the 2-cells should be natural transformations.

Any 2-category C makes use of three items C_0, C_1, and C_2. Elements of C_i are called i-cells i =0, 1 or 2. The 2-category is the three categories structure that consists of the so-called base category having C_0 as objects and C_1 as arrows, the horizontal category having C_0 as objects and C_2 as arrows, and the vertical category having C_1 as objects and C_2 as arrows.

The 2-cells are arrows in both the horizontal and the vertical category, thus they composes with two different composition operators, horizontal or vertical.

Cat is a strict 2-category, that is, all laws hold exactly, not just up to isomorphism.

Vertical composition corresponds to a sequential operation, while horizontal composition corresponds to a parallel operation. The 2-category is a category with morphisms between morphisms, that is, 2-morphisms.

There are also many weak categories. For example, a bicategory is a structure used to extend the notion of 2-category to handle the cases where the composition of morphisms is not strictly associative, but only associative up to an isomorphism.

Bicategories may be considered as result of the weakening of the definition of 2-categories. A similar process for 3-categories leads to tricategories, and more generally to weak n-categories for n-categories.

In an informal way a tricategory C is done by:

- A class C_0 of objects
- For any pair A, B $\in$ C_0 a bicategory C (A, B)
- For any triplet A, B, D$\in$ C_0 a bifunctor of composition c_{ABD}: C(A, B) x C(B,D)$\rightarrow$ C(A,D)
- For any object a bifunctor u_A:1 $\rightarrow$ C(A,A)

These elements verify several axioms (Gordon et al. 1995).

Higher-dimensional categories may be defined inductively in terms of the hom enriched categories (Street 1987, Street 2004). For instance a 2-category C is defined as a Cat-enriched category which means that if x and y are objects of C then the hom C(x, y) is a category its objects being the arrows from x to y and its arrows the 2-cells.

For any symmetric monoidal category V there is a symmetric monoidal category V-Cat whose objects are categories with homeomorphisms enriched in V. Starting with the category Set of sets and using Cartesian product for the monoidal structure we can iterate the process V$\rightarrow$V-Cat yielding the following sequence of definitions:

Set, Cat: =Set-Cat, 2-Cat: = Cat-Cat, 3-Cat: = (2-Cat)-Cat,…

All terms have Cartesian product as monoidal structure. Sets are called 0-categories, categories are called 1-categories, (Set-Cat)-Cat are called 2-categories and so on. There are inclusions: Set $\subset$ Cat $\subset$ 2-Cat $\subset$ 3-Cat $\subset$ …

The union of this chain is the category ω-Cat of strict ω-categories. Therefore, the ω-categories are understood as the directed limit of a sequence of iterated enrichments.

When V is closed, it is enriched in itself. Each n-Cat is Cartesian closed and hence n-Cat is itself naturally an (n+1)-category.

The n-cells in an ω-category can be defined recursively. The 0-cells of a set are its elements, the (n+1)-cells of C are the n-cells of some hom n-category C(x, y) for x, y objects of C. The theory of ω-categories, or ∞- categories, seeks to formalize the ideas of thing (object, device), process, meta-processes (process of processes), meta-meta-processes and so on.

A2.3 Periodic Table

PSM developments require understanding and running of computations for processes of processes, and so on.

The stabilisation hypothesis may be of help for this difficult task (Baez and Dolan 1995, Leinster 2004). This hypothesis refers to k-tuply monoidal n-categories.

A k-tuply monoidal n-category is an n-category in which objects can be multiplied in k ways, all of which interchange with each other up to isomorphism. This implies that these k ways all end up being equivalent, but that the single resulting operation is more and more commutative as k increases. The stabilization

hypothesis states that by the time we reach k=n+2, the multiplication has become maximally commutative.

The stabilization hypothesis says that each column in the periodic table of n-categories stabilizes at a certain precise point. The periodic table of Baez and Dolan for classifying n-categories is presented in Table A2.1. Table A2.1 is a periodic table for categories.

Table A2.1 Periodic table of categories

	n=0	n=1	n=2	n=3
k=0	sets	categories	2-categories	3-categories
k=1	monoidal	monoidal categories	monoidal 2-categories	monoidal 3-categories
k=2	commutative monoids	braided monoidal categories	braided monoidal 2-categories	braided monoidal 3-categories
k=3	“”	symmetric monoidal categories	sylleptic	sylleptic
k=4	“”	“”	symmetric monoidal 2-categories	involutory
k=5	“”	“”	“”	symmetric monoidal 3-categories
k=6	“”	“”	“”	“”

It contains the conjectured description of (n+k)-categories with only one j-morphism for j<k. The idea of the periodic table linked to stabilisation hypothesis is to study degenerate forms of n-category that is, n-categories that are trivial below a certain dimension k. Such an n-category only has non-trivial cells in the top (n-k) dimensions, so we can perform a dimension shift and regard this as an (n-k) category. The previous k-cells become the new 0-cells, the previous (k+1)-cells become the new 1-cells, and the previous n-cells become the new (n-k) cells. This is called a k-fold degenerate n-category.

Basically the Table A2.1 shows that (n+k) category with only one j-morphism for j<k can be reinterpreted as an n-category. But, it will be an n-category with k ways to multiply that is a k-tuply monoidal n-category. For example if n=1, k=1, a 2-category with one object is a monoidal category.

The Table A2.1 outlines properties as: monoidal, braided, sylleptic, involutory and symmetric. In the first row (k = 0), a 0-monoidal n-category is simply an n-category.

In the next row (k = 1), a 1-monoidal n-category is a monoidal n-category.

For instance, a 1-monoidal 0-category is a one-object category (a monoid), and a 1-monoidal 1-category is a one-object 2-category (a monoidal category). A monoidal 2-category can be defined as a one-object 3-category, or can be defined directly as a 2-category with tensor.

The third row (k = 2) allows observing that a degenerate monoidal category is a commutative monoid and a doubly-degenerate 3-category is a braided monoidal category.

Concerning the first column (n = 0) it was observed that one-object braided monoidal category is a commutative monoid together with extra data, for the braiding, satisfying some axioms.

This gives the entry for k = 3, n = 0, and the same applies all the way down the rest of the column. Similar results may be established for the second column (n = 1). Observe that for k ≥3, the k-monoidal 1-category is just a symmetric monoidal category. Then the column stabilizes, and the point of stabilization is the most symmetric object possible.

The same is valid for subsequent columns. The sylleptic characterization could be completed by more terms, as involutory for instance. It was observed that a braided category is a monoidal category with additional structure a sylleptic category is a braided category with additional structure and so on (Crans 2000).

A2.4 Categorification and Coherence

Categorification is the process of finding category-theoretic analogs of set-theoretic concepts by replacing elements with objects, sets with categories, functions with functors and equations between functions by natural isomorphisms between functors, which in turn should satisfy certain equations of their own, called coherence laws (MacLane 1971, Baez and Dolan 1998).

The correspondence between set theory and CT is presented in Table A2.2

Decategorification is the reverse process of categorification. Decategorification is a systematic process by which isomorphic objects in a category are identified as equal. Categorification is more complicated than decategorification, and requires insight into individual situations.

Table A2.2 Correspondence between sets and categories

Set theory	Category theory
Set elements	Objects
Sets	Categories
Functions	Functors
Equalities between morphisms	Natural isomorphisms of functors

The term vertical categorification refers roughly to a process in which ordinary categories are replaced by higher categories. Categorification implies moving from left to right in the periodic table while decategorification implies moving in the reverse direction.

In CT, the objects or identity arrows are elements within category, whereas the category compares objects, the functors compares categories and the natural transformation compares functors. For example, a monoid is a set with a product satisfying the associative law and a unit element satisfying the left and right unit laws. The categorified version of a monoid is a monoidal category. This is a category C with a product:$\otimes$: C x C$\rightarrow$ C and a unit object 1$\in$C. For categorization

we need to impose associativity and the left and right unit laws as equational laws only up to isomorphism. As part of the structure of a weak monoidal category we specify a natural isomorphism: a $_{x,y,z}$: (x ⊗ y) ⊗ z→x⊗(y ⊗ z) called the associator together with the natural isomorphisms: l_x: 1⊗x→ x and r_x: 1⊗x→ x.

Associativity means that, within a sequence containing two or more of the same sequencing operations in a row, the order that the operations are performed does not matter as long as the sequence to be operated is not changed.

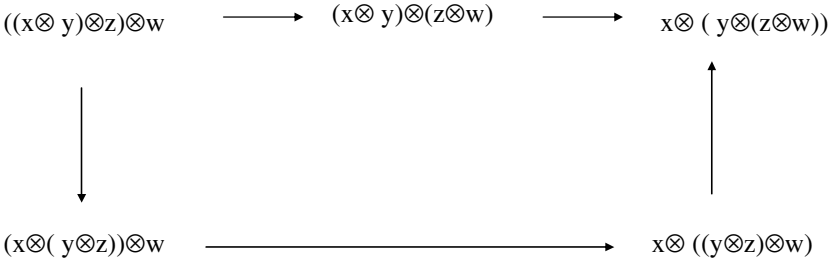

Fig. A2.1 Pentagon relations

Using the associator one can construct isomorphisms between any two parenthesized versions of the tensor product of several objects. For example there are five ways to parenthesize the tensor product of four objects, which are related by the associator as shown in Fig. A2.1. The coherence law called the pentagon identity, say that the diagram shown in Fig. A2.1 commutes. Pentagon relation concerns monoidal categories and associativity.

Suppose that we are looking to commutativity, that is, we want to categorify the notion of commutative monoid.

Consider a weak monoidal category equipped with a natural isomorphism:

$B_{x,y}$: x⊗y→y⊗x called the braiding and then impose coherence laws called hexagon identities (Fig. A2.2). The hexagon relations are illustrated by Fig. A2.2.

In physics there are processes allowing switching two systems by moving them around each other. The monoidal category in which we can do this sort of switch is called braided.

The first hexagon equation says the switching the object x past y⊗z all at once is the same as switching it past y and then past z.

The second hexagon is similar. It says switching x⊗y past z all at once is the same as doing it in two steps.

Hexagon relation concerns braided monoidal categories and braiding.

Consider as an example from the periodic table the case n=1, k=2 of a doubly monoidal 1-category, a braided monoidal category. The braiding is: $B_{x,y}$: x⊗y→y⊗x.

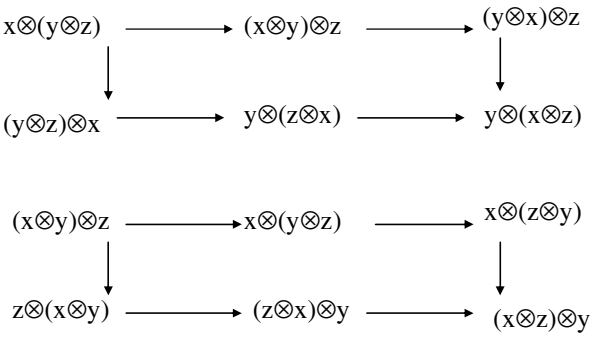

Fig. A2.2 Hexagon relations

The process of proving an equation becomes an isomorphism. This happens when we move one step right in the periodic table.

For codimension k=3 we should consider braiding versus inverse braiding. This introduces the notion of syllepsis.

Observe that we a faced with a hierarchy of higher braiding one for each codimension k≥2, each satisfying a hierarchy of laws.

A different proof of commutativity becomes a different isomorphism. $B^{-1}_{y,x}$: x⊗y→y⊗x This explains the existence of knots. A triply monoidal 1-category is a symmetric monoidal category. In this case we need three dimensions of space instead of just two. This makes the two ways of moving x past y equal. So the situation is more commutative. This happens when we move one step down in the periodic table.

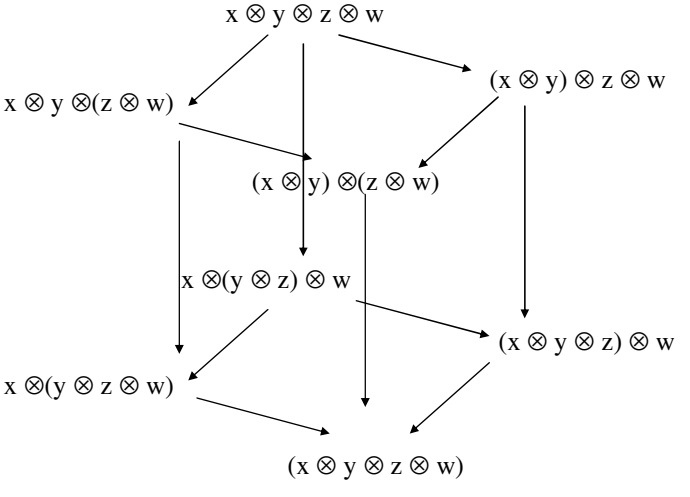

Fig. A2.3 Parity cube relations

It is interesting to lift the monoidal structure up a dimension into tricategories.

A tricategory may be defined on the basis of bicategories and these on the basis of categories. To characterize coherence the edges of the MacLane pentagon, shown in Fig. A2.1, becomes five sides of a cube as shown in Fig. A2.3. Fig. A2.3 illustrates the parity cube relations (Street 2004, Sheppeard 2007).

In this setting, the state composition "⊗" is the Gray tensor product denoted here by "Γ": (Crans 1999, 2000).

Gray defined for 2-categories a product analogous to the conventional product for 1-categories (Kelly and Street 1974, Gurski 2006).

Given two 2-categories C, D the Gray tensor C⊗D is informally defined to be the 2-category:

- With 0-cells given by products A⊗A' for all pairs $(A, A') \in C_0 \times D_0$
- With 1-cells given by products A⊗f' and f⊗A' for all pairs $(A, f') \in C_0 \times D_1$ and $(f, A') \in C_1 \times D_0$
- With 2-cells generated by products A⊗φ', f⊗f' and φ ⊗A' for all pairs $(A, \varphi') \in C_0 \times D_2$, $(f, f') \in C_1 \times D_1$ and $(\varphi, A') \in C_2 \times D_0$ were f⊗f' denotes a 2-cell with specific properties (Kelly and Street 1974).

The horizontal composition of two 2-arrows results in a three dimensional arrow.

The dimension raising aspect related to the Gray tensor product "Γ" should be emphasized.

A2.5 Toposes Modeling SDG

The formal notions necessary to understand categories and toposes may be found in Goldblatt (1979) monograph.

An informal presentation is due to Baez (Baez 2006).

An elementary topos *E* is a category such that:

i) *E* has all finite limits and colimits
ii) *E* has exponentiation
iii) *E* has a subobject classifier

The property i), says that there are: an initial object, a terminal object, binary coproducts, binary products, equalizers and coequalizers.

The property ii) says that for any objects x and y, there is an object y^x, called an "exponential", which acts like "the set of functions from x to y".

The property iii) says that there is an object called the "subobject classifier" that appears as the replacement for the usual Boolean "truth values" {true, false} from classical Boolean logics.

In order to treat the general relations of physics, it is necessary that the mathematical frame involves a Cartesian closed category *E* of smooth morphisms between smooth spaces. This is one of the reasons to use toposes in engineering.

Another reason is the need for constructivist mathematical study of complex systems. The logic in constructive mathematics is not the classical Boolean one.

Toposes may make use of a minimal more primitive logic, namely the constructive logic. Constructive logic, pioneered by Heyting, represents a logical framework for constructive mathematical models (Bell 1998). This logic rejects the law of excluded middle and allows characterizing fuzziness and vagueness in reasoning.

The prime example of toposes is the category Set. The conditions i) to iii) allows to the category *E* to be used as a model of constructive logic universe in much the same way as the category Set is used as a model of a conventional logic universe.

In any universe containing SDG, there exists an object of smooth reals *R* defined to expresses the idea that some aspects of the physical universe should be fundamentally smooth. It should be observed that all the function from *R* to itself must be smooth.

Some of the most relevant axioms for *R* are: (Moerdijk and Reyes 1991):

- (A1) *R* is a local commutative ring with unit
  Denote by $D = \{d \in R \mid d^2 = 0\}$ the first order infinitesimals.
- (A2) Derivation (Kock-Lawere): For each f: D→ *R*, there exists a unique b∈ *R*, such that for every d ∈ D, f (d) =f (0) +d.b
- (A3) Integration: For each f: $R \rightarrow R$, there exists a unique F: $R \rightarrow R$, such that F'(x) =f(x) with F (0) =0

Topos theory provides a framework in which it is possible to define a category which behaves like conventional sets and functions and which consists of smooth objects and morphisms. It should be emphasized that CT does much more than organize the mathematical materials furnished by classical set theory. Various topos models allow the study of the smoothly continuous incorporating actual infinitesimals which are inconsistent with set theory, a form of the continuous that cannot be reduced to discreteness.

References

Baez, J.: An introduction to n-categories. In: Moggi, E., Rosolini, G. (eds.) CTCS 1997. LNCS, vol. 1290. Springer, Heidelberg (1997)

Baez, J.: Topos theory in a nutshell (2006),
http://math.ucr.edu/home/baez/topos.html

Baez, J., Dolan, J.: Higher dimensional algebra and topological quantum field theory. Jour. Math. Phys. 36, 6073–6105 (1995)

Baez, J., Dolan, J.: Categorification. In: Getzler, E., Kapranov, M. (eds.) Higher Category Theory. Contemp Math., vol. 230, pp. 1–36. Amer. Math. Soc, Providence (1998)

Bell, J.L.: A Primer of Infinitesimal Analysis. Cambridge University Press, New York (1998)

Crans, S.: A tensor product for Gray categories. Theory and Applications of Categories 5(2), 12–69 (1999)

Crans, S.: On braidings, syllepses ans symmetries. Cahiers Topologie Geom Differentielle Categ. 41(1), 2–74 (2000)

Goldblatt, R.: Topoi. The Categorical Analysis of Logic. North-Holland Publishing Theory, Amsterdam (1979)
Gordon, R., Power, A.J., Street, R.: Coherence for tricategories. Memoirs Amer. Math. Soc. 117(558) (1995)
Gurski, N.: An algebraic theory of tricategories. PhD thesis, University of Chicago, IL (2006)
Kelly, G.M., Street, R.: Review of the elements of 2-categories. Lecture Notes in Math. 420, 75–103 (1974)
MacLane, S.: Categories for the Working Mathematician. Springer, New York (1971)
Moerdijk, I., Reyes, G.E.: Models for Smooth Infinitesimal Analysis. Springer, New York (1991)
Leinster, T.: Higher Operads, Higher Categories. Cambridge University Press, Cambridge (2004)
Sheppeard, M.D.: Gluon Phenomenology and a Linear Topos. Ph, D Thesis Univ. of Canterbury, New Zeeland (2007)
Street, R.: The algebra of oriented simplexes. J. Pure Appl. Algebra. 49, 283–335 (1987)
Street, R.: Categorical and combinatorial aspects of descent theory. Applied Categorical Structures 12, 537–576 (2004)

Index