Ralf Seppelt

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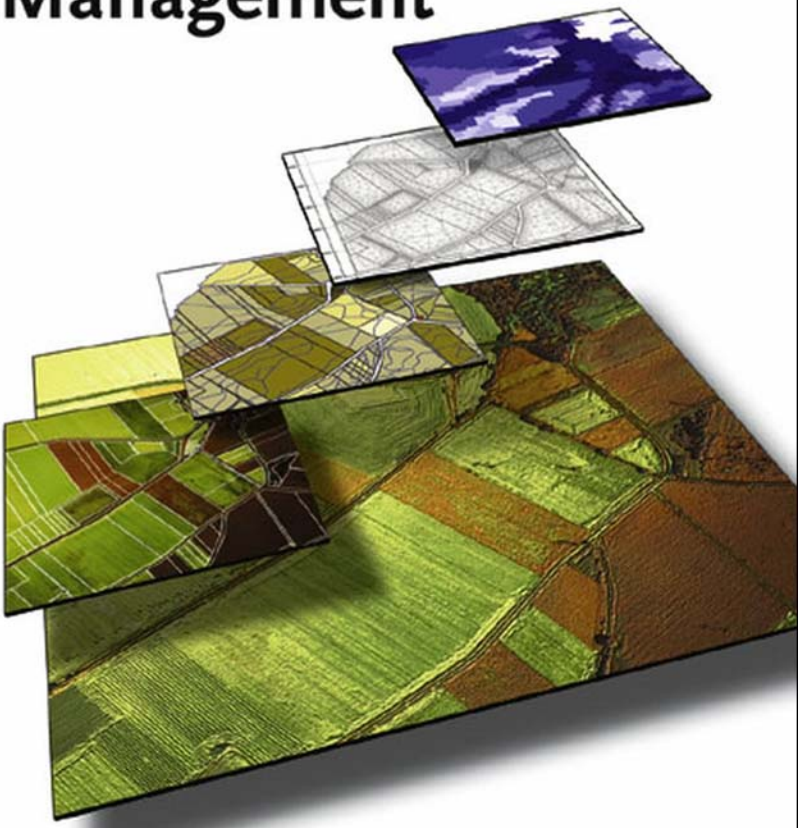
Computer-Based Environmental Management



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Foreword

As an active designer, user, and teacher of models and modeling, I'm always on the lookout for better tools. Ralf Seppelt's book is a unique and welcome addition to that toolbox. It is unique in its comprehensive integration of the theory and practice of environmental modeling and management.

Because of this integration, the book will appeal to three broad audiences and be useful:

(1) as an upper level or graduate course text in environmental modeling and management;

(2) as a guide for practitioners to get up to speed on the latest developments in computer modeling of the environment;

(3) as a guide for environmental managers to get a good handle on the latest developments in modeling and how they could be useful in making better environmental decisions.

As a teacher of environmental modeling, I've been searching for many years for the perfect text to use in courses. There are several books out there that are each very good in their own way, but which cover only some of the issues needed to get a good, comprehensive grasp of modeling and the uses of modeling in environmental management. It's also hard to find a text that is at just the right level — not so general as to be useless yet not so technical as to be useful only to a small, specialized

audience. My search has ended with the publication of Ralf Seppelt's book and I intend to use it as a core text in modeling courses.

As a practitioner of modeling as a method to achieve an integrated understanding of complex systems, I can appreciate the range of applications covered in the book. Ralf spent a sabbatical year at our Institute when were still at the University of Maryland and jointly developed several of the applications discussed in the book. That year was extremely productive for all of us, and helped to expand the envelope of spatially explicit environmental modeling, as reported in the book. I intend to use the book to make researchers in our Institute fully conversant with the theory and latest applications in environmental modeling so they can take the next steps forward.

As someone who interacts with environmental managers and tries to help them to use modeling effectively in their decision-making, I can see that the book will be very useful. Managers need a single source that can show them both how models work and how they can be useful in decision-making. By integrating theory and applications, this book can quickly bring environmental managers up to speed and help them to use existing models more effectively, to commission better models in the future, and to actively participate in the modeling process themselves. I intend to recommend this book to environmental managers as the best way to familiarize themselves with the latest theory and uses of environmental modeling.

Finally, as Ralf Seppelt makes clear in this book, modeling is an activity, and this activity is itself at least as important and valuable as the models themselves. Modeling as an activity can be seen as the essence of the scientific method. The unique integration that this book represents is thus also a good platform for talking about what science is at a very fundamental level. The links between science and policy are so tenuous today precisely because of some fundamental confusions about what science is, and how it can best inform decision-making. Science is *not* certainty, as it is often mischaracterized in the media. Science is about understanding *un*certainty, and modern science recognizes that complex systems can never be understood with certainty. Computer modeling is the best tool we currently have to describe and understand uncertainty in complex systems. By clarifying these confusions, this book will be a valuable and important tool at a very fundamental level, and will help to create a better link between science and policy in general.

July 2003

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Acknowledgments

Ecological modeling is a fast developing area in the field of environmental science in which substantial progress has been achieved in recent years. User-friendly software packages, including high performance numerical tools, enable environmental scientists to code complex systems and thus study environmental processes in a systematic fashion. Modeling has become an important part of environmental research. Redundancy and a confusing diversity, however, have been a frequent result of this development. In this book, the recent state of environmental modeling is presented in a concise manner, and model applications in environmental management are studied.

This project would have been impossible without the support of several colleagues and friends whom I would like to thank especially now that this project has been completed.

First of all, I would like to thank Otto Richter for his support and inspiring ideas. Special thanks go to the good humor of Dagmar Söndgerath and Boris Schröder for many fruitful discussions, suggestions and critical remarks, and — much more important — the resulting motivation.

The ideas and results presented in this publication are the outcome of numerous co-operations and projects. I appreciate having worked together closely with the following people (in alphabetic order): Robert Costanza, Michael Flake, Claudia Hiepe, Olaf Jensen, Verena Korr, Matthias Kuhnert, Tom Maxwell, Florian Stange, Christian Thiel, Christine Vogel, and Alexey Voinov. I gratefully appreciate their suggestions, inspiring discussions and ideas.

My thanks are due to Klaus-Jürgen Schmalstieg for his support related to GIS analysis and data management, to Wolfgang Max for his unfailing technical support as well as to Kerstin Schulze for technical assistance with figures, tables, bibliography and several simulation runs. Marko-Michael Temme and Conrad Hoffmann spent much of their spare time in programming and tweaking the software presented in this book.

I am very grateful to Wolfgang Pittroff, Leland J. Jackson and Charles A.S. Hall for their remarks and suggestions for this book in a very early stage of the project. Mary Korndorffer has carefully edited the final manuscript. Very special thanks to her, as well as to Carsten Dormann who provided many valuable comments on the final manuscript.

Finally, not only does environmental science make progress, so too did the situation of my private life. Since my first projects in environmental science several years ago Tim, Anika, and Moritz were born and changed our life fundamentally. Thus, most of all I owe a deep sense of gratitude to my wonderful family and especially to my wife Martina who supported me all these years.

R. S.

Contents

Introduction

> "and what is the use of a book," thought Alice,
> "without pictures or conversations?"
>
> —Lewis Carroll[1]

Modeling, . . .

Our environment with its dynamic and spatial processes is recognized as complex, highly interacting and spatially distributed. These properties make analyzing, describing, modeling and even simulating our environment a challenging task. A framework that enables us to study, for example, the consequences of human influences on ecological systems without even disturbing these is a valuable and important tool for environmental management. Models are therefore identified as important and necessary tools for studying and understanding ecological processes, testing hypotheses of the functioning of ecosystems in a systematic manner and for investigating environmental response to human impact.

This makes modeling an important part of the interdisciplinary research field of environmental science. Ecological modeling however is done less and less by mathematicians and more and more by practicing ecologists and environmental scientists.

[1] see p. 280 for references of quotations.

The present state of environmental modeling is characterized by a number of model developments. Several authors state that a general concept is missing in ecological or environmental modeling. Recent development of environmental models has shown that a multitude of possible approaches and theories have been developed. Some authors complain that *we have produced an enormous redundancy*. This multitude of different approaches refers to the considered temporal scale, the considered mathematical languages — such as differential equations (partial or ordinary), matrix models, fuzzy systems etc. — and the chosen concept of regionalization and spatial extent. The incorporation of spatial attributes into the modeling process causes a mismatch between the scale at which attributes are obtained, and the scale at which the processes occur.

The first part of the book (Chapters 1 to 3) gives a synthesis of model development concepts. Compiling mathematical equations and setting up simulation models is a complex and challenging task. Setting up ecological models requires a detailed system analysis of the processes of interest. A systematic way to achieve a concise and valid simulation model is to start with a conceptual model, which every scientist usually has in mind when investigating a process. Chapter 1 traces the path from conceptual models to validated regionalized environmental simulation models. The step of translating conceptual models into computer models is assisted by several development platforms. These platforms translate conceptual models into mathematical equations of a certain mathematical "dialect".

Focusing on processes of the abiotic environment as well as the first two trophic levels of the biotic environment, several different translations of conceptual diagrams into mathematical models are studied in Chapters 2 and 3. The first focuses on the dynamic patterns on different temporal scales such as nutrient flow, water transport, growth of crops and weed, population dynamics, competition, etc. Migration of species, vertical and horizontal fluxes of matter and information through a landscape are the characteristic properties of ecosystems. In Chapter 3 spatial interactions are discussed and the possible mathematical modeling concepts are presented, starting from highly aggregated mathematical models given by partial differential equation systems, we end up with with a discussion of cellular automata. For comparison, different mathematical "dialects" are used for modeling the same process to analyze and compare different methodologies.

Integration, . . .

Although there is consensus on a general methodology of model development, one needs to consider that environmental modeling is a diverse field of research. First of all because it is an interdisciplinary issue. Biologists, ecologists, computer scientists, mathematicians, physicists have to work together and to integrate their methodology to solve ecological problems of the 21st century. This diversity leads to a multitude of approaches solving similar or even identical tasks. Several scientists complain of a lack of theoretical foundation of environmental modeling.

For example, conceptual difficulties stem from the fact that processes of different dynamic quality interact. The dynamics of technical systems are mostly time discrete and their dynamics are closely related to discrete spatial structures, whereas many environmental processes are continuous in time and space. The whole system can be characterized as structured time discrete and time continuous. One is faced with a problem that can be summarized as mathematical heterogeneity. It is not feasible to model integrated systems in the framework of one mathematical "dialect".

An environmental model requires the integration of all these approaches. This requires a general theoretical framework. The subject of Part II of the book is to bring together modern mathematical methodologies to solve the task of integration. These concepts are used to assess the anthropogenic impacts of production and the use of goods and services on the environment. This life cycle impact assessment methodology comprises a system-wide analysis of mass- and energy flows, performed within the step of life cycle inventory. Distributions of emissions are estimated within an environmental fate model including dispersion–reaction modeling and impact assessment has to be performed for different impact categories. The product is a hybrid model which integrates different environmental techniques and demonstrates how these effects can be addressed in environmental assessment.

. . . and Management

Quantitative and qualitative analysis of environmental processes by computer models is one aspect of ecosystem modeling. Additionally, a very frequent application of ecological models is to study the consequences of anthropogenic impact on the ecosystem with respect to the environmental fate of substances, habitat suitability of species, persistence of populations etc. In this way different management strategies can be compared. The question of the degree of impact which nature can sustain without harm to the environment has already been posed. Ideas like most sustainable yield were introduced in the late 1960s. Ecosystem management has become now an important discipline of scientific research and is an important branch in the political decision-making process. Because ecological models are complex and highly interacting, as stated above, this decision making process requires methodological support. The third part of the book deals with applications of ecological models in the decision-making process: either by the use of scenario analysis technique or by the application of optimum control theory to an ecosystem model. Problems of ecosystem management are solved by the use of numerical optimization. This can be interpreted as the follow up of the most sustainable yield concept by the use of scientific computing.

With increasing complexity of ecosystem models, one becomes aware, that scenario analysis may not be the appropriate tool to vary all required control parameters. Systematically sorting through all possible combinations of control variables yields a desired optimal scenario. This is achieved by the optimization or optimum control approach. Chapter 8 introduces this third part of the book, offers an overview of

the approaches "scenario analysis" versus "optimization" and defines the tasks to be solved for optimum control of environmental systems.

Complexity of environmental models leads to an enormous computational effort, if these models are to be used in optimum control theory. Introducing certain hierarchies is one concept which can deal with increasing complexity. In Chapter 9 a framework is proposed for an application of environmental models in optimum control theory. This development focuses on spatially explicit models as well as models with a broad range of temporal patterns and dynamics. The generic code can cope with hybrid models. It requires appropriate numerical procedures, too. This is achieved by a hierarchical approach to the optimization problem and this decreases numerical effort.

Applications of this concept are presented in Chapters 10 to 12. Chapter 10 focuses on optimum temporal patterns of management strategies of an agroecosystem. Different results of optimum fertilizer input, pest management, weed control and crop rotation schemes are presented. Several scenarios of environmental assessment are compared using the tool of optimization. These results are then studied within a regionalized model. Beside the dynamic solution, Chapter 11 focuses on the regionalization of the optimum control problem. The task is solved by the identification of homogeneous units in the observed region by a geographic information system. The second innovative topic, which enables a regionalized solution of the optimum control problem, is the estimation of families of optimum solutions parameterized by spatial properties. The proposed methodology supports the step of decision support in site-specific farming.

In Chapter 12 all these concepts are applied to solve management problems of land use with a spatially explicit model on a landscape scale. Spatially explicit ecosystem models allow the calculation of water and matter dynamics in a landscape as functions of spatial localization of habitat structures and matter input. For a mainly agricultural region the nutrient balance as a function of different management schemes is studied in this chapter. The results are tested using Monte Carlo simulations which are based on different stochastic generators for the independent control variables. Gradient free optimization procedures are used to verify the simplifying assumptions. The framework offers tools for optimization with the computational effort independent of the size of the study area. As a result, important areas with high retention capabilities are identified and fertilizer maps are set up depending on soil properties. This shows that optimization methods can be a useful tool even in complex simulation models for systematic analysis of management strategies for ecosystem use.

Summary: How this Book is structured

Aspects of ecological modeling are of increasing importance in any branch of ecology, biology, landscape ecology, and environmental management. The book focuses on two main issues: the integration of different modeling approaches, together with applications in optimization and optimum control theory. It aims at supporting problems of environmental management and tries to bring together modern mathematical

methods with environmental ecological research. The concept of the book is to offer a theoretical and methodological platform for environmental modeling, that can provide a starting point for every environmental scientist to solve a particular modeling problem. This is achieved by using the level of conceptual models as a starting point for model development and explanes the types of models that can be derived from one conceptual diagram.

Recent progress in ecological modeling is presented in a concise way showing results of high standard mathematical methods, such as the use of numerical solutions of partial differential equations for modeling water and matter transport, as well as population dynamics and migration in real landscapes. This provides a foundation for aggregated spatially explicit models using geographic information systems. Finally these high standard mathematics are used to develop concepts of solving optimization and optimum control problems for environmental management.

This structure of the book follows these objectives. Chapter 1 introduces terms and methodologies and presents an overview of environmental modeling concepts. Chapters 2 and 3 can be understood as a toolbox for translating conceptual models into equations. These chapters provide the necessary functions and equations used in most ecological models. It must be noted that all equations presented are illustrated with examples and applications. Chapter 4 discusses the results obtained in the context of meta modeling and scientific theory. Further applications of hybrid models in biology as well as in environmental assessment are reported in Chapters 6 and 7. The focus in Chapters 5 and 9 is on the mathematical foundation of the integrating modeling concept as well as the application of environmental models in optimization. Applications of concepts are presented in Chapters 10 through 12, which are understandable without reading Chapters 5 or 9 in detail.

Part I

Setting the Scene: Diversity of Environmental Modeling

> The Analytical Engine has no pretensions whatever to originate anything. It can do whatever we know how to order it to perform. It can follow analysis; but it has no power of anticipating any analytical relations or truths.
>
> —Ada Byron

1

Tour d'horizon: from Conceptual Modeling to Computer Simulations

1.1 INTRODUCTION

Environmental models are tools which help us understand how ecological processes work and allow us to test hypotheses about ecological processes in a systematic manner. Setting up an ecological model requires detailed system analysis of the processes of interest. After this translation into mathematical equations is performed. Recent development of ecological and ecosystem models has provided a multitude of possible approaches and theories. Some authors complain that *we produced an enormous redundancy* (Müller, 1997).

Why? Environmental processes are recognized as complex, highly interacting and spatially distributed. These properties make analyzing, describing, modeling and even simulating our environment a challenging task. One probably intrinsic property of ecological models is that these models are hybrid or mathematically heterogeneous. For an explanation of this property it necessary first to analyze how mathematical models of ecological processes are set up in general.

Development of environmental models encompasses physical, mathematical, and conceptual modeling. All belong to the same process and none of the parts can be neglected in compiling a well-defined simulation model. Table 1.1 gives an explanation for this.

Two examples are chosen to illustrate this close relationship of conceptual, mathematical, and physical models. Let us consider the problem of modeling population dynamics of an insect species in a flood plain. The questions to be answered are, how do flooding events change habitat properties, and is it possible to identify a minimal viable population from this analysis?

Table 1.1 Conceptual, physical, and mathematical modeling. The table contains three sentences with three different options. Start reading with the first column and complete the sentence with the completion in the column (conceptual, physical, or mathematical) of your choice.

Models are ...	mental or conceptual.	physical.	mathematical.
System identification encompasses ...	definition of system boundary, components, interactions.		
The model is ...	a conceptual verbal description of system behavior.	a scaled reproduction of a real system.	coupling of functions, rules, equations.
Elements of a model are ...	premises, conclusions, syllogism.	a physical object.	mathematical functions and (state) variables.
With the plausibility check ...	conclusions are tested (for well-known situations).	an experiment in a well-known environment is performed.	model behavior is analysed using different methodologies (stability or sensitivity analysis).
Finally, a simulation is ...	a *Gedankenexperiment*.	a physical measurement by given boundary conditions.	a (numerical) solution of the mathematical equations or rules under given initial and boundary conditions.

The second example briefly discussed considers the problem of sediment erosion in a watershed and the question of which landscape elements can help to prevent soil loss at a given investigation site.

System analysis, as noted in Table 1.1, encompasses the definition of the system boundaries, important components and processes, and the interaction between them. The system boundary of our flood plain is bordered by the river and the embankment. The temporal system boundary is defined by a number of generations of the population. The more physical approach to answering the question raised may be either the location of traps in the investigation site, in which the abundances of the studied species can be counted, presumably as a function of abiotic parameters, or a laboratory experiment in which the parameters of the population dynamics are identified.

The system boundary of a hydrological catchment is defined by the hydrological watershed. The important component is an element of the landscape, which size is to be determined, characterized by the properties elevation, slope and roughness. Element size and its properties are strongly related. The question of scale comes up in this context and will be discussed later on. A physical model might focus on two issues. First, ground truth data may be derived from field experiments. The second idea of a physical model is to rebuild the landscape on a laboratory scale. A physical model of typical elements of the landscape under consideration is rebuilt. Knowledge of the sediment runoff process is derived from several laboratory experiments.

A mathematical model for both examples is based on the parameters derived from the physical models, from laboratory and field experiments and usually from literature data.

Note that compiling a mathematical model necessitates consideration of physical models and conceptual models. Without a clear specification of system boundaries of the parameters of interest, without knowledge of important and less important processes and without well-educated guesses of the values of sensitive parameters, an environmental model cannot be set up. We will now focus on the step of model development in detail, aiming at a mathematical model for an environmental process of interest.

1.2 THE MODELING PROCESS: FROM CONCEPTUAL MODELS TO COMPUTER SIMULATIONS

1.2.1 System Analysis: Conceptual Models

The starting point of any kind of model development is the design of a conceptual model. The conceptual model aggregates our knowledge of the system and implies a thorough (albeit subjective) selection of components and processes judged essential for the processes under study in a given spatio–temporal context.

An example is given in Figure 1.1. It shows three different conceptual models. Figure A displays possible migration pathways of a neozoan between the Galápagos archipelago. Figure B summarizes seven stages of development of a ground beetle (*Carabidae* species) that is possibly invading the Galápagos archipelago. Figure C displays the small and large circular flow of matter, in this case nutrients and pesticides, through an agricultural ecosystem together with abiotic parameters (such as precipitation and radiation) and anthropogenic disturbances (by harvesting, pest control and seed).

All these conceptualizations have this in common: certain components, here islands, containers, individuals, are connected by directed arrows. These arrows denote a flow of information, matter or substances. The graphical representation in a conceptual model helps to identify dependencies and helps to identify the processes that depend on each other. Feedback-loops are easily found.

Definition 1.1 (Conceptual Model) *A conceptual model is graphically presented in the form of a compartment system. Compartments are defined with respect to morphology and to physical, chemical and biological states. Connection between these compartments denotes exchange of matter or information between certain compartments or processes. Certain compartments may act as containers for sub-structures or sub-models.*

Jørgensen & Bendoricchio (2001) distinguish several types of conceptual models or diagrams. With some modifications, these authors list the following types of conceptualization:

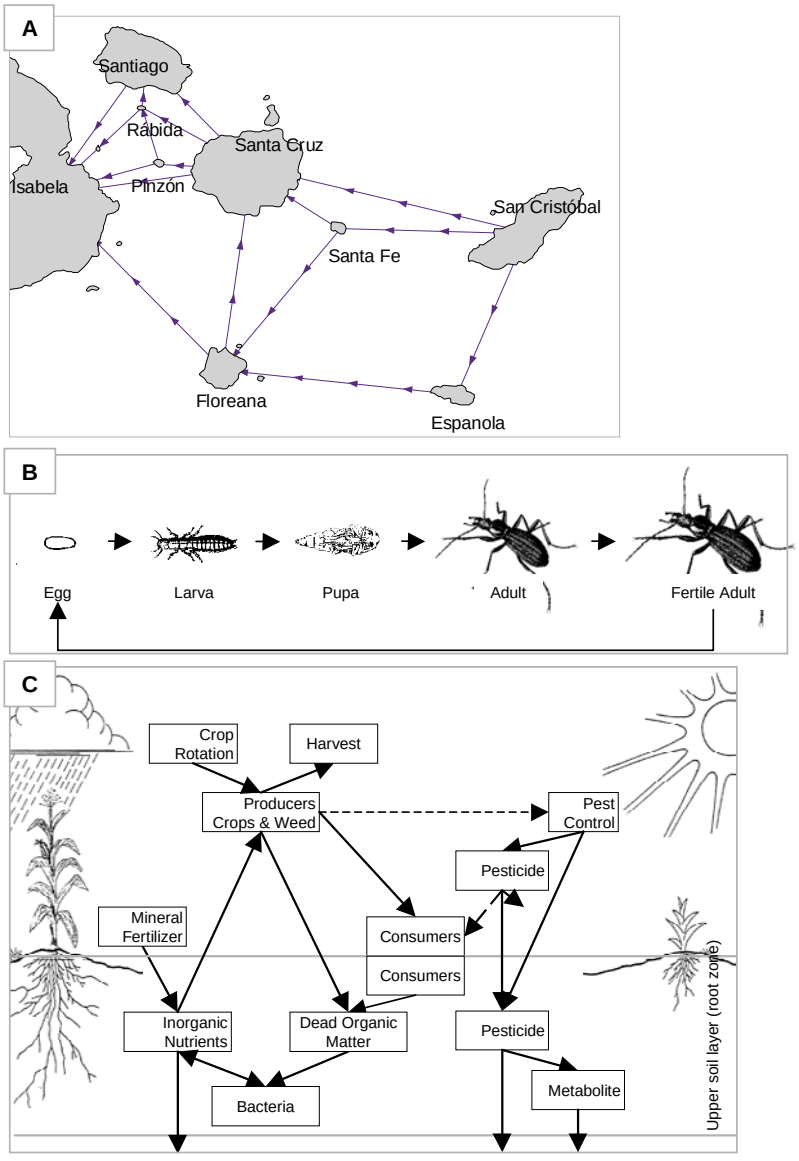

Fig. 1.1 Three different graphical representations of a conceptual model. Figure A shows spatial migration pathways of a neozoan species in the Galápagos archipelago. Figure B shows the development of a ground beetle (*Carabidae* species) simplified to a stage structured model. Finally, Figure C shows a conceptual scheme of mass and energy fluxes in an agricultural ecosystem.

Word models are based on language as a conceptualization tool and are a verbal description of the process. This concept is related to the *Gedankenexperiment* noted in Table 1.1.

Picture Models use illustration of components seen in nature and place them within a framework of spatial or temporal relationships. Figure 1.1.B is an example of this conceptualization method.

Signed Digraphs allow the display of qualitative dependencies between components, displayed by boxes. Influences between the components are specified by connections and a plus or minus sign denoting positive or negative influence.

Box-models Figure 1.1.C is an example of this commonly used conceptual design. Each box represents an compartment, arrows denote fluxes of matter, energy or information.

Input/Output Models, Black-box, White-box Models can be considered as box-models. However the term "input/output" suggest that everything between input and output is not of interest for the considered model.

In this context the terms "white-box" and "black-box" models will be discussed. Models are labeled black-box models if their internal functional relationships are derived from simple input/output relationships, e.g. statistical analysis, regression functions. Often these models are called input/output models, too.

White-box models are derived from basic physical or chemical laws and are constructed on causality for all processes. Obviously, there are many models that contain some causalities and some input/output relations. These models usually are termed grey-box models.

Feedback Dynamics are a symbolic language introduced by Forrester (1968). These diagrams are a special form of box-models, that allows automatic translation from the graphical representation of the system to a system of (nonlinear) differential equations.

Energy Circuit Diagrams were developed by Odum (1983). There diagrams give information of thermodynamic constraints, feedback mechanisms and energy flows.

What all these conceptualization methods have in common, is that the dynamic behavior of the system is implicitly defined by the topology of the network and the specification of the network element with their parameter. The growth of a crop, the amount of biomass added in a certain period of time, for instance in Figure 1.1.A, depends on the growth rate, that probably is also a function of nutrient availability (another component of the network), temperature, precipitation and CO_2 content.

The choice of a certain conceptualization method will depend on the modelers habits and preferences and on the modeling problem to be solved. However, what all these types of conceptual model have in common, is the issue of a graphical representation

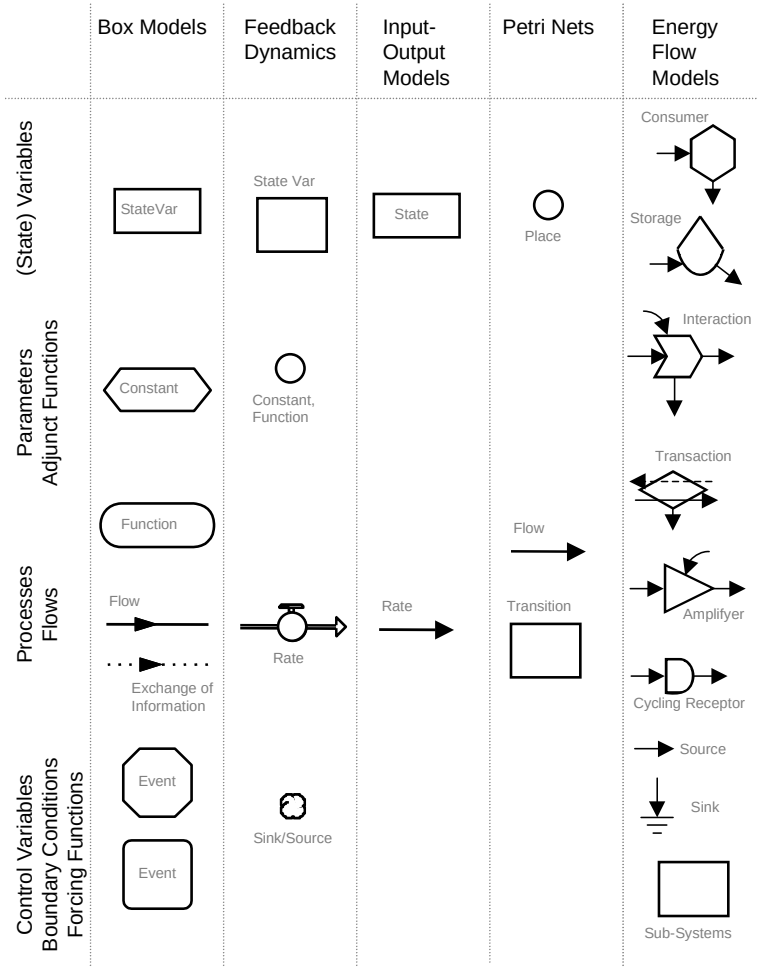

Fig. 1.2 Summary of icons in conceptual models used in deedback dynamics, energy flow models, box-models, Petri nets separated by the mathematical translation (state) variables, parameters, control and process.

of the system of interest. Figure 1.2 lists the most important icons of the conceptualization methods ordered by the operation performed with a dynamic model. In this diagram state variables, mathematical functions, parameters and boundary conditions are identified by different graphical icons. While these icons may differ from one type of conceptual model to another, the core concept remains the similar.

As information on the topology of the system is available at this stage, the first analysis of the system can be based on the resulting adjacence matrix. Based on the adjacence matrix, direct and indirect interactions can be identified. The adjacence or matrix model is first used as an intermediate step for translating the graphical representation of

a model into a mathematical notation and to support numerical solution of the resulting equations. Additionally, the matrix model is an intermediate format to translate between different conceptual models, see Chapter 4. Matrix conceptualization or matrix models are a tool for model description and analysis as well as an additional conceptualization methodology.

1.2.2 Properties: Granularity, Extent and Scale

Modeling environmental systems requires selection of a problem-specific set of processes, that is — as mentioned above — albeit and subjective. This focus is defined by the problem to be solved. For example, studying climate change needs consideration global temperature, atmospheric CO_2 concentration, radiation, vapor etc. Within this area processes like runoff, nutrient cycling in soil are neglected. However these variables determine the process. More crucially, depending on the spatial resolution, even clouds are described by a single parameter rather than a shadowed area.

The decision to exclude variables or processes from a model is based the modeler's experience, on expert knowledge: a variable may have an influence on the process studied, but this influence may be considered to be small compared to the other variables studied. Selecting variables for a process to be modeled defines a system boundary. System boundaries are defined in every modeling process. The important topic environmentalists are faced with is that environmental systems are *open systems*. A system boundary is defined only by the modelers and the scientist must decide which variables are important and which not.

Based on this selection of components — variables, processes and parameters, a precise definition will be given below — the conceptual model defines the scale of applicability. Conceptual modeling is therefore the step of model development in which processes and their granularity are defined and compartments are separated with respect to a specific problem-oriented scale. The question of scale of an ecological model finds widespread discussion in recent literature (Wu & David, 2002; Turner *et al.*, 2001).

Scale itself refers to temporal aspects of model dynamics, called *temporal scale*, and to the *spatial scale*. Temporal and spatial scale is determined by *granularity* or *grain*, which denotes the finest level of spatial or temporal resolution of a model or a given data set and the *extent*, which denotes the size of the study area or the duration of time under consideration. Spatial and temporal scale depend on each other in terms of modeling as well as in terms of data analysis: in general, one observes that if the domain of a certain model with respect to spatial and temporal scale is displayed within a diagram plotting spatial scale again temporal scale, model domains are arranged along the bisectrix, cf. Figure 1.3. Turner *et al.* (2001) presented examples for environmental disturbance regimes, biotic responses and vegetational patterns in this framework, see also (Levin, 2000).

Temporal Scale defines the time interval Δt or the characteristic time $\tau = 1/\Delta t$ which are valid for most of the dynamic process of the model. In entirely linear models

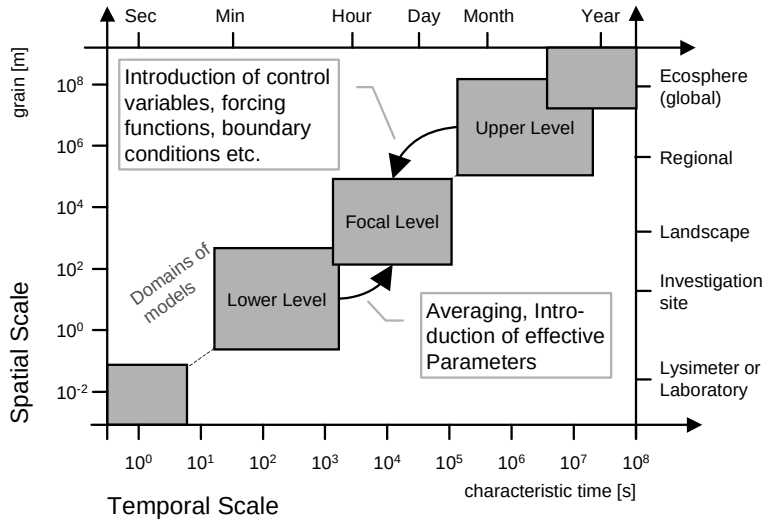

Fig. 1.3 Illustration of model domains with respect to temporal and spatial scales.

the characteristic times are given by the eigenvalues of the model systems. Eigenvalues are mostly used to analyze the general system behavior. There is an abundant literature in theoretical ecology on this methodology, see (Jørgensen & Bendoricchio, 2001, p. 274). Table 1.2 summarizes a list of processes related to agricultural ecosystems together with their characteristic times and the type of mathematical model used for simulation.

All eigenvalues define the *spectrum* of the system or model. If this spectrum has a wide range over several decades one speaks of a *stiff system*. This means, that models include very slow as well as very fast processes. In terms of Figure 1.3, the domain of the model would have a large horizontal extent. Stiff systems are usually difficult to solve numerically. Special procedures have to be applied (Hairer & Wanner, 1980). Model development tools as discussed in Section 1.5 rarely offer algorithms for dealing with stiffness. This is one of the reasons to focus on a specific temporal scale. In Chapter 9 we will analyze environmental models with respect to temporal scale and offer a methodology to group complex model by dynamics.

Spatial Scale With the spatial scale we denote the spatial extent or the spatial granularity that is chosen to develop a spatial model. At first glance one can think about the grid size in a grid based model or the average diameter of polygons in a vector based model. On the other hand the spatial scale is related to the size of the investigation area, for example an agricultural field, a small catchment, a region including large urbanized area or a continent or the world.

Spatially explicit modeling is always confronted with the question of how to handle, store and manage spatially explicit data — as well as acquiring — the data. Managing

Table 1.2 Agroecological processes on different time scales and the modeling approaches. Abbr.: ODE: ordinary differential equation; DAE: difference algebraic equation; DDE: delay differential equation; PDE: partial differential equation.

Process	Variables	Characteristic time	Mathematical model
Growth of microbial populations	Biomass, Nitrogen content, activity	30 minutes	ODE
Nitrification, denitrification	NH_4^+, NO_3^-, N_2O, N_2, microbial activity	1 day to 1 week	System of ODE
Degradation, volatilization of agrochemicals	Concentration in liquid and solute phase	Minutes to weeks	System of ODE
Populations dynamics	Density of eggs, juveniles, larvae, adults	Weeks to vegetation periods	Matrix equations, DAE, DDE
Crop growth	Organ biomass, nitrogen content, leaf area index	Month	(Systems of) ODE
Population dynamics of weed	Seed dispersal, coverage level	Vegetation period	DAE
Water transport in unsaturated soil zone	Water content	1 hour	PDE
Solute transport in unsaturated soil zone	Concentration in liquid and solute phase	Large spectrum	PDE coupled with ODE systems
Solute transport in aquifer	Concentration in liquid and solute phase	up to several years	PDE coupled with ODE systems

spatially explicit data requires the choice of an appropriate data model. All these issues will be discussed in Chapter 3.

Complexity Characterization of the spatial or temporal scale is related to the definition of a certain *degree of complexity* or simply *complexity*. Complexity of systems systems are characterized by four topics (Wu & Marceau, 2002). Complex systems:

- are thermodynamically open, they exchange energy, mass or information with their environment;
- are composed of a large number of of diverse components;
- have systems components that interact in a nonlinear way;
- exhibit a high degree of heterogeneity in time and space.

Integration of Scales Wu & David (2002) emphasis a second important property of environmental models. When selecting a certain spatial and temporal scale — the scale in this context is called the *focal level* — all related variables or processes from other scales or levels are denoted by special icons. For example components from

the level above the focal level, e.g. the larger time or spatial scale, are denoted by *context, constraints, control, driving forces* or *boundary conditions*.

Wu & David do not exemplify the same issue for levels below the focal level, considered scale, whereas Jørgensen & Bendoricchio (2001) distinguish between constraints "from below" and "from above". This is as important as the consideration of certain boundary conditions. To answer the question, what are the components of the lower level, we have to answer the question, what happened in system analysis when we neglected a certain scale that was much too detailed? We decided to neglect certain processes, as their temporal patterns do not influence the processes of the focal level. In this case we have the ability to parameterize the process in a different way. Usually a nonlinear function is introduced at the focal level. For example for degradation of a pesticide the high speed process of an enzymatic reaction is unimportant, and we can assume a nonlinear Michaelis–Menten kinetic, (Richter *et al.*, 1996).

When modeling environmental processes, one has to be aware of following facts related to scaling and levels:

- Notation of components changes through scales. A state variable of a large temporal scale model can be a boundary condition or driving force in a small temporal scale model. As scaling is frequently used with the task of integrating the model from a different scale this is an important topic.

- In general it holds true that, the more one steps away from the bisecting line, the less is the physical base of the model, the more phenomenological aspects enter the model. Or, we move away from a white-box to a black-box model. Scale therefore is also related to the distinction of black- and white-box models.

- Therefore spatial and temporal aggregation helps us to neglect low level scales. Mostly this aggregation leads to the incorporation of nonlinear processes in our model.

1.2.3 Toolbox and Language: Mathematical Models

Notations and Definitions Several notations have been used in the preceding paragraphs. A precise definition will be given in the following. Conceptual models consist of several components identified by their icons, cf. Figure 1.2. Although these icons differ from one conceptionalization method to another, all these components relate to certain mathematical elements. These are *state variables, parameters, control variables* and *mathematical equations*.

Definition 1.2 (State Variables) *All time- or space-dependent variables that are required to define the state of the system are denoted by* $\vec{x}$ *or* $\vec{X}$ *and are called state variables. Dependency to location is denoted by* $\vec{x}(\vec{z})$*. Time dependency is denoted by* $\vec{x}(t)$*.*

The set or vector of state variables is minimal, e.g. the vector collects all these variables that are necessary to derive the succeeding state of the system from the given state. Variables that can be derived from the state variable by an explicit or implicit equation do not belong to the state vector. These variables are called *auxiliary* or *adjunct variables* or *functions*.

The starting point for a simulation run is defined by a given set of state variables. This setup is called the *initial condition*. If a time interval from t_0 to t_{end} defined by $t \in [t_0, t_{end}]$ is considered, the vector with initial conditions shall be denoted by $\vec{x}_0 = \vec{x}(t_0)$.

Spatial dependency of a dynamic system is introduced, if the state variables depend on a location $\vec{z}$. In this case a certain study area is considered. Let us denote a study area or region by R. All locations are specified by location vectors $\vec{z} \in R \subset \mathbb{R}^{2,3}$. Usually R is a subset of the two-dimensional Euclidean space. The border of the study area is denoted by ∂R. Spatially explicit models are characterized by the fact that state variables show a functional dependency from state variable from a different — usually neighboring — location.

This raises the question of how to specify state variables that depend on the state of locations that are outside the study area. For those variables $x(\vec{z})$ with $\vec{z} \in \partial R$ *boundary conditions* are defined.

Processes of a considered system are translated into mathematical equations. These equations describe the exchange of information between the variables depending on space and time.

Definition 1.3 (Mathematical Model) *A dynamic model is defined by a set of mathematical equations, summarized with in a model equation $M_{\Delta t}$. The equation calculates a succeeding state $\vec{x}(t_1)$ from an initial state $\vec{x}(t_1)$ as a function of time t and location $\vec{z}$.*

A spatially explicit dynamic system is specified by a model equation M_t, an initial condition $\vec{x}_0$ and sufficient boundary conditions. A complete specification of the defined mathematical equations requires the specification of

Definition 1.4 (Coefficients, Parameters) *Parameters or coefficients are constant, e.g. not time-dependent, variables that specify mathematical functions. Parameters may depend on the spatial location. In the aggregated vector notation of a model system, we denote parameters by the vector $\vec{c}(\vec{z})$.*

The notations $\vec{c}$ or $\vec{x}$ for the vector of parameters or state variables are used if a model is discussed in a general way with respect to its structure or its application to different methodologies. In model development notations for the parameters are used that imply the function or meaning of the parameter or state variable. There is an abundant number of parameter notations, that have a more or less well-defined denotation or meaning, see Table 1.3. In general, parameters are notated by lower case, (state) variables by upper case letters.

Table 1.3 Some of the frequently used notations for state variables (upper part) and parameters (lower part of table) in environmental models.

Symbol	Denotation
P	Population
C	Concentration
Θ	Water content, Moisture
Ψ	Water pressure
T	Temperature
r	growth rate
F	Fertility, Fecundity
k, $k_{a,b}$	exchange rates, from compartment a to b
ρ	bulk density
p_i	transition probability, population dynamics modeling

With the choice of a relevant scale or level, certain components of the (open) environmental system acquire a special meaning.

Definition 1.5 (Control Variables) *Control variables or so-called forcing functions denote variables that incorporate influence in to a model that are driven by processes outside the model system boundary. These variables are to be defined before running a model. Control variables are* $\vec{u}(t, \vec{z})$ *and depend on time and space.*

The definition of the control variables is related to the definition of initial conditions and boundary conditions. All these three items are to be defined before running a simulation. A common interpretation of control variables in environmental modeling is the incorporation of anthropogenic influences into an ecological process. Differing parameterization of control variables define so-called *scenarios*, for a *scenario analysis*. Within the scope of optimization control variables have a special meaning, as these variables are estimated by special numerical procedures, see Part III.

1.2.4 Results: Computer Models

An adaptation from computer science and software engineering can illustrate the steps of model development in Figure 1.4: The "Water flow Model" summarizes the steps of system analysis, conceptualization, mathematical modeling and the result of a computer model. Running through these steps, different conceptualization methods are involved.

The resulting step of translating conceptual or graphical models into mathematical equations and solving these by the application of numerical algorithms leads to a computer model. The computer model then consists of *numerical codes* for the solution of initial value or initial boundary value problems.

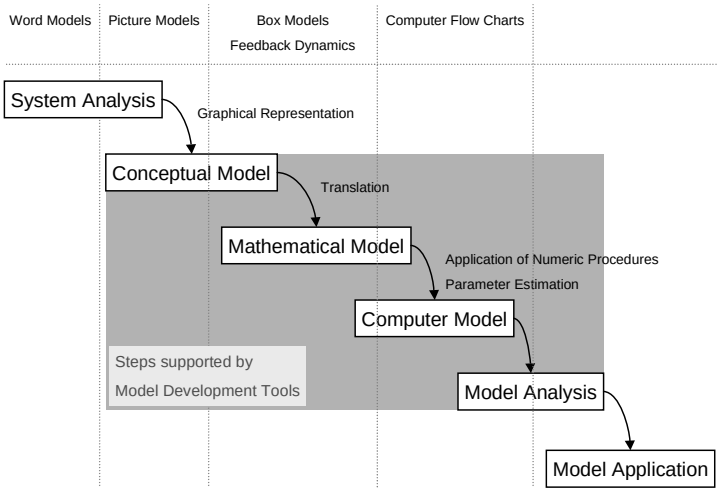

Fig. 1.4 An adaptation from computer science and software engendering: The "Water flow Model" clearly illustrates and summarizes the steps of model development in environmental system analysis: Starting with system analysis, conceptualization, mathematical modeling one derives a computer model. Several steps of model analysis may require us to step back and reformulate the previous step.

In general, the methodology of translating conceptual networks into equations is based on setting up the adjacence matrix — the matrix model — derived from the topology of the conceptual network. The matrix is then extended by parameters specifying the arcs between the graphical elements. Depending on the model concept chosen (see Figure 1.2) the resulting model consists of an equation system (input/output model), a time discrete, event-based model (Petri nets) or ordinary differential equation systems (box-model, feedback dynamics, energy flow models).

A common way of computer modeling (Richter *et al.*, 2001) is to start by designing the computer algorithm directly. The starting point of a model like this is a *computer flow chart*. Jørgensen & Bendoricchio (2001) add this to conceptualization methods, too. This is a common approach for *rule-based* models. The major difference from the conceptualization methods discussed above is that a computer flow chart defines a well-determined sequence of events whereas, for example, energy models define exchange rates of information and matter only. From this a sequence of computer instructions is derived thereafter.

In all cases, the final computer model is based on codes which are derived from mathematical models. Well-defined mathematical problems such as the solution of initial boundary value problems are a feasible starting point for simulation models, if the underlying processes are amenable to a direct formulation in a mathematically closed form. This is the case for most physical processes under controlled experimental conditions.

In environmental systems, where physical, chemical, biological, economic and other processes are interlocked at different scales and at different levels of complexity and information quality, codes cannot be derived via mathematical models, although the formulation of a general mathematical framework is still possible. In this case the code is a direct implementation of the conceptual model. Frequently encountered examples are *grid-based models* describing (mostly biological) spatial phenomena e.g. the spread of forest fires or of animal and plant populations, the migration of non-endemic species, the spread of pests and diseases or of certain genotypes. The latter example plays an important role in risk assessment of the spread of genetically modified organisms.

1.3 MODEL ANALYSIS

Whenever a computer model is finalized and ready to use, the question of model analysis arises. Two major issues are related to this topic. First, does the model cover all model processes correctly? This question will lead us to tasks such as, verification, validation, model testing. Second, how does the model behave if parameters, boundary conditions or initial values are specified from a domain that was not in the scope of model development? Or, in a different formulation, what does a model tell us in unknown situations? These may be either differing location or site condition, future states or different management strategies, differing anthropogenic input. The first question aims at a model analysis focusing on *intrinsic verification*, the second on *predictive power*.

1.3.1 Verification, Validation and Calibration

The use of the terms *verification*, *validation*, *confirmation*, and the *goodness of models* is the subject of ongoing debate in the literature. Oreskes *et al.* (1994) derived an explication of these terms from philosophy with special respect to environmental models. The term *verification* (from Latin, *versus*, meaning true) implies, that the truth of a model has been proven. This implies the reliability of the model as a basis for decision making. Understanding verification within this scope of philosophical logic, it is impossible to verify a model, as a model is per se a simplification of reality and the conditions under which a model need to be verified are infinite.

The term *verification* is also frequently used in terms of assessing numerical solutions of mathematical equations. With increasing availability of development tools for modeling, the underlying code of solving the derived equation system needs to be tested, too. In this context the verification of a numerically derived solution is done by a comparison of an analytical solution — usually obtained only for a simplified model — with the numerical solution.

In contrast to verification, *validation* denotes the establishment of legitimacy. For instance, a valid argument is one that does not contain obvious errors of logic,

cf. (Oreskes *et al.*, 1994). By analogy, a validated model is internally consistent and does not contain any flaws.

The term *calibration* is used, if certain parameters of a model are unknown, and may be derived only, if the model output is fitted to real world data. The mathematical problem of this task is *parameter estimation*. This precisely denotes a mathematical procedure of identification of parameter values based on experimental data using statistical methods. Calibration is usually used in a broader context. It also includes the choice of parameter values according to literature data. What can be done, if neither parameter estimations are possible, because field data is insufficient, and no literature data is present? If the considered process is identified as an important part of the modeled process, the only chance of continuing the model building process is to use well-educated guesses. Within the framework of model analysis one must test carefully, how the model reacts on modifications of these arbitrarily chosen parameters, cf. sensitivity analysis, model analysis, see below.

To continue with common denotation in literature the following can be found pretty frequently: After a model is "calibrated" based on training data, the model is "validated" comparing the model results with so far unused test data. If this step is successful, the model is classified as "verified". The outcome is that the terms of the section heading are frequently used in recent literature, rarely with a well-defined explanation.

To cope with the task of model analysis and to answer the question which introduced Section 1.3, we now consider intrinsic verification.

1.3.2 Intrinsic Verification and Predictive Power

The basic question of *intrinsic verification* is: Are model equations and the numerical methods correctly implemented?

One may derive an analytical solution of the mathematical model only for certain usually simplifying conditions. However, this is still a complex task and computer algebra systems may assist this step, see for instance Section 1.5.2. Care should be taken with nonlinear models, as special dynamic patterns may be lost, if the model is simplified too much. For these special cases comparison of numerical and analytical solutions yields benchmarks for goodness and correctness of the implemented numerical methods.

There are different ways to answer the question if the model outcomes match our (or some experts) prior knowledge of the system. If computer models are based on mathematical formulations, one is able to analyze the mathematical structure first. This type of system analysis focuses on the general system behavior. General properties of the dynamics system are analyzed, these are stationary points, or more general topological invariants (Arrowsmith & Place, 1994). It shows the capability of the model to describe processes which are qualitatively correct. This analysis may only be possible for simplified versions of the model — similar to the derivation of an analytical solution of the model. However, it is a worthwhile approach, as the derived

results are independent of parameter settings and allow a very general assessment and description of the system. For complex systems, systems that aim to be close to real systems, this approach is inappropriate.

Verification procedures and assessment of predictive power depend on the information available. If only expert knowledge is available the model can be analyzed using scenario analysis. Scenario simulations are set up by a defined set of input variables which characterize certain conditions (drought vs. wet climatic conditions, limited nutrients vs. sufficient nutrients). This is comparable to the *Gedankenexperiment* mentioned in Table 1.1. Using scenario analysis for intrinsic verification as well as assessing the predictive power the following recommendations are given:

- Crucial conditions as well as realistic conditions are recommended to test the robustness and the applicability of the model.
- Scenario simulations can be characterized as hypothesis testing. The hypothesis is that the model is capable of simulating certain situations known, and extrapolates to unknown situations in an appropriate way. The outcome of this type of scenario analysis is coarse. Either the simulations yield results expected by experts or not.
- If possible, scenario parameterization should cover the entire domain of a model in terms of temporal and spatial scale, refer to Figure 1.3.

For this step of model analysis algorithms exist that test all possible hypotheses, that are automatically generated from a knowledge base, which explain a lack of fit. As a result model parts are identified, which cause the differences of model output from observations. Additionally, information on processes not included in the model is identified. This analysis make use of the concept of *qualitative reasoning* (Struss & Heller, 1998). Ecological modeling applications are presented for instance by McIntosh (2003). This approach may be denoted as model verification in the strong definition given by Oreskes *et al.* (1994).

Results, acceptance and generality of model depend on the capability of the modeler to define appropriate characteristic scenarios. As the number of parameters increases with growing complexity of models, a sufficient analysis of model behavior to every parameter is hardly possible. Sensitivity analysis and Monte Carlo analysis are methodologies that allow an automated generation of model runs. Model output can be analyzed systematically based on predefined intervals or distributions that define the range of variation of parameters. Computational effort is high using these methodologies if the number of parameters increases. However, if knowledge on the distribution of parameters (Monte Carlo analysis) of parameter range (sensitivity analysis) are known or can be assumed, these methodologies offer an automatically estimation of model domain.

The predictive power can be analyzed by statistical tests if data from designed experiments are available at an ordinal scale or at a metric scale. *Cross-validation* is a widespread technique of model analysis in this case. This approach distinguishes

the steps of model calibration and assessment of predictive power. Two subsets of the underlying data set are selected randomly. The first subset is used for calibration (e.g. parameter estimation, see below). Assessment of predictive power is performed using the second subset. No changes are made to the model in this step. The results are statistical measures that assess the predictive power of the model.

1.3.3 Uncertainty

One has to be aware of the fact that *uncertainty* is an intrinsic property of environmental models, even if a model run through all steps of model analysis successfully. Jørgensen & Bendoricchio (2001, p. 80) propose an uncertainty relationship for ecological observations derived from Heisenberg's Uncertainty Principle, which can be applied to the energy balance of the world's ecosystem. They conclude that uncertainty cannot be avoided in principle in ecological studies. With a more theoretical focus, Haag & Kaupenjohann (2001) discuss the aspects of model uncertainty in the framework of philosophy of science. For practical purposes however, it is important to know the origin of uncertainty and the related consequences and conclusions.

Beven *et al.* (2001) collected several sources of uncertainty: lack of knowledge of the processes studied; lack of appropriate descriptive theories; errors in initial and boundary conditions; errors in inputting forcing data and calibration data; the difficulties in measuring the complex characteristics of the system at the scale of interest, and the limitations of numerical algorithms and computational power.

From this we identify three general different aspects that determine the degree of uncertainty of a model.

- Non-availability of data: Several steps in model definition and analysis require data to obtain statistical measurements of model performance, such as residual sum of squares (SQR), the correlation coefficient (r^2) or model efficiency (EF), (Loague & Green, 1991). Missing data or missing parameters lead to the uncertain specification of parts of the model, boundary or initial conditions. When we are assessing uncertainty therefore, we must take into account the uncertainty of the input data as well as the uncertainty of model parameters. Well-known statistical tools such as analysis of variation can assess uncertainty of data. Spatial data require geostatistical procedures. Uncertainty of model parameters can be assessed for instance by Monte Carlo analysis.

- Choice of scale: As mentioned in Section 1.2.2, the selection of the processes and the choice of the appropriate mathematical formulation and the chosen scale are arbitrary. Therefore, a specific selection of a certain mathematical notation of the process of interest incorporates uncertainty. Especially if processes of the level different from the focal level (see Figure 1.3) are to be incorporated into the model, several possible choices of model structures may be available. This is related to the question of uncertainty due to up- or down-scaling (Heuvelink, 1998).

An assessment of the uncertainty of the model is performed by different methodologies. First, well-known Monte Carlo analysis and sensitivity analysis are successful tools, cf. (Turner *et al.*, 2001). Based on these concepts Bärlund & Tattari (2001) used the tool UNCSAM to rank uncertainty of model parameters. Beven *et al.* (2001) suggest comparing different models to identify the correct *model structure* by applying the Generalised Likelihood Uncertainty Estimation (GLUE).

- Algorithms: Finally, uncertainty of simulation results is increased by the unknown error of numerical algorithms. Environmental models are very frequently coded by complex mathematical equations that require the application of one or more numerical procedures to obtain a solution. If possible one should select numerical procedures that are capable of controlling the error automatically, such as embedded Runge–Kutta formulae (RK) (Hairer *et al.*, 1980).

The three items above are inter-related. With a minimum of data or observations available one cannot develop a complex model with a large number of processes considered and a high degree of accuracy of the resulting simulation. The model is over-parameterized.

1.3.4 Categories and Classifications

Modeling is a problem driven methodology. This implies, that a model does not only depend on the selected spatial and temporal scale. The elements used for modeling also depend on the considered problem and on the viewpoint of the problem. The proceeding section summarized the methodology present for model development and model analysis.

As an addition to this one can identify categories that are applied to environmental modeling for characterization and classification of these models. Most of these categories or classifications are derived from recent publications, see for instance (Jørgensen & Bendoricchio, 2001). The most important classifications are summarized in the following starting from simple mathematical properties aiming at more general facts.

Autonomous vs. non-autonomous Models are a classification derived from mathematical analysis. An equation can be denoted as autonomous, if the model equation $M_{\Delta t}$ does explicitly not depend on the time t. This means for example for a linear model of matter flow, that reaction rates do not change with time.

Most of the more complex environmental models are non-autonomous, as basic processes depend on time, either direct or indirect, making use of variables like daily temperature, sun elevation etc. However, adding an adjunct variable $\frac{dx}{dt} = 1$ with $x(0) = 0$ and substituting t by x transforms any non-autonomous system into an autonomous system. This classification therefore is somewhat arbitrarry.

Static vs. Dynamic Models Static models do not depend on time. These models for example assess environmental parameters and derive variables or indicators important for further analysis. Habitat suitability models, which derive the probability of existence of a certain species as a function of abiotic conditions, are examples of these kinds of models.

Information on the static or steady state behavior of the dynamic model can be obtained by a stability analysis of a dynamic model. Information on stationary points with attractive or non-attractive behavior is the result of this analysis.

Deterministic vs. Stochastic Models Models entirely based on differential equations, matrix equations or algebraic equations are denoted as deterministic models. If a model contains a stochastic element, a random variable, the model is called stochastic. Monte Carlo simulation is a methodology that transforms a deterministic model into a stochastic model using assumptions on the stochastic distribution of selected model variables.

Distributed vs. Lumped Models This classification refers to the spatial scale and the spatial granularity of a model. Spatial processes may either be described by spatial distributed parameters and state variables, or one may identify so-called *effective parameters*. Effective parameters are derived from averaging over a certain spatial extent or domain (see *support of model* in Section 3.1.1). This is obtained by identifying the spatial distribution of the parameters and the estimation of the distribution function. A model that is based on effective parameters shows no spatial dependence and is frequently called a *lumped model*.

Complex vs. Aggregated Models Similar to the terms *distributed* and *lumped* the terms *complex* and *aggregated* are used. However, these terms are used more generally in literature and refer to temporal as well as to spatial scales. The meaning of the terms complex and aggregated has changed through the years with the increasing computer power, the support by development tools for modeling, and the availability of easy-to-use numerical algorithms.

Analytic vs. Numerical Models The categories analytic and numeric are more appropriate to characterize a model compared with the previous paragraph. An *analytic model* focuses on the mathematical structure and the system behavior of the developed model. It aims at presenting structures that are valid for a broad range of applications and can be studied without finalizing the specification of parameter to defined values. Well-known examples for these model types are the Lotka–Volterra equation in lots of different specifications of predator–prey modeling or the most sustainable yield problem for analyzing stability of harvest models, etc.

Numerical models require all parameters to be specified. These models are usually discussed within a certain framework of application and aspects of validation, calibration and verification (see above). In this context the chance of deriving an analytical

solution of a model equation may be discussed (Costanza *et al.*, 1993; Hall, 1988). With the available tools of model development and numerical solution of complex equations, this discussion has disappeared from recent publications.

Research vs. Management Models *Management models* aim at the application of models, whereas *research models* aim at identification of the environmental processes. The idea behind this classification is the observation that simulation models resulting from research projects are usually too complex, too large (and mostly too poorly documented) to be applied to questions of management.

Biosphere vs. Anthroposhere It is usual to distinguish between biosphere and anthroposphere as domains of certain models. However, knowing that mankind takes part in an ecosystem and mutually depends on the ecological environment, the distinction between the two spheres seems to be overcome. In my opinion, this classification may remain valid in the future, for reasons of perception, even though we should aim to overcome this anachronistic distinction. We should aim at an integrative rather than an anthropocentric view of our problems, and the same applies to our method of tackling the problem, the tool of modeling.

The difference of modeling a system from techosphere in comparison with an ecological system is that for the technical system, in most cases a conceptual model was present at the stage of building the system. For ecological systems the steps system analysis, conceptual models and parameter estimation must be performed, to assess if we know the system to a desired stage. One may argue, that even for a technical system, a system analysis is required to describe the system. The difference in system dynamics is more general. Beddington (1981) noted that “there are no Newtonian laws in ecology”. The following chapters will show that there is a multitude of methodologies to describe an ecological process appropriately, but this is rarely the case for technical systems.

The distinction between anthroposphere and biosphere is — besides the concept of scaling in time and space — another reason for the introduction of control variables. Control variables and forcing functions are frequently defined by a system boundary that separates of those two spheres.

Integrated Models In this context the term *integrated model* appears in recent literature. Integrated models aim at overcoming this separation of different disciplines. This means that these models aim at integration of anthropospheric as well as biotic processes. These models try to integrate aspects from such disciplines as ecology, economy and sociology. The system boundary of an integrated model is defined by the region studied rather than the processes of interest in the time scale.

1.4 LINKING REAL WORLD DATA AND MODELS

The problem of applying an environmental model to a real world situation shows a spatial and a temporal aspect. First, parameters and coefficients that show a dependency on spatial location — written as $\vec{x}_0(\vec{z})$ or $\vec{c}(\vec{z})$, cp. Definition 1.2, 1.4 — need to be set up. This implies the necessity of accessing spatially referenced data. The problem is denoted by regionalization of a simulation model. Second, process parameters must be identified: the dynamics of a model have to be identified. This aspect is related to parameter estimation.

1.4.1 Regionalization: Applications to Investigation Sites and Spatial Validity

Regionalization denotes the procedure of making a model depend on spatially distributed parameters or initial conditions. A methodology required to solve this task is *cartographic modeling* usually performed with the framework of a Geographic Information System (GIS), (Longley *et al.*, 2001). First, cartographic modeling is a tool in itself for processing spatial information, for instance creating new maps by the combination of information of several layers. Second, cartographic modeling is a tool for regionalization of local computer models by identifying basic spatial units, which are characterized by homogeneous attributes. These units are called for example elementary watersheds (hydrotopes) or elementary landscapes (ecotopes).

Before looking at different ways of regionalization, two different concepts of handling spatial data must be summarized. Two general approaches exist for regionalization of computer models using GIS.

- In the *vector representation* the boundary of any two-dimensional object is described by a sequence of point coordinates, a polygon. Attributes of the object are stored in a database.
- In *raster systems* the investigated area is set up by a regular grid of cells. For each cell, a representative feature attribute is stored as code value.

An application of one concept or the other depends on the task under consideration and on the identified spatial area of validity — the support — of the model. The *support* specifies the spatial extent for which a model is assumed to be valid (Heuvelink, 1998). Initial conditions as well as set up of model parameters are constant for the area of model support, a basic spatial unit.

The vector data approach is more flexible and has more prerequisites to the functionality of GIS. With this approach one is able to determine the appropriate areas for which a simulation model is valid. The GIS functions used are the intersection of a set of information layers (e.g. habitat suitability maps as intersection of vegetation maps, soil humidity maps and land use pattern maps), neighborhood analysis (computation of slopes or aspect), network analysis (shortest routes), etc.

For a raster based regionalization approach the support of the model is equal to the cell size. This data model has the advantage of a simple data structure. Additionally, neighborhood relationships are easy to derive, as there is a distinct number of neighbor cells. A cellular automaton (CA) has much in common with cartographic modeling using a raster based data structure. The raster approach is suitable for use in changing landscape patterns. Changing patterns, time depending land use or vegetation dynamics including migration processes can easily be implemented with the raster approach, as this can be performed by changing grid cell attributes only. Modeling the change of spatial patterns on the basis of vector data needs to dynamically change geometry information, which is a difficult task, and needs to modify the underlying GIS database.

In this context it becomes obvious, that coupling a dynamic simulation model with spatailly explicit data either for the specification of the location dependent parameters $\vec{c}(\vec{z})$ or location dependent initial conditions $\vec{x}_0(\vec{z})$ requires integration of a simulation model into a GIS. One can distinguish different approaches for this task:

- A loose integration uses the GIS to compile a data-set including parameter specification and feed this into the model and to start several model runs for every spatial unit;
- the integration of simulation functionality into a GIS;
- the integration of spatial data maintaining function into a model.

The first item can be used only if the simulation model does not include any interactions of processes between two models on different elementary landscapes. For example lateral, horizontal flow of matter and information, migration of species cannot be described by this approach. It is appropriate only if the model support can be identified in a way that there are no flows across the boundary of the support. This is for example the case in hydrological catchments. The time scale of the model must be considered for this analysis, too. For example, lateral flows can be neglected if studying degradation of substances in soil, if degradation and vertical transport is fast compared to lateral flows.

Integration of simulation functionality with a GIS is very expensive in terms of development costs. Some products can be found for distinct problems, such as ground water modeling or atmospheric transportation of substances.

Spatially explicit models, that cover both dynamic and spatial processes including flow of information, matter or energy across the boundary of model support, are usually set up by integrating GIS functionality into the model code. Additionally, modelers chose the raster data format, as this needs less effort to handle spatial data, as the topology of the raster data model is pretty simple. Chapter 3 focuses on spatially explicit environmental models.

1.4.2 Parameter Estimation

The crucial point in performing a realistic and convincing ecosystem simulation is the information of basic model parameters. Often, it is difficult even to assess the correct order of magnitude of important parameters (Richter & S öndgerath, 1990). *Parameter estimation* is a synonym for statistical procedures to obtain reasonable values for model parameters based on data. Dependent on the data available, different methods of parameter estimation can be applied.

The classical approach of parameter estimation are *regression methods* (Draper & Smith, 1966; Seber & Wild, 1989; Marsili-Libelli, 1992). With these methods parameter estimates are derived by minimizing the sum of squared deviations of model predictions and data. Numerical algorithms for the simple case of a linear model, as well as for nonlinear models, exist and are part of any statistical software package such as SPSS or SAS. Regression techniques to determine parameter values from underlying data are widely used (Kelpin *et al.*, 2000) and are embedded in software tools such as EASYFIT (Schittkowski, 1994) or MODELMAKER (Walker, 1997), even if the ecosystem model is given in terms of (ordinary or partial) differential equations with no explicit analytical solution. The goodness-of-fit can be judged by looking at the confidence regions and correlation matrix. However, successful application of regression techniques necessitates an appropriate experimental design. Measured data and model structure must fit together (Gubbins & Gilligan, 1996).

Other statistical approaches to obtain realistic parameter values are likelihood techniques which are based on a distribution assumption, or Bayesian methods which use some prior information (Foley, 2000). If there are no sufficient data, no prior information or if the model is not given in analytical form, other methods to obtain parameter values must be used instead. In these cases so-called *expert systems* can be derived. Current notations are also rule-based systems or knowledge-based systems (Salski, 1992). Roughly speaking these are sets of “if-then” rules built up with the help of practitioners or other experts. One example for gradient free optimization methods, which can be used for parameter estimation on rule-based model systems, are *genetic algorithms* (GA) (Wall, 1996).

If one is dealing with spatially explicit models additional problems arise with parameter estimation. This is because the number of parameters to be estimated for a grid-based model is proportional to the number of cells. Therefore methods have been developed to derive the model parameters from easy-to-determine cell properties e.g. via *transfer functions* (Tietje & Tapkenhinrichs, 1993). In soil science this technique is a common method to derive transport parameters from soil characteristics to avoid a huge experimental effort. It is also used in connection with scaling up of process models i.e. when applying process models to real landscapes.

1.5 MODELING LANGUAGES AND DEVELOPMENT PLATFORMS

1.5.1 Overview

Computer modeling is supported by a number of software packages, which support the previously described steps of model development from conceptual models to computer code, see for instance (Walker, 1997; Hulbert *et al.*, 2000; Heller & Struss, 1997; Struss & Heller, 1998; Wolfram, 1999; Muetzelfeld & Massheder, 2003; Soetart *et al.*, 2002; Lischke *et al.*, 2002). These software tools allow a (semi)-automatic translation from conceptual models to computer models, usually restricted to a certain mathematical language (ordinary differential equations, Petri-Nets, etc.). The use of development tools leads to the question, how to verify the software tool used. The steps of model verification described above are also valid for the *verification of development tools*. These tools consist of different functionality, like translation of conceptual models into mathematical models, numerical solution of differential equation system, analysis tools like sensitivity analysis or Monte Carlo analysis. The performance of these software systems can be assessed based on models with well-known system behavior. Problems frequently encountered are: stiff equation systems (Hairer *et al.*, 1980; Hairer & Wanner, 1980), robust parameter estimation (Schittkowski, 1994), mathematical heterogeneity.

Tools for computer modeling comprise one or more of the following functions:

- Graphical design of a conceptual model within a graphical user interface (GUI);
- Specification of compartments, definition of parameters, initial conditions;
- Definition and specification of mathematical function;
- Translation of fully specified conceptual network into set of mathematical equations;
- Export of set of equation into computer code of high level language or into meta-modeling language;
- Derivation of numerical solutions of derived mathematical equations, for instance numerical solution of differential equations;
- Specification of spatially referenced parameters by spatial databases, geographic information systems;
- Tools for visualization, plot of selected variables, plot of maps;
- Tools for model analysis, for instance sensitivity analysis, optimization, repeated runs, Monte Carlo analysis, parameter estimation.

Table 1.4 Comparison of model development tools. Part 1: General model development.

Name	MATHEMATICA	MATLAB
Company	Wolfram Research	The Mathwoks Inc.
URL	`http://www.wolfram.com`	`http://www.mathwoks.com`
Operating System	Win, Mac, Unix	Unix, Win
Mathematics	Large symbolic mathematics package, large numerical packages, e.g. analytical solutions of PDE, ODE, statistics	Large numerical mathematica toolbox, e.g. ODE, matrix equations etc.
Numerics	ODE, PDE solvers, (adaptive, stiff systems)	ODE solvers, (adaptive, stiff systems)
Model Analysis	several	several
Extendible	internal programming language, MathLINK interface	internal programming language
Graphical Front end	yes	yes

1.5.2 Mathematical Languages

Mathematics offers a general language for describing and analyzing complex environmental problems. Without a general language like mathematics it would hardly be possible to analyze any of the recent environmental problems. Complexity of systems has increased in the recent decades. This was supported by the good availability of mathematical and computer science support to environmental researchers. The crucial point with this is, that a multitude of methodologies exists, that compile a mathematical or computer model out of a conceptual model. So even if we identify a consensus on a conceptual model, the mathematical translation can look entirely different.

Let us examine some examples: for transport and reaction processes the mathematics are ordinary or partial differential equations. If compartments are regarded as spatially homogeneous, one is led to systems of ordinary differential equations. Another class of models is based on stochastic processes. In the context of environmental modeling, soil properties related to soil structure and soil composition determine transport and reactivity parameters. Each of these properties can be regarded as realizations of stochastic random processes. Once the process is specified, for example via a variogram, spatial realizations can be generated by a code (Deutsch & Journel, 1992; Cressie, 1991). All this leads to the problem of mathematical heterogeneity of environmental models, and this will be discussed in detail in Chapter 4.

Concerning the step automatic translation of graphical systems in mathematical equations, most of the available development tools choose a certain mathematical dialect. This means within a selected tool only time-discrete or matrix equations can be compiled, within another tool only systems of ordinary differential equations are generated and a third tool might focus on event-based Petri nets.

Table 1.5 Comparison of model development tools. Part 2: Development tools and environments for spatially explicit models.

Name	FemLAB	SME	SIMILE	ICMS
Author, organization, company	The Mathworks Inc.	Thomas Maxwell, Gund Institute of Ecological Economics, Univ. Vermont	Simulistics Ltd., Edinburgh Technology Transfer Centre	CSIRO Land and Water, Integrated Catchment Assessment and Management, ANU, Australia
URL	`http://www.mathworks.com`	`http://www.uvm.edu/giee/SME3`	`http://simulistics.com`	`http://www.cbr.clw.csiro.au/icms`
Operating system	Win, Unix	Unix, Linux	Win, Unix, Linux	Win
Mathematics	PDE	regionalized ODE	ODE, DAE, Matrix, object-oriented	object oriented user code
Numerics	FEM (adaptive, stiff systems)	2^{nd} order RK	1^{st} order RK, Euler	—
Programming language	within MATLAB	C++	C++	MICKL, C subset
Spatial data	vector	raster	implicit by spatial reference of multiple instances of model objects	vector, raster
Graphical front end	yes	optional, model development by STELLA etc.	yes	yes

This is a comprehensible way of restricting the required numerical procedures for solving the system generated. However, this restriction to a certain mathematical dialect often determines the ability of the modeler to describe a certain system. The strength and the functionality of the modeling toolbox strongly determines our perception of the system. The results of this issue is, that

- several models are developed, describing similar or even equal processes but with different methodologies. Redundancy is increased (Müller, 1997);
- it is hardly possible to define a general language for a meta-data environmental model that is capable of describing and documenting environmental model in general (Benz & Knorrenschild, 1997).

Therefore, mathematical models of environmental processes are mathematically heterogeneous, cf. Part II. In the following a brief overview of widespread development tools is given, that supports the steps of model development discussed in this chapter.

Tables 1.4–1.6 list some of the widespread tools used for development of environmental models, see also (Costanza & Voinov, 2001; Muetzelfeld & Massheder, 2003).

The table lists the program name, the company or institution responsible for maintenance and development and the related URL for further information. For detailed discussion the underlying mathematical dialect of the system is given, as well as some comments on the extendability of the system. Note, this is a more or less subjective choice based on the experiences of the author. There is much development in this area, which leads to new inventions of development systems. Compare for instance systems FEMME (Soetart *et al.*, 2002), RAMSES (Lischke *et al.*, 2002).

A distinction is made between conceptual modeling tools and programming tools. The former support a graphical representation of the considered processes and mostly support an automatic translation of conceptual models into mathematical equation systems. The latter support the steps of model development with a tool set of functions that are helpful for environmental model development. In the following some of the systems are described in more detail.

1.5.3 Generic Tools for Model Development

MATHEMATICA was developed in 1986 by Stephen Wolfram. It is a general symbolic and numeric solver, capable of performing a wide variety of mathematical computations. It uses its own programming language, which makes it a very flexible solver. Its internal functions can also be called by external programs, and the data output can be used by those programs. The MATHEMATICA programming language contains a rich set of commands, for solving calculus, algebra, differential equations, linear algebra, and trigonometric problems. MATHEMATICA performs very well as a differential equation solver for ODE as well as PDE, presenting solutions both numerically, if available analytically and of course graphically. MATHEMATICA has a wide variety of graphing capabilities, including 3D graphs and plots, which can be exported to Postscript (PS or EPS) documents.

While this diversity makes MATHEMATICA a very comprehensive solver system, it also makes MATHEMATICA a particularly difficult program to use, requiring a fairly long training period. As an aid in learning and using Mathematica, a number of "notebooks" are included with the package. A "notebook" is a collection of MATHEMATICA commands, textual documentation concerning those commands, and any data which might be used by those commands. It is the standard way MATHEMATICA organizes and saves a work session. MATHEMATICA also creates sub-groups of functions within notebooks, allowing for more flexibility in creating solutions. In fact, flexibility is the key word in describing Mathematica.

MATLAB is exclusively numerical, with no symbolic solving features incorporated. It is geared very much toward engineering and scientific applications. It comes with all necessary documentation, including many tutorial scripts and lessons. The main features of MATLAB are a very powerful and rich numerical mathematics package, and a relatively easy command syntax. For most applications, scripts can be written which use the solver tools provided, many applications can be created by dragging

and linking appropriate icons, which represent MATLAB's solver tools, to build the necessary application.

1.5.4 Conceptual Modeling Tools

Tools for conceptual modeling are often called graphical modeling environments. Systems like these have a long history starting from the first works by Forrester (1968) and Odum (1983). Recent developments encompass most of all functions for model development as listed above and displayed in Figure 1.4. Some systems even offer the functionality of model analysis and parameter estimation.

For the systems listed in Table 1.6 follows a short description.

EXTEND is used for discrete-event, continuous and hybrid simulations. Features of this system are the ability for the user to package up a sub-model with its own icon, which can then be used as a higher-level component. This supports hierarchical and modular model development.

MADONNA This system is very similar to MODELMAKER and STELLA. It is a system dynamics visual modeling package that generates very efficient models based on ODE systems.

MODELMAKER is a visual simulation modeling package designed for scientists and engineers (Walker, 1997). Based on system dynamics ODE systems can be graphically designed. Models can be structured hierarchically with the definition of sub-models. MODELMAKER offers — compared with the other systems listed in this section — a good functionality concerning the analysis of the defined model. Monte Carlo analysis, sensitivity analysis as well as parameter estimation and model optimization is implemented. Initial values of unknown model coefficients for parameter estimation can be calculated using a genetic algorithm approach or by a grid search strategy. Statistical documentation of a parameter estimation is profound, including correlation matrices and standard deviation of the parameters as well as statistical test.

POWERSIM offers a range of tools for building simulation models based on the system dynamics paradigm. The system is primarily aimed at the fast-growing business, Web-oriented market.

STELLA This is the best-established of the system dynamics visual modeling packages with a large number of users. STELLA offers a range of components in addition to the standard "stock" symbol. Model analysis functions are limited. Function for parameter estimation are missing. User-customizable interfaces are supported (Hulbert *et al.*, 2000).

VENSIM Originally VENSIM was designed as a tool for running STELLA models more efficiently. It is now a modeling package in its own right, combining causal loop and system dynamics elements.

SIMULINK MATLAB also comes with SIMULINK, which is a program for simulating dynamic systems. SIMULINK is graphic oriented, and the user can build the dynamic system by dragging and linking the appropriate icons. In contrast to the system dynamics platform, the icon concept in SIMULINK makes use of engineering concept, such as integrations, differentiator, etc. The dynamic nature of SIMULINK lends itself particularly well to solving differential equations systems.

FEMLAB In contrast to all mentioned systems above, FEMLAB offers the ability to setup models based on partial differential equations (Comsol AB, 2001). The required finite-element meshes are automatically generated and the underlying geometries may be imported from standard geometry files (DXF), for example exported from a geographic information system. As FEMLAB is embedded into the MATLAB framework, extendibility is given based on the programming facilities of MATLAB.

1.5.5 Modeling and Programming Environments

Restriction to a certain mathematical dialect requires us to code some part of an environmental model within the framework of a high level programming language. However, high-level programming languages (like C++ for instance) require specific extensions for environmental modeling. For example, the most frequent extensions reflect the spatial localization of environmental processes and the connection to database system for parameters specification. This is why most of the programming environments listed below support interactions and exchange with GIS. Several systems are in development that aim either at an integration of different models or at an support of spatially explicit model, see for instance the overview by Woodbury *et al.* (2002). For detailed discussion we focus on the Spatial Modelling Environment (SME), which is used for the case studies in this book and Simile, former known as AME.

Spatial Modeling Environment The Spatial Modeling Environment (SME) attempts to address the conceptual and computational complexity barriers to spatio–temporal model development. SME links icon-based graphical modeling environments with a generic object database (Costanza & Maxwell, 1991; Maxwell & Costanza, 1997a). This system allows us to create and share modular, reusable model components, and utilize advanced parallel computer architectures. The SME design has arisen from the need to support collaborative model development among a large, distributed network of scientists involved in creating a global-scale ecological and economic model. The system is designed to support a range of platforms, both in the front-end development environment and in the back-end parallel computing environment, cf. (Maxwell & Costanza, 1997a; Maxwell & Costanza, 1997b).

Table 1.6 Comparison of model development tools. Part 3: Icon-based modeling environments with graphical front ends for conceptional models

Name	STELLA	POWERSIM	MODELMAKER
Company	High Performance Systems Inc.	POWERSIM	Cherwell Scientific
URL	`http://www.hps-inc.com`	`http://www.powersim.com`	`http://www.cherwell.com`
Operating system	Mac, Win	Win	Win
Mathematics	ODE	ODE	ODE, DDE
Numerics	4^{th} order RK		up to 4^{th} order RK
Model Analysis	Repeated runs, unit analysis	Sensitivity analysis, optimization, scenario management, unit analysis	Parameter estimation, Sensitivity analysis
Extendible	no	no	DDL programming

Simile is a software environment for building and running simulation models in ecology, biology, environmental science and related disciplines. It features a powerful and expressive diagram-based language for designing models, including both system dynamics and object-based concepts. Simile also supports modular model construction, and modules can be nested to any depth.

The resulting models can be run very efficiently as compiled C programs, and delivered to others as stand-alone models. Simile provides a range of tools for displaying model behavior but also allows you to add your own, customized to your own needs.

One of the aims of Simile development is to show that it is possible to radically improve the way that modeling is undertaken within research programs, without restricting the ability of researchers to design the models they want.

1.5.6 Numerical Mathematics

These development platforms offer a good functionality for developing and running simulation models. With a graphical user interface several important functions are hidden from the user. However, these functions are very important for an understanding and correct assessment of the output derived. This section therefore sheds some light on the underlying methodologies implemented in model the development tool.

Having identified the mathematical elements induced by the conceptual model together with the topology defined by the conceptual network, two questions arise:

- How is a mathematical or computer model derived and (automatically) generated from the conceptual network?
- What mathematical procedures are required to perform a simulation based on the derived equations and what is required to solve the model equations?

Table 1.6 cont.

Name	SIMULINK	EXTEND	VENSIM
Company	Mathworks	Image That! Inc.	Ventana System Inc.
URL	`http://www.mathworks.com`	`http://www.imaginethatinc.com`	`http://www.vensim.com`
Operating system	Mac, Win, Unix	Mac, Win	Mac, Win
Math. languages	ODE	ODE	ODE
Numerics	see MATLAB		up to 4^{th} order RK
Model analysis		Optimization, Monte Carlo analysis, etc.	Monte Carlo analysis, optimization, sensitivity analysis
Extendible	within MATLAB	yes	DLL programming

These two questions are related together, as the numerical procedures available for the second item determine the methodology for translating a conceptual network into a mathematical model. For a model run of the derived model one or more algorithms related to the following numerical issues are required.

ODE Solutions The most common way of performing a simulation of a model based on a ordinary differential equation system is to apply a standard Runge–Kutta method to the system, see (Hairer *et al.*, 1980). Usually Runge–Kutta schemes up to order of 4 or 5 of the classical Runge–Kutta formulae are chosen. Good ODE solvers work with an embedded step size control, which aims at controlling the numerical error by applying two ODE solvers to the same system and comparing the solutions. If the solutions diverge the time step of the solution is decreased to limit the simulation error.

High performance model development packages additionally analyze the dynamics of the model system and identify the stiffness of the system. Note, stiffness is a dynamic property of the nonlinear systems. If stiffness is identified — a model incorporates processes with a large range of characteristic time — special ODE solvers are applied, e.g. GEAR or BDF scheme (Hairer & Wanner, 1980).

Implicit Equations come up if the result of a function is at the same time an argument of the same function. This type of equation is a typical outcome of flow networks, for instance recycling loops. Common model development platforms are not capable of solving these equation (STELLA, MODELMAKER, MADONNA, VENSIM). Iterative procedures, like regular–falsi or Newton are used to solve this type of equation. As these are iterative procedures an appropriate starting value for iteration is required (Stoer & Bulirsch, 1983).

Matrix Equations are usually solved by well-known procedure of numerical linear algebra. However, if the systems tend to be high-dimensional and the system matrices are sparse, it is recommended that a high performance equation solver be chosen that is capable of reducing error caused by floating point arithmetics.

Partial Differential Equations In general partial differential equations are not generated by translating conceptual models into mathematical equations if no spatial dependencies of variables are defined. These types of mathematical model are the outcome of a spatial referencation of state variables. These models are highly aggregated and incorporate a wide range of processes by a very limited set of parameters, cf. Chapter 3. Numerical solutions are derived by difference procedures, finite element methods of line methods.

Eigenvalue Problems Besides the foremost problems of estimating model solution the task of model analysis is related to numerical problems, too. Eigenvalue problems must be solved, if the dynamic properties of a model system are to be identified. The results are used to assess system dynamics, perform a stability analysis and calculate, for example, probability of species extinction (Stoer & Bulirsch, 1983).

Nonlinear Minimization or Maximization

Optimum Control or Optimization Optimization or the special topic of time-dependent control variables, optimum control aims at the identification of a set of control variables, that result in a desired system behavior. If the function is nonlinear but analytically derived, we have a nonlinear optimization problem, which is solvable by well-known Simplex or Levenberg–Marquardt algorithms (Press *et al.*, 1988; Stoer & Bulirsch, 1983). These procedures require at least a numerical approximation of the derivative of the goal function to the control variables. If these are not available or do not exist, derivative-free procedures like genetic algorithms may be an appropriate choice, see (Wall, 1996).

Several well-tested procedures for solving optimum control problems are available. These mostly focus on optimum control problems with underlying ODE for the dynamic system (Bulirsch *et al.*, 1993; Bulirsch & Kraft, 1994).

Parameter Estimation Optimization in terms of certain model parameters is a common feature of several model development tools, see tables. MODELMAKER offers the functionality of parameter estimation based on well-known Levenberg–Marquardt as well as Simplex algorithms, see (Press *et al.*, 1988). The general concept of numerically solving parameter estimation problems is to transform the given problem into a general nonlinear programming problem using a Gauss–Newton and quasi-Newton method. This is implemented in the algorithm DFNLP from Schittkowski (1983). The remaining optimization problem is solved by a sequential quadratic programming method (Schittkowski, 1980). These procedures calculate estimators for the parameters as well as standard deviations and covariance matrices.

More sophisticated algorithms that reflect on typical ecological problems such as sparse data of spatially explicit processes are developed and discussed by Bock (1983) (PARFIT) with applications in environmental fate modeling of pesticides by Altmann-Dieses *et al.* (2002) as well as Schittkowski (1980) with the toolbox EASYFIT.

In ecological models set up by different mathematical elements or dialects, more algorithms are presented for parameter estimation, that have fewer prerequisites on the model structure. The methodologies make use of gradient-free optimization algorithms such as genetic algorithmsq (Wang, 1997; Doherty, 1994).

1.6 SUMMARY

This chapter has given a general introduction to environmental modeling methodology. Important concepts are introduced such as the water flow concept for model development (see Figure 1.4) and the general criteria for model analysis and model performance assessment. These concepts are valid for a broad range of modeling problems and are independent from the considered spatial or temporal scale, see Figure 1.3.

The steps in the water flow model are supported by several software tools that support the development of environmental models. From this, two important conclusions can be drawn.

First, it is neither necessary to start modeling from scratch nor to perform all the steps of model development alone. That means development of environmental models has to make use of existing approaches. Available models can be used or integrated into a model that fulfills our needs. This also means that, compared with former documentations in ecological modeling, see for instance Jørgensen (1979), one does not need to consider for instance, the programming language or platform the model will be coded in. Abstraction to the mathematical formulation of the processes is a tremendous success in modeling. This is supported be the increasing capability of numerical algorithms in modern modeling platforms, see Section 1.5.

Second, even if modeling is supported by a broad range of tools, the material is still needed. This material is given by a set of mathematical equations that describe the most important environmental processes. In this context the next two chapters present a basic stock of important and frequently used models and modeling approaches for environmental processes.

2

Environmental Models: Dynamic Processes

2.1 INTRODUCTION

The main purpose of this chapter is to perform a system analysis of ecological processes of a general ecosystem in terms of fluxes of mass and information. The emphasis is on ecosystems with strong anthropogenic influences, for instance agricultural ecosystems. Several examples are given of possible translations of conceptual models into mathematical equations with special respect to non-spatial dynamic processes.

We focus on the first two trophic levels. The steps of model development as presented in Chapter 1 are run through on the first trophic levels of a general (agro)ecosystem model. The first trophic levels of the biotic sphere are analyzed in detail: interspecific competition between weeds and agricultural crops, and populations of phytophagous insects with age-structured population dynamics. Secondly, we focus on the mathematical heterogeneity, an intrinsic property of ecological models based on the variety of approaches capable of modeling the processes of interest. This is illustrated by presenting different possible mathematical translations for one conceptual model for selected processes.

2.2 FIRST TROPHIC LEVEL: PRIMARY PRODUCERS

Figure 2.1 shows a conceptual network of processes. This conceptual network focuses on the processes. More general foodwebs and conceptual systems of agricultural ecosystems can be found (Begon *et al.*, 1986).

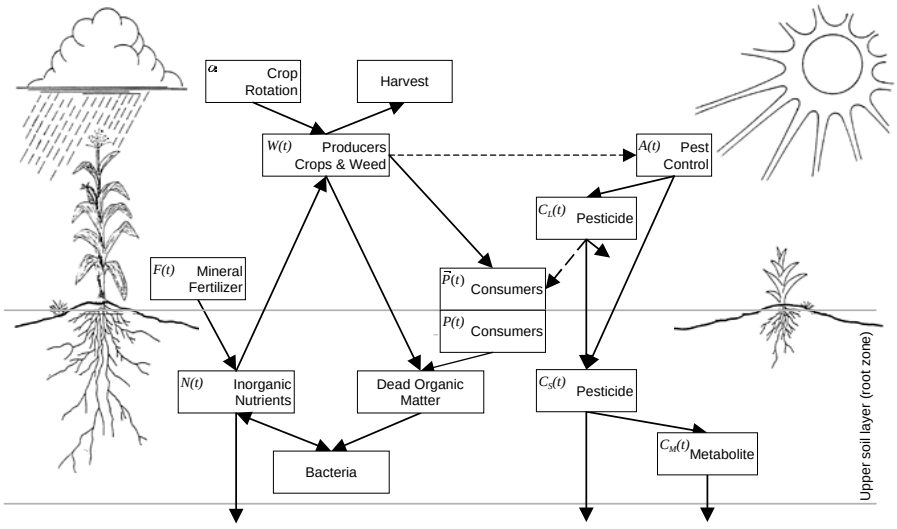

Fig. 2.1 Conceptual model of an agricultural ecosystem. The boxes denote compartments, arrows denote general transport of mass, energy. Dashed arrows denote dependencies or flow of information. State and control variables are noted at the upper left corner of the compartment boxes.

2.2.1 Crop Growth

Let $W(t)$ denote the weight of the above ground biomass in [kg/ha] of a specific crop, a primary producer, see Figure 2.1. We distinguish between crop biomass W_C and biomass of weeds W_W. The literature for modeling crop growth is abundant. The approach used here simulates crop growth in a single differential equation and covers the processes of growth (parameter r in [1/d]), mortality (μ_C in [1/d]) and senescence (function $f_s(t)$), cf. (Richter *et al.*, 1991). f_s is monotonically decreasing and equals unity at $t = 0$. It incorporates the reduction in dry matter biomass during maturity stages of crops into the model.

$$\frac{dW_C}{dt} = \Big(r_C f_s(t) - \mu_C\Big) W_C \tag{2.1}$$

The parameter r_C denotes the growth rate. The growth of a crop depends on the support of nitrogen, the rate of photosynthesis and the interspecific competition of weed or pests. All factors reduce a possible maximum growth rate $r_{C,max}$ [1/d]. These influences are described by reducing functions $r_N(N)$, and $r_{C,W}(W_C, W_W)$, which are normalized to one, if no reduction of the maximum growth rate takes place. The reductions functions $r_N(N), r_{C,P}(P_4) \in [0, 1]$ describe the dependence of growth on soil nitrogen and a pest population P_4, see below Section 2.6.2.

$$r_C = r_{C,max} \prod_i r_i(\vec{c}) = r_{C,\max} r_N(N)\, r_{C,W}(W_C, W_W)\, r_{C,P}(P_4) \tag{2.2}$$

The dependence of growth on nutrients is incorporated into the model via the function $r_N(N)$. It is reasonable to use a Michaelis–Menten form (Richter *et al.*, 1991).

$$r_N(N) = \frac{N}{N + k_N} \tag{2.3}$$

N in [kg/ha] denotes the amount of applied fertilizer, k_N in [kg/ha] the Michaelis–Menten constant.

Two effects of competition must be considered. First a higher amount of weed reduces crop growth. Second, the more crop biomass exists, the less influence on crop growth under weed is observed. Growth reduction by weed decreases, the more crop biomass is developed. This interaction can be incorporated into the model by the equation

$$r_{C,W}(W_C, W_W) = 1 - \left(\frac{l\, W_C}{W_W}\right)^s \tag{2.4}$$

with a shape parameter s [1] and a critical weed/crop relation l [1].

The possible extension concerns time and the physiological age of the crop. The concept of biological time (Cabelguenne *et al.*, 1999; Schröder & Söndgerath, 1995) can be used to incorporate a physiological age, depending on daily temperature. The biological time $t_{biol}(t)$ substitutes the logical time t in the senescence function f_s. This is a consistent extension to the concept of a general senescence function as described above, as t_{biol} increases monotonically which lets $f_s(t)$ decrease monotonically.

With a functional representation of the development rate $r_D(T)$ depending on the temperature $T(t)$ the biological time $t_{biol}(t)$ is evaluated by

$$t_{biol}(t) = \int_0^t r_D(T(\tau))\, d\tau \tag{2.5}$$

There are several mathematical functions which describe the nonlinear dependency between temperature and development rate $r_D(T)$, for instance the O'Neill function, see Section 2.4.2.

2.2.2 Temporal Patterns of Annual Plants

Annual plants show temporal patterns. For example, potato vine reaches its maximum of growth between blossom and berry-development. With yellowing of the plant, biomass starts to decrease continuously. With decreasing shading capacity weed biomass increases sharply. As a driving process or function for these patterns certain development stages have been identified. The temporal patterns are governed by

the function $f_s(t)$. It incorporates stages of senescence into the model where biomass decreases. It is reasonable to postulate the following properties of this control function

i) $f_s(t) > 0$ and $\lim_{t\to\infty} f_s(t) = 0$

ii) $f_s(t)$ may be normalized to unity, $f_s(0) = 1$.

Consider as an example the function

$$f_s(t) = \frac{(1+\rho_1)\, e^{-\rho_2 t}}{1+\rho_1 e^{-\rho_2 t}} \tag{2.6}$$

The characteristic temporal pattern is governed by the function $f_s(t)$. Its shape is defined by ρ_1 and ρ_2. The function $f_s(t)$ normalized by one and decreases in a sigmoid manner. In Equation (2.6) $f_s(t)$ incorporates a growth phase ($r_P f_s(t) > \mu_W$) and a loss of biomass in a phase of senescence.

Phenological stages of development, for instance the beginning of the tillering phase given by t_{DC} in winter crops such as winter wheat or winter barley are described by the function

$$f_{DC}(t) = \begin{cases} 0 & \text{if } t < t_{DC} \\ 1 & \text{else} \end{cases} \tag{2.7}$$

with t_{DC} denoting the beginning of a specific stage of phase of development of a crop. Note that f_{DC} is predestined to be used as a function of biological time t_{biol} as defined by Equation (2.5) rather than (system) time, cf. (Schröder & Söndgerath, 1995).

2.2.3 Nitrogen Uptake

The amount of nitrogen taken up by the crop is calculated using the reference content of nitrogen in the crop biomass $k_{cn}(t)$ derived from unlimited nutrient availability (Schröder & Richter, 1993). The function $k_{cn}(t)$ denotes the relative nitrogen reference content in the crop biomass $W_C(t)$. During the vegetation period a decrease of nitrogen content is observed. Therefore a function of the following form is used here

$$k_{cn}(t) = \begin{cases} k_1 & \text{if } t < t_{DC} \\ (k_{max} - k_0)e^{-\frac{t-t_{DC}}{\tau_2}^{\gamma_c}} - (k_{max} - k_1)e^{-\frac{t-t_{DC}}{\tau_1}^{\gamma_c}} + k_0 & \text{else} \end{cases} \tag{2.8}$$

with final relative nitrogen content in crop k_0 [1], the relative nitrogen content in crop in first development stages k_1 [1] and the maximum relative nitrogen content in crop k_{max} [1]. The temporal patterns of this function are defined by the development stages of the crop (cf. Equation (2.7)) as well as the parameters τ_1, that specify the time of maximum nitrogen content and τ_2 that holds the time of highest decrease of nitrogen content in crop. γ_c is a shape parameter of the function. The simplification of this ansatz $k_{max} = k_1$ leads to sigmoid behavior. It becomes constant with $k_{max} = k_0 = k_1$.

2.2.4 Interspecific Competition: Weeds and Weed Control

A growth model for weed must consider a whole population of weed species. A practicable approach for weed development is the classical

$$\frac{dW_W}{dt} = r_W W_W \left(1 - \frac{W_W}{K_w}\right) \tag{2.9}$$

with the weed biomass W_W [kg/ha], the specific growth rate r_W [1/d] and the capacity K_W [kg/ha]. Weed growth depends on the availability of nutrients, too. This dependency can be incorporated into the model via the function of $r_N(N)$ (see Equation (2.11) with a specific Michaelis–Menten constant $k_{N,W}$ for weeds.

A further reduction factor is introduced for the competition for light. Weed growth depends on the remaining photosynthetically-active radiation (PAR) on the ground, which depends on the leaf biomass of the crop biomass. Therefore the growth rate of weed is a product of a maximum growth rate r_Q and the factor $r_Q(Q)$ which depends on photosynthetically-active radiation denoted by Q in [W/m^2].

$$r_W = r_{W,\max} r_Q(Q). \tag{2.10}$$

The less radiation that reaches the ground between the crop, the more reduction has to be applied to the growth rate of weeds. This is applied by

$$r_Q(Q) = \left(\frac{Q}{Q_{\max}}\right)^c \tag{2.11}$$

with shape parameters Q_{max} in [W/m^2] and c [1] to the growth model of weeds. The function for the photosynthetically-active radiation depending on the crop biomass $Q(W_C)$ is defined by a 2nd order polynomial interpolation based on the observed data.

Weed biomass is reduced by a factor p_i at the time of weed control t^*. This reducing factor can be identified as surviving possibility of a selected treatment i for weed control. The application to the weed growth equation follows

$$W_W(t^* + \Delta t) = W_W(t^*)\, p_i \tag{2.12}$$

The coupled Equations (2.1) to (2.12) set up a simulation model for crop dynamics including nutrient-dependent growth, temporal patterns of annual crops as well as weed competition. See Section 2.7 for a summary of all model parts and Table 2.11 in this chapter on page 64, which lists all parameters introduced and their physiological interpretation.

2.3 PARAMETER ESTIMATION (PART I)

Before continuing the translation of the conceptual model of an agricultural ecosystem displayed in Figure 2.1, we first analyze the model in hand and try to specify

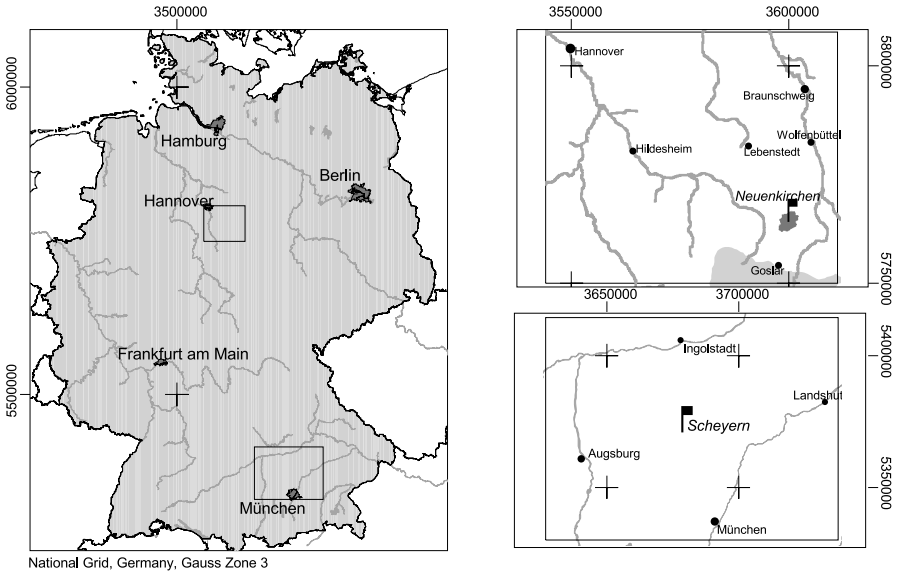

Fig. 2.2 Location of the study area "Neuenkirchen" of the Collaborative Research Project "Water- and Matter Dynamics of Agroecosystems" and the investigation site "Scheyern" of the Research Association for Agricultural Ecosystems Munich (FAM).

the parameters introduced. Most of the parameters are effective parameters of phenomenological patterns rather than biological parameters which are derivable by certain physical measurements. We therefore use the technique of parameter estimation based on field experiments to specify these parameter values.

2.3.1 Experimental Design of Field Experiments

Data for the parameter estimation was derived from two different investigation sites in Germany. The general methodology of measuring the above-ground biomass is: plant development (crop and weed) was determined by cutting biomass above ground and estimating ground coverage level every two to three weeks. Simultaneously, the shading capacity of the canopy was measured as photosynthetically-active radiation at ground level. Weeds were counted in defined periods.

Investigation Site "Neuenkirchen" Parameters of the simulation model are specified using data series from the Collaborative Research Project "Water- and Matter Dynamics in Agroecosystems" (CRP 179), project A2 "Modeling Crop Dynamics of Main Crops" of the Technical University of Braunschweig, Germany. Field experiments were carried out at one of the investigation areas of the CRP 179 "Neuenkirchen", located in the northern forelands of the Harz mountains in Lower Saxony (Niedersachsen), Germany. This investigation area is about 16 km^2 in area.

Soil parent material consists of a 1–2 m thick layer of loess topped by 0.2–1 m colluvial sediments, see McVoy *et al.* (1995) for a more detailed site description of the catchment. Figure 2.2 shows the location of this study area.

Investigation Site "FAM" Figure 2.2 show the location of the investigation site "Scheyern" of the Research Association for Agricultural Ecosystems Munich (FAM). Within the scope of the research project field trials on integrated weed management have been carried out from 1993 to 1995. Besides chemical and mechanical treatments, cultivation techniques that stimulate crop competitiveness were also included.

The field trials were located in the "Tertiärhügelland" about 40 km north of Munich on sandy loam soil about 450 m above sea level, see Figure 2.2. Climatic conditions are characterized by 815 mm annual precipitation and an annual average temperature of 7.4 ℃. Through all investigation years, weed infestation reached medium levels (about 27 weeds/m^2 before the second earthing up). The majority of weeds belonged to *Polygonum*- and *Chenopodium* species, typical for potato cultivation.

The potato variety "Selma" was cultivated with a fertilization rate of 60, 120 and 180 kg nitrogen per hectare [kg-N/ha]. Weed control was carried out as "chemical" (common herbicide), "mechanical intensive" (rigid-tine-weeder and a second late earthing up) and "mechanical extensive" (only a second late earthing up) treatment. The experiment was laid out in a split-plot design with four repetitions and a plot size of 27 m^2.

Direct weed control by herbicide application reached an average efficacy of 92%, compared to 77% by mechanical intensive treatment and 52% by mechanical extensive treatment. Nevertheless, at medium and high fertilizer levels no significant yield differences occurred between mechanical extensive and chemical treatment, while crop yield decreased by an average of 4% on the weedy, low fertilized plots. Even if no visible damage occured on potato vine, the use of the rigid-tine-weeder caused damage to roots and stolons of the potato plant. Therefore, yield decreased at all fertilizer levels by 7.5% with mechanical intensive weed control. Based on these results the following values for p_i ($i = 1, 2, 3$) are determined: $p_1 = 0.0$ (chemical treatment), $p_2 = 0.25$ (mechanical intensive treatment) and $p_3 = 0.54$ (mechanical extensive treatment), cmp. Equation (2.12).

2.3.2 Application of Algorithms

Some general remarks that hold true for all steps of parameter estimation presented in the following should be noted. The nonlinear ordinary differential equation system described has no analytical solution. Numerical procedures are used to solve the differential equation system and to solve the parameter estimation problem [1], see Sections 1.4.2 and 1.5.6 on page 32.

[1] Model development tools used in this chapter are MODELMAKER and EASYFIT.

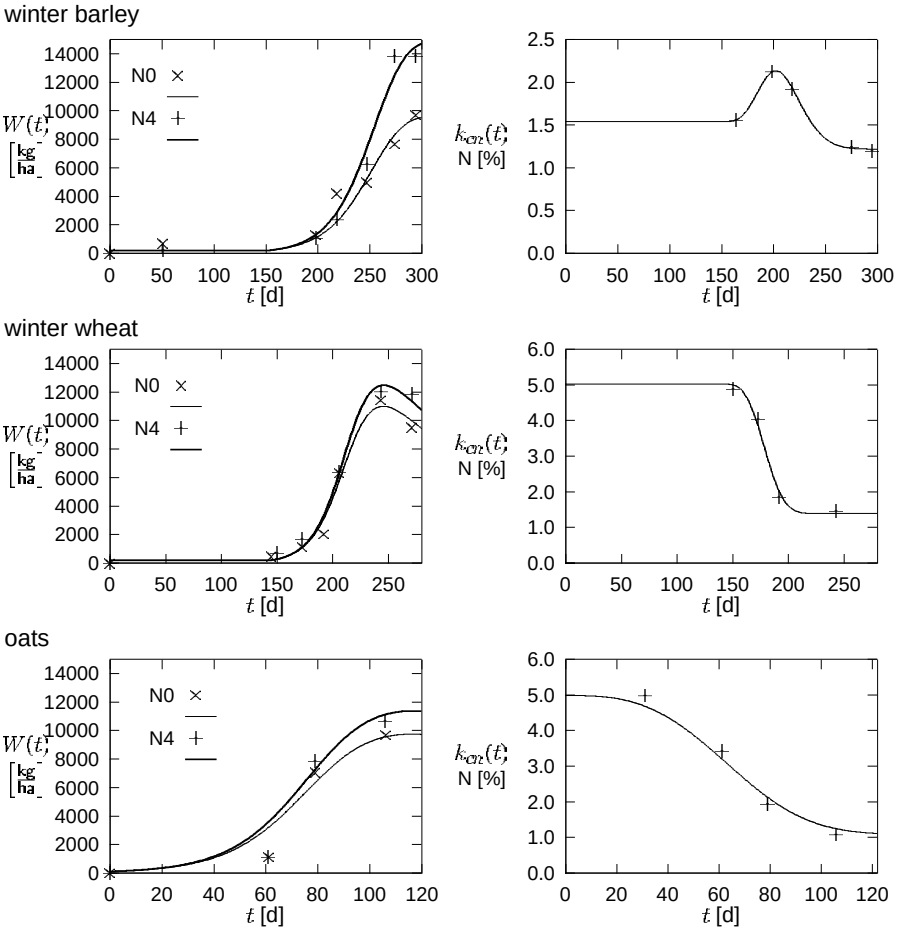

Fig. 2.3 Growth curves of winter wheat, winter and spring barley, sugar beets, oats and oil radish (non fertilized): measurement values (×, +) and results of models fits. left: biomass of N0 (no fertilization) and N4 (farmers usual fertilization). right: N-content of biomass in % of the variant N4. Part 1: winter wheat, winter barley, oats.

For the analysis of the results a convenient and widely-used performance criterion of the parameter estimation is used: the residual sum of squares r^2. From the statistical analysis of the estimators, denoted by x in the tables, values for the standard deviation σ can be obtained. The value is listed in round brackets in the tables. A large value of the standard deviation indicates that the underlying data does not allow a statistically sufficient estimation of the parameter. This is also related to the correlation coefficients derived from the statistical analysis. These coefficients are a suitable measure for the (stochastic) correlation between two random variables. These are

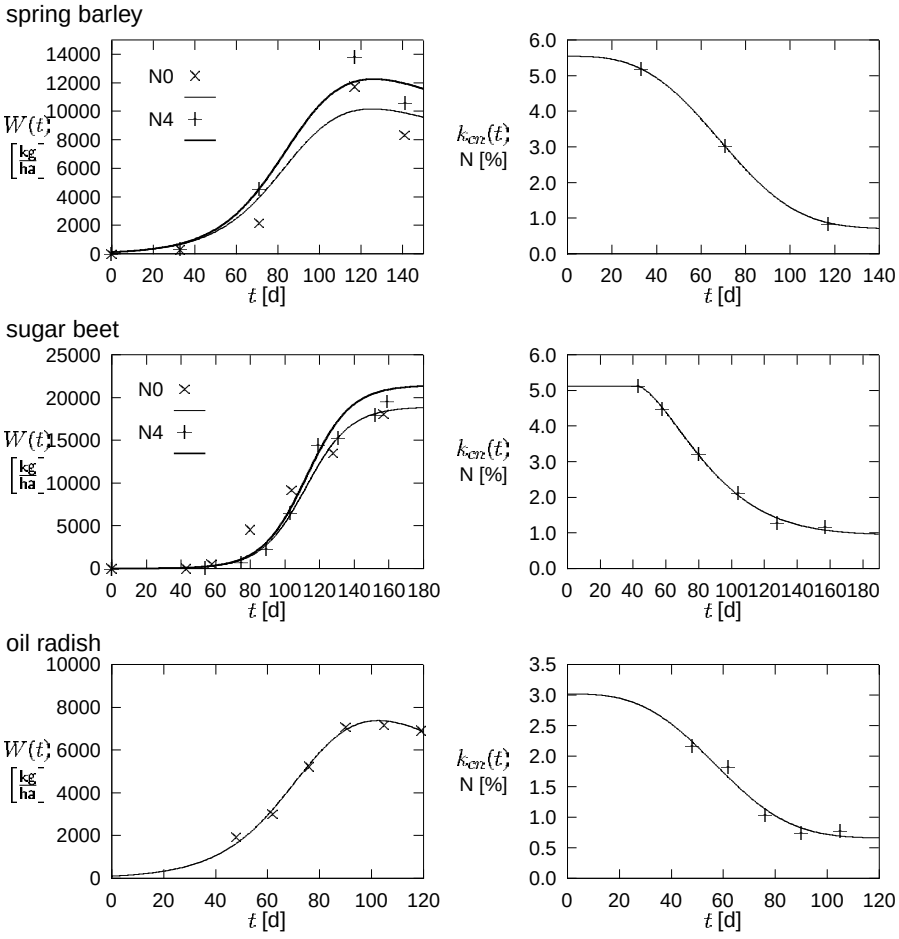

Fig. 2.3 contd. Part 2: spring barley, sugar beets and oil radish.

the unknown model parameters in terms of parameter estimation. Values close to ±1 indicate a strong dependence, whereas values close to zero indicate (stochastic) independence. Strong dependence, correlation is an indicator for a over-parameterization of the model, which may lead to misinterpretations of the results.

2.3.3 Parameters of Crop Growth

The results of model parameterization can be displayed only in summary without lengthening the topic too much. Figure 2.3 summarizes the results of the parameter estimation and Table 2.2 displays the results of the statistical analysis. Figure 2.4 and

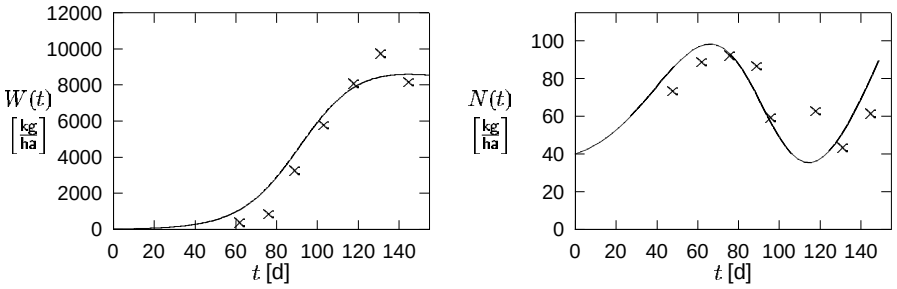

Fig. 2.4 Growth curve of the biomass of field beans (left) and nitrogen content in soil (right).

Table 2.1 Parameters of crop growth models. Fixed parameters (not estimated by parameter estimation procedure) are printed in *italics*.

Crop	Sugar beet	Spring barley	Oats	Winter wheat	Winter barley	Field beans	Oil radish	
Abbr. (α)	sub	spb	oa	ww	wb	fb	or	
Parameter								
W_0	*0.034*	*1.2*	*1.02*	*1.9*	*2.0*	*0.2*	*1.0*	[100 kg/ha]
$r_{max} = \rho_2$	0.0784	0.0615	0.0689	0.0709	0.0484	0.0682	0.0709	[1/d]
k_N	3.41	*5.0*	5.178	1.643	6.28	*0*	*1.0*	[kg-N/ha]
ρ_1	6930	227	251	154	205	590	256	[1]
μ_W	*0*	*0.005*	*0*	0.00732	*0.005*	0.002	0.0107	[1/d]
t_{DC}	43.4	—	—	144	153	—	—	[d]
k_0	0.937	0.698	1.08	1.39	1.22	2.85	0.657	N [%]
k_1	5.12	5.54	4.98	5.02	1.54	k_0	3.02	N [%]
k_{max}	k_1	k_1	k_1	k_1	2.84	k_1	k_1	N [%]
τ_1	—	—	—	—	41.6	—	—	[d]
τ_2	50.6	78.5	72.2	39.9	71.2	—	65.2	[d]
γ_c	*1.5*	*3.0*	*3.0*	*3.0*	*3.0*	—	*3.0*	[1]
r_f	0	0	0	0	0	2.42	0	[kg-N/d]
k_f	0	0	0	0	0	0.97	0	[dt/ha]
Fertil. N0	84	80	36	0	0	—	—	[kg-N/ha]
N4	108	130	126	216	171	—	—	[kg-N/ha]

Table 2.3 summarize results of the parameter estimation of the crop growth model for field beens including the sub-model of nitrogen fixation, see next Section 2.4.1.

Note that the growth curves of different fertilizing schemes are fitted simultaneously. All parameter estimations show good results. The estimated values of standard deviation are acceptably low and the correlation matrix shows that there are no correlations among the parameters, see Table 2.2. This shows that the problems are not ill-defined.

Table 2.2 Covariance matrix, estimator x and variance σ^2 (level of significance 5%) from the parameter estimations of the crop growth model Equation (2.1) and nitrogen content model Equation (2.8). All parameter values printed in *italics* are fixed.

	r_{max} $= \rho_2$	ρ_1	$t_{EC\,21}$	μ_W	k_1	t_2	t_1 t_{EC6}	k_{max}	x	σ^2
Sugar beet										
k_N	–0.26	–0.23							3.41	2.47
r_{max}		0.98							0.078	0.017
ρ_1									6930	11700
μ_W									*0.0*	
k_0					–0.055	–0.82	0.49		0.937	0.14
k_1						0.15	–0.43		5.12	0.073
t_2							–0.82		50.6	5.19
t_{DC}									43.4	2.94
Spring barley										
k_N	0.0186	0.0649							5.0	16.9
r_{max}		0.738							0.0615	0.0464
ρ_1									227	476
t_{DC}									*0.0*	
μ_W									*0.005*	
k_0					0.174	–0.561			0.698	0.0563
k_1						–0.585			5.54	0.0816
t_2									78.5	1.44
Oats										
k_N	–0.653	–0.833							5.18	8.76
r_{max}		0.744							0.0689	0.029
ρ_1									251	1930
t_{DC}									*0.0*	
μ_W									*0.005*	
k_0					0.286	–0.813			1.08	0.637
k_1						–0.58			4.98	0.53
t_2									72.2	11.7
Winter wheat										
k_N	0.51	–0.96	0.96	–0.24					1.64	8.02
r_{max}		–0.52	0.53	–0.63					0.071	0.013
ρ_1			–0.99	0.25					154	3510
t_{EC}				–0.25					144	328
μ_W									0.00732	0.0039
k_0					0.11	–0.605			1.39	0.26
k_1						–0.446			5.02	0.25
t_2									39.9	3.52
Winter barley										
k_N	–0.12	–0.97	0.863						6.278	6.59
r_{max}		0.128	0.225						0.0484	0.0098
ρ_1			–0.85						205	1000
t_{DC}									152	70
μ_W									*0.005*	
k_0					–0.060	–0.19	–0.42	–0.015	1.22	1.18
k_1						0.37	–0.63	–0.53	1.54	1.67
t_2							–0.25	–0.95	71.2	191
t_1								0.33	41.6	33.9
k_{max}									2.84	8.11

Table 2.3 Covariance matrix, estimator x and variance σ^2 (level of significance 5%) from the parameter estimations of the field been growth and nitrogen fixation model.

	x (σ^2)		ρ_1	μ_W	k_0	k_f	r_f
r_{max}	0.0682	(0.00146)	0.443	0.33	-0.513	-0.284	-0.306
ρ_1	590	(109)		0.91	-0.276	0.103	0.0794
μ_W	0.002	(0.00129)			0.11	0.012	0.0169
k_0	2.85	(0.23)				-0.05	0.0824
k_f	0.965	(0.485)					0.927
r_f	2.42	(0.211)					

Table 2.4 Parameter estimation results of crop growth (parameter values, variance in parentheses, and correlation matrix).

	x (σ^2)		ρ_1	k_N	μ_W
$r_{P,max} = \rho_2$	0.142	(0.146 10^{-3})	-0.912	0.377	-0.412
ρ_1	78.7	(4.68)		-0.187	0.694
k_N	12.6	(0.371)			-0.219
μ_W	0.0109	(0.31 10^{-3})			

2.3.4 Competition Models

A very convenient way of solving the problem of parameter estimation for the competition model is to solve the problem for sub-models or modules separately in several steps. For detailed study the field experiments on weed–potato competition from the "FAM" investgation site are selected.

Step 1: Sub-model Potato Growth Using the data sets of potato growth, which grew up without any weed influence, under chemical based weed control, leads to $r_{C,W} = 1$. This uncouples the crop growth equation from the weed growth model and enables a parameter estimation based on the data sets of the three different fertilizer amounts.

The parameter estimation of the potato growth sub-model is based on the data series of biomass weight and coverage under the chemical treatment in the year 1994. This treatment results in undisturbed potato growth without weed infestation. Growth parameters can be estimated without competition ($r_{C,W} = 1$). Table 2.4 shows the resulting parameter estimations together with the correlation matrix of the estimates. Figure 2.5 displays a plot of the data together with the fitted trajectories. The fit is satisfying as no estimates are correlated and the residual sum of squares results in $r^2 = 0.97$.

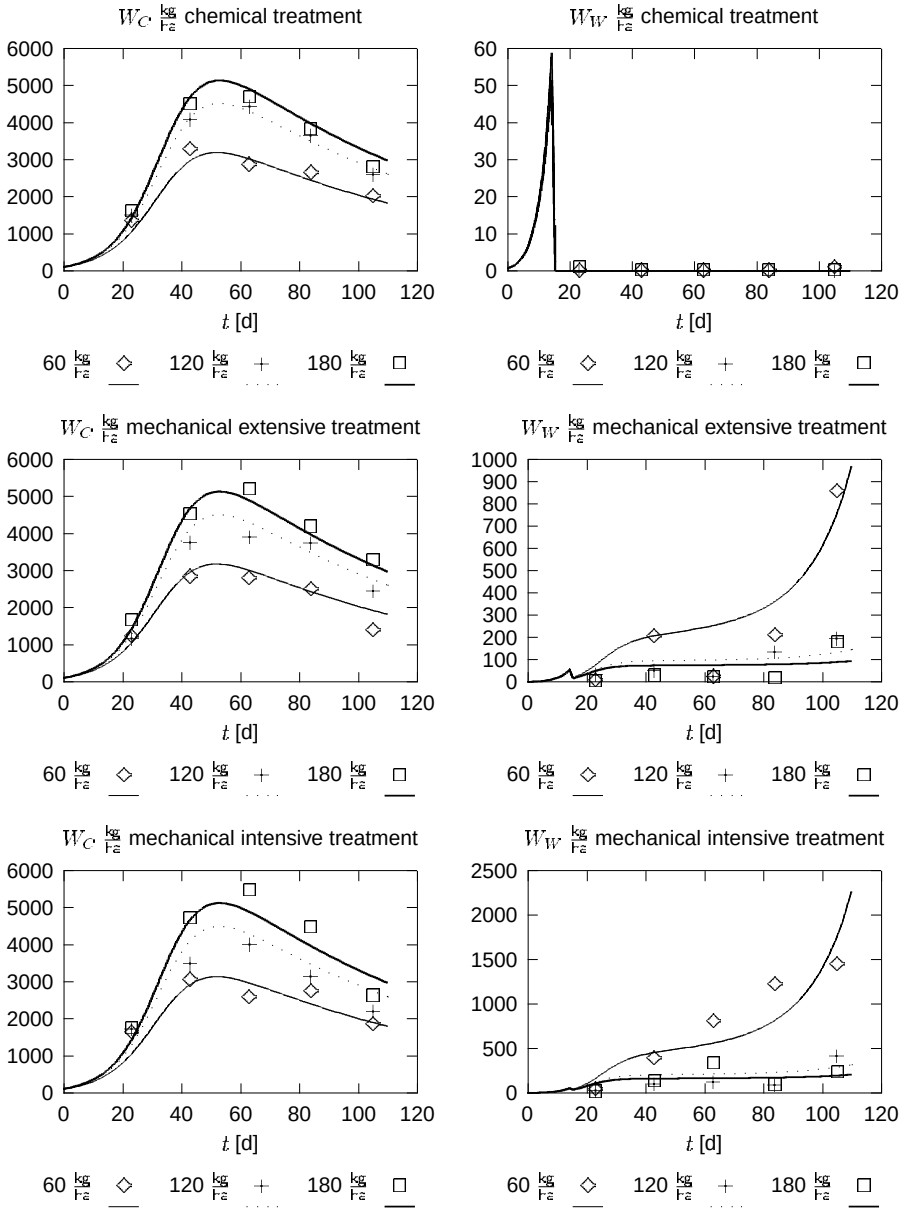

Fig. 2.5 Growth curves of potato biomass W_C (left column) and weed biomass W_W (right column) for different treatments of weed control for 1994.

Table 2.5 Parameter estimation results of weed growth (values, variance in parentheses, and correlation matrix).

	x (σ^2)		c	Q_{max}
$W_{W,0}$	0.0887	(0.0247)	0.963	0.921
c	2.85	(0.0807)		0.837
Q_{max}	29.0	(0.155)		
$r_{W,max}$	*0.4*			

Step 2: Sub-model Weed Growth In the second step of model development the parameters of weed growth are estimated. As stated before, weed growth depends on remaining photosynthetically-active radiation reaching the ground, and this depends on the standing biomass of potatoes. The reducing factor r_Q (Equation (2.11)) is a function of W_C. The potato biomass determines the PAR for weed. This function $Q(W_C)$ is derived by a 2nd order polynomial interpolation with the coefficients b_i ($i = 0, 1, 2$). With a resulting $r^2 = 0.61$, the parameters $b_0 = 30.8$, $b_1 = -9.4\ 10^{-3}$ and $b_2 = 8.5\ 10^{-7}$ are identified.

The parameter estimation of the weed growth part of the model is based on the mechanical extensive treatment. A higher weed infestation is observed here. Table 2.5 shows the resultant parameter estimation and correlation matrix. This good results are characterized by $r^2 = 0.79$, acceptable correlations and still extremely small standard deviations.

Sub-model Competition The previous parameter fits set up the basis for the estimation of the parameters l and s. The last step of model development incorporates the influence of weed into the crop growth model. It closes the feedback-loop from weed growth to the potato growth model. The parameter fit is necessarily based on all data-sets: chemical, mechanical extensive and intensive treatment incorporated by the surviving probabilities due to these treatments and fertilizing schemes. Growth parameters are not changed. Results of this parameter estimation are $l = 0.821$ (± 0.107) and $s = 2.42$ (± 0.134). With a correlation of 0.91 between s and l. These final results are summarized by an acceptable correlation between l and s and a residual sum of squares $r^2 = 0.81$.

Final Step: Full Model Parameter Estimation Finally a full parameter estimation can be performed. It uses all the parameters identified before as initial values. The approach can be summarized as stepwise identifying parameters of sub-models. It is the only way for identifying parameters in a model like this. An estimation of all parameters from scratch would lead to an ill-defined problem, as the underlying data does not fulfill the demands of parameter estimations of the full model. Using this stepwise approach we avoided the task of solving an ill-defined global optimization

problem by setting up several local optimization problems that construct appropriate starting values for the global optimization, see Chapter 8, Section 8.4.3 on page 170.

The process described in the previous steps may be continued in an iterative manner, till a sufficient result is achieved. The assessment of the goodness-of-fit should not solely be base on r^2 values. A visual interpretation should emphasis the stages of active growth of the canopy.

2.3.5 Results

Two general results are derived from parameter estimation. First, a capacity of dry matter biomass has never been reached by field experiments and K_W cannot be identified by means of parameter estimation. For this reason unlimited exponential growth was used, to describe weed growth.

Second, parameter estimation shows no dependency on available nutrients in weed growth. The introduction of a Michaelis–Menten function into Eqn (2.9) equally to Equation (2.2) yields high correlations (±1) between the Michaelis–Menten coefficient and the maximum growth rate of weeds. The parameter estimation of $k_{N,W}$ is not possible without correlations to other parameters. Therefore the influence of fertilizing on weed growth is not significant. However, in the field experiments it was observed that potato vine and shading capacity increased with higher doses of fertilization. For this reason, weed infestation in highly fertilized plots was significantly lower, which is reproduced by the model.

Predictive Power A major question, introduced in Chapter 1, is the question of the predictive power of a model and the applicability to new conditions. Model parameters were estimated based on data series from the experiments of the year 1993. To test the predictive power the model is applied to the data set of the year 1994. In this year no mechanical intensive treatment was carried out because of weather conditions. Without any modifications to the parameter values the resultant residual sum of squares $r^2 = 0.49$.

The following parameters depend on site and climatic conditions: the maximum growth rates, the parameterization of the senescence function, the initial weed infestation, and the attrition rate. The statistical analysis has been performed as follows. All parameters from the parameter estimation from year 1994 are used, and the parameters mentioned above are re-estimated. The results are shown in Table 2.6. The table lists the final parameters and the coefficient of correlation which is a measure of how precisely the algorithm of parameter estimation identifies a parameter value with respect to the underlying data.

This statistical analysis shows clearly that with the base of the data series from 1993 and 1994 no different parameter values can be estimated for $r_{C,max}$, ρ_1, ρ_2 and μ_W, see Table 2.6. Significantly differences are identified in the parameters $W_{W,0}$ and $r_{W,max}$. Both parameters are highly correlated. It shows that these different years have a significantly different initial weed infestation. This was observed during the

Table 2.6 Statistical analysis of the simulation model focusing on the question of application on different sites and years including the final parameter sets.

	1994		1993		
Parameter	x	(σ^2)	x	(σ^2)	Significant difference
ρ_1	80.1	(15.3)	92.5	(15.4)	no
c	3.20	(0.293)	3.20		
k_N	11.5	(0.209)	11.5		
l	0.358	(0.953)	0.358		
μ_W	0.0112	(0.0227)	0.0141	(0.000362)	no
Q_{max}	28.5	(1.16)	28.5		
ρ_2	0.127	(0.00446)	0.127	(0.00403)	no
$r_{C,max}$	0.139	(0.00177)	0.132	(0.00143)	no
$r_{W,max}$	0.307	(0.0359)	0.176	(0.00332)	yes
s	1.68	(0.714)	1.68		
$W_{W,0}$	0.705	(0.580)	14.3	(1.313)	yes

experiments but no measurement values were taken before weed control. Figure 2.6 shows the simulation results.

Model Analysis and Application A scenario: "What happens to crop growth, or yield depending on different initial weed infestations?" can be answered by the model. A simulation scenario is set up to answer that question. Assume different initial weed infestation from 0.5% to 7.5% coverage level before weed control, given by the initial condition $W_{W,0}$. Figure 2.7 shows a plot of the estimated potato biomass as a function of this initial weed infestation and fertilizer amount for the mechanical extensive treatment. This simulation scenario clearly shows the influence of fertilizing to potato–weed competition. With a fertilizing level of 180 N–kg/ha no reduction of yield can be found. This is caused by a quickly growing potato crop shadowing the weeds. A yield reduction greater than 5% occurs with an initial weed infestation of more than 8% with a fertilizing level of 120 kg–N/ha. A significant loss of yield can be found with the fertilizing level 60 kg–N/ha. These results of the simulation model extrapolate the data observed in the field experiments. This shows that sufficient fertilizing reduces weed infestation.

2.4 ABIOTIC ENVIRONMENT: WATER AND MATTER DYNAMICS

The second important part of the generic (agroecological) ecosystem model focuses on the abiotic parameters and the related processes that determine the environmental fate of nutrient and xenobiotica namely agrochemicals, pesticides.

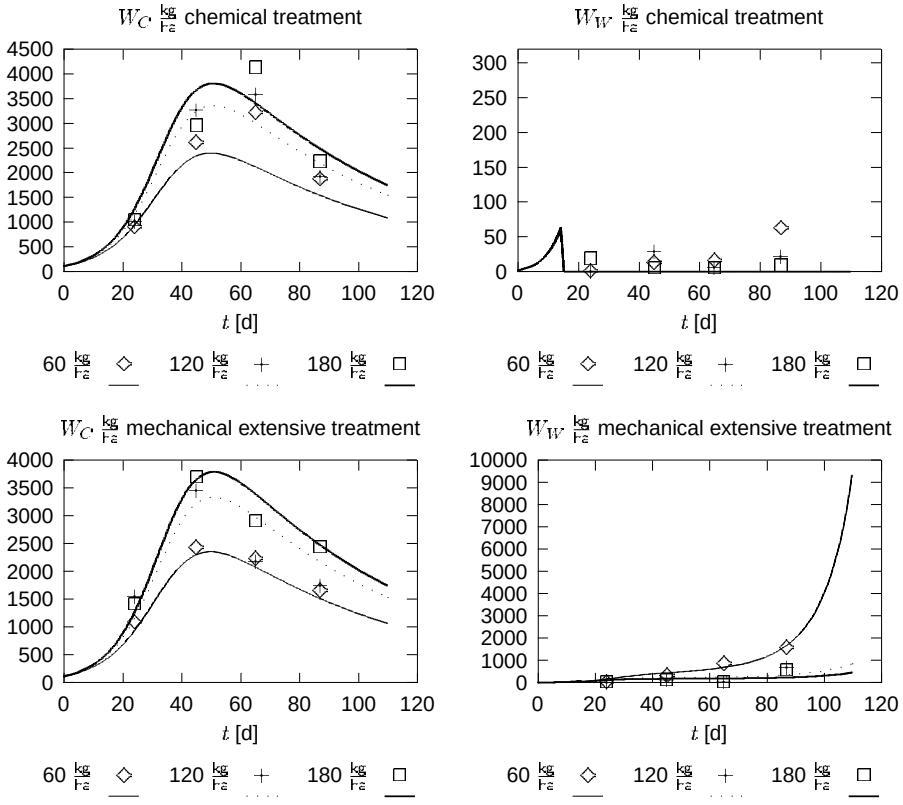

Fig. 2.6 Validation: Model application to data series of 1993. In this year no mechanical intensive treatment occurred ($W_C(t)$ potato biomass, $W_W(t)$ weed biomass).

2.4.1 Nutrient Cycle: Detritus

The plant-accessible pool of mineral nitrogen in soil is denoted by $N(t)$ in [kg/ha]. Plant growth depends on this pool. The simulation model couples the processes of nitrogen uptake by plants, nitrogen leaching out of the root zone, decomposition, mineralization, NO_2 fixation and fertilization.

$$\frac{dN}{dt} = -d(W,t) - k_l N + k_m \mu_W W + r_f \frac{W}{W + k_f} + F(t) \tag{2.13}$$

The above-ground biomass may be defined by either the crop biomass $W = W_C$, the weed biomass W_W or the sum of both $W = W_W + W_C$. Leaching and mineralization are modeled by linear flows with the rates k_l and k_m [1/d]. Fixation of NO_2 is modeled by a Michaelis–Menten function with the parameters r_f [1/d] and k_f [kg/ha]. The demand of nitrogen taken up by the crop $d(W,t)$ is calculated using the reference

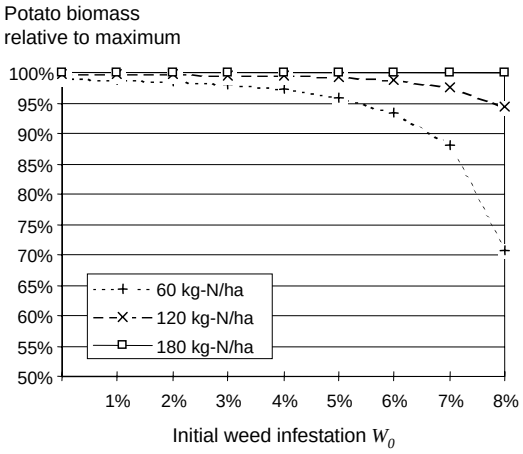

Fig. 2.7 Simulation experiment: Expected relative biomass depending on weed infestation observed at time of possible weed control and fertilization, to mechanical extensive treatment.

content of nitrogen in the crop biomass $k_{cn}(t)$ in [%] and is defined by:

$$d(W,t) = \frac{d}{dt}\left(k_{cn}(t)W(t)\right) = k_{cn}\frac{dW}{dt} + \frac{dk_{cn}}{dt}W \tag{2.14}$$

Decreasing biomass leads to negative values of $d(W,t)$. This may be interpreted as mineralization of dead biomass. This completely different process cannot be set up by the same parameter of nitrogen uptake. Therefore d is restricted to be positive or zero.

2.4.2 Xenobiotica Fate: Agrochemicals

The differential equations for the fate of agrochemicals are derived from the compartment scheme in Figure 2.1 with the assumption of linear fluxes. Let C_L denote the concentration [mg/l] of a pesticide on the crops' leaf and C_S the concentration [mg/l] in the upper soil layer. Precipitation is the driving force for transport from leaf surface to soil surface (k_w) and for leaching out of the upper soil horizon (k_l). Degradation of the chemicals is assumed as linear first order process (k_d).

$$\frac{dC_L}{dt} = -k_d C_L - k_w C_L + \nu(W)A(t) \tag{2.15}$$

$$\frac{dC_S}{dt} = -k_d C_S + k_w C_L - k_l C_S + (1-\nu(W))A(t) \tag{2.16}$$

The distribution of the amount of applied pesticide $A(t)$ [mg/l] depends on the current state of crop, on the leaf area index. The more leaf area is present, the more pesticide

reaches the plant leaf. This is expressed by the function, cf. (Schröder *et al.*, 1995)

$$\nu(W) = \frac{c_{LAI} W}{c_{LAI} W + 1} \tag{2.17}$$

Degradation or decay of chemicals in the environment is frequently a process that depends on a broad range of environmental factors. Focusing on degradation in soil, probably driven by microbial enzymes, depends on temperature T and humidity θ. The following approach is frequently used for modeling this bifactorial dependency:

$$k_d(T, \theta) = k_{d,max}\, k_T(T)\, k_\theta(\theta) \tag{2.18}$$

A maximum degradation rate $k_{d,max}$ is modified by two dimensionless factors that range between zero and unity and describe the univariate dependency to temperature $k_T(T)$ and soil moisture $k_\theta(\theta)$.

The classical form of temperature response curves is given by an Arrhenius temperature dependence function. Since degradation is mediated by biological processes at the level of micro-organisms and enzymes, it is evident that the Arrhenius law is valid only in a confined temperature range and should be replaced by a biological temperature law, if larger temperature ranges are considered:

$$k_T(T) = \left(\frac{T_{max} - T}{T_{max} - T_{opt}}\right)^{\beta} \exp\left(\beta \frac{T_{max} - T}{T_{max} - T_{opt}}\right) \tag{2.19}$$

However, since the shape of the curve at higher temperatures is determined by the two parameters, optimal temperature t_{opt} and lethal temperature t_{max}, biologically plausible values can be assigned to these parameters. The classical form of humidity response curves is given according to Walker, see (Richter *et al.*, 1996).

$$k_\theta(\theta) = \theta^a \tag{2.20}$$

It has also taken into account that degradation may decrease at water contents near saturation, so a more general form of a response surface is considered which takes into account both effects

$$k_\theta(\theta) = \left(\frac{\theta}{\theta_{opt}}\right)^a \exp\left(1 - \left(\frac{\theta}{\theta_{opt}}\right)^a\right) \tag{2.21}$$

2.5 PARAMETER ESTIMATION (PART II)

Identifying the parameters of the abiotic part of an ecosystem model has to make use of parameters that are physically measurable at the investigation. In the context of the model system developed, parameters of this type are the mineralization rate k_m, the leaching or percolation rate k_l and the rate of runoff k_w. These variables are highly dynamic and depend on precipitation and micro-meteorological data. These variables are also highly variable in space. Methodology for estimation of those parameters are presented in Chapter 3. For the moment we assume that effective parameter values, and appropriate averages are available, cmp. Section 3.1.1.

Table 2.7 Design of four slurry batch experiments for degradation studies of a pesticide.

Experiment	A	B	C	D	
Moisture θ	80	40	60	40	[%]
Temperature T	5	10	15	30	[°C]

Table 2.8 Statistical analysis of parameter estimation of pesticide degradation model.

	x (σ^2)	$k_{d,max}$	A:$C_{S,0}$	B:$C_{S,0}$	C:$C_{S,0}$	D:$C_{S,0}$	T_{opt}
$k_{d,max}$	0.77 (0.042)						
A:$C_{S,0}$	88.8 (5.23)	0.228					
B:$C_{S,0}$	62.3 (3.69)	0.0743	0.102				
C:$C_{S,0}$	90.5 (5.56)	-0.0189	0.0458	0.0914			
D:$C_{S,0}$	81 (6.2)	0.244	0.00702	0.00331	0.0256		
T_{opt}	37.8 (0.41)	0.909	0.288	0.120	-0.0236	-0.0825	
β	1.17 (0.11)	-0.849	-0.3132	-0.161	-0.00581	-0.0417	-0.987
a	*0.3*						
T_{max}	*45*						

2.5.1 Laboratory Experiments

As an example for the estimation of parameters of abiotic processes, the degradation of a pesticide is selected for detailed study. Degradation of the pesticide Idosulferon is studied as a function of temperature and moisture. A two-factorial laboratory experiment was set up. Table 2.7 lists the configuration of temperature T_i and moisture θ_j used for the degradation study. The underlying degradation studies using Iodosulfuron have been published elsewhere (Schraut, 2001). Temperature and humidity response curves of the degradation rate can be identified from data of degradation studies performed under different combinations of temperature T_i and moisture θ_j conditions. For several other examples the reader is referred to Richter *et al.* (1996) as well as (Diekkrüger *et al.*, 1995; Formsgaard, 1997; Vink *et al.*, 1994; Novozhilov *et al.*, 1995) and a general overview in (Richter, 1998).

2.5.2 Results

The simulation of the degradation curves assumes a linear first order degradation, as modeled by parameter k_d in Equation (2.16), with a degradation coefficient dependent on temperature and moisture from Equation (2.18). For temperature dependence the O'Neill approach according to Equation (2.19) is chosen. Moisture dependence follows the approach by Walker in Equation (2.20).

Based on the four data series (A, B, C, D) from the laboratory experiment, the unknown coefficients $k_{d,max}$, a, β, T_{opt} and T_{max} are to be identified by a multi-experiment

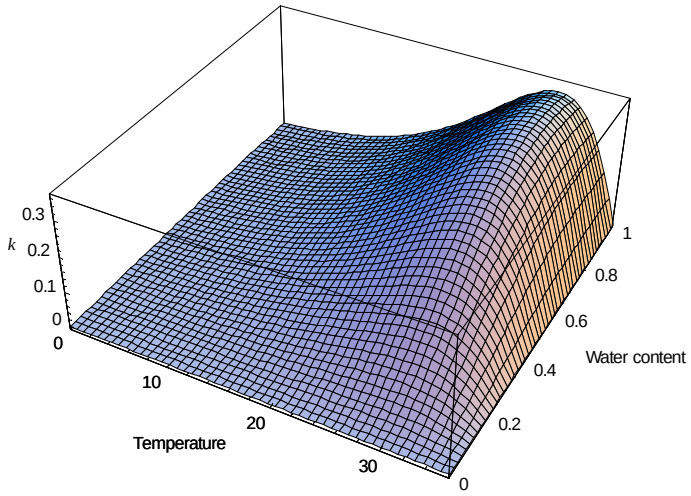

Fig. 2.8 Temperature and humidity response function $k_d(T, \theta)$ of Idosulforon.

regression analysis. The parameter estimation shows high correlations between the parameters determining the nonlinearities in the model: a, β and k_0. This problem can be solved by fixing one of the parameters a or β. Setting parameter $a = 0.3$ an acceptable parameter estimation can be performed. Table 2.8 documents these results. The underlying data is insufficient for significant identification of more parameters.

Figure 2.8 shows the response surface for Iodosulfuron derived from the two-factorial degradation study displayed in Figure 2.9. Note, Figure 2.9 use a semi-log scale that transforms the exponential decay curves into straight lines. The correlation of modeled and measured data is very good with $r^2 = 0.92$.

2.6 HIGHER TROPHIC LEVELS: CONSUMERS OR PEST INFESTATION

Modeling processes of higher trophic levels is related to the broad field of population dynamics modeling. With respect to our goal of setting up an (agro)ecosystem model we focus on examples of population dynamics modeling of the first trophic levels. More examples will be presented in the following chapters. In the context of agroecosystems the population dynamics of powdery mildew and a sugar beet cyst nematode will be analyzed.

2.6.1 Continuous Population Dynamics

An example of a pest is powdery mildew (*Erysiphe graminis*) which is both simple and aggregated. This population develops in distinct stages. However, we assume

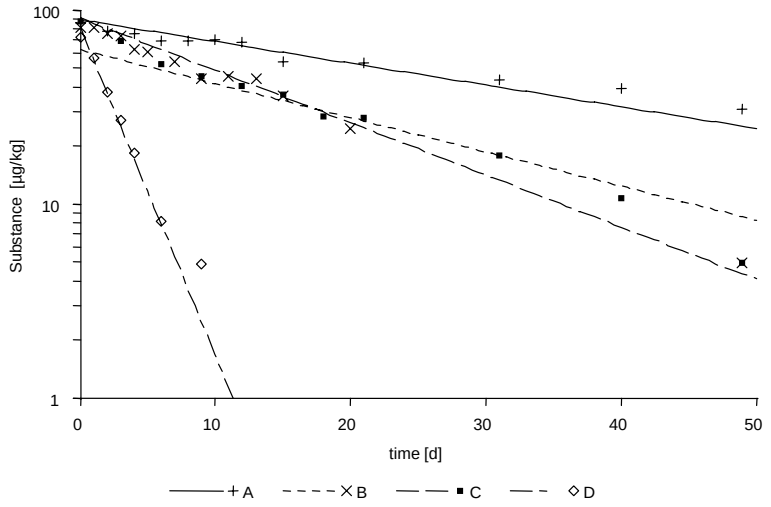

Fig. 2.9 Semi-log plot of degradation curves for Idosulforon obtained under different combinations of the factors temperature and humidity.

that we have no knowledge about the division into different stages, and assume a model for the entire population P in terms of a differential equation. Population growth depends of the ability to extract biomass from the host.

$$\frac{dP}{dt} = r_{P,max}\frac{W}{W+k_P}P - \mu_P P - \mu_P r_{P,C}(C_L)\,C_L P \tag{2.22}$$

Growth of the pest population depends on the available crop biomass using a function of Michaelis–Menten type. The parameter k_P [kg/ha] denotes the amount of biomass required to attain 50% of the maximum growth rate $r_{P,max}$ [1/d]. The parameters of degradation are introduced. μ_P specifies the natural mortality of the population in [1/d] and μ_C the mortality due to pesticide application. The latter depends on a critical pesticide concentration on the leaf, C_{crit} in [mg/m^2] using a nonlinear dose–response function

$$r_{P,C}(C_L) = 1 - \exp\left(-\left(\frac{C_L}{C_{crit}}\right)^2\right) \tag{2.23}$$

Besides the modification of a maximum growth rate of crop, see Equation (2.2), a flow of matter or energy from the hosting crop to the pest is an appropriate approach for modeling the influence of a pest on a crop. For powdery mildew we follow this approach and modify Equation (2.1) by another sink

$$\frac{dW}{dt} = \cdots - \gamma\frac{W}{W+k_p}P \tag{2.24}$$

γ can be interpreted as an efficiency parameter and specifies the fraction of biomass needed for population growth.

2.6.2 Age-structured Populations

Model Development Pest population modeling is a very good example of mathematical heterogeneity in ecological modeling. The first population of powdery mildew showed very fast exponential growth in one year and must be controlled by pesticide applications. In this second example a matrix model is set up. The second pest population considered shows a slow population dynamic, about one to three generations per vegetation period. A population like this must be taken into account in crop rotation design.

An example for this type of pest population is the sugar beet cyst nematode *Heterodera schachtii* population $\vec{P}(t_i)$. This population develops in distinct stages. For *H. schachtii* the stages: eggs and juveniles (P_1), hatched larvae (P_2), penetrated larvae (P_3) and adults (P_4) are distinguished. The population grows with the fertility F_0 of the individuals in the adult stage. This approach leads to a matrix-equation based on a Leslie matrix (Richter *et al.*, 1991; Schmidt *et al.*, 1993):

$$\vec{P}(t_{i+1}) = \begin{pmatrix} p_s & 0 & 0 & F_0 \\ p_h & 0 & 0 & 0 \\ 0 & p_p & 0 & 0 \\ 0 & 0 & p_d & 0 \end{pmatrix} \vec{P}(t_i) \tag{2.25}$$

Schmidt *et al.* (1993) define the following transition probabilities for hatching p_h, penetration p_p and adult development p_d

$$p_h(\vartheta_h, j) = \frac{p_{h0}}{j}\left(1 - e^{-\vartheta_h}\right) \tag{2.26}$$

$$p_p(\vartheta_{pdf}, \vartheta_h, P_2, j) = p_{p0}\vartheta_{pdf} \exp\left(-\left(\frac{P_2}{\vartheta_{pdf} D_p}\right)^{\gamma_p}\right) \tag{2.27}$$

$$p_d(\vartheta_{pdf}, \vartheta_h, P_3, j) = p_{d0}\vartheta_{pdf} \exp\left(-\left(\frac{P_3}{\vartheta_{pdf} D_d}\right)^{\gamma_d}\right) \tag{2.28}$$

with the maximum probabilities for hatching p_{h0}, penetration p_{p0} and adult development p_{d0} [1] and the critical density for penetration D_p and adult development D_d in [e.+j./100 g]. P_1 [e.+j./100 g] holds the number of eggs and juveniles per 100 g soil and j denotes the current generation of the year. The parameters γ_p, γ_d define the shape of the nonlinear functions.

From an agricultural point of view P_1, the number of eggs and juveniles in a unit soil in spring is decisive in determining potential crop damage. The adults P_4 influence crop growth of sugar beets, see Equation (2.2). This is modeled by an additional reducing factor of the maximum growth rate $r_{C,max}$. If the crop sugar beets are planted on the field the function

$$r_{C,P}(P_4) = r_0\left(e^{-\gamma_1(P_4 - P_r)^2} - e^{-\gamma_1 P_r^2}\right) + \frac{(1 + r_1)e^{-\gamma_2 P_4}}{1 + r_1 e^{-\gamma_2 P_4}} \tag{2.29}$$

modifies the maximum growth rates of the crop, with the factor of growth stimulation r_0 [1], the number of adults for growth stimulation P_r in number of larvae per 100 g

Table 2.9 List of parameters for specification of crop-dependent host suitability.

Crop	Sugar beet	Spring barley	Oats	Winter wheat	Winter-barley	Field beans	Oil radish	
Abbr. (α)	sub	spb	oa	ww	wb	fb	or	
ϑ_h	1.0	0.54	0.55	0.47	0.44	0.39	0.048	[1]
ϑ_z	ϑ_h	ϑ_h	ϑ_h	ϑ_h	ϑ_h	ϑ_h	0.87	[1]
γ_a	0	0	0	0	0	0	1.36	[1]
γ_b	0	0	0	0	0	0	-0.56	[1]
P_r	14.6	—	—	—	—	—	—	[e.+j./100 g]
r_0	0.146	—	—	—	—	—	—	[1]
γ_1	0.0164	0	0	0	0	0	0	[1]
r_1	59.5	0	0	0	0	0	0	[1]
γ_2	0.0261	—	—	—	—	—	—	[1]

soil and shape parameters r_1, γ_1 and γ_2 [1]. The function equals unity for $P_4 = 0$. Slight pest infestations stimulate crop growth (Schmidt *et al.*, 1993). For small values of P_4 the first term of the function models an increase of crop growth by $r_{C,P}(P_4) > 1$, higher values lead to a sigmoid decrease to zero.

All development stages of the nematode are influenced by the host, too. The parameters ϑ_{pdf} and ϑ_h for each development stage describe the potential suitability, as a host, of a crop. For sugar beet the parameter is arbitrarily set to 1, and all other crops or non-hosts are related to the sugar beet. For special crops, such as oil radish, Schmidt *et al.*(1993) calculates different values of ϑ_{pdf} and ϑ_h for the distinct stages by

$$\vartheta_{pdf} = \vartheta_z 10^{\gamma_a} P_k(t_i)^{\gamma_b} \quad (k = 2, 3) \tag{2.30}$$

with the suitability parameter ϑ_z and two additional shape parameters γ_a and γ_b. Table 2.9 list the crop-dependent parameters, see (Schmidt *et al.*, 1993).

The number of eggs and juveniles in a unit of soil $P_1(t_i)$ in spring is decisive in determining potential crop damage. The variable $P_1(t_{i+1})$ depends upon the development of the population in the previous year:

$$P_1(t_{i+1}) = P_1(t_i) p_{ov} \prod_{j=1}^{G(t_i)} \left(F_0 \vartheta_{pdf}(t_i) p_h p_p(j) p_d(j) + p_s(1 - p_h(j)) \right) \tag{2.31}$$

with number of generations $G(t_i)$ in year i and the probability of over-wintering p_{ov}. The number of generations G is determined by the overall environment conditions in a particular growing season t_i. The model is coupled to the crop growth model by the population of adult *H. schachtii* in the soil.

Model Analysis Model parameters are derived from a former publication (Schmidt *et al.*, 1993). Table 2.10 lists all parameters for the population dynamic model. This model is a very good example for demonstrating dynamic properties. There is no

Table 2.10 Summary of model parameters of the population dynamic model for *H. schachtii*.

Parameter	Value
Probability of over wintering	$p_{ov} = 0.6$
Survival probability	$p_s = 0.9$
Hatch probability	$p_{h0} = 0.8$
Penetration probability	$p_{d0} = 0.7$
Probability of adult development	$p_{d0} = 0.4$
Fertility	$F_0 = 10$ [e. + j./100 g]
Critical density for penetration	$D_p = 2500$ [e. + j./100 g]
Critical density for adult development	$D_d = 800$ [e. + j./100 g]
Shape parameters	$\gamma_p = 4.0$
	$\gamma_d = 2.5$

knowledge on system behavior for this model. No parameter estimation can be performed. No information on the goodness-of-fit or the correlation between model parameters can be derived from this step of model development. Therefore this is an excellent example to analyze the system with respect to dynamic behavior in the framework of a sensitivity analysis. For detailed study the parameter ϑ_h is chosen.

Figure 2.10 displays the asymptotic behavior of the population dynamics of referring to the number of eggs and juveniles in 100g soil. This so-called Ljapunov diagram displays the state of the variable after large number of iterations, e.g. a large number of generations G as a function of the host-crop suitability coefficient ϑ_h.

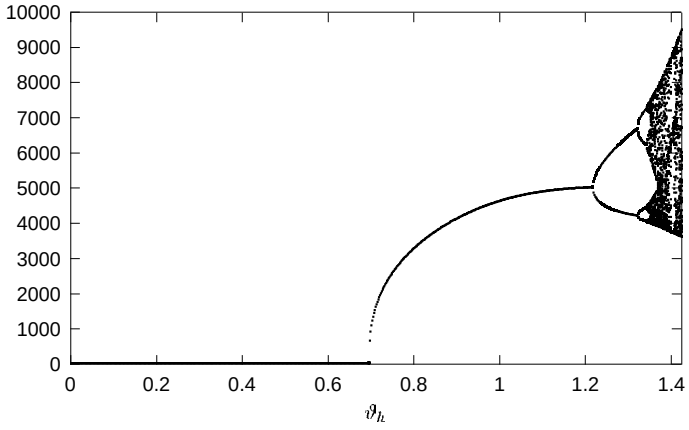

Fig. 2.10 Ljapunov diagram of asymptotic behavior of the population of eggs and juveniles in 100 g soil as a function of the parameter determining the host crop suitability ϑ_h.

2.6.3 Excursus: Types of Population Dynamic Models

Population dynamic modeling is an important aspect of ecological and environmental modeling. Matrix models are only one possible methodology, frequently used for clearly age-structured populations. However, for populations that show distinct age structure less clearly, different mathematical approaches are available. The following short excursus summarizes two additional mathematical approaches.

Partial Differential Equations We consider a population $P(a, t)$ which depends on time $t \geq 0$ with an age or length $a \in [0, A]$.

Together with the partial differential equation according to McKendrick and Foerster for age-structured population dynamics (Henson, 1999) this leads to the following general equation

$$\frac{\partial P}{\partial t} + \frac{\partial P}{\partial a} = -f(a, P, \vec{z})P. \tag{2.32}$$

The function $f(t, a, \vec{z}) \geq 0$ contains the per capita death rate due to different processes like mortality, harvesting or interspecific cannibalism.

The initial condition

$$P(0, a, \vec{z}) = P_0(a)$$

specifies an initial age-structured population. The boundary condition

$$P(t, 0) = r \int_0^A F(a)P(t, a)\, da$$

specifies the growth of the population P. r denotes the per capita growth rate, which may depend on the location $\vec{z}$. $F(a)$ denotes the fertility at age a. Section 3.2.2 (p. 76) discusses application of population dynamics modeling based on PDE.

Delay Differential Equations According to Kuang (1993) the application of delay-differential equations in population dynamics dates back to the 1920s, when Volterra (1927) investigated the well-known predator–prey model. It was only in the last three decades however that a greater interest in the mathematics of delay-differential equations and their application in the context of population dynamics and other areas of mathematical biology have arisen (MacDonald, 1989; Diekmann *et al.*, 1995).

Delay-differential equations have shown their usefulness in formulating population models for species with well-defined physiological stages, see for example (Gurney *et al.*, 1983; Nisbet & Gurney, 1983; Tuljapurkar & Caswell, 1997; Apel *et al.*, 2003). To illustrate how the introduction of time delays into the regulatory mechanisms of population dynamics is achieved through their stage structure, let us assume a simple stage-structured model of a closed population with only two stages, juveniles N_J and

adults N_A. The first step is to formulate the balance equations, which are

$$\left.\begin{aligned} \frac{dN_A}{dt} &= R_A(t) - D_A(t) \\ \frac{dN_J}{dt} &= R_J(t) - M_J(t) - D_J(t) \end{aligned}\right\} \tag{2.33}$$

with $R_J(t)$ and $R_A(t)$ being the respective recruitment rates, $D_J(t)$ and $D_A(t)$ the respective total death rates and $M_J(t)$ the total maturation rate from the juvenile stage at time t. This maturation rate $M_j(t)$ is equal to the recruitment rate of the adult population $R_A(t)$, $M_J(t) = R_A(t)$. The following model functions define the rate processes

$$\left.\begin{aligned} D_A(t) &= \mu_A N_A(t) \\ D_J(t) &= \mu_J N_J(t) \\ R_J(t) &= \beta N_A(t) \end{aligned}\right\} \tag{2.34}$$

μ_J and μ_A are the per capita death rates and β the fecundity.

Note that the maturation rate from the juvenile stage at time t is equal to the recruitment rate of the same stage but at the earlier time $t - \tau$. This is the important step, which will guide us to a delay-differential equation. The maturation rate from the juvenile stage $M_j(t)$ is equal to the number of matured juveniles, in mathematical terms:

$$M_J(t) = R_J(t-\tau)e^{-\mu_J\tau} = \beta N_A(t-\tau)e^{-\mu_J\tau} \tag{2.35}$$

Consequently τ defines the duration of the juvenile stage. System (2.33) can now be rewritten as follows:

$$\left.\begin{aligned} \frac{dN_A}{dt} &= \beta N_A(t-\tau)e^{-\mu_J\tau} - \mu_A N_A(t) \\ \frac{dN_J}{dt} &= \beta N_A(t) - \beta N_A(t-\tau)e^{-\mu_J\tau} - \mu_J N_J(t) \end{aligned}\right\} \tag{2.36}$$

In this form it becomes obvious that Equations (2.36) are delay-differential equations. The rate of change of N_A at any time t depends on its current state as well as on its state at time $t - \tau$. Equations (2.36) are of first order and linear. Besides the initial conditions, those kinds of equation require the definition of an initial history. This means, solving Equation (2.36) starting with $t = 0$, requires well-defined values for $N_A(t)$ for $t \in [-\tau, 0]$.

Summary This short excursion, together with the two examples for population dynamics modeling, clarifies an important statement from Chapter 1. Even if we start from a single conceptual diagram that is in some sense a consensus of different knowledge on the ecology of a population the resulting model does not only differ in parameters, equations of implementational details. The models differ entirely in their resulting structures.

These four different mathematical structures for population dynamics modeling cover the spectrum of approaches found in recent population ecology. However, one can

identify close relationships of these approaches and one can find intermediate types of models. For example the Leslie model makes it possible to separate the classical stages into a large number of "sub-stages" that can be compared to the delayed differential equation model.

2.7 MODEL INTEGRATION: GENERIC AGROECOSYSTEM MODEL

All the model equations introduced are ordinary differential equations or matrix equations. Interactions are defined by coupling functions of explicitly defined flows of matter from one compartment to another. Equations (2.1) to (2.31) define the following model system of an agroecosystem model. The following set of equations summarize this generic agroecosystem model. The main state variables and only the important functions are listed. If possible a short and aggregated formula is chosen, see this chapter for more detailed explanation.

$$\begin{aligned}
\frac{dW_C}{dt} &= \Big(r_{C,max}\, r_N(N)\, r_{C,W}(W_C, W_W)\, r_{C,P}(P_d)\, f_s(t) \\
&\qquad -\mu_W\Big) f_{DC}(t)\, W_C - \gamma \frac{W_C}{W_C + k_P} P \\
\frac{dW_W}{dt} &= r_{W,max} r_Q(Q) \left(1 - \frac{W_W}{K_W}\right) \\
\frac{dN}{dt} &= -k_l N - d(W,t) + k_m W_\mu + r_f \frac{W}{W + k_f} + F(t) \\
\frac{dC_L}{dt} &= -k_d C_L - k_w C_L + \nu(W) A(t) \\
\frac{dC_S}{dt} &= -k_d C_S + k_w C_L - k_l C_S + (1 - \nu(W)) A(t) \\
P_1(t_{i+1}) &= P_1(t_i) p_{ov} \prod_{j=1}^{G(t_i)} \Big(F_0 \vartheta_{pdf}(t_i) p_h p_p(j) p_d(j) + p_s(1 - p_h(j))\Big), \quad t_{i+1} - t_i = 1\text{a} \\
\frac{dP}{dt} &= r_{P,max} \frac{W}{W + k_P} P - \mu_P P - \mu_C r_{P,C}(C_L)\, C_L P
\end{aligned}$$

In some cases one cannot distinguish between crop or weed biomass. Here $W = W_W + W_C$ denotes the total above-ground biomass. Table 2.11 gives a summary of the processes considered, the modeling functions and the parameters and their physiological or physical meaning.

The model is specified by different control variables such as fertilization scheme F, application of pesticide A and weed control $p_i(t^*)$ as well as the crop selection, that is denoted by α.

$$F(t) = \sum_{i=0}^{q-1} F_i \delta(t - t_i)$$

$$
\begin{aligned}
A(t) &= \sum_{i=0}^{q-1} A_i \delta(t - t_i) \\
\alpha(t_i) &= (\alpha_1, \alpha_2, \ldots) \quad \alpha_i \in \{wheat, fallow, barley, \ldots\}
\end{aligned}
$$

Note that the model is parameterized and can be used to describe both abiotic and biotic processes of the first trophic levels for different species. Especially for different crops the model covers the dynamics of the sugar beet (abbreviated by "sub"), winter wheat ("ww"), winter barley ("wb"), oats ("oa"), spring barley ("spb") and potatoes ("pt") and the fallow seeds: oil radish ("or") and field beans ("fb") and weed. Simplifying parameterizations can be chosen for simulating bare soil or fallow.

The characteristic times of the model vary from years (population dynamics in $\vec{P}$) to weeks for growth of crop and weed, to days for degradation of pesticides. These are defined be the following parameters and parameter functions:

$$
\begin{aligned}
r_N &= \frac{N}{N + k_N} \\
r_{C,P}(P_4) &= r_0 \left(e^{-\gamma_1 (P_4 - P_r)^2} - e^{-\gamma_1 P_r^2} \right) + \frac{(1 + r_1) e^{-\gamma_2 P_4}}{1 + r_1 e^{-\gamma_2 P_4}} \\
&\quad \text{with } P_4(t_i) = p_h p_p p_d P_1(t_i) \\
r_{C,W}(W_C, W_W) &= 1 - \left(\frac{l W_C}{W_W} \right)^s \\
f_s(t) &= \begin{cases} 1 & \text{if } t < t_d \\ \frac{(1+\rho_1) e^{-\rho_2 t}}{1 + \rho_1 e^{-\rho_2 t}} & \text{else} \end{cases} \\
r_{P,C}(C_L) &= 1 - e^{-\left(\frac{C_L}{C_{crit}} \right)^2} \\
r_Q(Q) &= \left(\frac{Q}{Q_{max}} \right)^c \\
k_{cn}(t) &= \begin{cases} k_1 & \text{if } t < t_{DC} \\ (k_{max} - k_0) e^{-\frac{t - t_{DC}}{\tau_2}^{\gamma_c}} - (k_{max} - k_1) e^{-\frac{t - t_{DC}}{\tau_1}^{\gamma_c}} + k_0 & \text{else} \end{cases} \\
k_d(T, \theta) &= k_{d,max}\, k_T(T)\, k_\theta(\theta) \\
k_T(T) &= \left(\frac{T_{max} - T}{T_{max} - T_{opt}} \right)^\beta \exp\left(\beta \frac{T_{max} - T}{T_{max} - T_{opt}} \right) \\
k_\theta(\theta) &= \theta^a
\end{aligned}
$$

From this it follows that the control variable "crop planted" $\alpha(t_i)$ modifies the model parameters. Additionally, for special cases, such as "fallow", the structure of the model is also modified. The dependence from site-specific parameters introduces spatial aspects into the model, which require regional simulations.

Table 2.11 Summary of model parameters.

Compartment	Term	Parameter	Physiological meaning
Crops	W_C	$r_{C,max}$ [1/d]	maximum growth rate, relative increase of biomass per day
		$W_{W,0}$ [kg/ha]	initial crop biomass, biomass at time of planting
		μ_C [1/d]	attrition rate, relative decrease of biomass in stage of senescence
	r_N	k_N [kg/ha]	denotes amount of nitrogen necessary to attain half of the maximum growth rate (Michaelis–Menten parameter)
	$r_{C,W}$	l [1]	critical weed density relative to crop biomass
		s [1]	parameter of nonlinearity, equal behavior to c
	$r_{C,P}$	r_0	growth stimulation due to pest infestation
		P_r	density of pest for growth stimulation
		r_1, γ_1, γ_2 [1]	shape parameters
	f_s	ρ_1 [1/d], ρ_2 [1]	shape parameters
Weed	W_W	$r_{W,max}$ [1/d]	maximum growth rate, relative increase of biomass per day
		$W_{W,0}$ [kg/ha]	initial weed infestation, at time of planting
		k_W [kg/ha]	maximum carrying capacity of weed at observed site
	r_Q	Q_{max} [%]	critical level of photosynthetically-active radiation, in case of actual Q exceeds Q_{max} weed growth increases, otherwise weed growth decreases
		c [1]	parameter of nonlinearity, the dependency described in upper row to a more sensitive ($c > 1$) or insensitive ($c < 1$) behavior
Pest pop.	P	$r_{P,max}[1/d]$	maximum growth rate of pests
		k_P [kg/ha]	denotes amount of crop biomass necessary to attain half of the maximum growth rate (Michaelis–Menten parameter)
		μ_C [1/d]	natural mortality of pest population
		μ_P [1/d]	mortality of pest population due to pesticide treatment
	$r_{P,C}$	C_{crit} [kg/ha]	threshold value of pesticide on crop leaf that to attain a significant mortality of pest population
	$\vec{P}(t_i)$		see Table 2.10 for a parameter summary
Nutrients	N	k_l [1/d]	infiltration rate
		k_m [1/d]	rate of mineralization
		r_f [1/d]	maximum rate of N_2 fixation for legume crops
		k_f [kg/ha]	amount of crop biomass of legumes necessary to attain half of the maximum fixation rate
Pesticides	C_L	k_W [1/d]	runoff rate of pesticide from leaf to soil surface
	k_d	$k_{d,max}$ [1/d]	maximum degradation rate
	$k_\theta(\theta)$	a	shape parameter
	$k_T(T)$	T_{opt}	temperature of maximum degradation of pesticides
		T_{max}	maximum temperature from which no pesticide degradation occurs
		β	
	C_S	k_l [1/d]	infiltration rate

2.8 SUMMARY

This chapter has presented examples for the steps of model development presented in Chapter 1. The starting point is the conceptual diagram in Figure 2.1 that can be classified as a feedback model or box-model. From this a set of mathematical equations was derived summarized in the previous section. In this process of compiling the mathematical model we must clarify that the conceptual diagram is a guideline only. For example, some boxes are specified in detail by more than one differential equation (which is supported for example in the concept of energy diagrams of feedback diagrams).

Then we examine the steps of parameter identification and model analysis. It is typical for ecological modeling that the specification of parameters is obtained from

- Literature values and databases (such as (Jørgensen *et al.*, 2000)): k_l, ϑ_{pdf}, ϑ_h, γ_1, γ_2, γ_a, γ_b, r_0, r_1, etc.
- Field trials and following parameter estimation: $r_{C,max}$, $r_{C,max}$, $r_{WC,max}$, μ_C, μ_W, ρ_1, ρ_2, r_f, k_f, k_{max}, k_0, k_1, etc.
- Laboratory experiment together with parameter estimation: β, $k_{d,max}$, T_{opt}, etc.
- physical measurements and possible the aggregation to effective parameters: k_l, k_m, etc.
- and not to forget educated guesses: a, T_{max}, etc.

Specification of parameters is always subject to uncertainty. This uncertainty requires a detailed analysis of the derived model, focusing on dynamic properties and predictive power. Several examples in this chapter showed many possible results of dynamic behavior. The model shows different patterns in different temporal scales. Characteristic time vary from years (population dynamics) to weeks (crop growth) to days (pesticide degradation).

Patterns in reality are redrawn. Statistically this is measured by the r^2 values. Additionally statistical analysis showed that the model should be set up with a minimum number of parameters. This assists in applying the model to modified conditions (such as different crops) as well as different locations. Regionalization of the model is supported, cf. Section 1.4.1.

Besides this, the highly nonlinear model show chaotic patterns, which are rarely visible in reality in the form one can derive from a mathematical model. In this context, and knowing the uncertainty of model parameters, it should be noted that the domain of appropriate model parameters is a subset of biologically useful parameters (which again is a subset of the mathematically admissible parameters). The rejected domain with parameters, which may be biologically useful, but which does not lead to useful model output is a conjunction of two different domains: the domain of parameter that leads to chaotic patterns due to the mathematical structure of the model, and the

domain of parameters that lead to chaotic patterns due to the numerical solution of the underlying equation set. In most cases of environmental modeling one cannot distinguish between these two domains.

Several variables of the model, introduced management modeled by control variables. These variables denote the link of anthroposphere to biosphere. These variable are used to define scenarios. For example different amounts of fertilizer can be applied. Finally, a first management task was investigated within the weed control model. The concept of threshold values could be verified with a model with this kind of structure.

Besides the modification of different state variables, the control variable selected crop $\alpha(t_i)$ switches between different model types. This is possible because the model shows a very *general structure* that makes it applicable to different crops (and investigation sites). The minimum number of parameters is one prerequisite for obtaining a general or generic model. Additionally the model is generic. This means the model structure itself can change depending on control variables or parameters. For example the model structure can be used to simulate bare soil by setting all crop growth variables to zero or unity.

A second item that helped us to obtain such a generic model is the *modularity*. Modularity is important for achieving results in the parameter estimation step, and modularity is important for model integration of different building blocks in a model. Modularity is a very helpful property in the step of model analysis, too. The conclusion to be derived from this is that a model structure must be defined in an open way to allow a simple integration of an additional part or modify existing parts.

However, advocating an open and modular structure of dynamic simulation models, raises a difficult question. What is the appropriate mathematical tool, that can couple different mathematical models? As we have seen from this chapter, ecological models may be set up by different types of differential equations as well as different types of time-discrete equation sets. Possible relationships between time-discrete and time-continuous modeling approaches of dynamic processes are identified. Nevertheless, there is no formal theory which provides a link between continuous and discrete systems (Savill & Hogeweg, 1999). In environmental modeling we have to cope with both approaches. This mathematical heterogeneity so far is visible in forms of coupling matrix equations with nonlinear ordinary or partial differential equation systems. Additionally, environmental problems always refer to a spatial domain. So the question arises, what kind of system do we get, when introducing spatial dependencies?

3

Environmental Models: Spatial Interactions

3.1 SPATIAL REFERENCES IN ENVIRONMENTAL MODELS

3.1.1 Spatial Scales and Model Support

The models introduced in Chapter 2 depend on the properties of the investigation site being considered. For instance, growth parameters depend on radiation, exposition, nutrient availability. Population dynamics of species are a function of habitat suitability. This dependency on attributes of the investigation site is primarily introduced by a spatial dependency of the vector of model parameters from the location $\vec{c} = \vec{c}(\vec{z})$. As a consequence, state variables of a model acquire a spatial dependency, too $\vec{x}(t) = \vec{x}(t, \vec{z})$.

If a variable has a spatial dependency, this potentially requires an infinite amount of information for specification, since there are infinite variables at every point in any defined geographic area. A spatial discretization of the considered area for each layer of information, e.g. each variable and parameter, is required. The topic of spatial discretization can be approached from several directions. If good data is available, discretization of spatial data can be understood as a question of spatial data analysis. Several well-known mathematical procedures obtained from geostatistics are available, for example (Zhang & Griffith, 1997). For instance, variogram analysis of spatial data sets calculates indicators of the range of spatial variability. The reader is referred to (Cressie, 1991; Deutsch & Journel, 1992).

However, good data availability is rare, the larger the considered spatial scale of the modeling task is. In general the steps of model development and the step of acquiring

spatial information are two processes, that cannot be performed independently. The following issues are closely related:

1. A model is a simplification of real world processes with a certain purpose, cf. Chapter 1. This holds true for spatial discretization of information: a spatial model simplifies reality according to two dimensions: processes and spatial extension.

2. In most cases spatial data is often absent or of a much lower quality. Spatial discretization of data may be defined by the availability of spatial data, that determines the modeling process. For instance, data available from a remote sensing source is used frequently in raster-based models, with the data determining the raster cell size.

3. It follows that the process of model development is strongly influenced by the choice of an appropriate data model for spatial data. The translation of a conceptual diagram into mathematical equations depends on the chosen spatial data model. This glues several steps of model development together, that were introduced as independent steps in Chapter 1.

4. Even the processes considered and their mathematical formulation differs depending on the selected spatial scale. Different processes dominate at different scales, which leads to the fact that different processes are ignored in the step of conceptual modeling, which is the step of simplification in environmental modeling.

Models representing equal processes vary considerably across scales, even if environmental processes on large scales are to a great degree the result of processes at smaller scales, cmp. Figure 1.3 on page 8. In this context Heuvelink (1998) introduces the term model support:

Definition 3.1 (Support) *The support of a model denotes a spatial unit for which averaging in terms of model processes as well as data is admissible for the given modeling problem.*

The support of a model is closely related to "level of aggregation" or "sample volume". In this chapter results and solutions from several examples are discussed in the context of these three topics of spatial environmental modeling.

As an example for different types of spatial discretization and the resulting mathematical structure we focus on the processes of water- and matter dynamics in the unsaturated soil zone. Figure 3.1 displays the location of the investigation site called "Nienwohlde", an investigation site of the CRP 179, situated in Lower Saxony. Soil properties of this investigation site show a high spatial variability as this site is situated in a push terminal and ground moraine region, typical for northern Germany, see (Pollex *et al.*, 1995) for further information. Figure 3.2 displays a soil column for

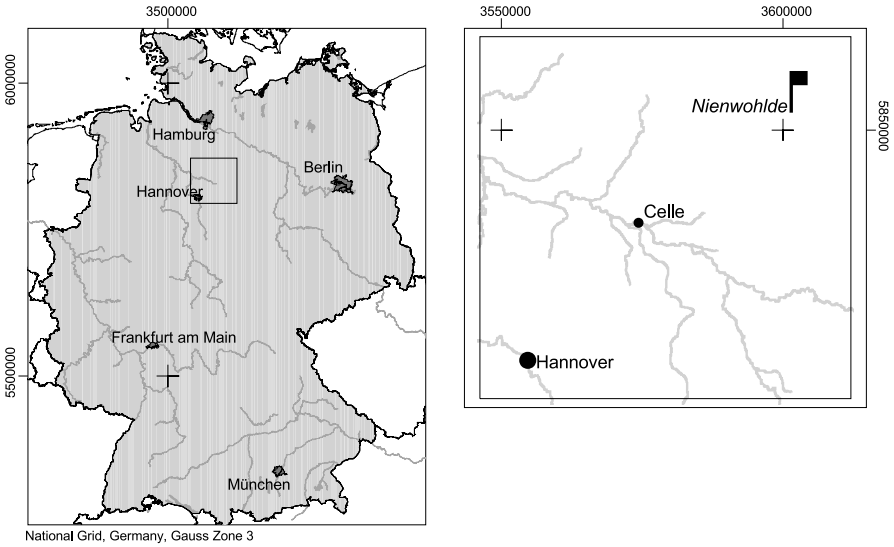

Fig. 3.1 Location of the investigation site "Nienwohlde" of the Collaborative Research Center "Water- and Matter Dynamics of Agroecosystems".

which the transport of water is to be modeled. Modeling of processes in soil (unsaturated or saturated) is subject to the problem of spatial variation on a very small range. Figure 3.2 gives an example of 1.80 m deep soil column located at this investigation site. Figure 3.2.a shows a photograph of the soil column after a tracer experiment using a conservative red-colored tracer. The flow region is colored by Rhodamine applied during the tracer experiment.

Starting from the photograph (Figure 3.2.a) of the soil column, different steps of discretization can be performed. First, homogeneous units, spatial units for which an averaging of soil parameters is appropriate, are identified. This leads to a map with several homogeneous units (Figure 3.2.b), the support of the model. This is performed within a GIS using a vector data model, see below.

For the next steps the chosen model or model structure has to be taken into account for spatial data management. If a partial differential equation in two dimensions is used for transport modeling a 2D-finite-element mesh has to be set up from the map of homogeneous soil regions, Figure 3.2.c. If a single soil column, is to be modeled by a 1D-PDE model based on the identification of a representative soil column a 1D-discretization has to be identified, Figure 3.2.d. Finally, if a system of ordinary differential equations, instead of a PDE, is used to solve the problem of simulation water flow through the soil column, a further aggregation of spatial information is required. The result is a conceptual diagram using a box for each spatially homogeneous region in soil, Figure 3.2.e.

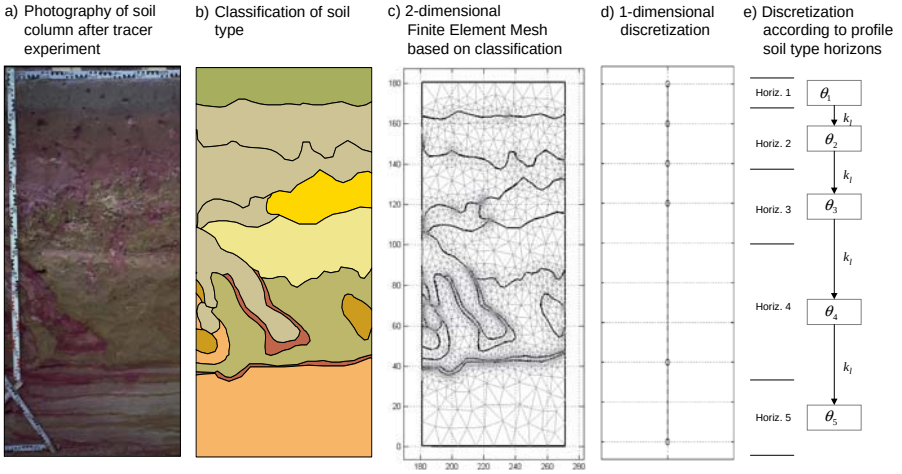

Fig. 3.2 Characterization of different modeling approaches together with different spatial resolution of spatial data. From left to right: a) Photograph of soil column, b) Spatial discretization of homogeneous units in soil (GIS), c) 2D-finite-element mesh, underlying discretization for numerical solving the PDE, d) 1D discretization for numerical solution of PDE, e) Discretization according to coarse classification of properties of the soil horizons ("bucket" model).

3.1.2 Models for Spatial Data Structures

The technical issue of storing, maintaining and analyzing spatial data is supported by geographic information systems (Longley *et al.*, 2001). Two concepts are used to reduce geographic information for making spatial information available by computer databases, that are required to develop models for a geographic area: *raster* and *vector* data (Longley *et al.*, 2001).

Raster Data In a raster representation of geographic space, that space is divided into an array of cells that are usually square. All geographic variation is expressed by assigning properties to theses cells. The striking advantage of this concept is the simplicity of the data model. Raster data sets can be handled as simple matrices, which are available in a broad range of programming languages.

For each property a separate layer of cells is introduced. The size of raster cells is the smallest possible unit with which spatial variability can be expressed, the smallest possible support of a model. Larger homogeneous areas are expressed by a cluster of raster cells with identical properties. In general an integration of several cells to one homogeneous object is not possible. However, there are concepts that make use of different raster cell sizes, such a multi grid or quad-tree approach (Nievergelt & Widmayer, 1991). No spatial variability is covered that appears below a raster cell size. Raster cell size therefore determines the precision with which spatial variability is covered within the model.

Table 3.1 Comparison of characteristic topics of vector- and raster-based data structure for environmental modeling.

Vector	Raster
Appropriate for modeling single, unique objects	Single objects (points or lines) are stored unstructured
Controllable precision of object location and shape	Approximization of object
High effort for data acquisition	Data acquisition "simple" in some cases, e.g. remote sensing
Low storage capacity required	High storage capacity required
Transformation of projection or co-ordinates simple	Projection transformations may change shape of raster cells and topology
Logical operation between several layers is complex function (intersection)	Implementation of logical operation or calculation simple, if raster maps show equal orientation and location

A spatial application of an environmental model is performed using a repeated simulation of the model for every grid cell. This is the reason why the raster cell size determines the complexity and computational effort of a model, too. The computational effort of a spatial model based on raster data increases quadratically with decreasing cell size.

Vector Data In a vector representation, all lines are captured as points connected by precisely straight lines. If spatial information is given using a vector-based data set, units with spatially homogeneous properties, for examples soil properties, or land cover, are given be a polygonal object, bordered by a polygon, a sequence of points. One can derive vector-based data sets from grid-based data sets by aggregating grid points with similar attributes using classification algorithms, see (Sadler *et al.*, 1998; Lu *et al.*, 1997; Weibel, 1997). The result, is a map S of homogeneous areas $s \in S$. Figure 3.2.b gives an example based on the photograph of a soil column.

Attributes, parameters are associated to this polygon using the layer concept. Every spatial layer holds a single piece of information, for example a soil parameter. Intersection different polygonal layers is a well-known function of GIS (Breunig, 1996, p. 77). This is displayed in the last row in Figure 3.9, see Section 3.3.1, p. 85.

Comparison Table 3.1 lists a short summary of several topics related to the use of raster or vector data. Both approaches are widely used in environmental modeling and are well supported by GIS. Transformation between the two data structures is possible. Transformation from raster to vector leads to the estimation of iso-surfaces, transformation from vector to raster data leads to discretization of the considered area defined by a given cell size.

3.1.3 Spatial Patterns

If dynamic models are set up using parameters, coefficients and state variables that show a spatial reference, the simulation results show temporal as well as spatial patterns. Two different sources of spatial patterns can be identified. Savill *et al.*(1999) distinguish between *exogenous* and *endogenous* spatial patterns. Exogenous spatial patterns are caused by external data fed into a simulation model. For instance soil properties, land use, biotope attributes. Endogenous pattern emerge, if spatial interactions are part of the model. Spatial interactions can be dispersal of species, diffusions of substances, migration along landscape gradients.

So spatially distributed parameters of models do not necessarily lead to endogenous patterns. On the other hand it is a necessary condition for obtaining endogenous patterns, that a model incorporates spatial interactions between state variables.

For example, Anderson *et al.* (2002) investigate the question: which patterns of driving forces cause which spatial patterns using different model systems? Their conclusion is, that in many cases, the local interactions are chosen so that the neighbors involved are within a fixed range and contribute equally. The choice of the neighborhood is not driven by realism.

From these introductory discussions one can distinguish two classes of spatial models. At this stage, a textual definition can be given for both types of models:

Definition 3.2 (Regionalized Model) *With the regionalization of a model, the following methodology is understood: all model parameters that describe environmental factors are identified and specified using georeferenced data, obtained from a GIS. The simulation is a repeated run of the model for each of the georeference data set* $\vec{z}_i$ *using the model parameters* $\vec{c}(\vec{z}_i)$ *and initial conditions* $\vec{x}_0(\vec{z}_i)$ *(*$i = 1, 2, 3 \ldots$*).*

Model structure may frequently change for different spatial patches. These models are suitable for discrete habitat, or patchy landscapes. Second, information exchange between state variables of different patches or homogeneous units is difficult, which complicates the implementation, for example, of horizontal fluxes.

For these types of models much effort is spent on the identification of effective model parameters and representative spatial units that show homogeneous attributes characterized by spatially constant parameters, see for instance (Bormann *et al.*, 1999; Beven & Kirkby, 1979; Wu & Levin, 1997). This may either be achieved within a grid-based or vector-based data structure.

Definition 3.3 (Spatially Explicit Model) *A spatially explicit model describes dynamic processes in a way that, for each arbitrarily chosen location vector* $\vec{z}$*, all state variables are well-defined. This methodology explicitly offers the ability to implement processes that are based on exchange of matter and information between the spatial units.*

Spatially explicit models make use of both types of spatial data structures: vector or grid data. Spatially explicit models based on vector data are presented for instance

by Krysanova *et al.* (2002), Beven *et al.* (1997), Kurz *et al.* (2000), and Wu & Levin (1997). From a survey of recent publications on spatially explicit models, the most frequent choice seems to be the grid-based data structure, see for instance (Rao *et al.*, 2000; Tyre *et al.*, 2001; Congleton *et al.*, 1997; Hargrove *et al.*, 2000; Boumans *et al.*, 2001; Voinov *et al.*, 1998; Voinov *et al.*, 1999; Thulke *et al.*, 1999; Yacoubi *et al.*, 2003).

Hybrid approaches combining vector and raster data structures, are presented by Tischendorf *et al.* (1997) who use a quad-tree approach for analysis of habitat fragmentation and Berger & Hildenbrandt (2000) who selected a hybrid data set combining point and raster data for a spatially explict mangrove tree growth model.

This chapter will present examples for both types of models and explains the differences between the two model classes. The starting point is an aggregated model with several examples for biotic and abiotic processes. After this several examples of integrated spatial models will be given.

3.2 AGGREGATED SPATIALLY EXPLICIT MODELS

Definition 3.4 *Aggregated spatially explicit models are spatially explicit models which are characterized by the use of a single mathematical "dialect" and a very limited number of equations.*

The important property of this definition is the uniqueness of the mathematical language. This distinguishes aggregated models from models, that integrate several different functions or equation systems, that probably change structurally for different spatial objects. The mathematical structure of aggregated models remains equal for all spatial objects (polygons or raster cells) of the investigation site.

In the following sections several examples of aggregated models are presented, focusing on mesoscalic applications and the relevant applications that are required for the following chapters of this book.

3.2.1 Abiotic Processes

Modeling transport processes of substances through different media has two principle components: modeling of transport and modeling of reaction. Both can be handled in different ways, which depend on the media, the considered scale and the mathematical dialect. For instance, transport of xenobiotica in soils may be modeled using box (or "bucket") models, which lead to ordinary differential equation systems or using the convection dispersion equation, which leads to a partial differential equation. Both approaches are based on an assumption of homogeneity of a certain volume of soil.

Water and Matter Transport in Soil Transport processes in soil are characterized by the number of phases or substances to be considered. In the upper soil

layer, water, soil substance as well as air set up the compartment of the *unsaturated soil zone*. Two different phases (water and air) are to be considered in a transport model. If there is also non-aquifer phase liquid (NAPL) the two-phase model changes to a multi-phase model. This holds true for the aquifer compartment which is characterized by the non-existence of air. One speaks of a multi-phase model for this compartment if water as well as NAPL media is present (Bear & Bachmat, 1990).

Modeling of processes in soil (unsaturated or saturated) is subject to spatial variation on a very small range. Figure 3.2.a shows a photograph of the soil column after a tracer experiment. Following the discussion from Section 3.1.1 the identification of the support of a transport model, that depends on highly variable parameters determining the transport velocities (such as conductivity, or sorption) the support of a soil transport model is defined by the assumption of an average or characteristic unit in which model parameters are homogeneous and constant. A porous medium domain is called homogeneous with respect to a macroscopic geometrical parameter characterizing the configuration of the void space or of any phase within the domain, if that parameter has the same value at all points of the domain. In this context a representative elementary volume (REV) is defined. Foremost is the requirement that the values of all averaged geometrical characteristics of the microstructure of the porous material at any point in the macro space of the porous medium domain be single valued function of the location of that point of time only, independent of the size of the REV (Bear & Bachmat, 1990).

The soil displayed in Figure 3.2 was analyzed in such a way. In a first step the photograph of 3.2.a was analyzed, homogeneous areas were identified and the soil structure was rebuilt using the vector data model for defining polygonal objects of homogeneous soil areas. In a second step a model was used to describe the process of water transport on such a geometry.

Richards Equation For unsaturated conditions the Richards equation describes the process of movement of water content in the unsaturated soil zone

$$\frac{\partial}{\partial t}\theta = \frac{\partial}{\partial x}\left(D(\theta)\frac{\partial \theta}{\partial x}\right) + \frac{\partial}{\partial y}\left(D(\theta)\frac{\partial \theta}{\partial y}\right) + \frac{\partial}{\partial z}\left(D(\theta)\frac{\partial \theta}{\partial z} - K(\theta)\right) + S \qquad (3.1)$$

where θ denotes the water content [%], K the conductivity and S a source or sink term. For a homogeneous, isotropic medium K is a scalar. In an anisotropic medium K is a tensor. This equation is derived from the mass conservation equation with the volumetric flux density $\vec{q}$

$$\frac{\partial}{\partial t}\theta = -\nabla \cdot \vec{q} + S \qquad (3.2)$$

which states that the rate of change of water content per unit volume equals the net gain of fluid per unit volume plus sink or source within the unit (REV), the *Darcy law*. The nabla operator abbreviates $\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right)$. The missing functional relationship between the flux density $\vec{q}$ and the water content θ in Equation (3.2) is derived from the equation

$$\vec{q} = -K(\theta)\nabla\Psi_h \qquad (3.3)$$

in which Ψ_h denotes the hydraulic potential in [hPa]. The hydraulic potential is an additive variable that is set up by the gravimetric potential Ψ_z, that is simply expressed by the vertical distance from a reference elevation, the matrix potential Ψ_m, which is due to the adsorptive forces of the soil matrix and depends on the water content of the soil: $\Psi_h = \Psi_z + \Psi_m$. Note, that in Equation (3.1) Ψ denotes the matrix potential Ψ_m (the index m will be dropped in the following) and it is set $\Psi_z = z$ with a negative sign below the surface (even if surface is chosen as the reference level).

Note, the conductivity K as well as Ψ_m depends on the water content. A functional relationship for both functions must be given that yields a specification of the unknown variable D in Equation (3.1). Using the capacity function $\partial\theta/\partial\Psi$ one gets

$$D(\theta) = K(\theta)\frac{\partial\Psi}{\partial\theta} \tag{3.4}$$

The conductivity function is written in the form $K = K_s K_r$, where K_s denotes the saturated conductivity, which is a parameter and K_r, which is referred to as normalized hydraulic conductivity, describes the functional relationship. Similarly θ_r denotes the residual water content, and θ_s the saturated water content, the normalized water content becomes

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} \tag{3.5}$$

Several parameterizations of empirical relationships for $\partial\theta/\partial\Psi$ and $K(\theta)$ are in use. As one example the parameterization according to vanGenuchten (1980) and Mualem (1976) is given here. It is a widely used flexible approach, that is applicable to a large number of soil types

$$\Theta(\Psi) = \begin{cases} \left(1 + (\alpha|\Psi|)^{\frac{1}{1-m}}\right)^{-m} & \text{for } \Psi \le 0 \\ 1 & \text{for } \Psi > 0 \end{cases} \tag{3.6}$$

$$K_r(\Theta) = \Theta^{1/2}\left(1 - \left(1 - \Theta^{1/m}\right)^m\right)^2 \tag{3.7}$$

with fitting parameters α and m.

Note, that the notation for the state variable water content Equation (3.1) is valid for unsaturated conditions only. A general overview of unsaturated soil and ground water reaction dispersion models can be found in Baer & Verruijt (1987) and Anderson & Woessner (1992).

Convection Dispersion Equation Based on the convective transport of solute matter in the soil water the convection dispersion equation (CDE) can be noted. Denoting the concentration of a substance by $C(t, \vec{z})$ the CDE is written as

$$\frac{\partial}{\partial t}C = \nabla \cdot \left(D\nabla C - \vec{q}C\right) + S \tag{3.8}$$

S denotes a sink or source term in the considered REV. $\vec{q}$ specifies the flux density derived from the Richards equation (3.2). D denotes the dispersion of the substance.

One assumes that movement of the solute along with the water is associated with a further effect arising from the random motion of the water through the porous medium. This effect is called mechanic dispersion and is treated in analogy to molecular diffusion. The classical approach is to relate the flux to a gradient of the concentration. The negative sign determines the direction of the flux from higher to lower concentration. The relation only holds in an isotropic medium. Additionally Equation (3.8) may be extended by sorption to the solid phase, and reactions such as degradation or transformation to metabolites. These processes are incorporated into the model by a modification of the sink/source term of ODE-type equations. The process model which define the sink/source term may be very complex. For instance Umgiesser *et al.* (2003) present a complex dynamic model for nutrient cycling in the Venice lagoon within the hydrodynamic model of the lagoon, solved by FEM numerics.

Boundary Conditions Spatially explicit models of any kind need the specification of boundary conditions. These conditions specify the behavior of a model at the edge of investigated region. In the theory of PDEs two important boundary condition types are distinguished. The *Dirichlet* type specifies a fixed, but possibly time depending, value of the state variable. The *VonNeumann* type specifies the values of the derivative of the state variable in the direction of the vector orthogonal to the system boundary.

Simulation Study Referring to the soil column displayed in Figure 3.2.a a simulation study[1] is performed that models the transport of a tracer substance through soil using a precise discretization of soil according to the 2D-finite-element mesh generation, Figure 3.2.c. Figure 3.3 displays the concentration of a fictive tracer for the time steps $t = 30$ h to $t = 240$ h (a) to (h). The initial condition is given by a homogeneous tracer wave in the first 10 cm of the soil. This wave moves slowly downwards. In the first 50 cm the initial shape remains. After $t = 120$ h the spatially distributed model parameters, such as conductivity, offer preferential flow paths for the substance. Finally the initial wave separated into two parts. Part of the applied substance reached the lower edge of the soil column at 1.80 m and part remained at partly impermeable layers at 1 m. These patterns are clearly exogenous, as these are a result of the specification of the conductivity parameters based on spatially referenced model parameters $\vec{c}(\vec{z})$.

3.2.2 Biotic Processes

Population Dynamics In Section 2.6.3 the PDE for age-structured population dynamics according to McKendrick and Foerster was introduced, cf. Equation (2.32). Introducing spatial explicitness to this equation makes P depend on time, age and location $\vec{z}$: $P(a, t, \vec{z})$. Without loss of generality we consider a 2-dimensional habitat.

[1] Nummerical solutions of PDE-type models presented in this book are calculated using the model development tool FEMLab, see Section 1.5.4, p. 29.

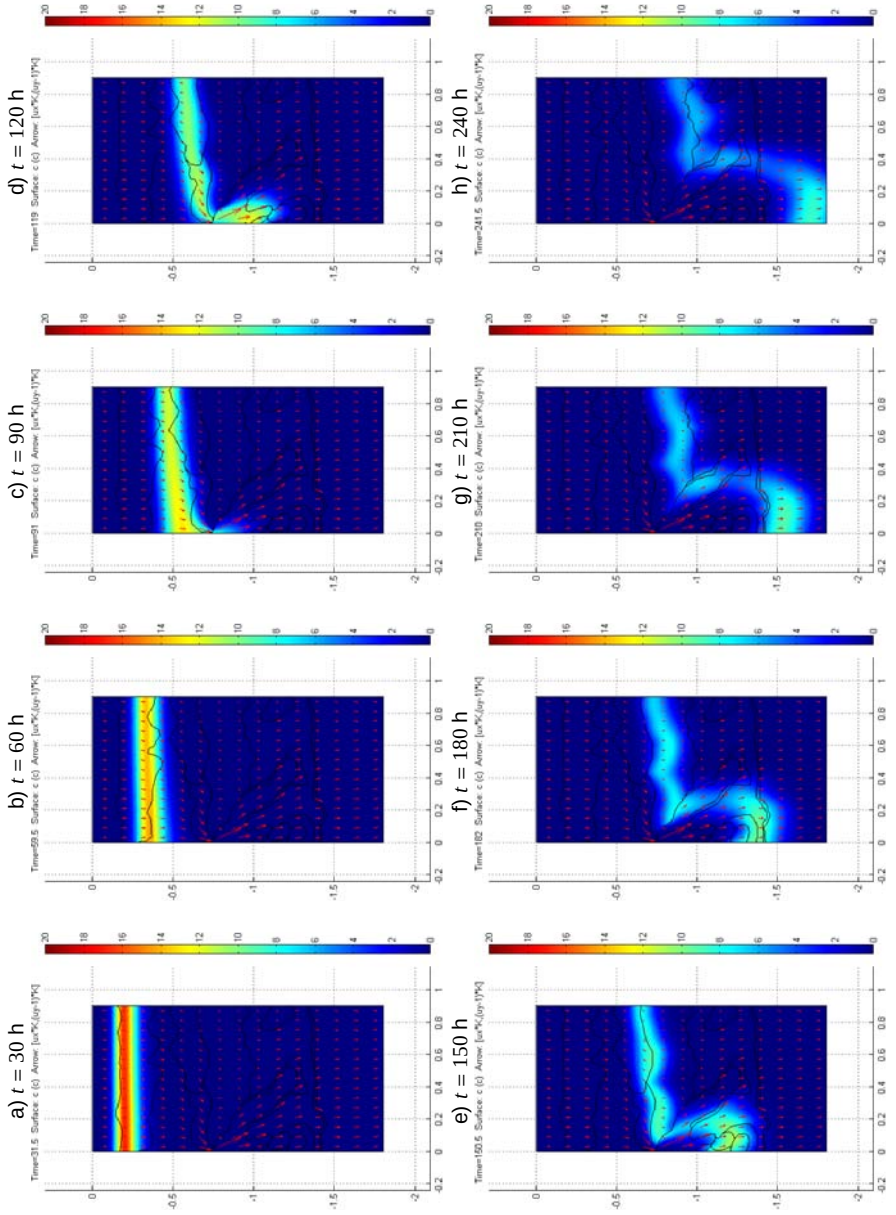

Fig. 3.3 Results of tracer transport modeling based on the soil of the "Nienwohlde" study area. The tracer substance is homogeneous distributed in the upper 10 cm of the soil in the initial condition. Figures a) to h) show the time steps 30, 60, . . . , 240 h. (See p. 279 for additional ressources.)

Spatial localization is given by a vector $\vec{z} = (x, y)$. An extension to a 3-dimensional approach can easily be set up. The latter is frequently used in marine ecology.

Let us first focus on the migration of species. The vector $\vec{j}$ denotes flow of population $P(t, a, \vec{z})$. $\vec{j}$ incorporates dispersion $\vec{j}_D$ and active movement to more suitable habitats $\vec{j}_H$ as well as advective drift by wind or current $\vec{j}_v$. It yields

$$\vec{j} = \vec{j}_D + \vec{j}_H + \vec{j}_v$$

Dispersion In analogy to the derivation of the convection dispersion equation, dispersion of the population denotes the spatial spread due to random motion of individuals. However, the behavior of a living organism differs from substances or solute. A frequent assumption in population dynamics modeling is that dispersal depends on the population density of the considered location. The more dense the population, the higher the the pressure to move to a different location. This leads to a density dependent-dispersal term

$$\vec{j}_D = -D_D \left(\frac{P}{P_{crit}} \right)^n \nabla P$$

P_{crit} denotes a critical density and n is a shape parameter. The negative sign denotes density-dependent migration directed to the lower population density. Note, that the operator does not include age.

Habitat Suitability Let $H(\vec{z})$ denote a function that describes the suitability of a given location $\vec{z}$ being a habitat for the considered species or community. There is an abundant literature on habitat modeling methodologies, see for instance (Guisan & Zimmermann, 2000; Tyre *et al.*, 2001). For the following we assume a given habitat suitability function obtained by an arbitrary model. The higher the value $H(\vec{z})$ returns, the more suitable the habitat is at location $\vec{z}$. It may depend on several environmental factors like availability or prey, or absence of predatory species. An example for population density is

$$H(\vec{z}) = 1 - \frac{P(\vec{z})}{P_{max}(\vec{z})}$$

where P_{max} denotes the carrying capacity of habitat in $\vec{z}$. Mobile species may have the ability to migrate to the more suitable habitat along a gradient of habitat suitability. The related vector $\vec{j}_H$ can be defined by

$$\vec{j}_H = D_H \; P \; \nabla H(\vec{z})$$

where D_H denotes the migration rate based on habitat gradients in the landscape. It is appropriate to assume that D_H is dependent on the habitat suitability $H(\vec{z})$. For instance for a less suitable habitat (low values of H) $D_H(H)$ may be large and vice versa.

Drift With the availability of a vector $\vec{v}$ holding the speed and direction of the surrounding medium (water or air) obtained from a convection model, the vector j_v can be specified by

$$\vec{j_v} = \vec{v}\, P$$

Together with Equation (2.32) describing age-structured population dynamics, the following general equation is derived

$$\frac{\partial P}{\partial t} + \frac{\partial P}{\partial a} + \nabla \cdot \left[D_H P \nabla H - D_D \left(\frac{P}{P_{crit}} \right)^n \nabla P + \vec{v} P \right] = -f(a, P, \vec{z}) P. \qquad (3.9)$$

The function $f(t, a, \vec{z}) \geq 0$ contains the per capita death rate due to different processes like mortality, harvesting, inter-specific cannibalism, environmental factors of habitat $\vec{z}$. Initial conditions are in accordance to the model in Section 2.6.3 and are extended by spatial references.

$$P(0, a, \vec{z}) = P_0(a, \vec{z})$$

specifies an initial age-structured population, which is — without loss of generality — equally distributed throughout the entire region. The boundary condition

$$P(t, 0, \vec{z}) = r(\vec{z}) \int_0^A F(a) P(t, a, \vec{z})\, da$$

specifies the growth of the population P at location $\vec{z}$. $r(\vec{z})$ denotes the per capita growth rate, which may depend on the location $\vec{z}$. $F(a)$ denotes the fertility at age a.

Considering aquatic species, for example, appropriate spatial boundary conditions are an impermeable boundary for coastline and Dirichlet boundary conditions for the oceanside, setting the population density zero for infinity. Because of the migration term of the model, it is guaranteed that the population will stay in a region of high habitat suitability.

Simplifications If we neglect age-structures Equation (3.9) can be rewritten by dropping the dependence on age a, its associated differential operator and by using a closed and analytical function for growth $f(P, \vec{z})$. We get

$$\frac{\partial P}{\partial t} + \nabla \cdot \left[D_H P \nabla H - D_D \left(\frac{P}{P_{crit}} \right)^n \nabla P + \vec{v} P \right] = r(\vec{z}) P \left(1 - \frac{P}{P_{max}(\vec{z})} \right) \qquad (3.10)$$

using a logistic growth equation with a location-dependent growth rate $r(\vec{z})$.

Simulation Study

Investigation Site "Sandau" The model is applied to an investigation site at the river Elbe in northern Germany. With a length of 1091 km and a catchment size of 148.300 km^2 the Elbe is one of the most important rivers of Central Europe. In contrast

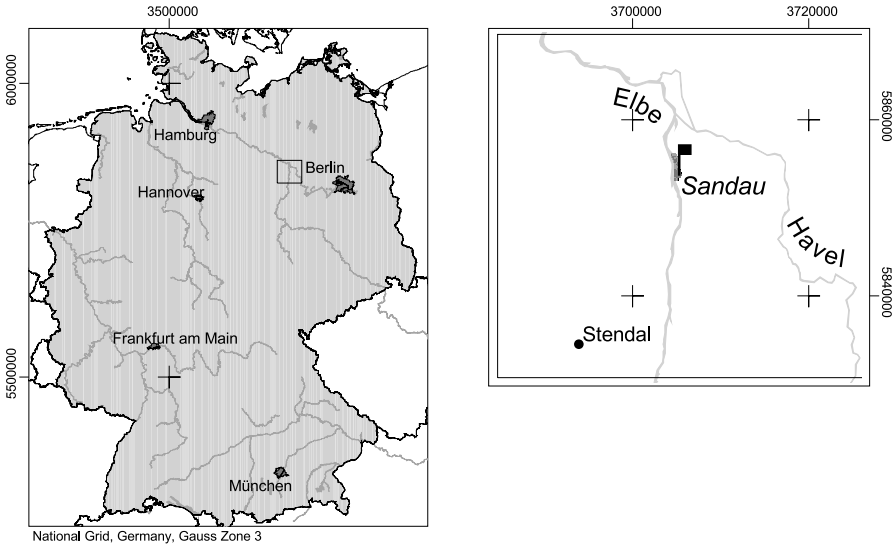

Fig. 3.4 Location of investigation site "Sandau" at river kilometer 417–418 of river Elbe, Germany.

to most other German rivers, the Elbe has maintained a relatively natural flood plain landscape because of its special situation of being a border river for several decades. The location of the investigation site, which was a bank section of the river Elbe near the small village Sandau (river kilometers 417–418) is shown in Figure 3.4. The banks of the stream are separated by groynes, which are stone structures built out transversely from the banks. This keeps the current in the middle of the embankment. Between them, the riverbanks are subject to dynamic hydro-morphological processes. From open soil patches of different soil textures and pioneer vegetation at the water's edge they go on to meadowland at higher altitudes. The study site is traversed by some branches of the main stream as well as by temporary alluvial channels and ponds because of the high water level in winter.

The first step in applying the model in Equation (3.10) is to set up an appropriate habitat suitability map for the investigation site. Figure 3.5 displays a map of the estimated carrying capacity of the ground beetle species *Agonum marginatum* derived from field observations (Vogel, 2002). The discretization of the spatial data is based on the vector-based biotope map with the associated carrying capacity values. From this a finite-element-mesh for the numerical solution of Equation (3.10) is generated, see Figure 3.6. Model parameters like growth rate r are estimated within laboratory experiments, see (Vogel, 2002).

Figure 3.7 displays four time steps of the spatially explicit population dynamic modeling for *A. marginatum* at the Elbe investigation site. The initial condition $t = 0$ is given by the upper left figure, the time steps $t = 30$ d, $t = 60$ d and $t = 90$ d follow from left to right and from top to bottom. The final stage shows abundances in the

same range as those identified by field experiments, and that are given by the habitat suitability, the carrying capacity, cp. Figure 3.5.

The important issue is to identify which dynamic patterns affect this final stage and what spatial patterns are responsible for these dynamic patterns. The initial population is given arbitrarily by an average abundance of 10 individuals per square meter at location $\vec{z}_0 = (4502600, 5852700)$. Two processes determine the spread of the population: growth and dispersal. The initial population is located at a less suitable habitat. Dispersal therefore proceeds only slowly. When the first individual reaches the most suitable habitat near the river, population growth speeds up and this habitat is occupied quickly. This very narrow-shaped habitat along the Elbe river acts as a migration highway. This is why most of the most suitable habitats are occupied by *A. marginatum* after 90 days, even if simple dispersal would have led to a migration to the intersection line "A" to "B" in Figure 3.7 lower right. This is in accordance to field observations (Vogel, 2002).

Spatially explicit Predator–Prey Models

The model The classical approach introduced by Volterra (1927) is widely used for modeling predator–prey interactions based on two coupled nonlinear ordinary differential equations, see for instance (Begon *et al.*, 1986, p. 356). A prey population denoted by P_1 and a predator population P_2 are considered. Several different types of predator–prey models have been discussed in recent literature. We focus on the

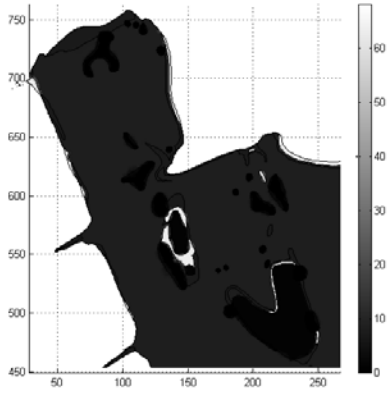

Fig. 3.5 Carrying capacity parameters derived from GIS. Coordinates denote the last three digit of the German Gauß–Krüger coordinate system (4502xxx, 5852xxx).

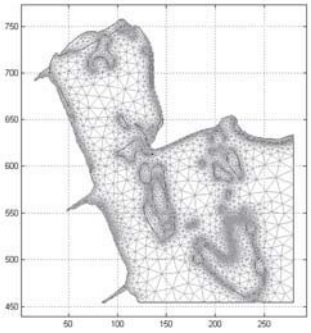

Fig. 3.6 Data preprocessing for spatially explicit solving or partial differential equation population dynamics modeling.

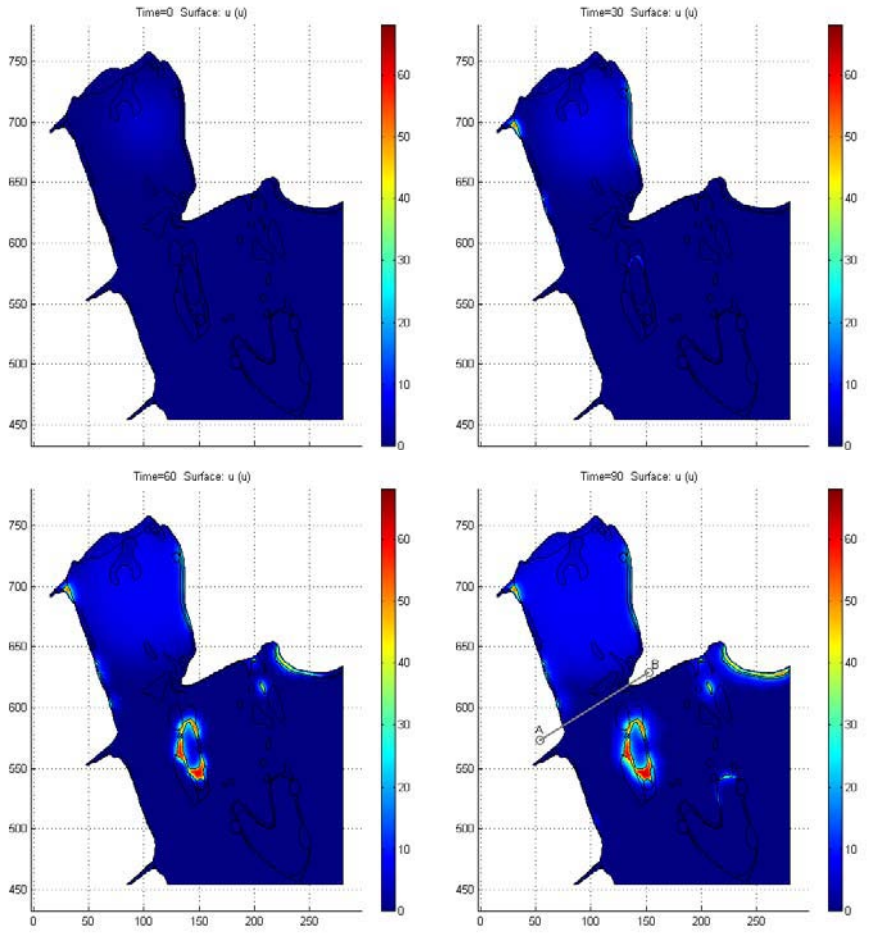

Fig. 3.7 Spatially explicit population dynamics for *A. marginatum* based on a partial differential equation model. Units are individuals per square meter. (See p. 279 for additional ressources.)

original predator–prey equation system introduced by Volterra (1927)

$$\left.\begin{aligned} \frac{dP_1}{dt} &= \beta P_1 - \sigma P_1 P_2 \\ \frac{dP_2}{dt} &= \alpha P_1 P_2 - \gamma P_2 \end{aligned}\right\} \tag{3.11}$$

in this ODE-system the term βP_1 denotes the (unlimited) growth of the prey population, $\sigma P_1 P_2$ death of prey by predation, $\alpha P_1 P_2$ growth of the predator population due to predation success and γP_2 mortality of predator population. The following specifications of the parameters are chosen: $\alpha = 0.05$, $\beta = 0.075$, $\gamma = 0.1$ and $\sigma = 0.2$. For detailed analysis we focus more qualitatively on the system behavior.

This ODE system can be used in the partial differential equation for spatially explicit modeling of predator–prey processes, simply by modifying the right hand side of Equation (3.10). This yields

$$\left.\begin{aligned} \frac{\partial P_1}{\partial t} - \nabla \cdot \left(D_{11} \nabla P_1 + D_{12}(P_2) \nabla P_1 \right) &= \beta P_1 - \sigma P_1 P_2 \\ \frac{\partial P_2}{\partial t} - \nabla \cdot \left(D_{21}(P_1) \nabla P_2 + D_{22} \nabla P_2 \right) &= \alpha P_1 P_2 - \gamma P_2 \end{aligned}\right\} \tag{3.12}$$

This equation system is solved for an artificial domain, a square with unit length. Boundary condition are of Neumann type, assuming population density is symmetrically at the boundaries.

Setting $D_{11} = D_{12} = 0$ neglects any random movement of the population. Dispersal is assumed to be density-dependent from the density of the second species. We assume that the prey escapes from high predator populations setting $D_{12} = -d_{12}P_2$ and assume that the predator population follows the prey population: $D_{21} = d_{21}P_1$.

Note, that the model has no dependencies on any coefficients and parameters that show spatial variability. If spatial patterns appear in this simulation study, these patterns are purely endogenous.

Results Figure 3.8.a displays the initial condition $t = 0$ of the density of prey and predator population. The initial population is set to $P_1 = 0.9$ and $P_2 = 0.4$ adding a small sinusoidal variation with amplitude 0.1, horizontally for P_1 and vertically for P_2. This introduces a slight variability and triggers the migration processes.

Figure 3.8.b shows the results after $t = 20$ time steps. The initial pattern changed. The results for the spatial pattern can be characterized clearly by the following properties:

- High prey population with less predators present (upper left corner);
- Low predator population with still large prey population (upper right corner);
- High predator population with less prey present (lower left corner);
- Low predator population with less predators present (lower right corner).

This is the spatial analog shown by the dynamic pattern of predator–prey systems, see Section 5.4.1 starting on page 118. Note that the initial variability increased to 0.7 units for P_1. Final results are plotted in the last row (Figure 3.8.c). In these last 80 time steps the spatial pattern finally changes to a pattern that will oscillate further on. The specific wavelength of approximate 0.2 units depends on the chosen coefficient of dispersal. Again spatial variability of the populations increased to 4 units for the prey population P_1 and 0.5 units for predator population P_2.

Summary The use of PDE leads to an aggregated description in the model. Within a two-dimensional equation system several processes are considered: growth, predation and dispersal. The model is derived from a strictly modular approach. Spatially explicit processes are derived from considerations described in Section 3.2.2. The interspecific relationships are modeled as source/sink terms of the PDE denoting growth processes see Equation (3.10), or reaction processes in the framework of the chemical fate modeling, cmp. Equation (3.8).

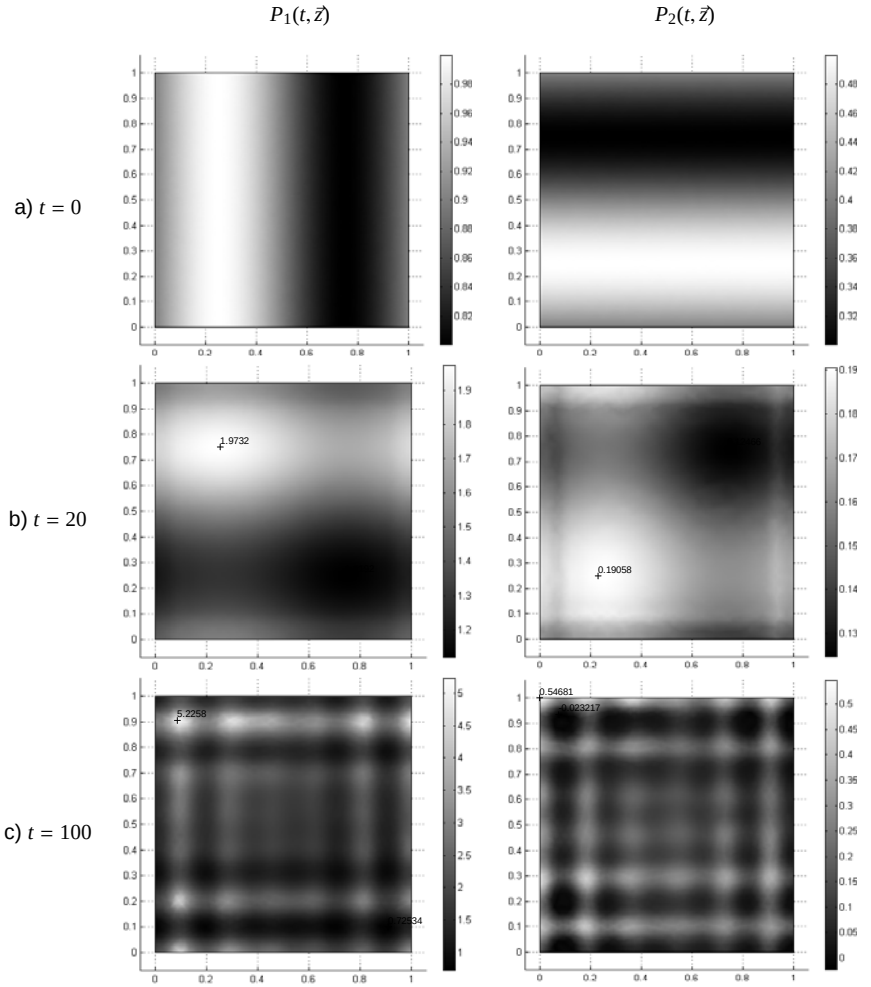

Fig. 3.8 Endogenous patterns derived from simple spatially explicit predator–prey model. From upper left to lower right the time steps $t = 0$, $t = 20$, and $t = 100$ are displayed. Note different scaling of shading. (See p. 279 for additional ressources.)

The most striking fact derived from this artificial simulation study is that spatial pattern could be derived based on *endogenous* processes only. Note, habitat suitability is not considered in Equation (3.12), respectively assumed to be constant in the artificial region. The patterns displayed in Figure 3.8 are solely derived from internal spatially dependencies. Second, endogenous patterns are obtained on different spatial scales, cmp. (Levine, 2000). Copious literature on theoretical biology focuses on the theoretical analysis of spatially explicit predator–prey models. We focus on the patterns only, the reader is referred to to these papers, see (Savill & Hogeweg, 1999; Kishimoto, 1982).

3.3 INTEGRATING SPATIALLY EXPLICIT MODELS

Philosophy of science proposes theories or theorems that explain most of the patterns studied with a minimum number of assumptions, hypotheses or axioms — in the framework of this book, with a minimum of mathematical equations or sub-models. From this point of view, an aggregated model as discussed in the foregoing section is the model of choice, as these models offer a large range of resulting patterns and processes with a minimum of input.

However, spatially explicit models are frequently set up by integration of many different equations. Spatially explicit models like these are not necessarily defined by PDE's. These are set up by systems of coupled (ordinary differential) equations with spatially referenced parameters.

In this case a general theoretical framework for spatial modeling cannot be given. This is why the following examples are structured by their methodological concept.

3.3.1 Regionalization of Site Models

Concept The first step for regionalization of a model is achieved by the identification of units with homogeneous environmental parameters for which a repeated run of model simulations based on varying initial conditions and parameters is performed, see Definition 3.2. This approach necessitates the identification of homogeneous regions. In a landscape ecological context, these areas may be denoted by *ecotopes* (Naveh & Lieberman, 1984). In terms of spatial model development these units are denoted by the support of a model, see Definition 3.1.

Both approaches can be compared as the underlying methodological is similar. Figure 3.9 illustrates this concept within a GIS framework. Focusing on a selected study area (red in all figures) four different layers of spatial vector-based information are displayed:

a) Sub-watersheds in the investigation site with the average elevation in [m];

b) Elevation, given by polygons with equal elevation in intervals of 20 m;

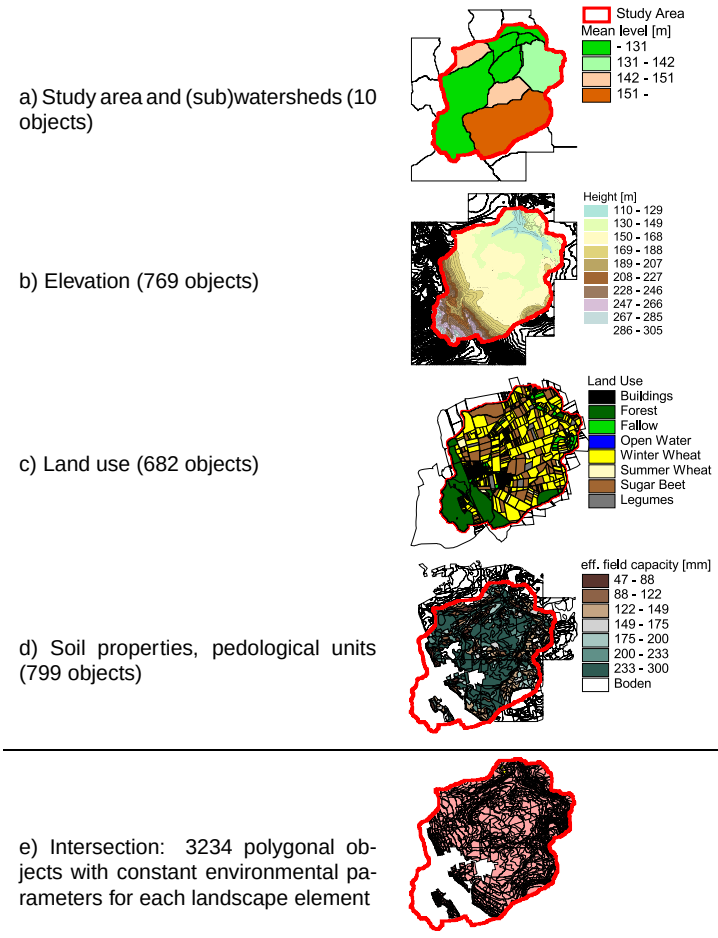

Fig. 3.9 Regionalization concept using vector-based spatial data based on derivation of smallest homogeneous unit: ecotopes.

c) Land use and habitat types (textual coding);

d) Soil properties, displaying effective field capacity in [mm].

Application of an agroecosystem model, as summarized in Section 2.7 for this investigation site using spatial references to different locations requires the identification of homogeneous spatial object. Calculating the largest spatial units with homogeneous properties derived from all input layers a) to d) is performed by an *map intersection*. The procedure of intersection is a GIS function (Breunig, 1996, p. 77) and (Gold *et al.*, 1997, p. 30). It generates new maps with shapes in particular polygons that have homogeneous attributes with respect to all input layers.

A map S of a layer, for example soil properties, is given by the tessellation of the studied region R. The map may consist of a set of n_i polygonal units s_j. The mathematical definition can be written as

$$S_i = \left\{ s_j \;\middle|\; j = 1, \ldots, n_i, \vec{z} \in s_j, g_i(\vec{z}) \in \mathbb{R} \right\}$$

Here g_i defines the attributes of map S_i. For all points located in a polygonal unit s_i of S_i the attribution fucntion g_i is constant.

Definition 3.5 (Intersection) *Considering a set of polygonal maps S_i $i = 1, 2 \ldots, m$ intersection can be defined by*

$$\begin{aligned} S_0 = \bigcap_{i=1,\ldots,m} S_i \quad = \quad & \left\{ s_{j_1} \cap \cdots \cap s_{j_m} \;\middle|\; j_i = 1, \ldots, n_i, \quad i = 1, \ldots, n \right. \\ & \left. \forall \vec{z} \in s_{j_1} \cap \cdots \cap s_{j_m} \forall i = 1, \ldots, n : \; g_i(\vec{z}) = const. \right\} \end{aligned} \tag{3.13}$$

Note, that this is a simplifying description. Intersection of maps requires a high computational effort. It exponentially increases with the number of vertices defining a single object. The calculation of intersection polygons leads to geometric units called *silver polygons* (Breunig, 1996) with a small area but long extent. Silver polygons are caused by similar but not necessarily identical input layers of maps. These silver polygons need to be removed or joined to similar regions to reduced computational effort.

Application

Agroecosystem Model Based on these considerations the agroecological simulation model developed in Chapter 2 can be regionalized by making all site-specific model parameters and initial conditions depend on the ecotope map, see Section 2.7. Figure 3.10 illustrates this concept for the investigation site “Neuenkirchen” introduced in Section 2.3.1, see Figure 2.2. The map in the lower left shows a detail from the 3234 element large ecotope map together with the identificator number used for accessing spatial parameters from the database. Model parameters like initial nitrogen content, field capacity and initial weed infestation are specified this way. Driving functions such as planted crop, applied fertilizer amount, weed control strategy depends on the considered field — the ecotope, too. Application of this regionalized agroecosystem model are discussed in Chapter 11.

Bucket Models These considerations aim at regionalization of models to a two-dimensional investigation site. Vertical transport of water and substances as introduced in Section 3.2.1 are not considered. The Richards Equation (3.1) and the convection dispersion Equation (3.8) can be coupled to the agroecosystem model. This integration can be performed by simply using the upper boundary condition and the source/sink term to couple the two models. Using the source/sink terms

in Equations (3.1) and (3.8) nitrogen uptake and transpiration is modeled. Infiltration, fertilization specifies the upper boundary condition (Diekkrüger *et al.*, 1995; Diekkrüger & Arning, 1995).

Second, water and matter transport is frequently modeled by systems of ordinary equations. These models simplify the underlying assumption of Darcy flow using the assumption of a field capacity in soil. A soil column is discretizised by units with equal field capacity. If water content in a layer reaches field capacity, an overflow of this "bucket" occurs and water flows down to the bucket below. This is illustrated by Figure 3.2.e. In this case the spatial discretization determines the conceptual model. This is an excellent example for the interdependence of spatial discretization and conceptual model design, as introduced in Section 3.1.1. These model types are frequently used for applications on a larger scales, especially if parameters of the Richards equation are not available through space.

Further Examples Similar approaches on larger scales, including hydrological aspects and surface runoff, which need to consider spatial interactions are introduced by (Beven & Kirkby, 1979; Krysanova *et al.*, 1989; Band *et al.*, 1991; Sasowsky & Gardner, 1991). With the tool TELSA Kurz *et al.* (2000) present a toolbox for spatially explicit modeling of agricultural landscapes together with the analysis of scenario simulation, see Chapter 8 based on a vector data set.

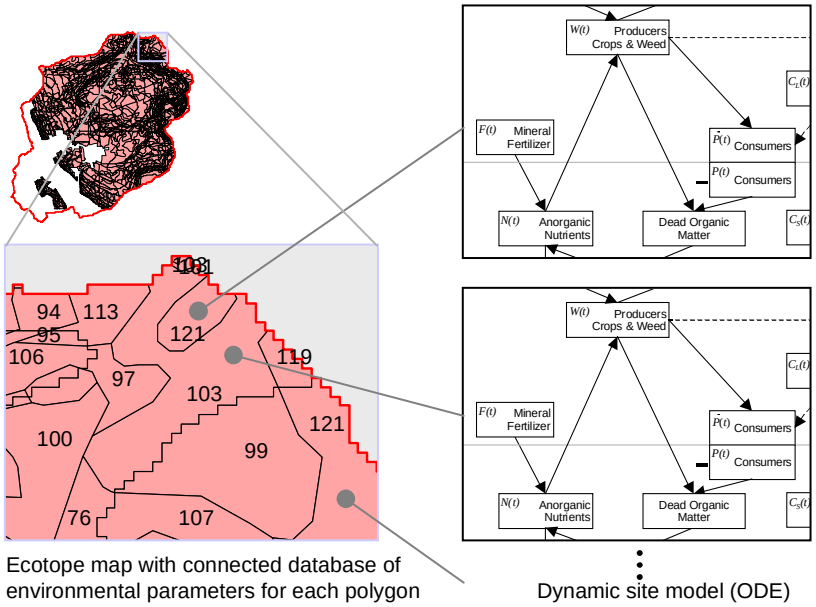

Fig. 3.10 Regionalization of environmental models based on the ecotope concept, that assume model parameters and initial conditions depending on homogeneous units and performs a repeated run of an equal model structure.

If we are to consider scenarios of land use change, generated by economic considerations, which were not envisioned in the design of the elementary spatial units, this approach is inappropriate. The boundaries between spatial units are fixed and cannot be modified during the course of the simulation, which may be somewhat restrictive.

3.3.2 Cellular Automata

Concept A widely used grid-based model is the cellular automata approach (Ermentrout & Edelstein-Keshet, 1993). A cellular automaton consists of a regular lattice of cells. Each cell can hold a finite number of possible states, which can be expressed by a scalar, a vector, a matrix or other mathematical objects, an information or any other property. In the simplest case, the state is expressed as a binary variable.

In mathematical terms, the observed region is modeled by a set of discrete grid points $R = \{(i, j) \mid n_i < i < N_i; m_j < j < M_j\}$. A grid cell of the map is denoted by $\vec{z} \in \mathbb{R}$. The notation is used for the description of spatially explicit models too, see next section.

The states of the ensemble of cells are updated synchronously in discrete time steps according to a set of local, identical interaction rules. The rules can be formulated both in a rigorous mathematical or in a more qualitative way, e.g. with the help of *fuzzy sets* (Zadeh, 1965). Apart from its own previous state, the state of a cell is determined by the previous states of a surrounding neighborhood of cells. There are different ways

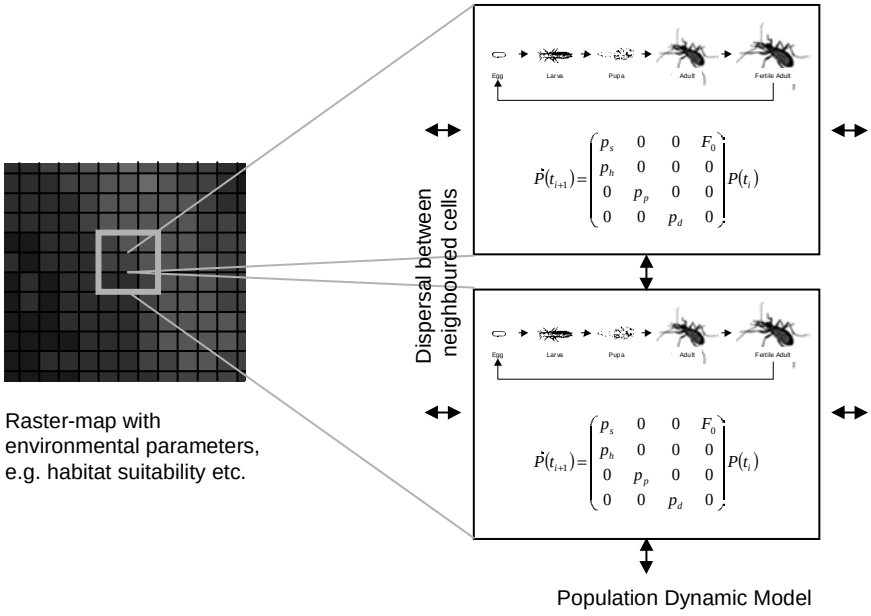

Fig. 3.11 Regionalization of integrated models based on cellular automaton model approach.

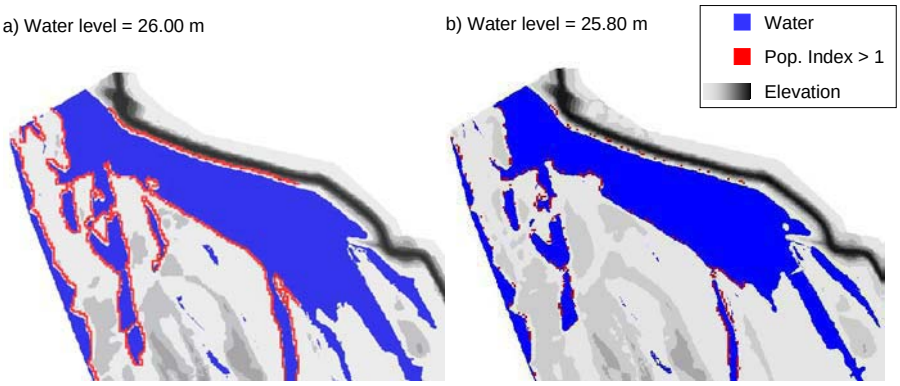

Fig. 3.12 Results of population index derived from spatially explicit population dynamics model of *A. marginatum* using a CA approach.

of defining neighborhoods. The *vonNeuman neighborhood* consists of all adjacent cells, the *Moore neighborhood* also includes the diagonal cells. These definitions can be extended by enlarging the distance to the next adjacent cells. However, the characteristic property of the cellular automaton approach is that this neighborhood is limited to a small number of cells. It is impossible to change the state of the considered cell by accessing all other cells or cells far beyond the neighborhood radius.

A second important property is, that CA models usually are autonomous models, see Section 1.3.4. The new state of a cell only depends on the recent state and the state of the cells in the defined neighborhood. Cellular automaton models with memory were introduced by Alonzo-Sanz (2003). These are examples of systems with endogenous patterns.

Figure 3.11 illustrates this concept, assuming a population dynamic model as a matrix-based dynamic system for the dynamic process of each grid cell. This example will be used in the following application.

Application Based on the parameter of the population dynamic model for *A. marginatum* a cellular automaton model for the "Sandau" investigation site of the river Elbe is run, compare Section 3.2.2. In this example, the population dynamic model is set up by a matrix equation (Leslie model), compare Section 2.6.2. Dispersal of species was modeled by the neighborhood radius in the cellular automaton model (Vogel, 2002). From the results in Section 3.2.2 we know that the important habitats are the sandy area with less vegetation near the river Elbe and the branches. For the application of the cellular automaton model, the focus is on changing water levels. For aggregated display of the result the *population index* is calculated. This index calculated by the quotient of the final population divided by the initial population at the beginning of the year for each grid cell. An index above unity denotes a suitable habitat, as population is growing, an index below unity denotes a habitat with decreasing suitability for *A. marginatum*. Figure 3.12 displays the results for two

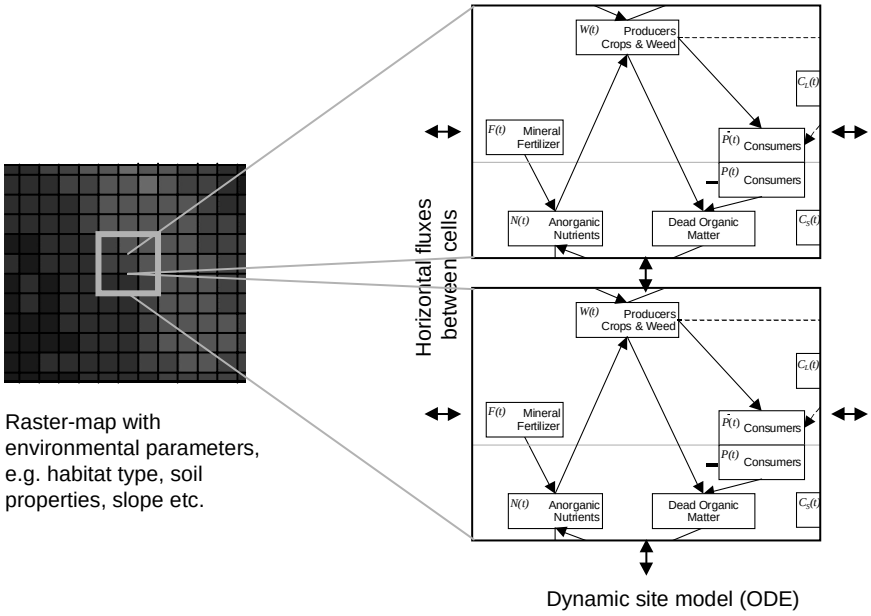

Fig. 3.13 Regionalization of integrated models based on cellular automaton model approach.

different water levels 26 m and 25.8 m. Note, for the higher water level more suitable habitats are available. This is because water level and vegetation together build up an ideal pattern for *A. marginatum*, cf. (Vogel, 2002).

3.3.3 Generic Landscape Models

The generic landscape modeling concept, introduced first for the Everglades ecosystem by (Fitz *et al.*, 1996) followed by an abundant list for further publications on the concept (Voinov *et al.*, 1999; Maxwell & Costanza, 1997a; Maxwell & Costanza, 1997b) integrates the two approaches discussed before. The general idea is to use a grid-based topology introduced for cellular automaton models but extend the domain of possible cell state and process models. Additionally, the strict limitation to a defined neighborhood is dropped. Figure 3.13 illustrates this concept.

Concept The ecosystem model used for the regional model covers the processes of hydrology (above ground, unsaturated soil zone, ground water), macrophytes and consumers as well as and nutrient cycling (Voinov *et al.*, 1999). In this approach the modeled landscape is partitioned into a spatial grid of square unit cells. The landscape is modeled as a grid of relatively small homogeneous cells and run simulations for each cell with relatively simple rules for material fluxing between the cells (Sklar *et al.*, 1985; Burke *et al.*, 1990; Costanza *et al.*, 1990; Maxwell & Costanza, 1997a).

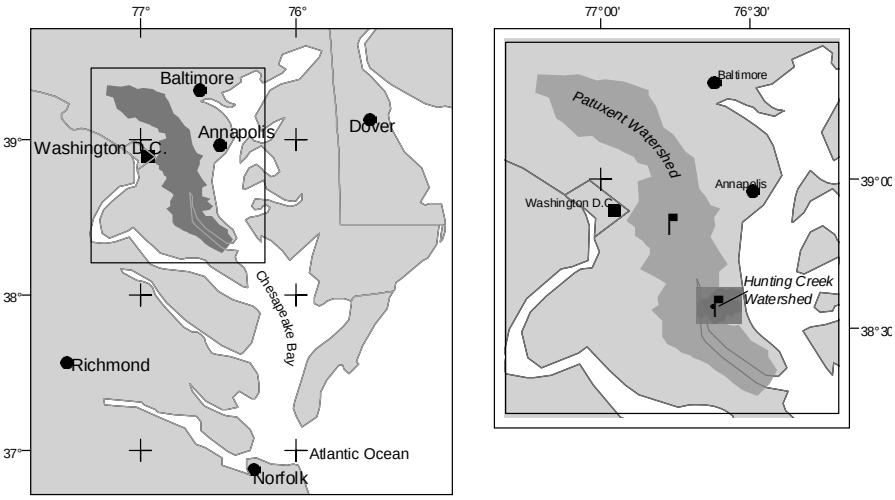

Fig. 3.14 Location of Patuxent river within the catchment of the Chesapeake Bay region.

This approach requires extensive spatial data sets and high computational capabilities in terms of both storage and speed. Note, the approach allows quasi-continuous modifications of the landscape, where habitat boundaries may change in response to socioeconomic transformations. This is one of the prerequisites for spatial scenario analysis, since it allows one to modify the spatial arrangement of the model endogenously, within the simulation procedures. With this approach, the model builds on the format of a raster-based geographic information system, which is used to store all the spatially referenced data included in the model.

Model Description The model is designed to simulate a variety of ecosystem types using a fixed model structure for each habitat type, cf. the generic agroecosystem model in Chapter 2, Figure 2.1, p. 36. The model captures the response of macrophyte and algae communities to nutrient concentrations, water and environmental inputs. These processes are driven by hydrological algorithms for upland, wetland and shallow-water habitats. It explicitly incorporates ecological processes that determine water levels or content of surface water and the saturated and unsaturated soil zone, plant production, nutrient cycling associated with organic matter decomposition and consumer dynamics. Therefore the simulation model for a habitat consists of a system of coupled nonlinear ordinary differential equations, solved with a 1 day time step.

The model is hierarchical in structure, incorporating the ecosystem-level unit model that is replicated in each of the unit cells representing the landscape. Although the same unit model runs in each cell, individual models are parameterized according to habitat type and georeferenced information for a particular cell, see Figure 2.1 for a general compartment scheme of the generic model. The habitat-dependent

information is stored in a parameter database, which includes initial conditions, rate parameters, stoichiometric ratios, etc. The habitat type and other location-dependent characteristics are referenced through links to GIS files.

The unit models in each cell exchange matter and information across space. Surface and subsurface hydrology define the horizontal fluxes. This joins the unit models together. The spatial hydrology module calculates the amount of water fluxed over the surface and in the saturated sediment. The fluxes are driven by cell-to-cell head differences of surface water and saturated sediment water, respectively. Dissolved and suspended material (nutrients) is carried by water fluxes between cells. At each time step, first the unit model updates the stocks within each cell caused by vertical fluxing and then cells communicate to flux matter horizontally, simulating flows and determining ecological conditions across the landscape.

This model approach has been used to construct the Hunting Creek model (HCM), a sub-watershed of the Patuxent. The local dynamics in the Hunting Creek Model were similar to those developed in Patuxent landscape model (Voinov *et al.*, 1999), but the spatial implementation, defined by the study area, and the spatial resolution were different. By focusing on a smaller sub-watershed, we could make many more model runs, calibrate the model more precisely, and refine our understanding of some of the crucial ecological processes and spatial flows in the ecosystem. Use of a relatively small study area was especially essential for the optimization procedures that require numerous computer runs of the model.

The problem is analyzed on different scales. For the largest study area, the entire Patuxent watershed, a lattice with a grid size of 1 km to 1 km is chosen. For detailed study the Hunting Creek sub-watershed is selected. Simulations for this area are based on a 200 to 200 m grid. Figure 3.14 displays GIS maps with the underlying land use data sets of 1990. For more detailed analysis a sub-watershed of Hunting Creek with an equal grid size is selected.

Validation Validation of this complex model was performed using a stepwise approach. First, calibration of the hydrologic module was conducted against the USGS (1997) data for one gaging station on the watershed. The model was calibrated for the 1990 data and afterwards tested for 7 consecutive years (1990–1996). The results are in fairly good agreement with the data and may be considered as model verification, because none of the parameters have been changed after the initial calibration stage for 1990. No reliable data was available to calibrate the spatial dynamics of ground water. Nevertheless, the general hydrologic trends seem to be captured well by the model.

Once the watershed hydrology was mimicked with sufficient accuracy, the calibration of the water quality component was performed. Finally, the model was able to reproduce the trends of nitrogen concentration at the gaging station (USGS, 1995). In addition to the daily nitrogen dynamics we obtained a fairly good fit for the annual average concentration. For detailed documentation of the validation results, see (Voinov *et al.*, 1999). Overall, the model seems to do a good job in predicting the integral and distributed fluxes of nutrients over the watershed.

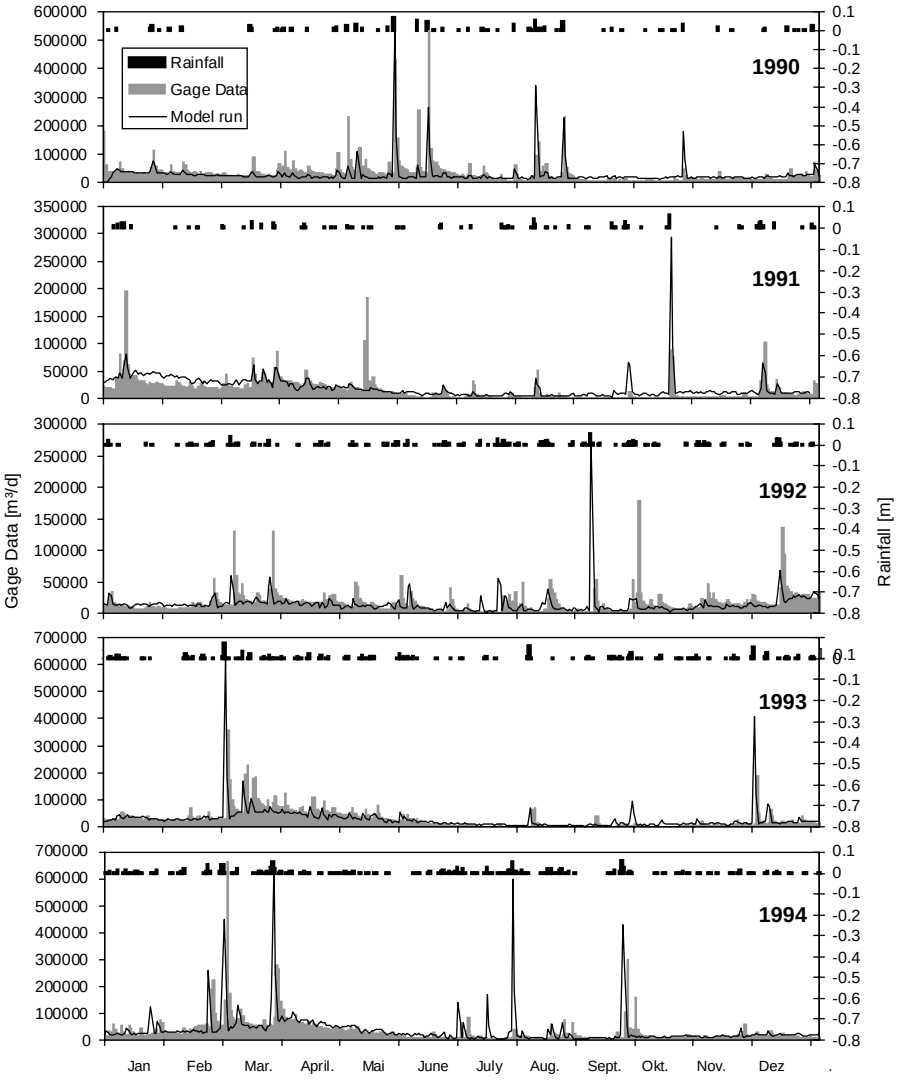

Fig. 3.15 Hydrology calibration for 1990/91 and further runs of the model for 1992–1996. The later model runs may be considered as model test in terms of its predictive power, since the parameters derived from the 1990/91 calibrations were not changed any more.

3.4 DISCUSSION

The last two chapters, which complete the first part of the book, have clarified that the recent state of environmental modeling shows a trend away from analytically treatable models towards complex integrated models systems. One can hardly list

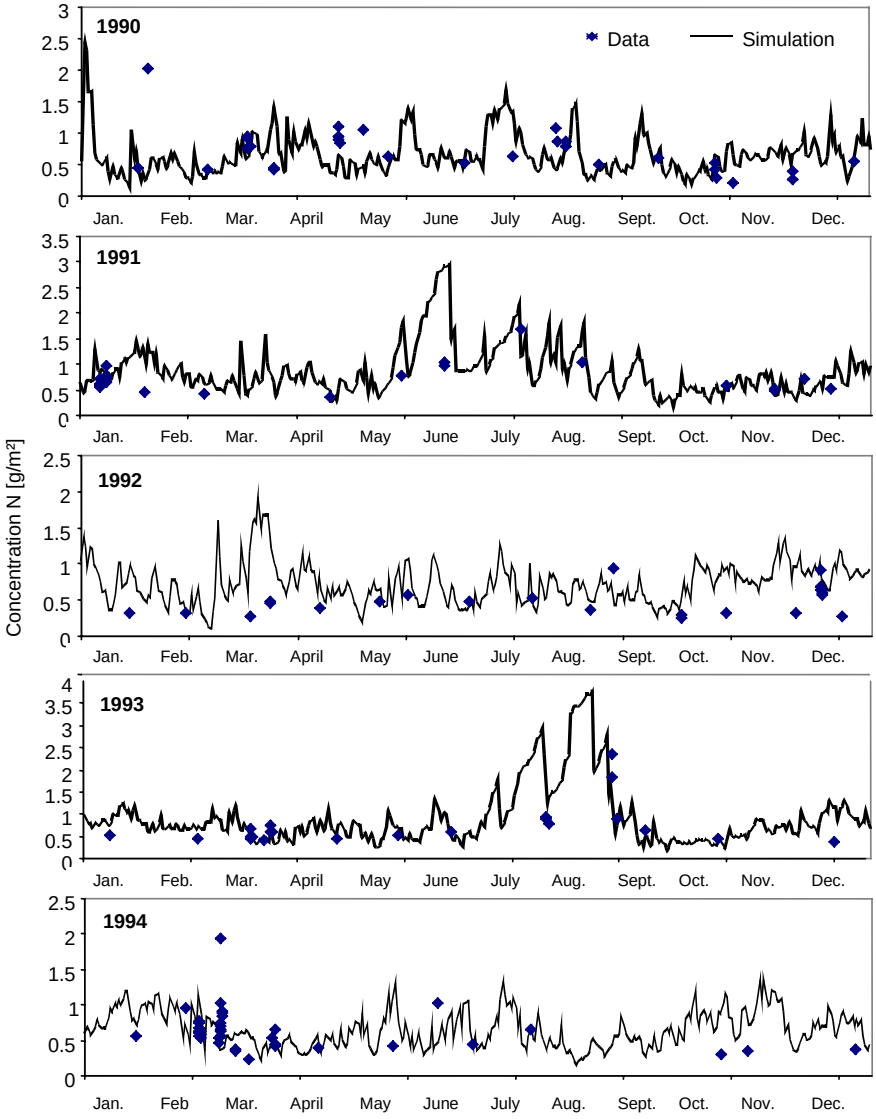

Fig. 3.16 Nitrogen calibration for the data at the USGS gaging station.

all equations coded in an integrated model as well as all conditions tested to start or solve these implemented equations.

Before discussing the related problems, we first focus on the general results from this chapter. Spatially explicit models can be derived from different mathematical approaches. Partial differential equations seem to be the most aggregated and the most sophisticated approach. These systems require an enormous numerical effort.

Related software tools are highly sophisticated. High standard numerics are required to solve these system. A profound mathematical knowledge is required for the correct setup of these models. This may be one reason why this approach did not find its way into recent modeling in landscape ecology, even though these are highly aggregated and easily transferable to different site conditions. In this context, the important summary is that the link between geometry in the landscape and the topology with respect to the considered species or substance is derived using a GIS. Spatial patterns are then derived from aggregated equations for processes of convection, growth or dispersal. This shows the strength of the PDE methodology for real landscapes.

Using these PDE systems as a starting point, one can interpret all other solutions as possible discretization of these system. For example, spatial discretization using an equal step size vertically and horizontally, leads us to the concept of cellular automata. Second, discretizing an age-structured population dynamics equation from McKendrick–Foerster leads to a (extended) Leslie matrix.

However, aggregated spatially explicit models can become integrated models, just by discretization in space. Soil process modeling is a good example for this statement. With the use of discretization, models become more and more integrated and different additional sub-models and equations can be coupled. Integrated models therefore seem to be the logical consequence. Integrated models offer the extendibility necessary to cope with all important environmental processes derived from different disciplines and coded by different mathematical approaches. In this context it seems as if the most favorable data structure is the raster data set when choosing integrated model approaches. In any case, GIS is the important tool for data preprocessing and supporting spatially explicit modeling.

Finally, spatial patterns are the most important result of spatially explicit models. Opdam *et al.* (2002) state that *the future of landscape ecology lies in the understanding of how landscape pattern is related to the functioning of the landscape system, placed in the context of (changing) social values and land use*. Modeling and simulating processes with a spatial reference together with analysis of the resulting patterns is the methodological concept that can cope with this task. Studying the results from this chapter, the most important result is that spatially explicit models encompass exogenous as well as endogenous patterns. These two pattern types are superimposed on the final result of a model. From this it follows, that a final answer to Opdam *et al.*'s (2002) question needs identification of what the endogenous and exogenous patterns of a system are.

Part II

Integrated Models

"Pathetic," he said. "That's what it is. Pathetic." He turned and walked slowly down the stream for twenty yards, splashed across it, and walked slowly back on the other side. Then he looked at himself in the water again. "As I thought," he said. "No better from this side. But nobody minds. Nobody cares. Pathetic, that's what it is."

—A.A. Milne

4

Multi-paradigm Modeling

4.1 INTRODUCTION

Translation of conceptual models into mathematical equations so far ends up either in aggregated spatially explicit models defined by partial differential equations (see Section 3.4) or by models integrating different mathematical equations on the basis of a spatial discretization by grid or vector data (see Section 3.3). Most environmental models are a mixture of these two possible categories. Müller (1997) published an overview and characterized development of ecological modeling by a lack of theoretical background, and a missing general concept in ecological or environmental modeling.

There are different reasons for this development. First, environmental models are set up by different approaches. The last chapter exemplified that population dynamics are described by algebraic difference or matrix equations, while process models are expressed by systems of ordinary differential equations. If spatial processes are to be considered, partial differential equations have to be included. In an environmental model, these processes have to be integrated.

Second, environmental models frequently trace flows of substances through different media. For instance, substances are emitted from a production site, transported, probably transformed by chemical reactions, and dispersed in the lower atmosphere, then disposed and maybe suspended in an aquatic ecosystem and finally taken up by a species, see Chapter 7. It is very difficult or even impossible to find a model that covers all these processes within a general mathematical structure and to give an aggregated notation of the mathematical model. Multi-media models cause mathematical heterogeneity.

Third, a conceptual difficulty arises stemming from the fact that processes of different dynamic quality interact. The dynamics of technical systems are mostly time-discrete and their dynamics are closely related to discrete spatial structures, whereas many environmental processes are continuous in time and space. The whole system can be characterized as structured time-discrete and time-continuous. An illustrative example is crop production where continuous biological processes such as crop growths or water transport in soil are embedded into time-discrete agrotechnical management procedures.

One is faced with the problem of *mathematical heterogeneity* (Seppelt & Temme, 2001) or *multi-paradigm models* (Villa, 2001). It is not feasible to model integrated systems in the framework of one mathematical theory like ordinary differential equations. More general methodologies will be developed by integration of heterogeneous systems (McIntosh, 2003). Besides this an important consequence of mathematical heterogeneity is, that the number of applicable procedures for model analysis is reduced, the more heterogeneous a model is. From this background some additional criteria for assessing the performance of a model are to be studied. These criteria can be derived from philosophy of science. The aspects offer a methodological framework for developing general methodologies for model integration and for developing mathematically heterogeneous or hybrid models.

4.2 FUNDAMENTAL ASPECTS OF ENVIRONMENTAL MODELING

The important questions stemming from this observation on environmental models are: Is there a theoretical foundation of ecological modeling that can offer a guideline for model development? Can mathematical heterogeneity be reduced? Can a theoretical foundation help us to choose the appropriate mathematical structure? Shortly, how can the translation from conceptual models to mathematical models be guided and theoretically founded?

From an analysis of the process of environmental or ecological modeling as briefly summarized in the preceding chapters the following important topics can be obtained:

1. Modeling the entire system in an integrative way requires input from modeling approaches of different disciplines, such as soil science, biology, chemistry, physics etc. This multi-disciplinarity of environmental modeling results in different conceptualizations of environmental processes, in different viewpoints on the step of transferring and in a broad spectrum of underlying theoretical concepts.

   Environmental modeling can be approached in many different ways. Depending on the scale of interest, on the accessibility and usability of data sets, and of the aim and scope of the problem to be solved, different simulations models have been developed and used. Some authors complain about an enormous redundancy (Müller, 1997).

2. The considered processes show a broad spectrum of time scales as well as spatial scales. It seems as if the chosen temporal and spatial scale (cmp. Figure 1.3) determines the conceptual model, the structure of the equation and the mathematical dialect chosen, see (Levin, 2000).

3. This motivated Beddington *et al.* (1981) to state that "there are no Newtonian laws in ecology". A similar statement is, that ecological modeling lacks so-called first principles.

   Of course the basic laws of thermodynamics and physics are valid in environmental systems. However, equal processes can be described by different modeling approaches, while looking at the phenomena at different levels of aggregation.

4. Finally, Wu & Hobbs (2002) advocate an application of methods from complexity theory and associated methods, such as self-organizations, fractals, cellular automata, genetic algorithms or neural networks in environmental modeling, see also (Jørgensen & Bendoricchio, 2001).

The conclusion from these observations is that environmental modeling has to cope with reductionistic as well as holistic approaches. Reductionistic approaches make use of first principles for example derived from thermodynamics, or physics wherever applicable to the considered scale. Holistic approaches intend to describe entire patterns on the considered scale and tend to be treated as black box models. A good environmental model therefore is characterized by an appropriate combination of reductionistic and holistic approaches.

Well-known measures of model goodness and statistical tests are used to identify the fraction of variability in real world data that is reproduced by the model, see Section 1.3. However, these procedures are difficult to apply to integrated and spatially explicit models, see for instance (Boumans *et al.*, 2001). More important, these measures require data available for the comparison of real world data and model output.

From this background the questions are raised: How can model performance be assessed with reduced or missing real world data? How can model assessment be extended to the entire process of model development? Model applications are understood also in terms hypothesis testing (Jørgensen & Bendoricchio, 2001). Following this idea the answer to the above question can be derived from some consideration of scientific theory.

Developing a hybrid or integrated model by adding or coupling different modules has to fulfill *inner consistency*, which means that a new model shows no contradictions within the model itself. The new model has to fulfill *outer consistency*, too, which means that a new model has no contradictions to other consistent models. This is in accordance with the criteria developed in Chapter 1 for testing and analyzing a model. The following criteria are new from this perspective. Adding a new module must describe a new issue, a new feature or process, new in terms of environmental

issues, issues of scale, or of hierarchy, and which can be tested by experiments or applications. These are necessary conditions in model development.

Important optional criteria that can be derived from scientific theory are generality, depth, minimality, precision and accuracy of prognosis. Transferred to the methodological of environmental modeling, the following recommendations can be derived:

Precision and Accuracy aim at a minimum of deviation of the model results from the data observed. Denoting this property as an optional criterion is no contradiction to the explanations of Section 1.4.2, as there is an abundant list of examples in which the derived patterns are of more interest than the precise values of the state variables.

Generality denotes the size of the domain for which the model is applicable. A modeler always aims at a large domain and a high generality.

Depth and Minimality are criteria that are very frequently used to assess models. Models that offer a deep insight into the functioning of processes or that use a minimum of equations are very good and preferred models. Examples for these kinds of models are the spatially explicit population dynamic models introduced in Section 3.2.2.

A scientific theory oriented assessment of models would prefer an aggregated model, that needs less parameters, variables and functions and is able to describe the same spatial and temporal patters as a complex, integrated model.

These criteria may be guidelines for developing a theoretical scaffolding of environmental modeling frameworks. These criteria are very important and valuable for those hybrid or integrated models for which less analytical and numerical procedures are available for model testing, as shown in Section 1.3.

4.3 MATHEMATICS OF ENVIRONMENTAL MODELING

4.3.1 General Model Equation

Once we have identified that environmental models show this intrinsic property of mathematical heterogeneity, we still need to apply these models in procedures for model analysis or model application, even if criteria for assessment are available. This requires us to abstract from all possible mathematical dialects integrated in a mathematical model. To abstract from all these properties and to achieve a treatment of the system on a more general level a general model equation is introduced:

Definition 4.1 *Consider a dynamic system with the state variable $\vec{x}$, the control variables $\vec{u}$, a vector of parameters $\vec{c}$ and a right-hand side $M_{\Delta t}$ the equation*

$$\vec{x}(t_{i+1}, \vec{z}) = M_{\Delta t}\left(\vec{x}(t, \vec{z}), \vec{u}(t, \vec{z}), \vec{c}(\vec{z}), \vec{z}\right) \quad \vec{z} \in R \tag{4.1}$$

defines a General Model Equation (GME), where Δt is defined by $\Delta t = t_{i+1} - t_i$ with an arbitrarily separation $(t_i)_{i=1,2,\ldots}$ of the time interval of simulation.

The initial condition is given by $\vec{x}_0(\vec{z})$. All model variables (state, control and parameter) may vary in space. This may be true for the system equation $M_{\Delta t}$ that may also depend on space $\vec{z}$. Boundary conditions are defined for all $\vec{z} \in \partial R$.

In this definition a distinction is made between control variables $\vec{u}$ and model parameters $\vec{c}$. $\vec{c}$ collects all parameters, which specify the model due to site conditions, such as soil conductivity, site-specific growth rates, precipitation etc. Whereas, the control vector $\vec{u}$ sets up all those variables of the simulation model, which may be defined by different scenarios, by possible impact or control of an experiment or by management strategies, such as fertilizer amounts, pesticide application, etc. In Equation (4.1) $M_{\Delta t}$ integrates all mathematical equations, rules etc., which set up the entire simulation model as well as numerical code, which is required to solve the mathematical equation. Some examples of how to specify $M_{\Delta t}$:

- In the case of pure matrix models (population dynamics, Leslie models) or pure algebraic models, Equation (4.1) can be applied directly.
- In the case of ordinary differential equation systems, the estimation of the succeeding state $\vec{x}(t_{i+1})$ involves the numerical solution of the differential equation system (Hairer *et al.*, 1980; Hairer & Wanner, 1980). $M_{\Delta t}$ integrates the ODE-system as well as the system solver. In this case $M_{\Delta t}$ is called the flux of the dynamic system (Arrowsmith & Place, 1994).
- In the case of a cellular automaton model $M_{\Delta t}$ also incorporates spatial interaction, e.g. $\vec{x}$ depends on a vector of location $\vec{z}$. However, cellular automaton models are defined by a fixed neighborhood radius (which is often small, 1 to 2 cells), $M_{\Delta t}$ is structured, and can be written as a band matrix for their spatially dependencies.

4.3.2 Integrated Models

Section 3.3 summarized three different types of spatial models, that make use of a number of different equations or functions in spite of an aggregated spatially explicit model defined using a PDE. Integration in this context was meant by coupling the models by a spatial data model.

Integration can be understood in a more general context, too. Integrated models aim at a consistent description of economic as well as ecological processes (Boumans *et al.*, 2002), at integration of anthroposphere and biosphere processes. In general integrated models we aim at overcoming the classifications and characterization introduced in Section 1.3.4. From this basic idea, and the explanations given up to this point, some recommendations can be derived for the process of developing complex, spatially explicit environmental models set up by many processes from different disciplines:

Modeling can hardly begin from scratch. While defining a conceptual model, available models or modules need to be considered. Environmental models should be set up by single modules or sub-models. System behavior, admissible domain of initial variables, parameters and control variables and spatial and temporal grain and extent must be available and need to be well documented. The module itself must be robust for the given domains known, see Figure 1.3. This refers to the mathematical part of the model as well as to the numerical procedures implemented to derived model solutions if present.

Using predefined modules reduces redundancy in a model, as well as redundancy in environmental modeling. Vice versa, a conceptual diagram may be used to identify where to start with the development of sub-models first. The modularity derived in this way helps to integrate, couple and document models. It supports achievement of the recommended depth or minimality of a model.

Note that, even if the single modules are properly tested and sub-models system behavior is known, it is hardly possible to derive system behavior of the coupled system. Model analysis techniques such as Monte Carlo simulation, sensitivity analysis, stability analysis, see Section 1.3, can and should be applied to integrated models, too. The most important prerequisite of re-usability of models and modules seems to be the documentation, there are several solutions available (see next section).

4.4 MODEL DOCUMENTATION AND MODEL DATABASES

4.4.1 Introduction

The major prerequisite of model integration and usability of modules in different models is appropriate model documentation. This documentation has to cover the process models, dynamics and patterns implemented and the domain to which the model can be applied. Available model documentation methodologies can be classified by the following topics:

- Model documentation treats the model as black box. Information on the included processes, the meaning of input and output variables as well as the domain of the state variables and parameters are given. If available, information on the investigation sites, from which data for model development was obtained, is added, too. This approach neglects any mathematical structures. Information on the domain of application and on the expected dynamic behavior (spatial and temporal patterns) is limited.

- The mathematical structure of a model is documented by listing the equations, parameters and initial conditions. This documentation includes results of model analysis, results from parameters estimation and the system behavior. Chapters 2 and 3 present examples for this type of model documentations.

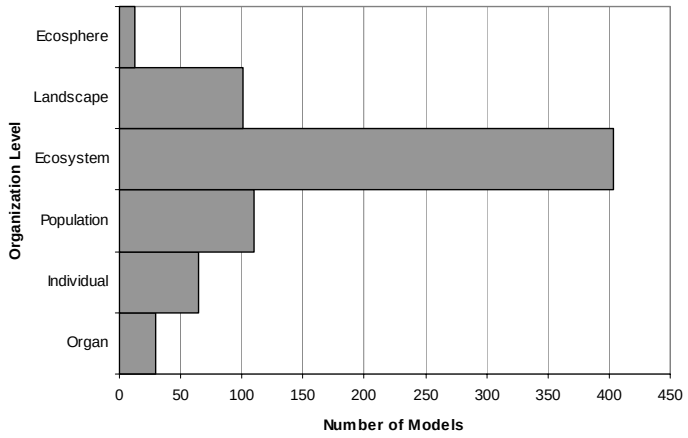

Fig. 4.1 Distribution of meta-documentation entries of models in the Register of Ecological Models for different levels of organization.

- The most convenient (and less frequently chosen) procedure in documenting environmental models is to include information on the development procedure according to the decisions and considerations made, when going through all steps of the water flow model (Figure 1.4), presented in Chapter 1, page 13. As these decisions and considerations determine the mathematical structure and the heterogeneity, this is a very important step of model documentation.

In recent literature model documentation usually covers the first topic of this list. Documentation in terms of the remaining item is understood as so-called *meta-documentation* or *meta-modeling*. Different concepts for these tasks are available. The following sections give a short overview of these concepts.

Meta-modeling concepts are used to solve two major problems. The first task is to set up appropriate databases on model documentations, that allow us to browse through a list of available models and retrieve models that solve the problem of interest. These databases are either meta-databases, e.g. databases that offer documentation on models and the contact address of the modeler, only. Or, these databases permit us to download the model code or run the model interactively. The following section briefly summarizes some concepts and examples.

4.4.2 Model Databases

Register of Ecological Models The register of ecological models (REM) is the result of the union of the databases of the REM database in its first stage of development and the Environmental Research Information System (UFIS), (Hoch *et al.*, 1998). REM provides easy access to and information on more than 600 ecosystem models at different organization levels. Figure 4.1 shows the results of the screening

review of this database. Depending on the specified level of organization a model is developed for, the number of available meta-information entries is displayed. One may think that modeling ecosystem process is of most interest in ecological modeling.

REM is a meta-database for existing ecological models and is designed to offer information on ecological models as a whole. The goal is to provide a tool that supports interdisciplinary work among modelers as well as to give administrative bodies an overview of national and international activities in ecological modeling. The availability of such an information system is believed to be crucial to international coordination of modeling activities, and to reduce redundancy in environmental modeling. REM pay particular attention to data requirements of models, areas of application, and scales of the model. REM as a meta-database is open to all modelers for submitting information on new model development. Figure 4.2 displays an excerpt of the web page for entering model information. The part related to model structure and mathematical characterization is shown (Benz, 2003).

A part of REM which is closely linked to model documentation focuses on the description of data. Since there is no modeling without data it is natural to combine information systems on data and models in one unit. UFIS does not intend to keep data, but will keep information on where and how to access data (meta-data). Descriptions of data in the model information system will be compatible with the ones in the meta-data information system such that relations between models and data can be easily recovered (Knorrenschild *et al.*, 1996).

The CAMASE Register of Agroecosystems Models The project CAMASE (Plentinger & de Vries, 2001) develop a comprehensive register of agroecosystems models. The aim is to

- increase awareness among scientists of existing models and reduce redundancy in model development, prevent reinvention-of-the-wheel effect;
- increase accessibility of these models;
- stimulate harmonization and compatibility of models;
- stimulate use of models.

The project aims to collect 80% of relevant models used in Europe for research, education and application in intensively and extensively produced agricultural crops, grasslands, forests, and their environments, cropping and farming systems, farm households, land use. Additionally shells for such models and tools for such models in decision support applications (e.g. micro-climate profiles for irrigation scheduling) are listed. Models in the CAMASE Register need to be documented on a scientific level and need to be validated, at least partially. Software tools are listed in the database if they are closely related to agroecological modeling (Plentiger & de Vries, 1997).

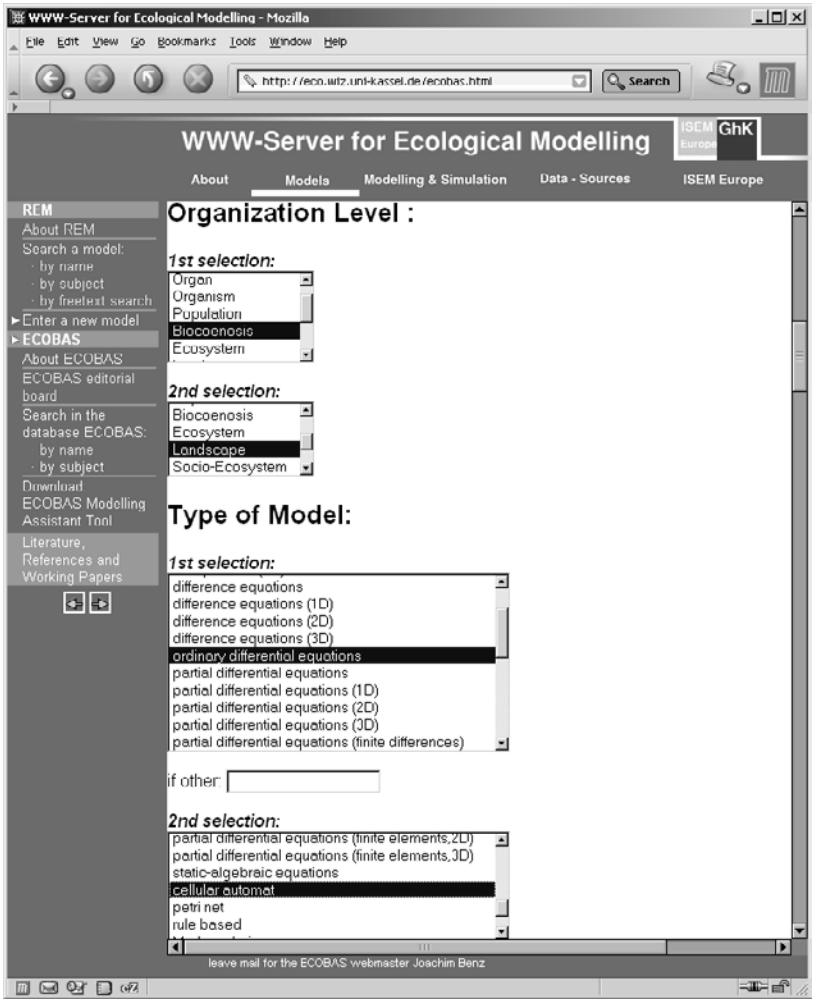

Fig. 4.2 REM/ECOBAS web page for entering meta-information on ecological models. URL: `http://eco.wiz.uni-kassel.de/ecobas.html` [July 2003].

4.4.3 Meta-modeling Concepts

The second major problem that requires an appropriate methodology on meta-modeling is the integration and model coupling of sub-models or modules. An automatic integration and coupling of different (heterogeneous) models necessitates access and work with data structures that make information on the type of model, variables and domain accessible. The general idea for solving this problem is to identify models, or the processes described, as objects using an object-oriented concept for modeling the data structures of the meta-data as well as the model integration tools (Hoch *et al.*,

1998; Villa, 2001; Maxwell & Costanza, 1997a). The following examples briefly discusses implemented solutions without focusing too much on a highly sophisticated computer science realization.

ECOBAS — Model Interchange Format The `ECOBAS_MIF` model interchange format is used for model documentation as well as for supporting the model database ECOBAS. The project aims at complete and consistent documentation of models as well as to make them accessible and comparable (Benz *et al.*, 1997). The MIF file is an easily portable ASCII file and holds complete documentation of a model including:

- General information for the specification of the ecological process and source of the mathematical description;
- Declaration and identifications of the attributes and quantities (inputs, outputs, states and constraints) of the process modeled;
- Complete and consistent formulation of all input-output relations (functions and equations);
- Information about the environment for which the documented model has developed.

Based on a properly defined model using a MIF file the following functions can be used within the associated framework (Hoch *et al.*, 1998):

- Compilation of documentation in RTF, TEX, or HTML;
- Use the MIF file as source for modeling platforms such as MATLAB–SIMULINK, cf. Section 1.5.3. p. 29.

The creation and maintenance of MIF based models is supported by a graphical front end editor that supports editing all components of a MIF file.

Modular Modeling Language Maxwell (1997a) presented the modular modeling language (MML). This modular modeling concept set up the foundation for the spatial modeling environment, see Section 3.3.3. Similar to a MIF file, the MML acts as an intermediate layer supporting the communication and interchange between the model description layer and model implementation. As an important addition to the MIF concept the spatial modeling environment offers a tool for translating output from graphic model development platforms (STELLA) to MML file. The key properties of a model description in MML are (Maxwell & Costanza, 1997a):

- Simplicity: Only the important details relevant to the dynamics of the models are coded using MML. Implementational aspects are neglected.

- Modularity: Components, sub-models or modules are separately represented using this languages. These modules encapsulate their data and dynamics in the sense that they can only be interfaced through their inputs and output.
- Encapsulation hierarchy: Modules may include or encapsulate other modules. The scope of the encapsulated module cannot access modules declared outside the encapsulating module.
- The inheritance hierarchy allows modules to inherit some of the functionality of other modules. This property facilitates the construction of specialization hierarchies.
- Connections: MML declares connections of input/output variables between modules.

These properties of the MML are in accordance with the requirements listed above. The major focus of this development is the integration of models and the construction of spatially explicit models rather then the documentation of models and model retrieval. For instance, much information coded into a STELLA model, like documentation, units of variables etc., is dropped in the translation to a MML confirm model.

Integrated Modeling Architecture Villa (2001) extends this concept by the integrated modeling architecture (IMA). It specially focuses on the problem of mathematical heterogeneity and the problem of multi-paradigm and multi-scale environmental models. The major characterization of environmental models follows the three categories of representation, domain and scale. Referring to these categories the concept of IMA offers a framework for making different modules comparable and supports interaction between different modeling paradigms.

This is achieved by an open source modeling toolkit (Integrating Modeling Toolkit, IMT) that offers several functions for translating, storing and coupling different modules based on a general mark-up language using the extensible mark-up language XML. An example for a definition of a ordinary differential equation can be look like, compare Section 3.2.2.

```
<STOCK NAME="P1">
  <INIT> 10 </INIT>
  <INFLOW NAME="BIRTH">
    BETA*P1
  </INFLOW>
  <OUTFLOW NAME="PREDATION">
    SIGMA*P1*P2
  </OUTFLOW>
</STOCK>

<STOCK NAME="P2">
  <INIT> 10 </INIT>
```

```
    <INFLOW NAME="PREDATION">
      ALPHA*P1*P2
    </INFLOW>
    <OUTFLOW NAME="MORTALITY">
      GAMMA*P2
    </OUTFLOW>
  </STOCK>
```

A model documentation may be added to different module entities by adding an URL to the object specification. IMA and IMT are under development. Neither IMT nor MML can cope with modules that base on partial differential equations.

4.5 SUMMARY AND OUTLOOK

As a summary from this short overview it becomes clear, that model based solution of environmental problems and computer-based management of environmental systems requires the setting up of models that satisfy the needs of the given problem, but that are not developed from scratch. Sufficient resources will rarely be available for developing entirely new model systems. Model integration has been identified as the important step. Several approaches show different possible implementations of model integration and model coupling. Second, several criteria are derived from scientific theory, that help to assess models and that support the step of model analysis described in Section 1.3, and that are appropriate especially from models that are mathematically heterogeneous because they are derived from different modeling paradigms.

This part of the book aims at an integration of the modeling languages presented in Chapters 2 and 3 focusing on the problem of integrating anthroposphere and biosphere processes. A possible methodological framework for this is the use of hybrid Petri nets presented in the following chapter. Applications for hybrid ecological models based on Petri nets are presented in Chapter 6. Finally, Chapter 7 then gives a real world application to a problem of integrating anthroposphere and biosphere processes including a environmental impact assessment.

5

Concepts: Hybrid Petri Nets

5.1 INTRODUCTION

5.1.1 Concepts of Hybrid Model Development

Several applications of Petri nets can be found, which model mathematically heterogeneous or hybrid systems. Most of them originate in engineering science. Kluwe *et al.* (1995) state that a combined "three-layer-model" may achieve an overall optimum in modeling of quantitative and qualitative knowledge. The three-layer-model consists of a rule-based qualitative layer; an event-based qualitative layer, which is set up by Petri nets, and a quantitative model layer set up by differential equation systems. Jávor (1995) proposes the lumping of Petri nets, and methodologies of artificial intelligence. Rodrigo *et al.* (1998) emphasize the interdisciplinary nature of the modeling task.

Chouikha (1998) proposes the integration of differential equations with Petri nets. Following this approach there is a relationship between net structure and structure of a system matrix, which represents a differential equation system whose solution is given by the fundamental matrix. In this way, it is possible to formulate a basic equation for the description of continuous net behavior on the basis of the initial marking and the fundamental matrix. The basic equation provides a formal basis of this new description, which is necessary for the formal analysis and verification of system behavior.

Applications in ecological modeling by hybrid systems are proposed in (Gronewold & Sonnenschein, 1998). They offer an object-oriented system modeling cellular

automata. Petri nets are used here for asynchronous migration of species in cellular automata. Ewing *et al.* (2002) suggest Petri nets in event-driven population dynamics modeling and assess competing risks.

5.1.2 Aim and Scope of the Development

Requirements for a general integrating concept of hybrid or heterogeneous models are met, for example, by Petri net theory. Hybrid low level Petri nets offer the basis for a general theory, which combines structure and dynamics and is amenable to various kinds of extensions (Chouikha & Schnieder, 1998). We follow most of the suggestions from Chouikha and extend them by several properties. The latter comprise time-weighted and stochastic transitions and integration of differential equation systems.

Petri nets with these extended properties are capable of simulating the dynamics of mathematically heterogeneous systems, which are structured by net topologies. They serve as a theoretical basis for the analysis of topological properties and enable the efficient simulation of complex integrated technical–ecological systems. A simulation tool has been developed, which allows graphical creation of the Petri nets and includes the above-mentioned functionalities.

5.2 THEORETICAL BACKGROUND

5.2.1 Hybrid Low Level Petri Nets

The purpose of modeling environmental systems, requires the introduction of a non-standard form of a Petri net with places and transitions. Extensions to the mathematical formulation of Petri nets are the association of time to transitions, and stochastic and dynamic behavior of transitions in terms of ordinary differential equation systems and time-discrete systems.

Structure and Topology A Petri net is a directed graph with two types of nodes, i.e. places $p_i \in P$ and transitions $t_j \in T$. Alternate nodes are connected with arcs $a \in A \subseteq (P \times T) \cup (T \times P)$ (i.e. a place connected to a transition and vice versa).

Places are locations that hold tokens. The information carried by the token is transformed by the transition nodes of the Petri net.

The state of a Petri net is given by the information of the tokens, the mapping $m : P \times \mathbb{R}^+ \rightarrow \mathbb{R}$. It is defined by the distribution of values m_i in the places p_i in time $\tau \in \mathbb{R}^+$ of the Petri net: $m(p_i, \tau) = m_i(\tau)$. Real values are allowed for the marking, which is a non standard extension. Places are also associated with attributes like capacity $c : P \rightarrow \mathbb{R}^+$.

Definition 5.1 (Petri net) *A 5-tuple $N = (P, m, T, A_M, A_I)$ defines a hybrid low level Petri net N with*

$$\left.\begin{array}{rl} P = \{p_1, p_2, \ldots\} & \textit{places} \\ m : P \to \mathbb{R} & \textit{marking} \\ c : P \to \mathbb{R} & \textit{capacity} \\ T = \{t_1, t_2, \ldots\} & \textit{transitions} \\ A_M, A_I \subseteq (P \times T) \cup (T \times P) & \textit{arcs} \end{array}\right\} \tag{5.1}$$

We distinguish between arcs which identify mass flow A_M, and flow of information A_I.

Definition 5.1 up to this point incorporates the structural and qualitative description, the interconnection of events and processes: topology or a so-called *conceptual network*.

Let $I : T \to P$ denote all input places and $O : T \to P$ denote all output places of a given transition $t \in T$:

$$\left.\begin{array}{rcl} I_I(t) & := & \{p \in P \,|\, (p,t) \in A_I\} \\ I_M(t) & := & \{p \in P \,|\, (p,t) \in A_M\} \\ O(t) & := & \{p \in P \,|\, (t,p) \in A_I \cup A_M\} \end{array}\right\} \tag{5.2}$$

The functional and quantitative behavior of a Petri net is defined by the specification of transitions and the weights associated with the arcs.

If processes which show different time characteristics are considered, transitions have to be extended by an attribute $\Delta\tau > 0$. One can interpret $\Delta\tau$ as switching or processing time or duration of execution.

Definition 5.2 *Each transition $t \in T$ is associated with a switching period $\Delta\tau : T \to \mathbb{R}^+$. If $\Delta\tau$ is defined for a transition t, the last time of switching is also stored: $\tau : T \to \mathbb{R}$.*

Flux of mass or information is defined by weights associated with the arcs by a function $w : A_M, A_I \to \mathbb{R}$. Arcs from places to transitions are held in a matrix $W^- = \left(w^-_{ij}\right)_{i,j=1,2,\ldots}$, and arcs from transitions are hold in a matrix $W^+ = \left(w^+_{ij}\right)_{i,j=1,2,\ldots}$. The flow from places to transitions is denoted by a negative sign; the flow from transitions to places is denoted by a positive sign. The incidence matrix is derived by calculating $W = W^+ - W^-$.

Because we want to include extensions, four different types of weighting have to be considered:

Definition 5.3 (Weights) *Let $t_j \in T$ be a free but fixed transition:*

1. *Information is not "removed" from places*

$$w^-(p_i, t_j) := 0 \textit{ for } (p_i, t_j) \in A_I$$

2. *Weights are defined by constant values*

$$\begin{aligned} w^-(p_i, t_j) &:= w_{ij} \in \mathbb{R}^+ \text{ for each } p_i \in I_M(t_j) \\ w^+(t_j, p_k) &:= w_{jk} \in \mathbb{R}^+ \text{ for each } p_k \in O(t_k) \end{aligned}$$

3. *Weights can be defined by a linear relationship to the connected place*

$$w^-(p_i, t_j) := \widetilde{w}_{ij} m_i(\tau) \text{ for } p_i \in P \text{ and } \widetilde{w}_{ij} \in \mathbb{R}^+$$

4. *Variable weights are defined by functions which are associated with the connected transition:*

$$w^+(t_j, p_k) := f_{jk}(\tau, w_{j1}, \ldots, w_{jn}) \text{ for all } p_k \in O(t_j), n = |I_I(t_j) \cup I_M(t_j)|$$

Two additional remarks need to be added here. If weights are defined in terms of item 3 or 4 of Definition 5.3, the mass balance may be invalid in the net. Second, so-called "reset arcs" may be defined by setting $\widetilde{w}_{ij} = 1$ in step 3 of the definition. The definition of weights introduces quantitative dependencies to the structural information of the network. The quantitative relations induce the dynamics of the system.

5.2.2 Functional Behavior

Switching Conditions The functional behavior is defined by the transitions. Tokens are moved from input places to output places if three conditions are fulfilled. According to the input weights, all input places contain a sufficient amount of tokens, and according to the output weights, all output places must be able to store the results if capacities are defined. This is summarized by the definition:

Definition 5.4 *Consider the transition $t_j \in T$ and the time of simulation $\tau' \geq 0$. If the following conditions are fulfilled*

$$\left.\begin{array}{lcl} \forall p_i \in I_M(t_j) & : & m_i(\tau) \geq w_{ij} \\ \forall p_k \in O(t_j) & : & m_k(\tau) + w^+(t_j, p_k) \leq c(p_k) \\ & & \tau' \geq \tau(t_j) + \Delta\tau(t_j) \end{array}\right\} \tag{5.3}$$

the transition switches, which means the following equations are calculated:

$$\left.\begin{array}{lcl} \forall p_i \in I(t_j) \backslash O(t_j) & : & m(p_i, \tau') = m(p_i, \tau) - w^-(p_i, t_j) \\ \forall p_k \in O(t_j) \backslash I(t_j) & : & m(p_k, \tau') = m(p_k, \tau) + w^+(t_j, p_k) \\ \forall p \in I(t_j) \cap O(t_j) & : & m(p, \tau') = m(p, \tau) - w^-(p, t_j) + w^+(t_j, p) \\ & & \tau(t_j) = \tau' \end{array}\right\} \tag{5.4}$$

The Definitions 5.1 to 5.4 set up a dynamic system in a very special manner. In contrast to dynamic systems e.g. based on differential equations the sequence of processes started is not obvious after model initialization. The sequence is determined by testing the conditions in Equation (5.3) for all transition $t \in T$ and each state $\tau > 0$ of the given Petri net N.

Stochastic Time Weighting and Ordinary Differential Equation Systems
This section gives an explanation of the important functional extensions to standard Petri nets which are introduced by items 3 and 4 of Definition 5.3.

Let Z be a stochastic variable. The coefficients of its distribution function depend on the state of the connected places. The switching time $\Delta\tau$ of transition t_j can be estimated, using a random number generator, by

$$\Delta\tau(t_j) := Z(w_{1j}, \ldots, w_{nj}) \text{ with } (p_i, t_j) \in A_I, n = |I_I(t_j)| \tag{5.5}$$

Definition 5.5 *Let* $\frac{d\vec{y}}{d\tau} = \vec{g}(\tau, \vec{c}, \vec{y})$ *specify a nonlinear ordinary differential equation system with the initial condition* $\vec{y}(0) = \vec{y}_0$ *and a set of parameters* $\vec{c} \in \mathbb{R}^n$. *The (numerical) solution can be noted by the concept of flux (Arrowsmith & Place, 1994) by* $\vec{y}(\tau) = \vec{\varphi}_\tau(\vec{y}_0, \vec{c})$

In most cases the given differential equation system may be nonlinear. Therefore the solution noted by the flux $\vec{\varphi}$ incorporates a procedure of numerical integration (Hairer *et al.*, 1980; Hairer & Wanner, 1980).

In the notation of the Petri net, a differential equation system is applied to a transition t_j by the following steps.

$$\left.\begin{array}{rcl} \vec{y}_0 & := & \left(w^-(p_i, t_j)\right)_{i=1,\ldots,|I_M(t_j)|} \text{ and } \widetilde{w}^-(p_i, t_j) := 1 \\ & & \text{for } (p_i, t_j) \in A_M \\ \vec{c} & := & \left(w^-(p_i, t_j)\right)_{i=1,\ldots,|I_I(t_j)|} \text{ with } (p_i, t_j) \in A_I \\ w^+(t_j, p_k) & := & f_{jk} := \varphi_{j,\Delta\tau}(\tau, \vec{c}, \vec{y}_0) \text{ for } (t_j, p_k) \in A_I \cup A_M, \\ & & k = 1, \ldots, |O(t_j)| \end{array}\right\} \tag{5.6}$$

5.3 DEVELOPMENT PLATFORM

5.3.1 Overview

This theoretical framework is embedded into a graphical user interface, which forms the development platform for development of hybrid low level Petri nets [1] (hPEN). It allows graphical development and controls the simulation run. Figure 5.1 gives an impression of model development. The following list summarizes the capabilities of the platform:

- Graphical construction of a Petri net with transitions, places, arcs, and bidirectional arcs.

[1] See p. 279 for availability of software.

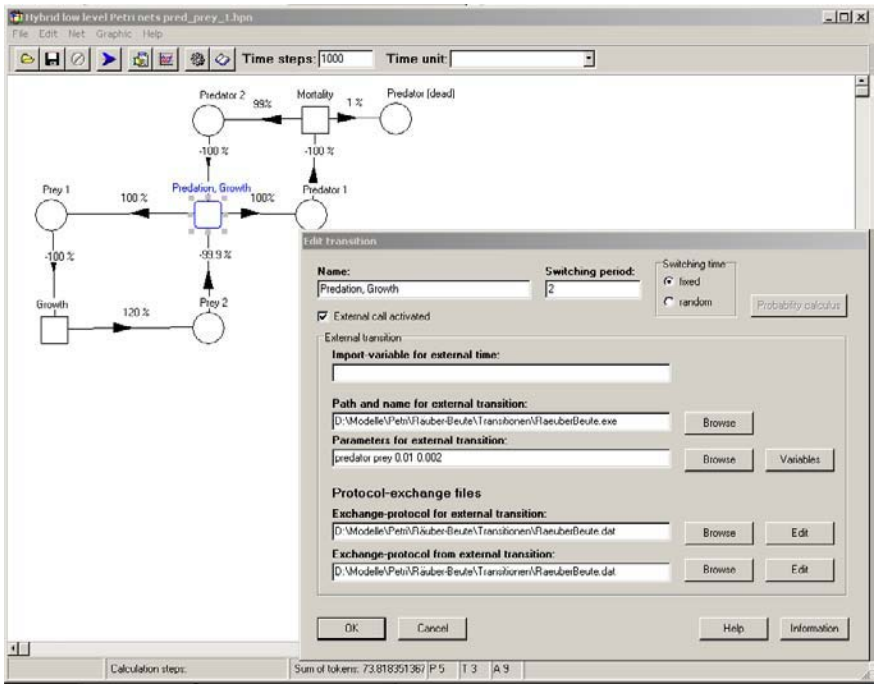

Fig. 5.1 Graphical User Interface (GUI) for development of hybrid low level Petri nets. The development platform runs on any Windows operating system. The Petri net shown represents a predator–prey model using two stages for population dynamics modeling and the specification of a hybrid transition "predation". (See p. 279 for availability of software.)

- Specifications of places with capacities and interconnections to external tabular data (measurement values, temperature data, etc.), see Equation (5.1).
- Definition of transitions with static switching time, Equation (5.2), and stochastic switching times using Erlang-k, exponential, equal and normal distributed stochastic variables, see Equation (5.5).
- Coupling of external models (ordinary differential equation systems, etc.) to transitions. Initial and parameter values and results are exchanged during run time, see Equation (5.6).
- Graphical display of simulation results.
- Logging results for each time step to a file.
- Analysis of the system- or net-comitants, see next section.
- Export of incidence matrices W^+, W^- in different formats (esp. Mathematica) for further analysis.

5.3.2 Meta-modeling Concept

Integration of different models defined by other development tools or methodologies than the Petri net concept requires the definition of an appropriate interchange format. For instance, the transfer of initial conditions and parameters to a differential equation solver that solves equations defined according to Equation (5.6) requires a well-defined protocol. This is a task of meta-modeling and model documentation, see Section 4.4.1.

Figure 5.1 displays how this is performed within the Petri net development platform. External models are integrated in the Petri net by the specification of the command line sequence which starts the external computer model with the command line parameters. Additionally, interface files may be used to exchange information such as initial conditions and parameters. The modification of these interface files follows a very flexible concept. Parameter values to be read or written by the Petri net development platform are replaced by user defined keywords. This enables data exchange based on text files and command line instruction.

5.3.3 Core Simulation Algorithm and Model Analysis

The Petri net can be defined using graphical representations. Transitions are identified with squares, places with circles and arcs with arrows. Boxes with rounded corners identify an external model, e.g. an integrated differential equation system. See for instance in Figure 5.1 the population dynamics model for the predator–prey interaction. In addtion, the notation in the development platform one might use solid arrows to denote mass flow and dashed arrows to identify flow of information. Transitions and places may be named and comments may be added to each model element (p, t).

The core algorithm, which evaluates Equations (5.4) to (5.6), is displayed in Figure 5.2, which summarizes the actions performed for running a dynamic simulation based on a hybrid Petri net in a very aggregated way. The extensions to standard Petri nets require precise formulation of the calculation sequence. The main loop starts with the activation of all transitions and an input of external data. In the next step the flow of mass and information is set up using the incidence matrix W^- according to items 2 and 3 of Definition 5.3, where item 2 is prior to item 3. After this, all simulation tasks in external transitions are performed. This evaluates item 4 and the second equation of item 2 in Definition 5.3. From this W^+ is obtained and the new marking can be calculated.

For further analysis net invariant properties, so-called comitants, can be derived from the incidence matrix W. For instance, the number n_i of switching events of each transition t_i $(i = 1, \ldots, |T|)$ can be derived by estimating nontrivial solutions of the equation $W \cdot \vec{n} = 0$ (Chouikha & Schnieder, 1998).

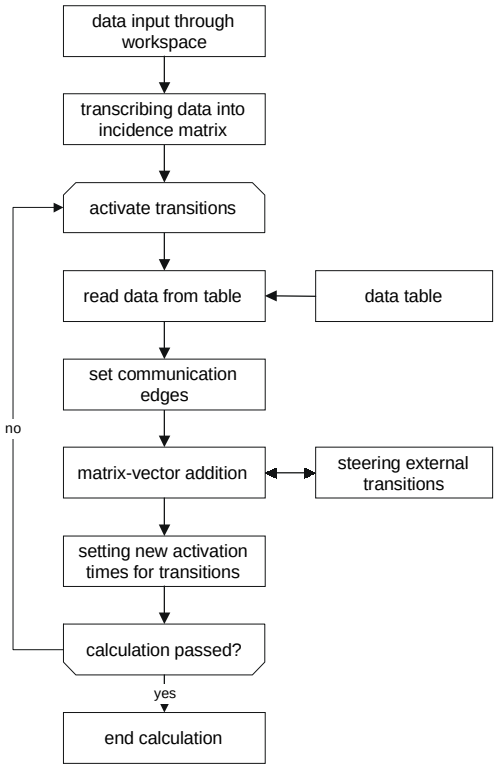

Fig. 5.2 Flow diagram of core algorithm for simulation of hybrid Petri nets.

5.4 AN ECOLOGICAL MODELING EXAMPLE

5.4.1 Predator–Prey Interactions

The classical predator–prey model (Volterra, 1927) was introduced in Section 3.2.2 on page 81. Denoting the prey population by P_1 and the predator population by P_2, the following system models predator–prey interaction by a nonlinear ODE system

$$\left.\begin{aligned} \frac{dP_1}{dt} &= \beta P_1 - \sigma P_1 P_2 \\ \frac{dP_2}{dt} &= \alpha P_1 P_2 - \gamma P_2 \end{aligned}\right\} \tag{5.7}$$

Refer to page 81 for the description of the terms and parameters. The following parameters are assumed for this case study: $\alpha = 0.002, \beta = 0.09, \gamma = 0.01, P_1(0) = 10$, $P_2(0) = 15$. For detailed analysis we focus on the system behavior more qualitatively.

The common results are oscillating phase-displaced population densities. The system produces several stable tori or cycles in phase space depending on the initial condition.

A close look at the underlying processes shows that the process of predating can be considered as a event "lynx meets rabbit" in the system. In the following the predator–prey system is described by an event-based Petri net.

5.4.2 Event-based Modeling of Predator–Prey Interactions

Looking at predator–prey interaction as an event-based system using the conceptualization of a hybrid Petri net leads the following considerations: Populations of prey and predator are described in one or more places. If we consider age-structured populations we may want to introduce more than one place for a population, see Figure 5.1. In this case the "life-cycle" of a species is clearly specified by arrows. The places are connected via transitions that denote simple growth (for the prey), simple mortality (for the predators) and the interacting transition of predation. The latter is specified by a analytical function — the terms $\sigma P_1 P_2$ and $\alpha P_1 P_2$ — all other transitions are specified by parameters introduced in the classical Petri net framework.

This approach can be aggregated or condensed to a version displayed in Figure 5.3. Using bidirectional arrows the system can be reduced to three places: "predator

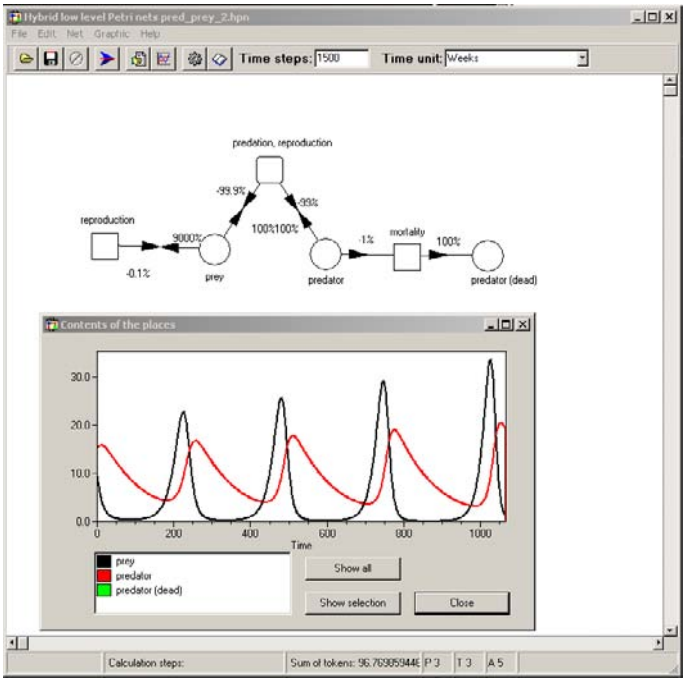

Fig. 5.3 Example of an aggregated Petri net model using one place for the population "prey" (P_1) and "predator" (P_2). The simulation results as presented within the development platform are displayed in the pop-up window below.

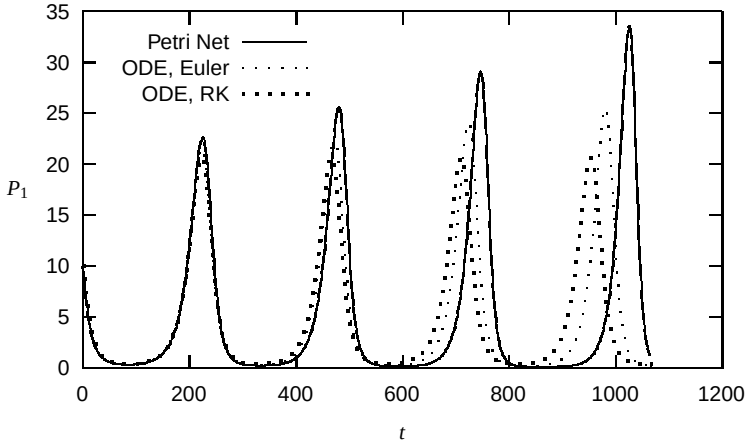

Fig. 5.4 Simulation results of predator–prey models. The results from the hybrid Petri net model and the differential equation model are displayed. Note that from the simulation, results vary depending on the numerical procedure chosen for solving the ODE system.

population", "prey population" and "dead predators". A meeting of predator and prey is again modeled by a nonlinear external transition.

5.4.3 Simulation Results

Figure 5.4 displays the population dynamics of the prey population P_1. The solid line gives the results from the hybrid Petri net model. The simulations result in the well-known fluctuating population densities. Figure 5.5 uses the state phase plane to summarize the simulation results for the two populations P_1 and P_2. A striking fact is that the numerical solution based on the ODE from Equation (3.11) is identical to the solution from the Petri net. Using equal parameters but changing the model structure does not change the results.

A closer look at Figure 5.4 shows that there are differences between the two methodologies. Figure 5.4 compares the simulation of the Petri net with the solutions obtained from the ODE system in Equation (3.11) by a standard Euler method with no step size control and by a Runge–Kutta 4^{th} order scheme and embedded step size control. Note, all solutions differ. The solution derived from the RK solution of the ODE is the only solution that is consistent with stability analysis of the system. The qualitative result from stability analysis is a stable tori or cycle depending on the initial condition (Jørgensen & Bendoricchio, 2001). An increase of oscillation with continuing simulation is a numerical artifact and not a property of the mathematical structure. This is an example for the usually unknown domain of the numerically and structurally unintended patterns of dynamic systems, as described in Section 2.8.

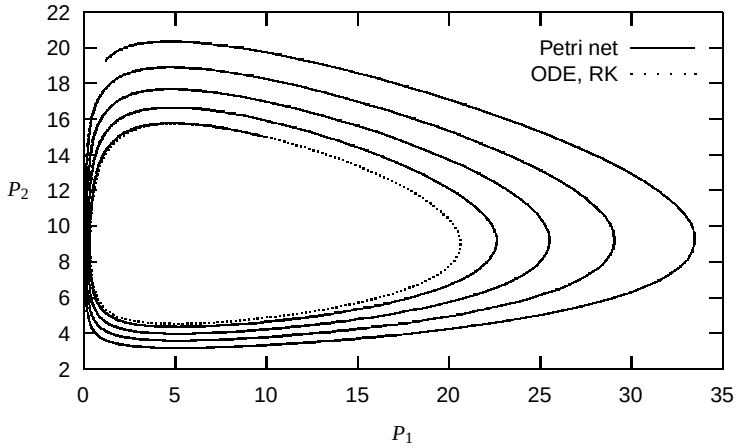

Fig. 5.5 Results of Petri net model in state phase plane. The dotted line shows the reference solution estimated by a Runge–Kutta scheme.

It follows that the Petri net simulation can be interpreted as a numerical solution of the classical predator–prey model, showing that control of domains of stability in discrete or event-based model is difficult. This is supported by the information on the stability analysis of the procedure for numerical approximation of the ordinary differential equation system. An important requirement for the application of a numerical integration procedure to a model system is that the domain of stability of the numerical differential equation solver (the eigenvalue spectrum) is in the same range as the eigenvalues of the dynamic system to be solved (Hairer *et al.*, 1980). If this is not the case, the numerical solution can be anything except the solution of the differential equation modeled.

5.4.4 Discussion and Extensions

There is a broad range of possible extensions to the classical predator–prey model, see for instance (Jørgensen & Bendoricchio, 2001). These extensions can be made to the ODE model as well as to the Petri net. As expected, the way of introducing an extension clearly varies between the modeling types.

Limitation of Growth Abiotic factors of a habitat determine the maximum density of a population carried or supported by this habitat. Capacity limited growth is introduced into the ODE model by adding the factor $(P_{max} - P)$ to the growth terms of the model. This introduces a stable attractor P_{max} to the system behavior. Starting from $P(0) < P_{max}$ growth will not exceed P_{max}.

For the Petri net such a limitation can be incorporated by the definition of a maximum size of a place. This a standard attribute of Petri nets. The consequence of such a

limited storage capacity of a place, is that, if the place carries its maximum capacity, all preceding transitions will stop switching. The dynamic behavior of the system changes, as this is an event-based model.

Density-dependent Predation Density-dependent predation rates are incorporated into the model by a modification of the predation term P_1P_2 in both equations. Multiplication of this term by a term such as $1 - \exp(-(P_1/P_{crit})^c)$ reduces predator growth, as well as prey death, if prey density is very low. In the Petri net model we can define a density-dependent probability of predation success by using different switching times of the predation transition. Using a stochastic time weighting with a density-dependent mean introduces the desired density dependence. In addition, by choosing the distribution one can extend the model with statistical knowledge of the predation success of the species being studied.

Harvesting Harvesting a population is denoted by adding a sink term like $-H$ to the harvested or hunted population. In the conceptual framework of feedback dynamic modeling (ODE-type models) this formulation leads to the problem of identifying the optimum or most sustainable yield (MSY). Sustainability in this context means the stable survival of all populations. It is defined by a threshold level of harvesting rate that must not be exceeded in order to maintain the population. Frequently this threshold level itself depends on the population density (of the considered or all populations). The Petri net allows a very intuitive approach here. In the framework of Petri nets this modeling task can simply be solved by adding a transition that withdraws a specified amount of yield, or number of individuals only if a sustainable configuration of populations is present. Harvesting depends on the event "populations are sustainable" not on a certain time.

5.5 CONCLUDING REMARKS

An obvious advantage of the techniques introduced here is the graphical representation, which allows systems to be described in a detailed but clear manner. The extension of hybrid low level Petri nets offers an integrating platform for hybrid modeling in ecology. With this conceptualization scheme an integration of any model based on arbitrary mathematical dialects is supported. Second, with Petri nets the classical deterministic concept of model development is broadened by event-driven models. Actions and processes started in the Petri net model, depend highly on the configuration of states in the system. This is the basic principle of a event-based model and must be distinguished from all modeling approaches presented in the previous chapters. Even with this first example from ecological modeling, the possible functional spectrum of the concept of hybrid Petri nets has been illustrated. The capability of this system will be analyzed in detail in the following chapter in different case studies.

6

Case Studies: Hybrid Systems in Ecology

6.1 INTRODUCTION

The concept of hybrid low level Petri nets as integrating platforms for environmental models can be used to study examples from ecological modeling. The first case study extends the crop growth sub-model of the agroecosystem model from Section 2.2.1 to an event-triggered model with changing structure. The second case study presents a meta-population model analysis of species invasion in fragmented landscapes and compares this approach with the spatially explicit model based on PDE, as discussed in Section 3.2.2.

6.2 HYBRID CROP GROWTH MODELS

6.2.1 Modeling of Crop Growth with Dynamically Changing Model Structures

Crop development depends on biological, chemical, and physical processes and is related to air temperature, humidity, nutrients, and density of growth. Section 2.2.1 introduced modeling approaches for the underlying processes in detail. The generic model in Section 2.2.1 was applied to a large number of crops and different data sets. However, two issues were neglected in this section:

- Crop growth models have to cope with distinct biological stages of annual crop growth.

- Within these stages structural changes have to be considered (e.g. appearance of new plant organs).

The simulation of agricultural yield necessitates the prediction of the harvest biomass. For example, in a wheat growth model, modeling the total biomass is not a suitable solution, because one has to differentiate between leaf, stem, and ear components. The emergence of these different components depends on the development stage of the crop. Crop development is separated into three stages, denoted by development codes (DC) (see (Zadoks *et al.*, 1974) for encoding of DC): growth during the winter period from seed to tillering phase (development stages DC01 to DC21); development up to stem elongation (to DC31); and growth from ear emergence (DC51) to maturity.

Figure 6.1 displays a hybrid Petri net which sets up the framework for modeling three different development stages with three different organs of the crop. Entering a new development stage is modeled by an event in the Petri net. These events are triggered by entering a new physiological stage. Physiological stages can be identified using the concept of biological time $t_{biol}(t)$ as defined by Equation (2.5), see Section 2.2.1 on p. 37. Biological time is defined as the integral over the development rate. This nonlinear dependency between temperature and development rate can be described by the O'Neill function, see Equation (2.19). The progress of the O'Neill function describes the rising of the development rate from a temperature of 0 °C until a specific optimum temperature is reached and the adjacent decreasing of the rate until lethal temperature. This equation is based upon parameters, which are easily derived from experimental data.

The differential equation system for the dynamically changing structure is given by

$$\frac{dW_L}{dt} = \begin{cases} 100\, r_L \left(1 - \frac{W_L}{W_{L,max}}\right) & \text{if } t_{biol}(t) < t_{DC21} \\ W_L\,(r_L f_s(t) - \mu) & \text{else} \end{cases} \tag{6.1}$$

$$\frac{dW_S}{dt} = \begin{cases} r_S\ W_L\ \left(\lambda - \frac{W_S}{W_L}\right) & \text{if } t_{biol}(t) \geq t_{DC31} \\ 0 & \text{else} \end{cases} \tag{6.2}$$

$$\frac{dW_E}{dt} = \begin{cases} r_E\ W_L & \text{if } t_{biol}(t) \geq t_{dc51} \\ 0 & \text{else} \end{cases} \tag{6.3}$$

The biomass in [kg/ha] of leaf, stem and ear is given by W_L, W_S and W_E. Note, the leaf compartment can be interpreted as photosynthetically-active component, as growth of all other compartments depend on the leaf biomass present. For a detailed discussion on the phenomenology of the crop see (Schröder *et al.*, 1995).

Based on experiments in the investigation site "Neunkirchen" (see page 40) the biological time for entering the development stages DC21, DC31 and DC51 were determined: $t_{DC21} = 4.81$, $t_{DC31} = 6.41$ and $t_{DC51} = 12.7$. From this investigation parameters for development rate r_D using the O'Neill function Equation (2.19) were determined: $T_{opt} = 16.8\,℃$, $T_{max} = 35.0\,℃$, $r_{D,max} = 0.054$ and $\beta = 14.7$.

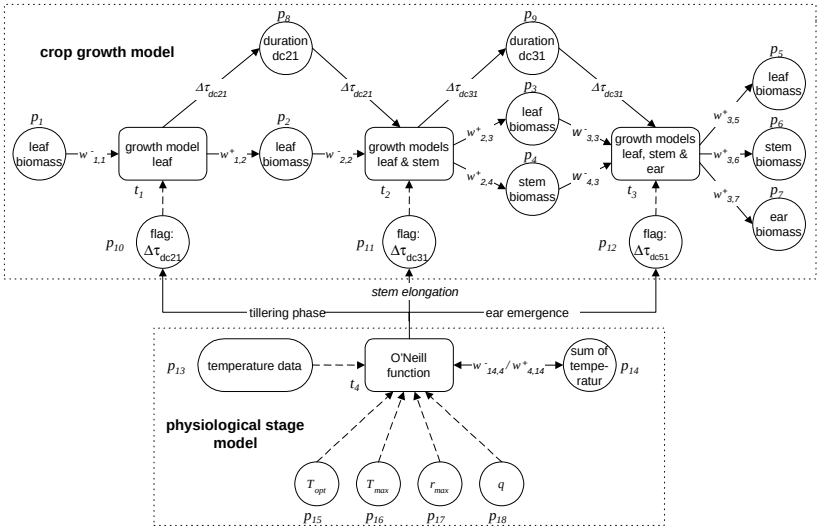

Fig. 6.1 Petri net model for integration of discrete development stages derived by a continuous model for biological time (physiological stage model, lower part of figure) and crop development (upper part of figure).

All the remaining parameters of organ growth are determined by parameter estimation, as documented in Section 2.3.3. Results are $r_L = 0.085$ d^{-1}, $r_E = 0.174$ d^{-1}, $r_S = 0.0091$ d^{-1}, $\mu = 0.0681$ d^{-1}, $W_{L,max} = 395$ kg/ha and $\lambda = 10.6$.

Based on this specification, the differential equation for the biological time is used by the Petri net to synchronize all the differential equation systems coupled by the hybrid Petri net.

6.2.2 Hybrid Petri Net

Structure and Topology The following processes must be coupled:

- physiological stage model;
- model for biomass production.

The model for biomass production underlies structural changes during the simulation period. In the first two development stages (to DC31) only one compartment can be identified (leaf biomass). With the stage of stem elongation (DC31–DC51) two

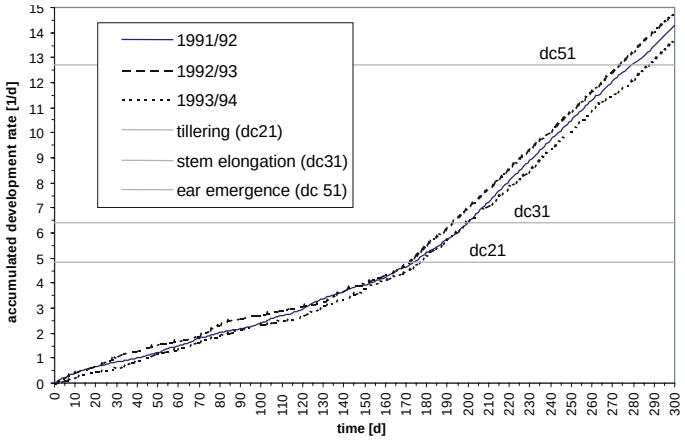

Fig. 6.2 Biological time as a function of different climatic conditions.

compartments are needed to describe crop growth, and in the maturity stage (from DC51) three compartments are used to describe the processes. The physiological model determines the structure of the growth model. The length of the different phases is determined by an external variable, the climate.

Subnet: Physiological Stage Model In the physiological stage model, the daily temperatures from sowing till harvest are stored in a table connected with the transition t_4, which calculates the biological time t_{biol}. This is performed using an external transition, which integrates the development rate depending on the daily temperature value and the parameters of the O'Neill function.

A token is put in one of the places p_{10}, p_{11}, or p_{12}, when a development stage is entered. This activates the transition of the crop growth model, which means that the differential equation system of the specific stage is solved numerically.

Subnet: Crop Growth Three distinct growth models define the transitions t_1, t_2, and t_3. The differential equations for $\vec{y} = (W_L)^T$, $\vec{y} = (W_L, W_S)^T$ and $\vec{y} = (W_L, W_S, W_E)^T$ are solved, when the transitions are activated. This activation of the transitions is done by the places p_{10}, p_{11}, and p_{12}, which contain a token, if the specific stage is reached. The calculation time, switching time in terms of the Petri net, depends on the length of the physiological stage. This $\Delta\tau$–value is handed over to the crop growth transition of the preceding stage by the places p_8 and p_9. The results of the simulation are the harvest biomasses in p_5 to p_7 at the maturity stage.

6.2.3 Results

The development of the biological time is shown in Figure 6.2 for the years 1991/92 to 1993/94. One can see that the beginning of the tillering phase is reached almost

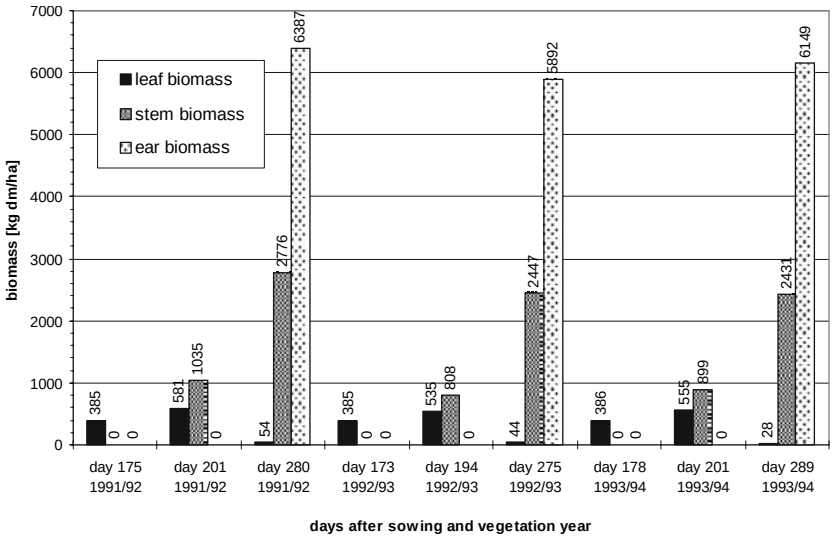

Fig. 6.3 Results of crop growth based on climate date from the years 1991/92 to 94/94.

at the same day of crop development each year. The end of the tillering phase in the vegetation years 1991/92 and 1993/94 was reached after the same number of days but in 1992/93, it ended one week earlier.

In 1992/93 maturity was observed 275 days after sowing, in 1991/92 after 280 days, but because of the low temperatures in the summer of 1994 not before 289 days after sowing (Figure 6.2). As with the biological time, the crop biomass shows a maximum in 1991/92. This was caused by the mild temperatures during winter and summer. In 1992/93, the biological time runs more quickly in comparison to the other years. Wheat reached its maturity stage earlier but with less biomass. The cold winter and spring of 1993/94 caused a slow development, so the wheat needed a long time for development but with middle maturity at harvest. Figure 6.3 shows the results of the simulated biomass for the years 1991 to 1994 for each organ.

This example demonstrates the capability of hybrid low level Petri nets for integration of continuous and discrete processes including a structural change of the mathematical model. The Petri net is used to synchronize the specific stages with its processes.

Possible extensions in this first case study are:

- a transition for a carbohydrate pool;
- retranslocation at the maturity stage;
- nutrient dependency, as described in Section 2.2.1, may be integrated into the transition, and
- the integration of event-based management, see Chapter 10.

All these extensions can be supported by the proposed modeling framework of hybrid low level Petri nets.

6.3 THE GALÁPAGOS ARCHIPELAGO AND THE BLUE-WINGED GRASSHOPPER

6.3.1 Meta-population in Island Biogeography

Insular Zoogeography Colonization of an island, persistence and extinction of a species depends on the habitat suitability and the distance to the next island or habitat (MacArthur & Wilson, 1963). Simulation models for colonization therefore comprise two processes: migration in spatial irregular structures and population dynamics on each island or habitat.

The probability for new species to settle on a particular island decreases exponentially with the distance to the living space. On the other hand, the probability for extinction increases with the number of species resident in a habitat. Species have to surmount inhospitable areas like oceans, deserts or mountains to reach a new island. Small, unsuitable habitats may support migration to suitable areas, because two small migration steps may be more successful than one big step. These islands are called *stepping stones*.

The larger the target island's cross-section, the likelier is a colonization (MacArthur & Wilson, 1963). The following discrete equation is used to calculate the number n of individuals that reach an island p_1 from the source region p_2:

$$n(p_1, p_2) = \alpha\, A(p_2)\, e^{-\lambda\, d(p_1,p_2)} \frac{1}{\pi} \arctan\left(\frac{1}{2}\frac{\mathrm{diam}(p_1, p_2)}{d(p_1, p_2)}\right) \tag{6.4}$$

This equation uses the area of source island p_2 denoted by $A(p_2)$, the mean distance $d(p_1, p_2)$ from island p_1 to p_2 and the diameter $\mathrm{diam}(p_1, p_2)$ of recipient island p_1 taken at a right angle to the direction from p_1 to p_2. This information is calculated using a geographic information system. The calculated number of individuals reaching

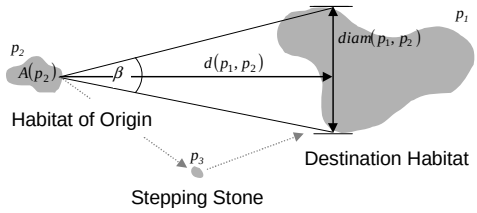

Fig. 6.4 Visual representation of the angle of visibility of a species migration from habitat p_2 to p_1. Additionally the migration path using a stepping stone island is sketched.

an island p_1 from p_2 per time step $n(p_1, p_2)$ requires the specification of the parameter λ which denotes the reciprocal of mean travel distance per time step and the number of individually leaving recipient island α. These parameters are species-dependent.

Figure 6.4 visualizes the approach by MacArthur & Wilson (1963). The angle or visibility of the destination habitat β is estimated by

$$\beta = 2 \arctan \left(\frac{1}{2} \frac{\text{diam}(p_1, p_2)}{d(p_1, p_2)} \right) \tag{6.5}$$

If we divide this expression by the angle of a fullcircle, 2π, we can derive the fraction of destination habitat that take part, with respect to all possible direction of migration, the full cirlce.

Reproduction Reproduction of individuals is estimated by the logarithmic growth

$$\frac{dP(p)}{dt} = r\, P(p) \left(1 - \frac{P(p)}{C(p)} \right) \tag{6.6}$$

$P(p)$ denotes population density on island p. Parameters of habitat suitability are introduced by the carrying capacity $C(p)$ of habitat p and the growth rate r. The latter is assumed to be constant for all islands. This continuous approach is suitable for most insect populations and many other species (Richter & Söndgerath, 1990).

In this first approach $C(p)$ is assumed to be linear depending on the island area $C(p) = \gamma A(p)$, with a fixed coefficient $\gamma > 0$. For this first case study the parameters were arbitrarily set to $\gamma = 0.1$ and $r = 0.06$ 1/h.

Case Study For detailed analysis the Ecuadorian Galápagos islands were selected as a typical oceanic archipelago. The Galápagos archipelago is located 1050 km west of the shoulder of South America and contains 13 large islands, 6 small islands, and 42 islets with a total area of 8006 km^2. Isabela, the largest one, is 4278 km^2. The distances between the islands range from 4 to 68 km. The archipelago's geology is completely volcanic and the vegetation ecosystem varies from rain forest to dry habitats with sparse vegetation. 378 species are endemic: 60% have been introduced by birds, 31% by wind, and 9% have been floated across the ocean. Nearly 800 species have been introduced by humans since 900 AD.

However, even if the Galápagos' ecosystems suffered from several non-endemic species, intruding the archipelago, this is clearly an artificial simulation experiment: The blue-winged grasshopper, *Oedipoda caerulescens* (Linnaeus, 1758) is a palaearctic species with a distribution from North Africa and the Canary Islands in the south to Central Europe in the north. Eastwards the distribution reaches Southwest Asia and China (Harz, 1975). The xerothermophilous species can be found in regions from plains up to mountains with sparse vegetation. These grasshoppers move about 10 m daily on average, but migration distances of 800 m per day have been recorded (Appelt, 1996; Appelt & Poethke, 1997). In 1996 it was observed that *Oedipoda*

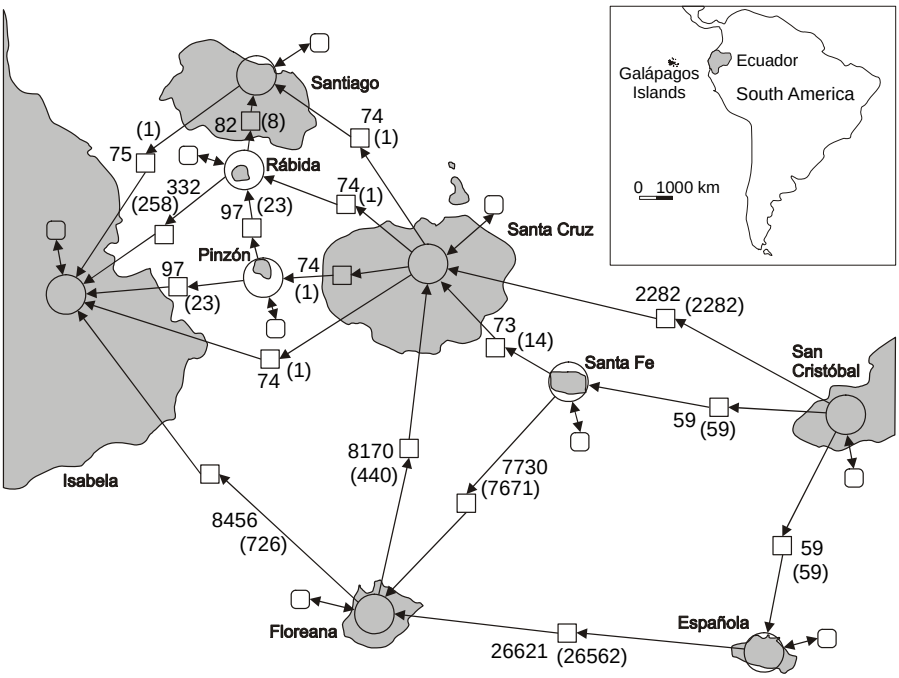

Fig. 6.5 Map of the Galápagos archipelago overlaid with the Petri net of a meta-population model. Transitions with rounded corners specify the continuous population dynamic model, differential equation. The numbers on the arcs denote the first possible colonization of an island. The numbers in brackets denote the average time in years grasshoppers need to migrate from one island p_1 to another p_2: $n(p_1, p_2)^{-1}$.

caerulescens have expanded their habitat from the island Rottumeroog to the island Borkum, both located in the North Sea. The distance between these two islands is 4.7 km. From these observations we derived $\alpha = 0.11/\text{km}^2$ and $1/\lambda = 6$ km using digital maps of the Galápagos archipelago in a GIS for the estimation of $A(p)$, $d(p)$, and $diam(p)$.

6.3.2 Spatially Explicit Hybrid Petri nets

Figure 6.5 shows a map of the larger islands of the Galápagos archipelago overlaid by the Petri net developed to estimate the expansion and population dynamics of *O. caerulescens*. Each place represents the species' population on an island. The transitions with rounded edges are connected by bidirectional arcs to the island places. They model the population dynamics based on Equation (6.6).

The process of migration is modeled by stochastic transitions, which connect the island places. Switching time of a migration transition is defined by an equally

distributed stochastic variable with the expectation value

$$n(p_i, p_j)^{-1} : \Delta\tau(t_j) = Z\left(n(p_i, p_j)^{-1}\right) \text{ with } p_i \in I(t_j), p_k \in O(t_j).$$

In Figure 6.5 numbers at the arcs denote the mean travel time from one island to another (numbers in brackets) and the date of the first possible appearance at an island after individuals have been released on San Cristóbal. Calculating the shortest route in the network using GIS functionality derives the latter.

6.3.3 Results

The following behavior is a typical result of the simulation experiments of intra-archipelagic migration: reproduction starts as soon as the first two grasshoppers are released on San Cristóbal. Santa Fe is the first island reached after a few years, but a small grasshopper population is no guarantee for a durable colonization. Grasshoppers may vanish on Santa Fe a few years after their settlement. Nevertheless, some individuals made the step from Santa Fe to Santa Cruz. There they were able to establish themselves and their population grew. Thereafter the first individuals reached the largest island Isabela using Santiago, Rábida, or Pinzón as stepping stones.

The right-hand part of Figure 6.6 demonstrates that on smaller islands the population is more often extinct than on larger ones. Reasons are the smaller population size and the emigration rate. The left part of Figure 6.6 shows the population sizes for all considered islands. For clarity, the population sizes of some selected islands can be seen in the right part of Figure 6.6. On some islands, the number of individuals varies widely depending on time. This effect has been observed in many field studies and is caused by the migration and immigration of grasshoppers.

The importance of the stepping stones can be quantified by analysis of the switching frequency of the migration transitions (part of net comitant). Figure 6.7 shows different pathways from the island San Cristóbal to Isabela using different stepping stones. The thickness of the arrows denotes the relative importance of the migration route with respect to the total number of migration events. The absolute number of events is noted on the arrows.

One can see that the settlement of the island Isabela is mainly caused by the population dynamics on the Island Santa Cruz and Santiago. The stepping stones Pinzón and Rábida are used to reach Isabela.

This case study shows that

- the framework of hybrid low level Petri nets enables the integration of dynamic population models with migration or meta-population models based on statistic approaches;
- the net structure and network parameters may easily be set up by information derived from GIS, which enables spatial simulations; and
- net comitants of Petri nets support an analysis of the developed model.

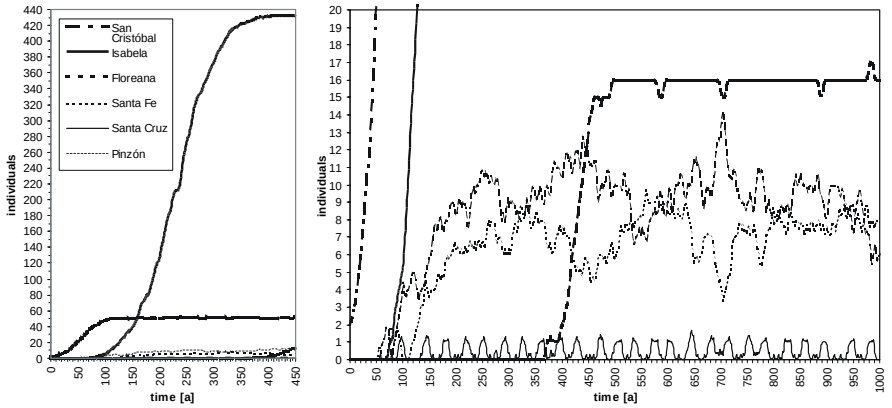

Fig. 6.6 Results of population dynamics on different islands of the Galápagos archipelago. The left figure shows the number of individuals of the larger islands Isabela and San Cristóbal. The right figure shows the population dynamics of possible stepping stone habitats like Floreana or Pinzón.

6.3.4 Comparison

Spatially explicit population dynamics can be modeled by a partial differential equations system, see Section 3.2.2. This approach is applied to this Galápagos example. The parameterization of the PDE can easily be performed. Most of the required information is available from the model development. Parameters required for a single species PDE-migration model are the growth rate r, carrying capacity C and migration distance of dispersal coefficient. The Petri net model uses a logistic growth model which is specified by a growth rate and a carrying capacity. The latter depends on the size of an island. This information is sufficient for specification of the right hand side of Equation (3.10). The dispersal coefficient D can be specified from the average migration distance known for *O. caerulescens*.

Figure 6.8 displays six time frames of this simulation. The upper left picture shows the initial population defined on San Cristóbal. With $t = 75$ a because of migration or dispersal the population density on this island decreased. It needs the same time for an establishment of the population on the first big stepping stone Santa Cruz ($t = 150$ a), as habitat is more suitable for the grasshopper population growth. The next islands are settled very quickly as several smaller islands support migration by their stepping stone function. The last time steps chosen are $t = 225$ a and $t = 250$ a. Note the population at Isabela reaches 250 individuals in accordance with the results from the Petri net model. Note, the scale for the density plots in Figure 6.8 is defined according to the population densities of the early time steps.

Using the partial differential equation model, an analysis of the migration pathways can be derived from a grasshopper-tracking analysis, a function most FEM-solver programs are capable of, usually known as *particle tracking*. Figure 6.9 shows such

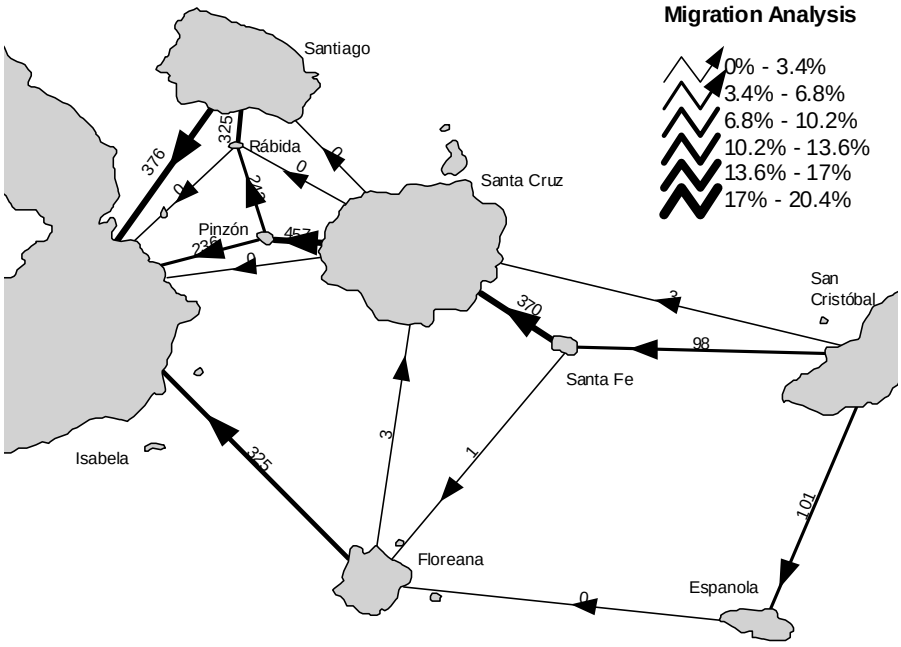

Fig. 6.7 Analysis of migration pathways of *O. caerulescens* in the Galápagos archipelago. Based on a 2.500 year simulation the movement of individuals between two islands are counted and noted at the arrows.

a *grasshopper tracking* analysis for time step $t = 142.5$ a. Each line displays the migration pathway for an interval of 100 years. A general statement compared to Figure 6.7 is difficult to derive from the PDE-model. In the simulation the most frequent (San Cristóbal, Santa Fe, Santa Cruz, Isabela) paths are displayed, which is in accordance to the Petri net model.

Both modeling approaches may be applied to the problem in hand. Both methodologies show advantages and disadvantages. For detailed comparison of the two modeling approaches Table 6.1 gives a summary of different aspects. In terms of scientific theory the partial differential equation system is the more concise, more aggregate model with a broad range of resulting explanations (compared to the parameters fed into the model). This equation collects the processes in one core equation. On the other hand, with this model we can run into more problems concerning numerics and interpretation. For instance, how shall we interpret positive population values (below unity) for open water regions? Shall we suggest the more phenomenological Petri net model, which has no physical explanation of Equation (3.10)? Or, is Equation (3.10) the *building block* for the migration process in patchy habitats?

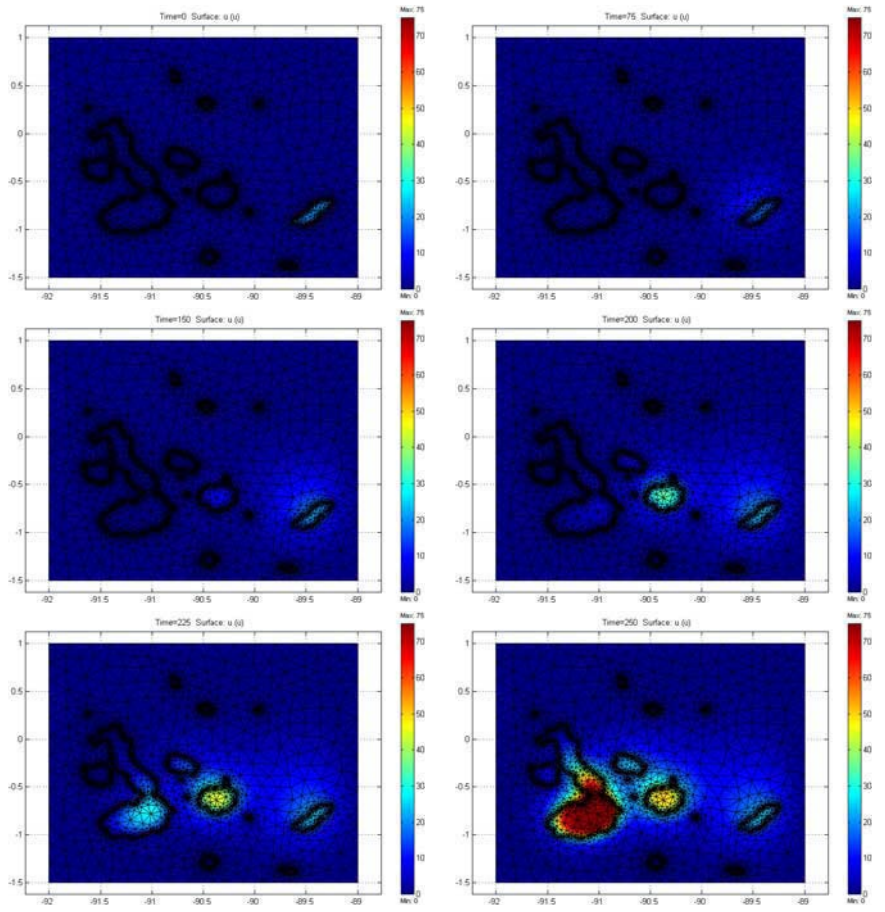

Fig. 6.8 Six time steps of spatially explicit population dynamics of *O. caerulescens* based on partial differential equation. Shown are (from upper left to lower right) the time steps $t = 0, 75, 150, 200, 225, 250$ a. (See p. 279 for additional resources.)

Modeling biological systems requires the development of mathematically heterogeneous or hybrid systems. This is because temporal or spatial processes show both discrete and continuous behavior. Hybrid models based on different mathematical modeling languages are the common result in ecological modeling. One possible general approach to these is the concept of hybrid Petri nets as described in the here. Analysis of the dynamic behavior of systems like these is indispensable when comparing and assessing different modeling approaches. The examples in this chapter showed that entirely different modeling approaches produced qualitatively, and to a certain degree quantitatively, equal dynamic behavior.

However, this can only be a starting point. Analysis of dynamic behavior includes concepts of stability analysis and dynamic and spatial invariant properties. This may

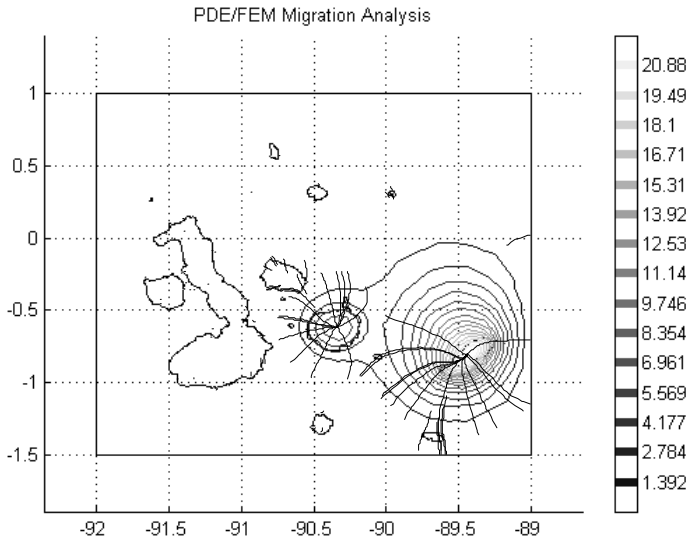

Fig. 6.9 Example of migration analysis based on partial differential equation system: A grasshopper tracking analysis.

be achieved by comparing the topologies derived from different dynamic simulation models.

For more detailed studies the methodology presented — comparing different modeling approaches — allows dynamic properties of models derived from different hybrid mathematical approaches to be studied, and enables the building blocks of ecological models to be identified. This might be a fruitful research topic, as it offers a deep insight into the relationship of different approaches in ecological modeling and might help to identify the building blocks of ecological models.

6.4 SUMMARY

Both applications show capabilities characteristic of the system. The application focussing on the hybrid crop growth model shows how a discrete system controls the state and structure of a continuous differential equation system depending on the states of a second differential equation. The application of the Gal ápagos meta-population model shows how stochastic discrete systems of migration are coupled with continuous systems for population dynamics. Furthermore, in this example properties of places are extended by spatial properties derived from geographic information systems. Additionally, Petri net theory supports the examination of these systems. Besides the analysis of the system behavior of differential equation systems (stability), the topology of the network can be investigated by the incidence matrix and dynamic structure can be analyzed using the net comitants.

Table 6.1 Comparison of the two modeling methodologies.

	Petri net	Partial Differential Equation
Processes		
Dynamics	Continuous (growth)	Continuous
Spatial	Stochastic, discrete (migration)	Continuous
Data		
Topology of habitats	The only information implemented into the Petri net is the topological relation between the habitats/islands	No information on topology of habitat patches deducible from FEM-mesh
Geometry of habitats	Only aggregated indicators on the geometry of the archipelago are fed into the PN-model: distance, diameter of a habitat.	FEM-mesh directly derived from habitat borders, imported from GIS.
Analysis, Results	– Stochastic analysis, Monte Carlo analysis – Event-based model – stepping stones – Migration distance	– Numerical solution by FEM using adaptive mesh generation – Experimental migration pathways – Migration distance – Nonnegative populations for open water regions
Classification	Empirical approach	Physical foundation on well-known diffusion/migration and growth models.

The important capability of the system is model development for anthroposphere–biosphere interactions. A general concept at global scale is presented by Schellnhuber (1998) based on a theoretical system approach in terms of ordinary differential equations. In classical ecosystem models, anthropogenic effects enter the system as environmental covariables or indirectly via the control parameters. Models of technical systems are primarily devised for process control and optimization and yield at most the order of magnitude of emission rates. In reality both systems are closely interlocked and should be treated as a whole at least at higher scales, see Section 1.3.4, p. 20. Environmental impact assessment of human activities necessitates a comprehensive analysis of both industrial and ecological systems.

7

Applications: Environmental Impact Assessment

7.1 INTRODUCTION

Life cycle assessment (LCA) is widely used as a tool for assessing the environmental aspects and potential impacts of products and services. While the methodology is well developed for the steps goal definition and life cycle inventory (LCI), impact assessment is still under discussion (Pohl *et al.*, 1996; ISO, 1997).

The Society of Environmental Toxicology and Chemistry (SETAC) called for the development of models which integrate the fate and impact of emissions in the assessment of the life cycle of products (SETAC, 1993). There is also a need for expert systems which facilitate the step of impact assessment within LCA (SETAC, 1993). German Federal Environmental Agency (Umweltbundesamt) requests consideration of global and local impacts within life cycle assessment (LCIA). The SETAC LCA impact assessment work group asks for an integration of different techniques to conduct a more complete and holistic environmental assessment (SETAC, 1997). Suitable quantification parameters exist for the calculation of the potential environmental impact of emissions on a global scale such as global warming or tropospherical ozone depletion. Impact potentials like global warming potential (GWP) or ozone depletion potential (ODP) are already widely used in LCA.

The intensity of local and regional impacts, for example acidification or eutrophication, depends on variable environmental conditions and is therefore *site dependent*. Hence many authors, for instance Owens (1996), Tolle (1997) and Krewitt *et al.* (1998), state that the concept of global parameters is not useful for the LCIA of local and regional impacts. A research goal is then to develop and evaluate suitable methods for assessing local and regional impacts within LCA.

7.2 AIM AND SCOPE

An appropriate methodological concept that can solve the problem of site-dependent impact assessment of goods and services requires an integrated spatially explicit model. The required integration can be achieved by the use of a hybrid Petri net. The intention of this case study was to develop a generic concept for an integrated approach for environmental assessment where LCI, environmental fate modeling, and environmental impact assessment together can be used as a tool to assess local and regional impacts of emissions released along the life cycle of products. The actual impacts at the point of emission for several impact categories ought be addressed site-dependently. This approach is unusual, as it suggests a truly integrated approach. It reaches far beyond LCIA by the use of other environmental modeling techniques. This study was carried out in a co-operation with the Department of Environment and Transportation of Volkswagen AG, Wolfsburg (Thiel *et al.*, 1999). The following section summarizes the basic concept of the general assessment model followed by the description of a prototypical implementation of an application and the results.

7.3 METHODOLOGY

To meet the required extensions for a truly integrated approach, a general method was developed which consists of three modules. These are:

- life cycle inventory;
- environmental fate modeling, comprising chemical reactions and the spatial spread of emissions;
- a detailed environmental impact assessment based on the results of the previous step and operated by fuzzy expert systems, which allow an assessment of ecological impacts for several categories at one site involved in the system life cycle.

Figure 7.1 summarizes this methodological concept. In the upper part of the figure the LCI phase is symbolized by a small Petri net. Petri nets are suitable for modeling production processes, as these processes are frequently discrete and show all the properties of event-based systems. Moreover, the Petri net model can be extended to represent the entire life cycle of the product.

Production, use, and deposition as well as recycling of products, leads to emissions. In this integrated concept emissions are traced by an environmental fate model. The environmental fate model covers the processes of transport through different media (atmosphere, soil, or water) and possible reactions the substances go through during transport. Finally a substance reach environmental sinks, which are identified as *receptors* of immissions. In this case study the focus is on atmospheric transport

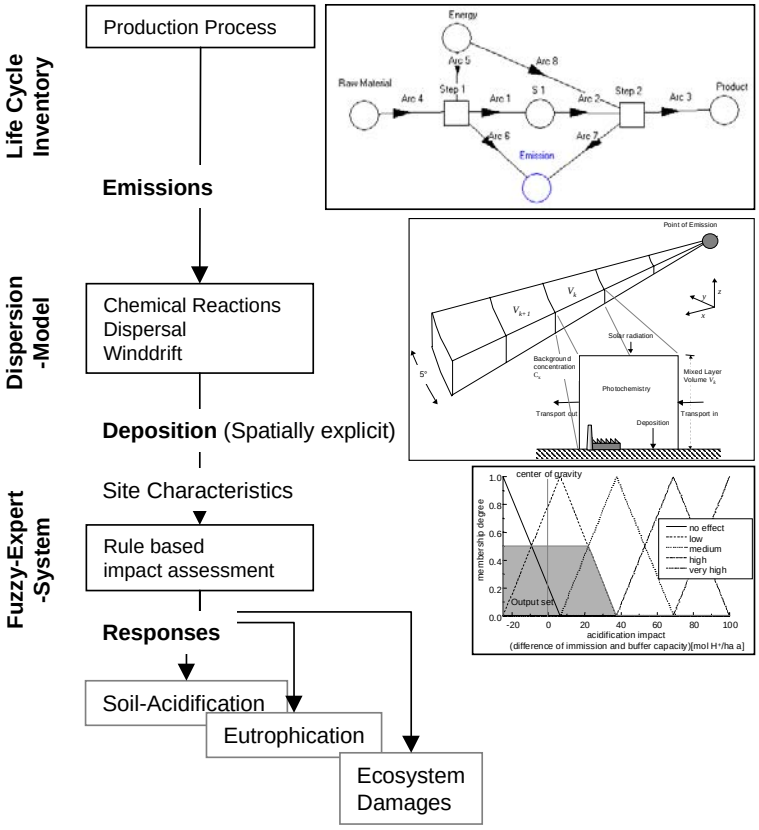

Fig. 7.1 Methodological concept of the integrated approach for life cycle impact assessment.

of NO_x. Soil, ecosystem, and plant are used as examples. They may be replaced by any other receptor whose potential impacts have either a regional or local spatial environmental sensitivity, see bottom of Figure 7.1.

Note, that from top to bottom of Figure 7.1 several methodological boundaries are crossed. This methodological spectrum covers deterministic modeling (event-based and continuous) and application of soft-computing methods. Soft-computing methods, in this example fuzzy expert systems, are used for the assessment of environmental impact on soil acidification, eutrophication, and plant damage. The uncertainty of the knowledge and the imprecision of the information increases from top to bottom of the figure.

7.3.1 Life Cycle Inventory

LCI was performed using the theoretical background of Petri nets, cf. Chapter 5. Material and flow analysis are modeled by a network approach based on the Petri

nets. Production and transport processes are identified with transitions. The transitions are the graphical representations of the mass and energy flow equations of the different processes. Storage places, products, raw material deposits, and emissions are identified with places.

To undertake a LCI of a product, the sites of production are usually known (otherwise the transport distances could not be determined). We did not aggregate the same processes at different sites to unit processes but designed the Petri net in such a way that we could calculate the site-specific mass flows of the stationary emission sources. Knowing annual production for the studied product, the mass flow values can be transformed into mean annual in- and output values. The site-specific emissions or output places define the interface between the LCI and environmental fate modeling.

7.3.2 The Link: Environmental Fate Modeling

Environmental fate models support the calculation of the spatial spread of emissions starting from the point of emission, providing the results as concentrations and immissions in space and time. It thus models the source–receptor relationship. The environmental fate of emissions can be modeled by different approaches for the media soil, water, or air. All dispersion models are based upon systems of differential equations which contain terms for transport, chemical reactions, and deposition processes, see Chapter 3.

The sites of emission from the LCI have to be geographically localized. Their mass flows are identified as sources in the context of a dispersion model. Output places from the LCI may be mobile (e.g. transports) or stationary point sources (e.g. stacks) or diffuse inputs (such as nitrogen leaching out of agricultural sites). It depends on the observed process (in the transitions) of the LCI. The GIS supports these different types of information exchange from LCI results to reaction dispersion models.

Modeling the spatial spread of emission also depends on the observed media. Several modeling approaches exist for transport modeling in atmosphere, water, or saturated and unsaturated soil horizons, see Chapter 3. It is useful to couple models for different media. In most cases the emitted substances pass from one medium to the other.

7.3.3 Fuzzy Expert Systems for Impact Assessment

Basic Concept The results of the environmental fate modeling are used to assess the exposure of environmental components to a certain substance or burden, cf. Figure 7.1. In the integrated approach the assessment is performed by a fuzzy expert system, which links the results of transport modeling and environmental receptors. The first two phases of the integrated LCA approach, presented in Sections 7.3.1 and 7.3.2, describe physical and chemical processes which can be simulated by deterministic models. The ecological impacts of immissions are a result of complex interactions, which can often be described only by heuristic approaches (Kelly &

Harwell, 1989). Nevertheless, the causality between the exposure to a burden and the response of a receptor can often be described by expert knowledge.

An environmental impact assessment tool must be capable of dealing with imprecise data and must be able to come to a conclusion despite the uncertainty. An adequate method for mathematical modeling of processes which deal with uncertainty is *fuzzy logic*. In classical set theory the membership of an object x to a set A out of a class X is defined by the two values 1 if x belongs to A: $x \in A$ and 0 if $x \notin A$. In fuzzy set theory a set A is characterized by a membership function $\mu : X \rightarrow [0, 1]$ which assigns to each object $x \in X$ a grade of membership to the set A ranging between zero and one. This property of fuzzy sets can be useful in environmental impact assessment. For example, the transition from favorable to unfavorable environmental conditions for a receptor is often not crisp but fuzzy. The notions and operators of classical logic have been extended to fuzzy sets within the theory of fuzzy logic allowing approximative reasoning under uncertainty (Yager & Zadeh, 1992). The theory of fuzzy fogic is outlined in Zadeh (1965).

One of the first application of fuzzy logic in modeling social systems with non-measurable variables was presented by Seppelt (1998). Based on these principal ideas, a generalized exposure–response model using fuzzy logic was developed to assess the environmental effects of the calculated immissions. Figure 7.2 shows the structure of the generalized model. The use of fuzzy set theory in expert systems not only allows crisp values from LCI to be used as input variables, but also linguistic terms can be used in the database. In ecological assessment this is a particularly important advantage.

Generic Expert System for Impact Assessment In the first step, the sensitivity of a receptor to a certain exposure is defined by a *buffering capacity*. This concept is well-known in soil science and agrochemistry, where it means the capability of the soil to neutralize acid input or withdrawal of nutrients. For the integrated approach we generalized this concept. The buffering capacity takes into account the ability of the receptor in most of the exposure–response relationships, to buffer exposures without showing any measurable effect. The buffering capacity depends on regional characteristics. In Figure 7.2 the sub-model which calculates the buffering capacity is shown in the box named *environmental conditions*. Here, the parameters 1 to n represent environmental characteristics and determine the buffering capacity. The sub-model for the calculation of the buffering capacity is applied to the different impact categories, for example soil acidification or eutrophication. The interdependence of the environmental characteristics and the buffering capacity has to be deduced from expert knowledge.

In the second step, the possible response of the receptor is assessed by comparing the buffering capacity with the immission values. If the immission values exceed the buffering capacity, a measure for the potential ecological impact of the immission is derived.

The environmental assessment is performed by fuzzy expert systems in the integrated LCA approach. In Figure 7.2 the squares represent variables whose different expres-

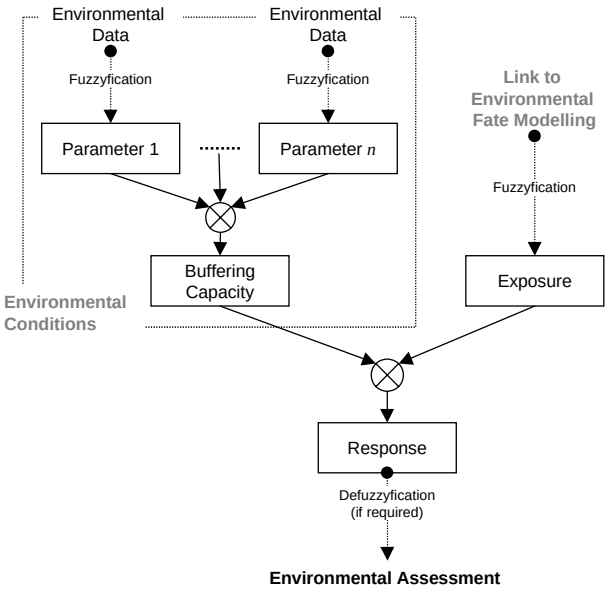

Fig. 7.2 Structure of the generalized fuzzy expert system for environmental assessment of substances exposure as an extension of a dose–response framework based on critical load concept.

sions are defined by fuzzy sets. The triangles represent rule nodes. A typical rule could be: "if parameter 1 is low and parameter 2 is low, then the buffering capacity is low". The membership functions of the generalized response variable are defined as follows: If the membership degree of the fuzzy sets of "no effect" and "low" are equal, then the defuzzyfication of the result by center of gravity leads to the value 0, see Figure 7.3. The response variable can easily be adapted to different receptors by rescaling of the *x*-axis. Units for the *x*-axis should be chosen so that defuzzyfication leads to crisp values which represent determinable effects.

The fuzzy sets of the immission, the buffering capacity and the response variable are defined in connection with the rule node in a way that, when the immission exceeds the buffering capacity, this leads to positive response values (i.e. negative effects). In the opposite case the output of the response variable is "no effect".

There are two alternatives for the interpretation of the resulting output:

- The first possibility is to have the output as linguistic variables. As the resulting output the fuzzy set with highest membership value is chosen. This could be for example: "possible damage is very high" with the membership degree 0.6.
- The second alternative is a crisp value after defuzzyfication. This is a theoretical value which represents the difference between immission and buffering capacity. Hence the impact on the receptor can be quantified and model estimates can even be evaluated in on-site measurements.

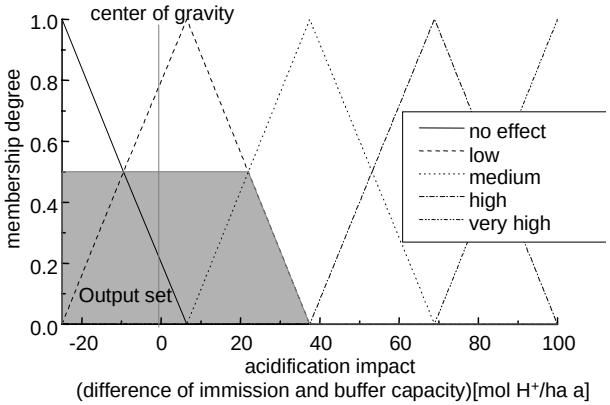

Fig. 7.3 Membership functions of the response-variable soil-acidification.

System Specification The implementation of a fuzzy system requires the specification of a considerable number of parameters and options. The observance of all the criteria described above leads to transparent and plausible conclusions within the systems. For the development of the LCIA fuzzy expert systems the following rules are used to minimize the number of free parameters in the fuzzy expert systems:

- definition of five fuzzy sets with normalized membership-functions per variable: sets from "very low" (respective to "no effect" for the response sets) up to "very high", see also Figure 7.3;
- sum of all membership values over all fuzzy sets per variable equals one;
- definition of the membership functions in a way that one value can belong at most to two different fuzzy sets;
- use of minimum operator for modeling of an "and"-connection in the premises;
- use of maximum operator for modeling of an "or"-connection in the premises;
- use of Mamdani implication for the conclusion procedure;
- use of supremum-minimum operator for the propagation;
- (if desired:) final calculation of a crisp value ("defuzzyfication") by the center-of-gravity method.

7.4 LIFE CYCLE INVENTORY OF THE PRODUCTION PROCESS

The following section sheds light on the application of the modeling and assessment concept presented above. The approach was applied to the life cycle of car components produced by Volkswagen AG. A life cycle inventory has been prepared for the

planned production of magnesium (Mg) door parts using the annual Polo production in Wolfsburg of 1995. The environmental fate modeling focused on the fate of emitted nitrogen oxides as they cause several typically regional or local impacts. In the environmental assessment of the NO_x-emissions the possible response of the three receptors crop, soil, and ecosystem were assessed.

The following processes were investigated in the LCI for the planned production of the magnesium door parts:

- raw magnesia production,
- production of the alloy Mg-AM 60,
- smelter,
- die casting,
- part finishing,
- chromate treatment,
- recycling of the production residues (leading to input of secondary Mg-AM 60 in the smelter),
- transportation between the different production sites as well as the recycling facilities.

The Mg-production and alloy production take place in Israel at the Dead Sea Works plant, cf. Figure 7.4. The other processes from smelter to chromate treatment take place in Germany. The data for the production activities were provided by Volkswagen. The transportation processes between the production sites were calculated using databases from the underlying LCI tool Umberto. The portion of secondary Mg-AM 60 input in the smelter was assumed to be 24.7%.

NO_x-emissions are chosen for detailed study: The results of the LCI show that more than 80% of the NO_x-emissions are released in the first two processes at the Dead Sea Works in Israel. The remaining NO_x-emissions occur at energy production sites in Germany (16.8%) and in other operations (1.9%). The high share of NO_x-emissions in Israel is mostly due to the fact that at Dead Sea Works the energy demand is covered by a power plant burning residual oil. The power plant is located in Israel at the southern end of the *Dead Sea*. Hence, in the environmental fate modeling, we focused our attention on the environment of this site. The emission results of the LCI yield the input flow of the reaction–dispersion model. We made calculations for the annual Mg production of approximately 30000 t at Dead Sea Works. The annual demand due to VW-Polo production is only about 8.2% of this amount. However, to estimate the potential impact of the NO_x-emissions on the environment near the power plant, the calculations should be based on the energy demand for the entire annual Mg production at this site.

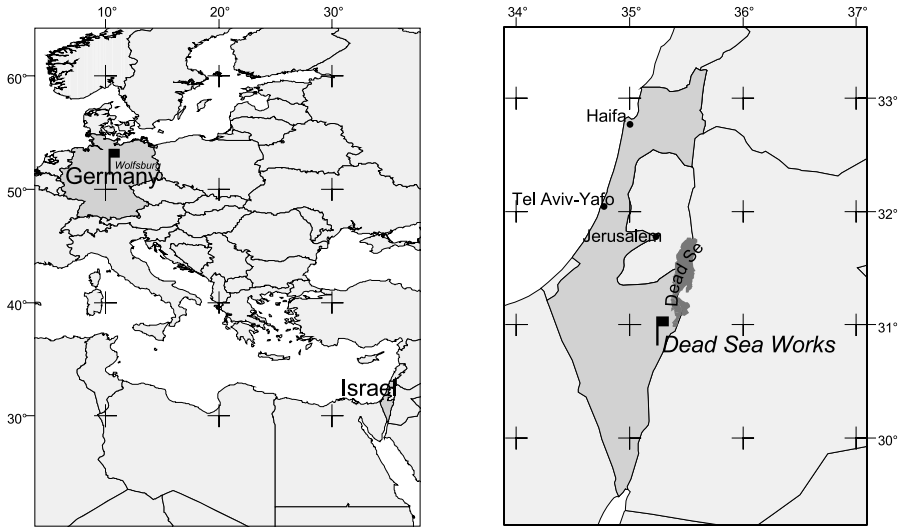

Fig. 7.4 Location of Dead Sea Works plant south of Dead Sea, Israel. Assessment of emissions as a consequence of the production located at Wolfsburg factory in Germany. From this plant have to refer to the environmental conditions of the surrounding study area.

7.5 ENVIRONMENTAL FATE MODELING OF NO_x-EMISSIONS

7.5.1 Overview

Three different concepts can be distinguished for modeling atmospheric transport of substances.

1. Physical models, that describe the processes of the Ekman layer with its turbulent processes based on Navier–Stokes equation (Seinfeld & Pandis, 1998). Using this methodological concept for the problem in hand, one has to solve a system 3D partial differential equation, one equation for every substance. These equations are coupled by their reaction terms. This approach therefore creates an enormous numerical effort.

2. Stochastic models, that represent the process of dispersal by a spatially explicit stochastic variable, that gives several realizations of a random function describing a puff (Liu & Du, 2003).

3. Aggregated models, that use analytical solutions of the Navier–Stokes equation, or an arbitrarily chosen discretization of the spatial variable, together with knowledge of the stochastic process of dispersal to parameterize analytical equations (Seinfeld & Pandis, 1998).

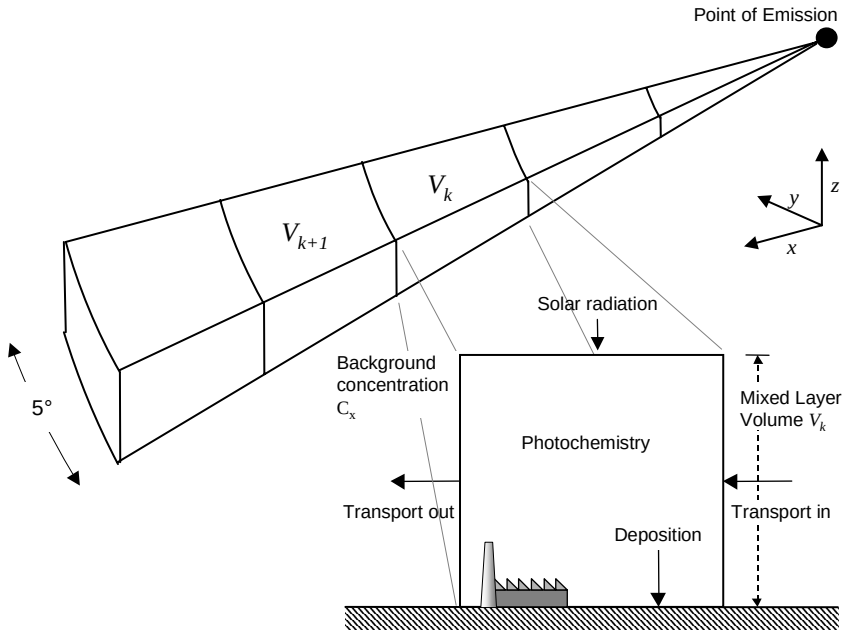

Fig. 7.5 Concept of atmospheric transport model for the processes of diffusion and wind spread according to the box-model approach. Conceptual model of environmental fate model. The processes of transport, reactions and deposition are assumed to be constant for a defined box of the atmosphere.

Integrated models result from modeling processes, that use discretization of aggregated partial equations. Similar to the matter transport example from Section 3.2.1 environmental fate modeling of substances in the atmosphere requires consideration of the two processes, transport and reaction.

7.5.2 Atmospheric Transport Model

The environmental fate modeling of the emitted NO_x has been performed by a box-model approach, (Fisher & Smith, 1987; Russell, 1988). The emission smoke plume is numerically separated into several discrete compartments with a trapezoid surface (x- and y-axis) and a constant height of 1000 m (z-axis). Figure 7.5 illustrates this approach. The trapezoid surface takes into account the increasing width of the plume (as a function of the distance to the emission source). The limitation to the height of 1000 m is due to the observed mean height of the boundary layer (Stull, 1988). This limitation of the boundary layer is caused by a temperature inversion in the lower troposphere. The inversion has the effect of an exchange barrier between the atmospheric layers above and below, cf. Figure 7.5.

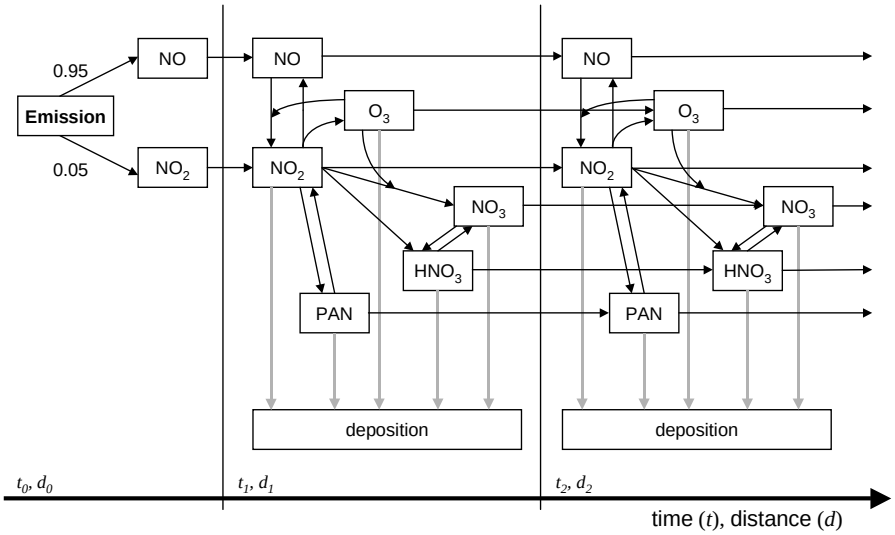

Fig. 7.6 Conceptual model of NO_x environmental fate: chemical reactions and deposition processes of the NO_x dispersion–reaction model.

Most frequently meteorological situations based on long term meteorological mean values are used to set up the base for reaction dispersion modeling scenarios. Furthermore different scenarios can be defined by possible future production of the car components. For detailed study, production is assumed to be constant and different meteorological scenarios are defined.

For environmental fate modeling a box-model was chosen that couples the transport processes of NO_x with the chemical reactions in the atmosphere. Stack emissions are approximated assuming continuous operation of the power plant. Mean wind speed and direction for the site are taken from Adler (1985). Dispersion was calculated with discrete time steps of 1 hour.

Chemical reactions and deposition are calculated for each numerical compartment of the plume. Figure 7.6 shows the chemical reactions and substances which are taken into account. The chemical reactions and deposition processes are modeled based on an ordinary differential equation system. The box-model simulates the matter transport by successive numerical solution of the initial value problem. Initial values for the background concentrations were taken from Krüger & Graßl (1994). Chemical reactions are a function of ambient temperature and concentrations. Parameterization of those functions is according to Simpson *et al.* (1990) and Krüger & Graßl (1994). Deposition rates are assumed to be constant, cf. (Grennfelt *et al.*, 1987; Krüger & Graßl, 1994). A practical assumption for long-term prediction in the considered dry region is, to aggregate wet and dry deposition to a total deposition rate. Properties of the boundary layer are different for day and night and in winter and summer.

7.5.3 Process Model

This section gives a summary of all model equations, parameters and background concentrations of the model. The ODE system is run for each box-compartment, cmp. Figure 7.5.

General Notations The following general notations hold. Time t dependent concentrations of a substance i in a box-compartment $k = 1, 2, \ldots$ is denoted by $C_{i,k}(t)$ holding the concentration in $[\mathrm{mol/cm^3}]$. The box-compartment k has a volume V_k in $[\mathrm{cm^3}]$. Reaction coefficients k_i may depend on temperature T in kelvin [K]. Depositions rates d_i are given in [1/d].

General Initial Condition Convection and dispersion is modeled by a general initial condition, which presents the concentrations of a substance i in the following box-compartment.

$$C_{i,k+1}(0) = C_i(0) + \frac{1}{V_{k+1}} C_{i,k}(t) V_k \left(1 - \frac{C_i(0)}{C_{i,k}(0)}\right) \tag{7.1}$$

This equation defines that the initial condition of compartment $k + 1$ is calculated by the background concentration C_i plus the non-background fraction of substance moving from compartment k, given by $C_{i,k}V_k$ into compartment $k + 1$, considering the attenuation by the larger box volume $(1/V_{k+1})$.

System of Reaction Equations The translation of the conceptual model in Figure 7.6 into mathematical equations results in the following system of ODEs. The system is linear, as all reactions are assumed to be linear. This equation system is

Table 7.1 Background concentration values $C_i(0)$ and deposition rates d_i for substance i used for the environmental fate model.

Substance	NO	NO_2	PAN	HNO_3	NO_3	O_3	
$C_i(0)$	0.987	1.93	0.196	0.654	1.88	189000	$10^{-17}[\mathrm{mol/cm^3}]$
d_i		0.036	0.144	0.0072	0.0036	0.018 (daytime) 0.0018 (at night)	[1/h]

Table 7.2 Parameters of reaction rates for environmental fate model of NO_x.

	Day			Night			
	[OH·] [mol/cm^3]	[CH_3COO_2·] [mol/cm^3]	T [K]	[OH·] [mol/cm^3]	[CH_3COO_2·] [mol/cm^3]	T [K]	α solstice
Summer	$2.67 \cdot 10^{-18}$	$4.78 \cdot 10^{-18}$	308	$2.62 \cdot 10^{-20}$	$4.35 \cdot 10^{-19}$	298	82.5°
Winter	$2.32 \cdot 10^{-18}$	$6.67 \cdot 10^{-18}$	291	$2.32 \cdot 10^{-20}$	$6.06 \cdot 10^{-19}$	282	35.5°

solved for each box-compartment k. The index k is not printed.

$$
\left.
\begin{aligned}
\frac{dC_{NO}}{dt} &= k_{NO_2\,NO}(t)C_{NO_2} - k_{NO\,NO_2}(T)C_{NO}C_{O_3} \\
\frac{dC_{NO_2}}{dt} &= k_{NO\,NO_2}(T)C_{NO}C_{O_3} + k_{PAN\,NO_2}(T)C_{PAN} \\
&\quad -\Big(k_{NO_2\,NO}(t)k_{NO_2NO_3}(t,T)C_{O_3} + k_{NO_2\,HNO_3}[OH\cdot] \\
&\quad +k_{NO_2\,PAN}[CH_3COO_2\cdot] + d_{NO_2}\Big)C_{NO_2} \\
\frac{dC_{HNO_3}}{dt} &= k_{NO_2\,HNO_3}[OH\cdot]C_{NO_2} + k_{NO_3\,HNO_3}C_{NO_3} \\
&\quad -\left(k_{HNO_3\,NO_3} + d_{HNO_3}\right)C_{HNO_3} \\
\frac{dC_{PAN}}{dt} &= k_{NO_2\,PAN}C_{NO_2}[CH_3COO_2\cdot] \\
&\quad -\left(k_{PAN\,NO_2}(T) + d_{PAN}\right)C_{PAN} \\
\frac{dC_{NO_3}}{dt} &= k_{NO_2\,NO_3}(t,T)C_{NO_2}C_{O_3} + k_{HNO_3\,NO_3}C_{HNO_3} \\
&\quad -\left(k_{NO_3\,HNO_3} + d_{NO_3}\right)C_{NO_3} \\
\frac{dC_{O_3}}{dt} &= -\left(k_{NO\,NO_2}(T)C_{NO} + k_{NO_2\,NO_3}(t,T)C_{NO_2} + d_{O_3}(t)\right)C_{O_3} \\
&\quad k_{NO_2\,NO}(t)C_{NO_2}
\end{aligned}
\right\} \quad (7.2)
$$

Coefficients Parameter values for background concentration of the molecules considered are listed in Table 7.1. Values for the reaction coefficients of the system (7.2) are obtained from (Krüger & Graßl, 1994; Simpson *et al.*, 1990). Table 7.2 gives an overview of all parameters needed for a model run. Several reaction rates depend on time or temperature:

$$
\begin{aligned}
k_{NO\,NO_2}(T) &= 7.56\,10^{-9}\exp\left(-1450\frac{1}{T}\right) \quad [cm^3/mol/h] \\
k_{NO_2NO}(t) &= \begin{cases} 18\exp\left(-0.39\frac{1}{\sin(\alpha)}\right) & \text{daytime} \\ 0 & \text{else} \end{cases} \quad [1/h] \quad \text{(desert area)} \\
k_{NO_2\,PAN} &= 1.15 \cdot 10^{-8} \ [cm^3/mol/h]
\end{aligned}
$$

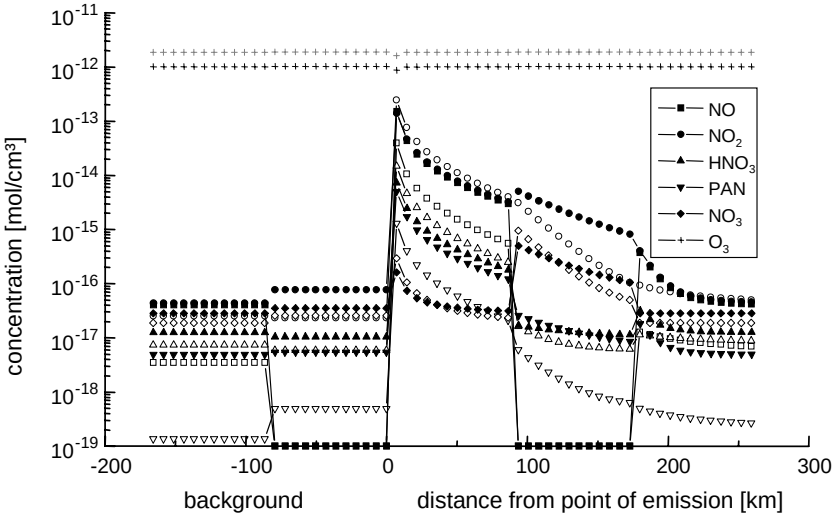

Fig. 7.7 Results from long term forecasts of concentrations. For a comparison of the climatic situation of winter and summer, the corresponding graphs are juxtaoposted: winter: dark dots, summer: small circles.

$$
\begin{aligned}
k_{\mathrm{NO_2\,HNO_3}} &= 3.96 \cdot 10^{-8} \ \ [\mathrm{cm^3/mol/h}] \\
k_{\mathrm{PAN\,NO_2}}(T) &= 2.7 \cdot 10^{18} \exp\left(-12530 \frac{1}{T}\right) \ \ [1/\mathrm{h}] \\
k_{\mathrm{NO_2\,NO_3}}(T,t) &= \begin{cases} 8.64 \cdot 10^{-10} \exp\left(-2450 \frac{1}{T}\right) & \text{at night} \\ 0 & \text{else} \end{cases} \quad [\mathrm{cm^3/mol/h}] \\
k_{\mathrm{HNO_3\,NO_3}} &= 3.6 \cdot 10^{-2} \ \ [1/\mathrm{h}] \\
k_{\mathrm{NO_3\,HNO_3}} &= 1.8 \cdot 10^{-2} \ \ [1/\mathrm{h}]
\end{aligned}
$$

7.5.4 Results

The results of this simulation are long-term forecasts of concentrations. Long-term forecast is here understood as annual mean values in the time range of several years. Figure 7.7 shows the results of the environmental fate modeling given as concentrations in the plume. To demonstrate the difference in the reaction dynamics in winter and summer, the corresponding graphs are juxtaposed. Windwards of the stack (left portion in Figure 7.7) the daily variation of the background concentrations can be observed. Steady state conditions are presumed during the day and during the night. Leewards of the stack (right portion in Figure 7.7) the plume's influence on the atmospheric concentrations of the considered substances is shown. The NO_x-concentrations near the stack are significantly higher than the presumed background

values. Nevertheless, the NO_x-concentrations caused by magnesium production do not exceed the average NO_x-concentrations of Jerusalem, a NO_x-burdened site in Israel (Luria *et al.*, 1985). About 250 km leewards of the stack, the NO_x-concentrations are almost down to the background level again. Note that in summer the reactions are faster than in winter because temperatures and levels of oxidants (e.g. ozone) are both higher. For the subsequent environmental impact assessment step, the mean concentration and deposition values which were derived from the different winter/summer and day/night scenarios, are used.

7.6 ENVIRONMENTAL IMPACT ASSESSMENT

From the generic fuzzy expert system discussed in Section 7.3.3 three models are specified, that assess the impact of immissions on the ecosystem characterized by selected indicators. The selected indicators are *plant damage*, *soil acidification*, and *eutrophication*.

7.6.1 Soil Acidification

The model for soil acidification caused by NO_x is presented in detail below. It is based on an expert system developed by Kuylensstierna *et al.* (1995). The fuzzy expert system is illustrated in Figure 7.8. In this model, average soil pH values and ambient precipitation/evaporation indices determine the buffering capacity of the soils.

High pH values of the soil obviously result in a high buffering capacity. A low precipitation/evaporation index also leads to a high buffering capacity, because, in semiarid or arid regions, we observe mostly ascending movements of the soil-water, which leads to increase in calcium carbonates in the upper soil horizons. This eventually contributes to the development of Pedocals (Eyre, 1968). High deposition of protons (acids) and low buffering capacities lead to high acidification impact and vice versa.

Figure 7.9 shows the result of the case study employed on the fuzzy expert system for soil acidification. In this scenario, impact for wind direction North-West is calculated,

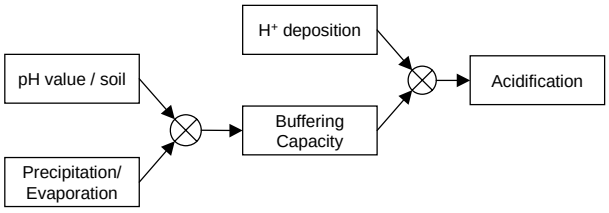

Fig. 7.8 Structure of the fuzzy expert system for soil acidification.

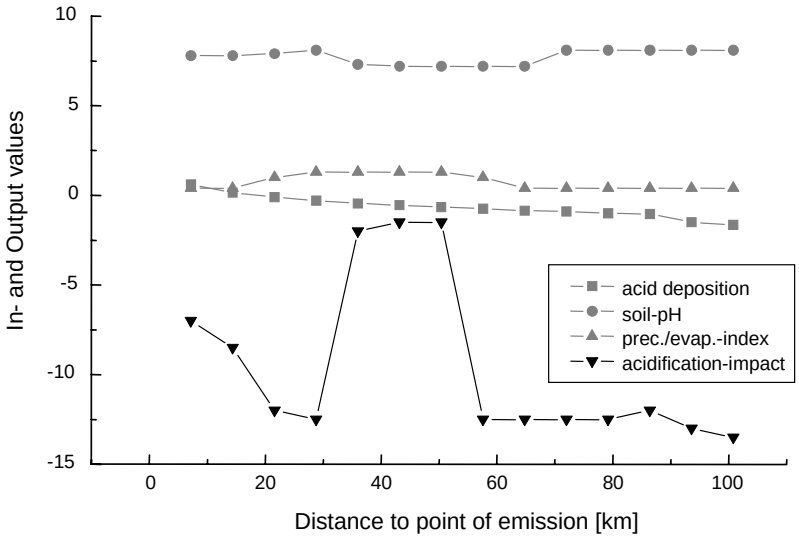

Fig. 7.9 Possible soil-acidification impact in the scenario "South-East of the stock" (see text for explanations of input and output values).

which means that the plume spreads in direction South-East of the stack. Data for the environmental conditions is taken from Adler (1985). Units in this figure are:

H^+-deposition	log[mol H^+/ha/a]
pH-value	-log[H^+]
precipitation/evaporation index	dimensionless [mm/mm]
possible impact	[mol H^+/ha/a]

Here the impact is always below 0 which means that the H^+-deposition due to the NO_x-emissions caused by the power plant is below the buffering capacity of the soil. This example illustrates the high sensitivity of the model to changes in the environmental conditions. From km 30 to km 50 the plume traverses the Jordan mountainous region. The soils of this region are slightly more acid than the soils in the Jordan valley and East of the mountains. The values for the possible acidification-impact change with the soil-pH. The calculations for the other 7 directions lead also to the result that the H^+-deposition due to the NO_x-emissions caused by the power plant is below the buffering capacity of the soil.

7.6.2 Eutrophication

The fuzzy expert system for eutrophication is based on the critical loads concept, see (Nilsson, 1986). In this model, the different soil characteristics cation exchange capacity (CEC), moisture, temperature and C/N-ratio determine the main N-buffers: biomass, denitrification and humus. In the model, the capacity of the biomass to

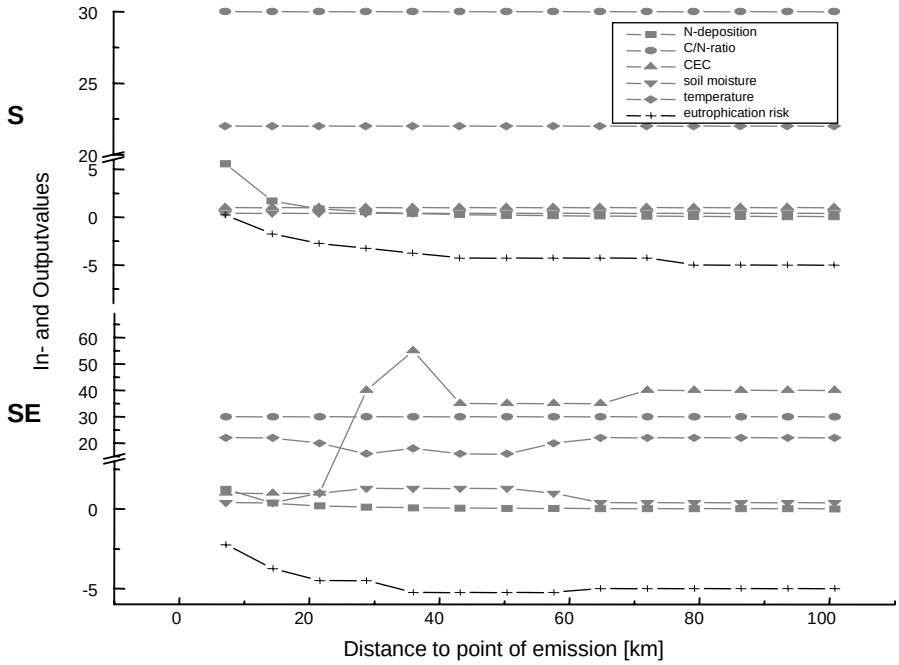

Fig. 7.10 Possible eutrophication impact in the scenario "South" (upper part of figure) and "South-East" (lower part) of the stack.

buffer an additional N-input is determined by the application of the minimum principle of Liebig. The capacity is limited on the one hand by the CEC which represents the availability of nutrients and on the other hand by the precipitation/evaporation index which indicates the availability of soil water. A high precipitation/evaporation index and a high CEC have a positive effect on the biomass buffer and vice versa. The denitrification performance of the microorganisms is influenced by the temperature and the precipitation/evaporation index. High values of both factors lead to a good denitrification performance. The immobilization of nitrogen within the humus fraction is increased by a high C/N-ratio and vice versa (Gundersen, 1992).

The three N-buffers determine the buffering capacity of the ecosystem with respect to nitrogen input. Supplementary N-input by microbiological fixation of N_2 is not considered, according to (Posch, 1993). Loss of nitrogen by leaching is negligible due to the aridity of the region studied, cf. (Noy-Meir & Harpaz, 1977).

The model for eutrophication of soils forecasts low impacts which are negligible. The predicted ecological effects in this model also show a high sensitivity to the variability of soil characteristics across the mountainous region of Jordan.

This is illustrated in Figure 7.10. In the upper part of the figure, the results are shown for the possible impact South of the stack. In the lower part, the assessment results South-East of the stack are indicated. The values for the environmental conditions are

taken from Adler (1985). In Figure 7.10 the N-deposition is given as total nitrogen in [kg/ha/a], the C/N-ratio and the precipitation/evaporation index are dimensionless, the CEC is given as meq/100 g soil. The unit for the mean ambient temperature near the soil is °C. The possible eutrophication impact is given as [kg-N/ha/a]. It represents the difference between N-deposition and buffering capacity.

Eutrophication impacts for the other six directions are negligible. This is mostly due to the fact that the wind regime is dominated by the wind directions North and North-West and therefore the highest NO_x-immission values are South and South-East of the power plant.

7.6.3 Plant Damage

NO- and NO_2-immissions can have adverse effects on the development and physiology of plants (Sanders *et al.*, 1995). However, as nitrogen compounds are also nutrients for plant growth, low doses of NO_x can have positive effects on plants (Curtiss & Rabl, 1996). Within the fuzzy expert system for possible plant damage, three different fuzzy sets have been defined for the susceptibility of plants to NO_x. These sets represent the dose–response relationships of the three plant categories: "very susceptible", "susceptible" and "less susceptible" to NO_x-immissions. The threshold values for adverse effects due to NO_x-immissions have been defined in accordance to Kolar (1990) as follows: very susceptible plants: 100 $\mu g/m^3$ (given as mean value over six months), susceptible plants: 160 $\mu g/m^3$ and less susceptible plants: 250 $\mu g/m^3$. The possible nutritional effect of low NO_x-immissions has been taken into account within the fuzzy expert system.

In the first step of the environmental impact assessment for possible plant damage the different crops in the vicinity of the power plant (up to 250 km distance) are assigned to their respective fuzzy sets of susceptibility and in the second step their response to the NO_x-immissions is estimated.

The model for plant effects forecasts a slight increase of potential crop yield South of the power plant. The effects in the other 7 directions for which calculations have been made are negligible.

7.7 DISCUSSION

LCIA faces spatial and temporal difficulties as well as problems concerning threshold values and dose–response relationships for many impact categories. In order to achieve a more extensive and accurate environmental assessment of product systems, the combined use of relative assessment techniques such as LCA and absolute assessing techniques such as environmental fate modeling and environmental impact assessment is a solution (de Haes & Owens, 1998). To further investigate the advantages and difficulties of such an integrated approach an environmental impact assessment in conjunction with LCA was employed.

As a result of the methodological extensions and the application of regional impact assessment for improving the accuracy of LCIA discussed above, the following conclusions can be made:

- An important methodological extension is the coupling of heterogeneous mathematical modeling developments: Petri nets for technical systems, ODE or PDE systems for reaction dispersion modeling and fuzzy expert systems for indicator development and assessment.
- This methodological extension allows the integration of different kinds of information: technically measurable data in LCI, chemical reactions and spatial spread which is often difficult to measure, as well as ecological impact assessment which is based on expert knowledge and is difficult to quantify.
- The first two steps of the integrated approach allow the derivation of indicator systems which assess spatial heterogeneous ecological situations.
- The approach circumvents one of the major limitations of LCIA. It can now address actual impacts at the site of emission, for instance the observed power plant. The suggested solution integrates absolute environmental assessment techniques into LCA.

The modular structure of the integrated approach and the well-defined interfaces between the parts allow the exchange and improvement of each module separately. For instance, it may be is necessary to expand the model of environmental fate for other substances with their reactions or for a more complex geometries in other landscapes. An application of the described approach to other impact categories needs an extension of the fuzzy expert system. The use of fuzzy expert systems for assessment allows the possible input of linguistic data, which is an important feature for ecological and non-measurable data. A regional decision system for environmental impact assessment of anthropogenic emissions should therefore consist of the four elements LCA, fate modeling, assessing expert systems and geographic information systems.

We are now able to cope with mathematically heterogeneous systems for environmental models integrating interrelationships of anthroposphere and biosphere. This lays the foundation for a systematic search for optimum environmental management strategies assessed by environmental indicators and described by spatially explicit dynamic systems.

Part III

The Big Picture: Environmental Management

Ja mach nur einen Plan
Sei nur ein großes Licht!
Und mach dann noch ’nen zweiten Plan
Gehn tun sie beide nicht.

—Berthold Brecht

8

Scenario Analysis and Optimization

8.1 INTRODUCTION

A frequent application of ecological models is to support decisions on the anthropogenic impact on the ecosystem and to assess certain different management strategies for ecosystems. The question as to how much impact nature can bear without harming our environment is quite old. Ideas like "most sustainable yield" were introduced in the late 1960s. Ecosystem management has now become an important discipline of scientific research and is an important branch in the political decision-making process. Simulation models are recognized as efficient tools for the analysis of environmental processes, education, and decision-making. The most fascinating ability of a model is the possibility of performing non-intrusive experiments over a system based on the theoretical and practical knowledge about processes and interactions.

Because ecological models are complex and highly interactive, this decision-making process requires methodological support. The third part of this book deals with applications of ecological models in the decision-making process: either by the use of the scenario analysis technique, or by the application of optimum control to ecosystem models. Applications of ecological and environmental models are studied. Problems of ecosystem management are solved by the use of numerical optimization methodology. This can be interpreted as the follow-up of the most sustainable yield concept by the use of scientific computing.

In this context a model consists of a *simulator* which represents the environmental processes and connects *control variables* (also known as forcing functions or inputs) to output variables, cf. Chapter 1. The former ones, the control parameters, may

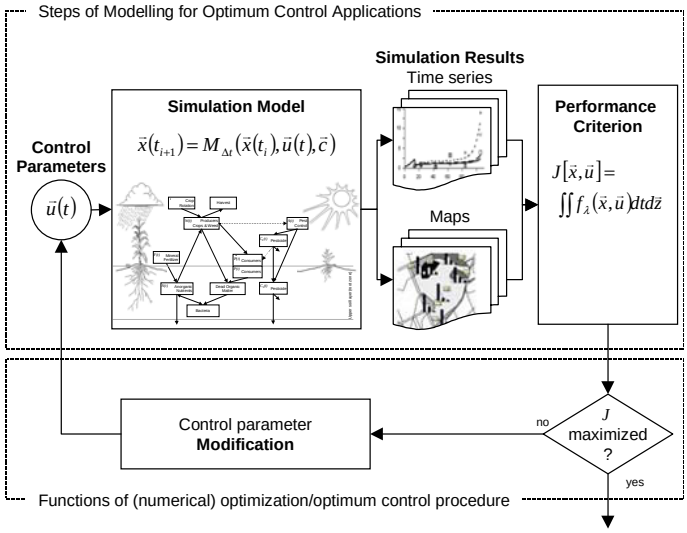

Fig. 8.1 Concept of applications of environmental models in numerical optimum control procedures. Basic elements of the modeling part are simulation models — displayed by the conceptual model of an agroecosystem — and the performance criterion. Important part of the optimization procedure is an intelligent modification of the control vector driven by the estimation of the performance criterion. Note, compared to the scenario analysis methodology, which one could compare with an open control system, this is a control loop.

be used to define management strategies in terms of the model variables. The latter ones, output variables, are used to describe the system behavior and to assess the management strategies being studied. One or more of these output variables are used to assess the simulation, the results of the modeling experiment. Because of this, these variables are often called *indicators*. Figure 8.1 illustrates this concept.

To analyze the system and define the most appropriate management practices, usually a number of scenarios are formulated and then fed into the model. The output results are then compared to choose the one that fits the requirements, the management goals, best of all. The formulation of a management scenario, assessment and comparison of results requires considerable effort. Scenario definition requires knowledge on the modeled system, which probably may not be available due to the complexity of the investigated system (Jakeman & Letcher, 2003).

Instead of running numerous scenarios through the model and then comparing the results, see for instance (Costanza *et al.*, 2001; Kurz *et al.*, 2000; Rao *et al.*, 2000), we may formulate a certain goal that we want the ecosystem to reach, and then let the computer sort through the numerous parameter and pattern combinations to reach that goal. In this case the variations of parameters and functions in the model input (control) are performed automatically, as well as the processing of the output. The core of this process is the algorithm of numerical optimization, which makes the decision on how to define the next scenario to analyze, based on the available information about the

of this process is the algorithm of numerical optimization, which makes the decision on how to define the next scenario to analyze, based on the available information about the results of previous model runs. This optimization procedure connects the scenarios, the simulation process and the *performance criterion*. Algorithms of optimization are capable of performing a systematic search in the space of control variables to find an input vector which controls the systems in the desired way, specified by the goal function.

This is the basic idea of *optimization* — or if temporal patterns are considered — *optimum control*, that are illustrated by Figure 8.1. The basic difference between optimization and scenario analysis is the closed feedback loop in the figure. This feedback loop is closed by the condition if the performance criterion "J is maximized" and the modification of control parameters.

In the following this concept will be analyzed with respect to environmental processes. The reader may guess that integrated models, mathematical heterogeneity, use of several temporal and spatial scales as well as spatially explicit models lead to methodological problems. To approach the problem the steps of model development, modeling a performance criterion, and implementation of optimization procedures are separated. In the following chapters we will focus on the set up of appropriate algorithms for optimization and optimum control of environmental systems as well as the development of general performance criteria for environmental systems.

8.2 OPTIMIZATION AND ENVIRONMENTAL MODELING

8.2.1 Analytical Treatment and Non-spatial Applications

Analytical solutions of optimum control problems were first presented by van Dyne *et al.* (1970). The importance of nonlinear models was noted, but there was no methodology capable of solving nonlinear systems in terms of control theory. Clark (1976) and Clark *et al.* (1979) laid the foundation for investigating ecological optimum control problems. Forest management and fisheries were the first applications, which initiated a large number of publications on agricultural models (Cohen, 1987b; Cohen, 1987a; Falkovitz & Feinerman, 1994; Velten & Richter, 1993; Velten & Richter, 1995) and ecological economics (Doherty Jr. *et al.*, 1999). DeGee and Grasmann (1998) studied sustainable use of renewable resources using analytical solutions of optimum control problems based on Lotka–Volterra-type systems. The underlying simulation models in the these papers were set up using systems of ordinary differential equations.

In terms of ecosystem management, more complex model systems, which cannot be treated analytically will now be considered. Recent developments in numerical procedures of optimum control focus on high performance real-time optimization of large systems of ordinary differential equation systems, which can be written in the form $d\vec{x}/dt = \vec{f}(\vec{x}, t)$; see, for instance, Bulirsch *et al.* (1993). Environmental models do not fulfill the prerequisites. It is difficult to transform ecological models

into this notation. This hints at reasons for this lack of optimization applications in environmental modeling, although it seems to be a very promising branch of system theory and ecosystem management.

8.2.2 Spatially Explicit Applications

Table 8.1 summarizes recent publications on ecosystem management based on spatially explicit or regionalized simulation models. We look at the model structure, the control variables, the goal function, the processes, and the spatial database used. The last column lists the location of the study area, if any.

The scope of ecosystem management problems ranges from forest management and timber harvest (Loehle, 2000; Tarp & Helles, 1997) to agricultural problems (Nevo & Garcia, 1996; Makowski *et al.*, 2000) to general issues of land use change (Martinez-Falero *et al.*, 1998), and to habitat suitability (Bevers *et al.*, 1997). The models used differ in terms of mathematical structure. Modeling methodology ranges from aggregated dynamic models based on difference equations of exponential growth (Bevers *et al.*, 1997; Loehle, 2000) to complex models based on systems of nonlinear differential equations (Randhir *et al.*, 2000). In terms of optimization methodology one can find a broad spectrum of approaches.

Hof & Bevers (1998) published an overview of application of optimization to landscape management problems. Together with Clark they are aware of the problem of complex and spatially explicit systems. They use linear programming and nonlinear program methodology to solve problems of pest management, re-establishment of population forest treatment, and runoff by storms etc., mostly within artificial landscapes. They are aware of the difficulties in defining and solving optimizations problem with highly complex nonlinear models in real landscapes.

8.3 ASSESSING THE ENVIRONMENT VARIABLES

8.3.1 Indicators . . .

In order to assess the results of a scenario analysis in terms of environmental, economic, toxic, or social aspects, we need to consider more than one output variable. To compare different simulation scenarios we then need to integrate output variables into a scalar value. The other option would be to analyze a multi-dimensional decision problem. This function aggregates several output variables and is called a *goal function* or *performance criterion*. In the mathematical formalization this function must be maximized or minimized to reach the desired state.

The definition an appropriate performance criterion can be separated into two main questions, which will be discussed later on in Section 8.4.1. The first concerns the technical aspects and the mathematical properties. Second, the more general aspect

Table 8.1 Application of spatial optimization in landscape ecology.

Reference	Model structure, process	Control variables	Performance criterion	Optimization algorithms	Spatial DB, Scale, GIS	Case Studies, Applications
Bevers *et al.* (1997)	Time discrete migration & population dynamics	– Location of reintroduction – Rodiacid treatment	Habitat sustainability function	Nonlinear programming, stochastic variation	Raster	Badlands National Park, Buffalo Gap National Park, South Dakota, US
Hof *et al.* (1999)	Population dynamics	Timing of habitat protection for prairie orchid	—	—	Raster, ArcINFO	Sheyenne National Grassland, South East North Dakota, US
Loehle (2000)	Exp. growth of forests	Timber harvest	Timber harvest, water quality	0–1 integer programming	Raster	—
Makowski *et al.* (2000)	—	Spatial distribution of agricultural land use	—	Hierarchical structured linear programming	—	European Union
Martínez *et al.* (Martinez-Falero *et al.*, 1998)	Linear model, eqn. system	Land use modification	Ecological sustainability, economic costs, social constraints	Baye's approach to land use changes	Raster	Torrelague township, Spain, 2787 ha
Nevo & Garcia (1996)	—	Spatial distribution of agricultural land use	Habitat sustainability to wildlife species	Two stage nonlinear optimization	—	Lonetree Wildlife Management Area, North Dakota, US
Tarp & Helles (1997)	—	Timber harvest	Sustainable forest management	Simulated annealing, linear programming	Vector	Boendernes Hegn, Denmark
Randhir *et al.* (2000)	EPIC (Williams *et al.*, 1983)	Landuse	Water quality erosion	Spatial dynamic programming	Raster, GRASS	Experimental watershed

of a performance criterion is how to measure the state of an ecosystem. This refers to an ongoing discussion about indicators of an ecosystem, in which many scientists from different disciplines have presented valuable input.

Recent definitions of indicators and the use of terminology in this area are particularly confusing (Gallopín, 1997). Many authors and institutions give different definitions and explanations what indicators are, what they should perform, and what properties they should have. Three examples of definitions or explications are given, which are presented from different origins.

Example 8.1 ((United States Environmental Protection Agency, 1995)) *An environmental indicator is a parameter (i.e. a measurement or observed property), or some value derived from parameters (e.g. via an index or model), which provides managerially significant information about patterns or trends (changes) in the state of the environment, in human activities that affect or are affected by the environment, or about relationships among such variables. As defined here, indicators include geographical (spatial referenced) information, and information used in environmental management at any scale, i.e. not just for high-level policy makers.*

This definition covers most of the issues discussed in the previous chapters. US EPA recognizes the importance of models to be used within environmental assessment, as models allow the derivation of unmeasurable variables. Second, this definition also notes the importance of spatially referenced indicators, as shown in Chapter 7. Azar *et al.* identify two problems in the definition of indicators. With special respect to indicators assessing sustainability, they write

Example 8.2 ((Azar *et al.*, 1996)) *There are in many cases long time delays between a specific activity and the corresponding environmental damage. This means that indicators based on the environmental state may give a warning too late, and in many cases only indicate whether past social activities were sustainable or not.*

The complexity of the ecosystem makes it impossible to predict all possible effects of a certain social activity. Some damages are well-known, but others have not yet been identified. Models of sustainability indicators suggested in literature are formulated with respect to known effects in the environment.

These two topics clearly relate to the development of dynamic models describing environmental processes of concern. First, because dynamic models can cope with long time delays. Second, because models can handle and structure complex systems. Refering to the second topic of Example 8.2, uncertainty is an inherent property of indicators comparable to models, as not all processes may be known or may not be considered in the definition an indicator or the underlying model, see Section 1.3.3.

However, from this one can conclude that indicator definition requires the use of dynamic environmental models. Winograd extends these considerations and suggests

Example 8.3 ((Winograd, 1997)) *The function of indicators would be to:*

- *determine the condition of, or change in, the environment in relation to society and the development process.*
- *diagnose the actual causes and effects of existing problems that have been detected, in order to elaborate responses and actions.*
- *predict future impacts of human responses and actions.*

Winograd extends the definition from the US EPA by the recommendation that indicators should offer cause-effect relationships, the necessity to predict the future, as well as the basis to derive management strategies. With the background of the methodology of environmental modeling (see for instance Figure 3.11) this seems to ask too much of an indicator concept. Predicting future impacts is related to environmental modeling, and elaboration of responses and actions will be a result of optimization or optimum control. Indicators have to focus on the problem of assessment and comparison. This is what Hunsaker (1993) is focusing on:

Example 8.4 ((Hunsaker *et al.*, 1993)) *Candidate indicators can be evaluated with regard to the following criteria:*

- *The indicator must be operationally defined and readily measured;*
- *The indicator must be sensitive to changes in pollutant deposition;*
- *The response of the indicator must be stable over the spatial and temporal ranges of the assessment end point and of pollutant exposure;*
- *The indicator must be contained in the output of predictive models if it is to be used as a predictor of future response;*
- *The indicator must be contained in databases that allow the resource to be mapped or quantitatively characterized;*
- *Changes in indicator status should result in a willingness to change the regulations of sources.*

All these definitions aim at an identification of the environmental state and its changes. This is achieved either by the application of a model or by measuring an environmental variable. This variable (either from model or measured) has to be stable over the considered spatial and temporal range on the one hand, and sensitive to changes on the other hand. To fulfill these recommendations it might be helpful to have a look on what environmental models offer.

8.3.2 . . . and Applications for Optimization

What can be derived from this discussion for the application of environmental models aiming at an estimation of optimum management strategies?

First, the indicator concepts help to define performance criteria J, cmp. Figure 8.1. Several recommendations in Examples 8.1 to 8.4 hold true for the modeling of performance criterion. The performance criterion

- is defined as a function of the model output, e.g. a function of state variables or derived auxiliary variables;
- is therefore a quantification of the system state;
- depends on geographically referenced information, or aggregated/integrated information for a specific region;
- should be sensitive to changes of the system state.

Additionally, environmental simulation models enlarge the spectrum of possible definitions of performance criteria. Using ecological models one is even able to use unmeasurable variables for assessing management scenarios.

A definition of indicators and performance criteria must solve the problem of comparing and aggregating different variables with units that are difficult to compare. For instance, how can nitrogen loss and the probability of nitrogen in drinking water reservoirs be compared with prices for agricultural products? Or, as a more landscape ecological example, how can habitat maintenance for certain species be compared with real estate prices for dwelling units?

Ecological systems are open systems. In a performance criterion variables can be used which are represented in the simulation model. For instance, an assessment of possible ground water contamination with nitrate can only be assessed by the possible outflow of nitrogen out of the plant-accessible root zone. In economic terms this means, that *external costs have to be internalized*. Note that the definition of the system boundary determines whether variables and costs are external or internal. For example, the integration of the ecological impact at the production site at the Jordan river in the environmental impact assessment study in Chapter 7 integrated these "costs" to the impact study of the car production in Wolfsburg. However, environmental models cannot cover all possible effects. Because of this a methodological treatment of externalities is required.

This problem does not only occur when comparing state variables from biosphere and anthroposphere. Even in assessing variables only from the biosphere, it is difficult to compare different variables on an equal level of information. There are two approaches to solve this problem. Concerning anthroposphere-biosphere interaction, some authors advocate the use of monetary units for comparison. Giving prices for ecosystem functions has been very successful (Costanza, 2000; Costanza *et al.*, 1997;

Scheffer *et al.*, 2000). Authors believe that this approach increases awareness of the services provided by ecosystems to maintain life on earth.

Second, by comparing different ecosystem functions, one can make use of evolutionary concepts underlying most of the patterns identified in ecology. Ecosystems tend to use the *energy available* (from solar radiation) very efficiently. The means on the other hand, that ecosystems tend to minimize unstructured energy, so-called *entropy*. Several authors suggets using concepts like exergy, emergy etc. for assessing ecosystem state (Jørgensen *et al.*, 1998; Müller, 1998).

The basic ideas obtained from this discussion are that two possible strategies can be followed for defining performance criteria. Either try to compare anthropogenic and biosphere processes using monetary units, or use energy or entropy respectively to compare processes for the definition of a goal function.

8.4 GENERAL OPTIMIZATION TASK

8.4.1 Performance Criteria

Considering the models presented in this publication, the following variables or processes can set up performance criteria for optimization

1. leachate of hazardous substances into the environment (which is to be minimized in terms of optimization):
    - nitrate below rooting depth (agricultural production), cf. Sections 2.2.3, 2.4.1
    - phosporous at the watershed mouth, from sewage input or caused by erosion, see Section 3.3.3
    - emitted substances like NO_x or sulfur at a certain distance from an industrial production site, cf. Chapter 7
    - other xenobiotic substances, for instance pesticides, cf. Section 2.4.2
2. maintaining ecosystem functions
    - maintaining habitat suitability for species, preserving biodiversity, cf. Sections 3.2.2 and 3.3.2
    - supporting CO_2 retention capability, cf. Chapter 3
    - maximizing nett primary production, cf. Chapter 2
3. maintain and support production by
    - maximization of agricultural yield, cf. Section 2.2.1

- minimization of input of energy, of work power, or minimizing of production steps, for instance weed control or fertilization (Section 2.2.4, 2.4.1), or in terms of industrial production, see Chapter 7
- assessing yield stability considering a long term period
- minimization of weeds, cf. Section 2.2.4

4. support human life (recreation, housing, etc.)

Performance criteria aggregate different indicators. A performance criterion comprises a broad spectrum of different state variables for assessment with different origins like economy, ecology, and social aspects. In the above list items 1 and 2 can be associated to ecological aspects; item 3 lists economic indicators; and item 4 belongs to social assessment. In most cases these are contradictory goals.

From a methodological point of view, two different approaches are available to cope with this problem. Optimization problems may be formulated as scalar optimization problems. The second approach is to define a multi-criteria optimization problem. Both approaches will be considered in the following, starting with scalar optimization problems. A mathematical definition for a scalar performance criterion is given by the following definition:

Definition 8.1 (Performance Criterion) *Consider a general environmental model given by Equation (4.1). $\vec{x}$ denotes the vector of state variables. $\vec{u}$ denotes the vector of control variables. Both depend on time t and location $\vec{z}$. A performance criterion maps a trajectory from state and policy space to a real number $J[\vec{x}, \vec{u}] \in \mathbb{R}$.*

This mapping requires an aggregation in time as well as in space. The general transformation is achieved by the following function

$$J[\vec{x}, \vec{u}] = \int_0^{t_{end}} \int_R f_\lambda \begin{pmatrix} \vec{x}(t, \vec{z}) \\ \vec{u}(t, \vec{z}) \end{pmatrix} dt \; d\vec{z} \tag{8.1}$$

where R denotes the study area and t_{end} the upper limit of simulation interval.

Assuming that f_λ simply performs a linear combination of its arguments with a vector of weighting coefficients Equation (8.1) can be rewritten as follows

$$J[\vec{x}, \vec{u}] = \int_0^{t_{end}} \int_R \vec{\lambda}^T \begin{pmatrix} \vec{x}(t, \vec{z}) \\ \vec{u}(t, \vec{z}) \end{pmatrix} dt \; d\vec{z} = \int_0^{t_{end}} \int_R \sum_{i=1}^{n} \lambda_i x_i(t, \vec{z}) + \sum_{i=1}^{m} \lambda_{i+n} u_i(t, \vec{z}) dt \; d\vec{z} \tag{8.2}$$

Additionally certain constraints or boundary condition may be defined. A general formulation is

$$f_0(\vec{x}(t, \vec{z}), \vec{u}(t, \vec{z})) \leq 0 \text{ for all } \vec{z} \in R, t \in [0, T] \tag{8.3}$$

An application of Equation (8.2) can be found in the well-known example of energy minimization while landing a moon vessel. This is why this equation often is considered as *energy norm*.

The definition of the weighting scheme $\vec{\lambda}$ turns out to be the crucial problem in modeling performance criteria for environmental problems and the application of Equation (8.2) to an optimization problem. Nutrient contents, habitat suitability for certain species, or net primary production denote ecological variables. Model variables like harvest biomass and fertilizer input from/to a field denote purely economic variables. The crucial question is: How to integrate these indicators to a scalar value by a single constant vector $\vec{\lambda}$? One might note that using the more general Equation (8.1) might offer more freedom for aggregation of these different variables. A nonlinear function of assessment of indication does not simplify nor solve the problem. The following chapter will show how to work with this technique of optimization based on scalar performance criteria based on Equation (8.2).

A different aspect, which is to be noted here, is that more freedom in assessing the processes is achieved, if multi-criteria approaches are used for assessing the process. However, we will see that with certain techniques of optimization and by solving the (so far undefined optimization problems), a multi-criteria analysis using a scalar performance criteria can be analyzed.

8.4.2 General Optimization Task

Based on the definitions of a general environmental model, cf. Equation (4.1), and the performance criterion in Definition 8.1 we can now formulate the mathematical problem of identifying optimum management strategies in environmental problems in a general notation.

Task 8.1 (General Optimum Control Problem) *Let $M_{\Delta t}$ define a simulation model according to the General Model Equation (4.1): Calculate $\vec{u}^*$, so that*

$$\begin{array}{rcl} \vec{x}(t) & = & M_{\Delta t}\left(\vec{x}_0, \vec{u}^*, \vec{c}\right) \\ J[\vec{x}, \vec{u}^*] & \geq & J[\vec{x}, \vec{u}] \end{array} \quad \text{for all } t \in [0, T], \vec{u} \in U \tag{8.4}$$

where U denotes the set of admissible sets of control variables.

Note $\vec{u} \in U$ as well as $\vec{x}$ depend on time and space. This task in general defines a *spatio–temporal optimization problem*:

Task 8.2 (Regionalized Optimum Control) *Calculate $\vec{u}^*(t, \vec{z})$ so that*

$$\begin{array}{rcl} \vec{x}(t, \vec{z}) & = & M_{\Delta t}\left(\vec{x}_0(\vec{z}), \vec{u}^*(t, \vec{z}), \vec{c}(\vec{z})\right) \\ J[\vec{x}(\cdot, \vec{z}), \vec{u}(\cdot, \vec{z})^*] & \geq & J[\vec{x}(\cdot, \vec{z}), \vec{u}(\cdot, \vec{z})] \end{array} \quad \text{for all } t \in [0, T], \vec{u} \in U \tag{8.5}$$

for all $\vec{z} \in R$.

8.4.3 Methodology

The general form used in this definition together with the general notation of an environmental model, see Definition 4.1, faces us with a number of problems concerning the numerical solution of the problem notes in Task 8.1.

Numerical solutions for optimization problems usually make use of the structure of the system. For instance, linear problems based on explicit solutions can be solved analytically using linear programming methodology (Tarp & Helles, 1997). Nonlinear optimization problems make use of the linearization of the problem of an iterative procedure for identification of the maximum or minimum of J as a function of the control variable (Press *et al.*, 1988; Stoer & Bulirsch, 1983).

Concerning optimum control, several solutions have been presented that required the dynamic system to be set up by ordinary differential equation systems only (Bulirsch *et al.*, 1993; Bulirsch & Kraft, 1994). Optimization or optimum control based on partial differential equation makes use of a discretization in space transforming the problem into a system of ordinary differential equations (Altmann-Dieses *et al.*, 2002), see Section 1.5.6.

In general one can distinguish two different approaches for solving the optimization problems.

Global optimization procedures are able to identify the global optimum. This means, that these procedures search through the entire space of control and state variables, finally identifying this (spatio–temporal) control vector, that maximizes or minimizes the performance criterion under the given boundary conditions.

The enormous computational effort required for these procedures means that they are only applicable to low dimensional systems.

Local Optimization procedures are based on an iterative procedure that improves an initial solution stepwise in the direction of the increasing (or decreasing) performance criterion — depending on maximization or minimization.

These procedures are applicable to a broad spectrum of models. Depending on the implementation of the procedure, more or less prerequisites are required such as the derivative of the performance criterion with respect to the control variables.

The major drawback of this iteration is that these procedures stop if no change of the performance criterion value can be identified. This does not necessarily mean that the estimated control vector holds the set of control variables that globally maximize or minimize the performance criterion.

Application of general environmental models in optimum control and optimization applications requires the development of a methodology that can handle these mathematically heterogeneous systems. Dynamic programming (Bellman, 1957; Angel &

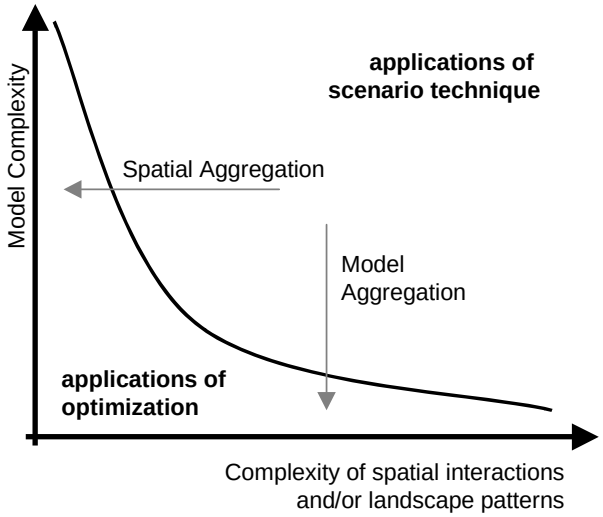

Fig. 8.2 Graphical representation of the present state of the art in concepts of regional optimization solutions.

Bellman, 1972) is a suitable methodology, which identifies the global optimum of the problem and has less restrictions to the underlying model. Chapter 9 will summarize this concept together with several extensions and modifications required for environmental models. The property of spatial explicitness of an environmental model makes these problems even worse. The spatial explicitness of the model increases the space of control variables and state variables exponentially. Because of this, local optimization methodologies are required to solve optimization problems using environmental models. For the successful application of these algorithms strategies have to be found that give a good starting point for the iterative search in control space. These questions will be discussed in the second part of the next chapter.

8.5 DISCUSSION

In environmental modeling the idea of applying simulation models to numerical optimization algorithms in terms of optimum control theory is quite new, cmp. Table 8.1. For this application it is necessary to use well-validated simulation models within the framework of a robust and flexible optimum control procedure. Both items are difficult to achieve in environmental modeling. The first — validating an environmental simulation model — is a complex task, cf. Chapter 1. The second, because modeling environmental processes leads leads to mathematically heterogeneous mathematical models as shown in the earlier part of this book.

The complexity of an optimization task depends on two factors: the complexity of the ecosystem model (number of state variables, degree of nonlinearity etc.) and the

spatial complexity (size of study area, grid cell size, number of spatially interacting processes). The more complex the simulation model is and the more spatial relationships are considered, the lower are the chances of success in the optimization. For such complex models, scenario analysis is usually the only feasible method. Figure 8.2 illustrates this relationship.

Scenario analysis compares the outcome of a given number of scenarios, which are identified with possible management strategies. Optimization procedures perform a systematic search over the whole control space automatically, whereas optimization tasks require much less effort in preprocessing and formulating the numerous scenario options, their computational complexity is incredibly high. The models described in Table 8.1 are considered in an optimization context. Therefore they all required certain simplification or aggregation to allow optimization, cf. Figure 8.2. This was achieved either by aggregation of the model or aggregation of the study area, or both. Chapter 9 will introduce a set of methodological tools that extends the domain of environmental model applicable in optimization and optimum control theory — they move the boundary line in Figure 8.2 to the upper right. The following chapters then present several case studies and applications of spatially explicit environmental models and the estimation of management strategies.

9

Prerequisites: Temporal Hierarchies and Spatial Scales

9.1 INTRODUCTION

Environmental models are complex for different reasons. First of all the number of state and control variables is an indicator for complexity of models. Second, the number of mathematical "dialects" used to set up the model is a measure of the mathematical heterogeneity. The more heterogeneous a model, the smaller is the spectrum of possible numerical methods of optimization tasks. This is because the number of fulfilled prerequisites of numerical methods is decreasing. Third, spatial explicitness of regionalized models allows the space of state and control variables to increase exponentially. This again lets computational effort increase in an additional dimension.

One concept that can offer solutions to this problem is the introduction of different temporal hierarchies as well as different spatial scales. This concept was introduced in Chapter 1 with Figure 1.3 (p. 8). In that chapter scales were used to characterize and classify models. In this chapter this concept will be used to develop solutions for the application of complex environmental models to optimization theory. A methodological framework is proposed for the application of environmental models in optimum control theory. Dynamic programming algorithms are used based on general dynamic systems. Numerical effort is decreased by making use of properties of environmental models. In the second part of this chapter spatially explicit models will be considered in the process of optimization.

9.2 HIERARCHICAL DYNAMIC PROGRAMMING

9.2.1 Introduction

Formulation of optimum control problems and the numerical methods require a general notation for simulation models. This formal representation needs to abstract from mathematical properties of the underlying simulation model, e.g. ODE, DAE, PDE.

Consider a dynamic system with the state variables $\vec{x}(t)$, the control variables $\vec{u}(t)$ and the right-hand side $\vec{\varphi}(\vec{x}, \vec{u})$ on a time interval $t_i \in [0, T] = I$. $\vec{\varphi}(\vec{x}, \vec{u})$ is called the flux of the dynamic system (Arrowsmith & Place, 1994, ch. 1). On this system a q-stage process can be defined:

Definition 9.1 (q-stage-process) *q stages are defined by $0 \leq t_0 < t_1 \cdots < t_{q-1} < t_q = T$, e.g. q events of possible control. The sequence of control $\left(\vec{u}(t_i)\right)_{i=0,\ldots,q-1}$ modifies the dynamic system so, that*

$$\vec{x}(t_{i+1}) = \vec{\varphi}_{\Delta t}(\vec{x}(t_i), \vec{u}(t_i)) \tag{9.1}$$

with $\Delta t = t_{i+1} - t_i$ for $i = 0, \ldots, q-1$.

Equation (9.1) can be applied directly to a dynamic system, which is defined by a time-discrete algebraic equation. In the case of a differential equation system, the estimation of the succeeding state $\vec{x}(t_{i+1})$ involves the numerical solution of the differential equation system (Hairer *et al.*, 1980; Hairer & Wanner, 1980).

Application of optimum control theory to simulation models with the described properties requires methods that do not restrict the class of applicable models by strong assumptions; for instance, derivatives of the model functions may not exist. Bellman (1957) offered *dynamic programming* as a flexible optimization approach applicable to heterogeneous mathematical systems. Equation (9.1) sets up the bases for an application of the algorithm of dynamic programming. Bellman (1962, p. 15) denotes $\vec{u}^*(t)$ an *optimal policy* if it maximizes a given performance criterion $J[\vec{x}, \vec{u}]$. J is a functional defined on the space of state and control functions. For an application of dynamic programming it is necessary to write J in a *recurrence equation* in the stages $i = 0, 1, \ldots, q$.

Definition 9.2 (Performance Criterion (recurrence equation))

$$J[\vec{x}, \vec{u}] = J\left(\vec{x}(t_1), \ldots, \vec{x}(t_q), \vec{u}(t_0), \ldots, \vec{u}(t_{q-1})\right)$$

denotes the assessment of the entire process. J has Markoff property, if J can be separated by continuous functions K_i in the stages $i = 1, 2, \ldots, q$ and $J_i(\vec{x}(t_i), \vec{u}(t_{i-1}))$

can be set up by

$$\left.\begin{aligned} J &= \widetilde{J}_q\Big(J_1(\vec{x}(t_1),\vec{u}(t_0)),\ldots,J_q(\vec{x}(t_q),\vec{u}(t_{q-1}))\Big) \\ \widetilde{J}_{q-i}(J_{i+1},\ldots,J_q) &= K_{q-i}\left(J_{i+1},\widetilde{J}_{q-i-1}(J_{i+1},\ldots,J_q)\right) \\ &\qquad\qquad \textit{for } i=0,\ldots,q-2 \\ \widetilde{J}_1(J_q) &= J_q \qquad\qquad \textit{for } i=q-1. \end{aligned}\right\} \tag{9.2}$$

Definition 9.3 *With the notation from Definitions 9.1 and 9.2 state functions ξ_i are defined by*

$$\left.\begin{aligned} \xi_1(\vec{x}(t_{q-1})) &= \max_{\vec{u}(t_{q-1})} \widetilde{J}_1(J_q) \\ &\vdots \\ \xi_{q-1}(\vec{x}(t_1)) &= \max_{\vec{u}(t_1),\ldots,\vec{u}(t_{q-1})} \widetilde{J}_{q-1}(J_2,\ldots,J_q) \\ \xi_q(\vec{x}(t_0)) &= \max_{\vec{u}(t_0),\vec{u}(t_1),\ldots,\vec{u}(t_{q-1})} \widetilde{J}_q(J_1,\ldots,J_q) \end{aligned}\right\} \tag{9.3}$$

Principle of Optimality as proposed by Bellman & Dreyfus (1962, p. 15): *An optimal policy has the property that whatever the initial stage and initial conditions are, the remaining decisions must constitute an optimum policy with regard to the state resulting from the first decision.*

In the notation $\vec{u}(t_i)$ with $i = j,\ldots,q-1$ denote the remaining decisions. From this principle a computational scheme can be derived:

Algorithm 9.1 (Dynamic Programming (DP)) *Equation (9.2) is used to estimate $\xi_{q-i}(\vec{x}(t_i))$ for all possible $\vec{x}(t_i)$ for $i = q-1,\ldots,0$. At each stage i the optimum control vector $\vec{u}^*(t_i)$ is stored as a function of $\vec{x}(t_i)$. For the evaluation of J_{i+1} depending on $\vec{x}(t_{i+1})$ Equation (9.1) is solved for a general dynamic system. The complete sequence derived from that $\left(\vec{u}^*(t_i)\right)_{i=0,\ldots,q-1}$ is the solution of the optimum control problem for a given initial condition $\vec{x}_0$. The mathematical notation of this procedure is summarized by:*

$$\left.\begin{aligned} \xi_1(\vec{x}(t_{q-1})) &= \max_{\vec{u}(t_{q-1})} J_q(\vec{\varphi}_{\Delta t}(\vec{x}(t_{q-1}),\vec{u}(t_{q-1}))) \qquad \textit{for } i=q-1 \\ \xi_{q-i}(\vec{x}(t_i)) &= \max_{\vec{u}(t_i)} K_{q-i}\Big(J_{i+1}(\vec{\varphi}_{\Delta t}(\vec{x}(t_i),\vec{u}(t_i))), \\ &\qquad \xi_{q-i-1}(\vec{\varphi}_{\Delta t}(\vec{x}(t_i),\vec{u}(t_i)))\Big) \textit{ for } i=0,\ldots,q-2 \end{aligned}\right\} \tag{9.4}$$

The procedure estimates the global optimum solution of the optimum control problem. Additionally, this procedure may be used to estimate the the *k*th-best solution ($k = 1,2,\ldots$). See the contradictory proofs in Bellman & Kalaba (1960).

Note, the sequence of optimum control vectors $\left(\vec{u}(t_i)\right)_{i=0,\ldots,q-1}$ is estimated as a function of the initial condition $\vec{x}(t_0)$. This is an outcome of the principle of optimality.

In terms of numerical aspects this allows the derivation of an optimum control sequence from *any* initial condition $\vec{x}(t_0)$ using the calculated $\xi_1, \ldots, \xi_q$ *without* any computational effort (Bellman & Dreyfus, 1962).

The computational effort of estimating $\xi_1, \ldots, \xi_q$ increases polynomially with the increasing dimensions of state or policy space. Let n, m denote the dimensions of state and policy space and n_i $(i = 1, \ldots, n)$, m_i $(i = 1, \ldots, m)$ the number of possible values of each state/control variable. The estimation of $\xi_1, \ldots, \xi_n$ according to Algorithm 9.1 requires

$$S_{DP} = q \prod_{i=1}^{n} n_i \prod_{i=1}^{m} m_i \tag{9.5}$$

evaluations of Equation (9.1). Bellman (1957) calls this property "dilemma of dimensionality".

9.2.2 Hierarchies and Temporal Scales

The problem of hierarchy can be faced if one takes into account that environmental systems are structured with respect to characteristic times. Ecological systems show characteristic times from hours to years or decades, see Chapters 1 and 2, Table 1.2, Figure 1.3. This property can be formalized for dynamic systems: only a few state variables have to be considered for simulation and optimization, if the remaining state variables stay approximately constant. Formally, this means the observed simulation and optimization interval I has to be subdivided in a special manner. For the aims of this contribution a Hierarchical Dynamic System HDS may be formalized by:

Definition 9.4 (Hierarchical Dynamic System (HDS)) *If a pairwise disjunct partition of sub-intervals $I = \cup I_k = [0, T]$ can be found, with the property that a subset $(X_{n'+1}, \ldots, X_N)$ of all state variables $(X_1, \ldots, X_{n'}, X_{n'+1}, \ldots, X_N)$ stays approximately constant on each of the sub-intervals, a local simulation interval is defined.*

The variables of the local system are denoted with small symbols: $\vec{x}, q, \vec{u}, \vec{\varphi}, \xi$. The variables of the global system are denoted with capital symbols $\vec{X}, Q, \vec{U}, \vec{\Phi}, \Xi$. The function Ψ maps the entire dynamic system $\vec{X}' = \vec{\Phi}(\vec{X}, \vec{U})$ to the local system

$$(X_1, \ldots, X_{n'}) = \Psi(\vec{X}) = \vec{x} = \vec{\varphi}(\vec{x}(t_0), \vec{u}) \text{ and } \Psi(\vec{U}) = \vec{u}$$

"Staying approximately constant" means that for a given $\varepsilon > 0$

$$\| (X_{n'+1}, \ldots, X_n) \| \leq \varepsilon \text{ for all } t \in I_k$$

for each simulation interval I_k.

This procedure can be applied recursively to every sub-interval I_k. A hierarchy of simulation intervals is defined by the characteristic time patterns of the simulation model. This approach is known as the *slavery principle* and was first described by

Haken (1983). With this set-up an error of simulation is introduced. One can show that this error depends on the length of simulation sub-intervals I_k and the dynamics of the simulation model. For linear systems one can show that a very efficient set-up of subintervals can be created if the eigenvalue spectrum shows distinct gaps (Seppelt, 1997, Chapter 4).

This approach is applied to the DP algorithm and offers a solution to the "dilemma of dimensionality". The computational effort for a solution of the optimum control problem of the entire system is diminished, if Algorithm 9.1 can be modified to a hierarchical dynamic system from Definition 9.4. Note that all above-mentioned Definitions 9.1–9.3 can be applied to the local as well as to the global system. The basic idea is to solve a local optimum control problem by DP once, and to use the calculated state functions ξ_i every time a local problem has to be solved again.

Algorithm 9.2 (Hierarchical Dynamic Programming (HDP)) *According to the dynamic programming procedure for $i = Q-1, \ldots, 0$ the state functions $\Xi_{Q-i}(\vec{X}(t_i))$ are calculated and the optimum control vectors $\vec{U}^*(t_i)$ are stored as a function of the system state $\vec{X}(t_i)$. The estimation of Equation (9.1) requires either estimation of the flux or solution of a local optimum control problem on $\Psi(\vec{X})$. In the last case an optimization procedure according to Algorithm 9.1 is started, if no previously estimated state functions $\Psi(\Xi_i) = \xi_i(\Psi(\vec{X}))$ are found. Once ξ_i are calculated, every further request for a solution of the local optimum control problem makes use of the previously calculated set of state functions.*

This procedure diminishes the computational effort, as the recurrence equation (9.4) has to be estimated for the local processes only *once*. All stage assessments $\xi_{q-i}(\vec{x}(t_i))$ of the local problem are stored and can be used in the global optimization procedure.

For Algorithm 9.2 one can show that the global optimum solution is derived in a similar manner as for Algorithm 9.1 (Seppelt, 1997, annex a.3). In addition to the contradictory proof (Bellman & Kalaba, 1960), one has to find an estimation for the simulation error. This simulation error is caused by the assumption that several state variables stay approximately constant, for numerical analysis see (Seppelt, 1997, annex a.2).

With the introduction of HDS the computational effort of the DP procedures can be diminished. Efficiency depends on how the HDS is set up. Consider a global state/policy space of N/M variables with N_i, M_i possible values. An application of the basic DP procedure requires

$$S = qQ \prod_{i=1}^{N} N_i \prod_{j=1}^{M} M_j$$

steps to estimate $\Xi_i, \ldots, \Xi_Q$, cmp. Equation (9.5). If local variables $\vec{x}$, $\vec{u}$ with the dimension $n < N, m < M$ and $n_i < N_i (i = 1, \ldots, N), m_j < M_j (j = 1, \ldots, M)$ are

defined, the computational effort is given by

$$S_{HDP} = q \prod_{i=1}^{n} n_i \prod_{j=1}^{m} m_j + Q \prod_{i=n+1}^{N} N_i \prod_{j=m+1}^{M} M_j \tag{9.6}$$

A crucial point of the hierarchical structuring of a multi-scale dynamic process in terms of optimum control theory is that the identified time hierarchy may depend on the current stage and the control vector. With a modification of Equations (9.4) Algorithm 9.2 can solve optimum control problems with a changing time schedule. Let ν be a function that estimates the index of the succeeding stage of control j for a given control vector $\vec{u}(t_i)$ and the current stage i so that $j = \nu(i, \vec{u}(t_i))$. In Equation (9.4) the index i is replaced by ν:

$$\xi_{q-i}(\vec{x}(t_i)) = \max_{\vec{u}(t_i)} K_{q-i}\left(J_{\nu(i,\vec{u}(t_i))}(\ \cdots\ ), \xi_{q-\nu(i,\vec{u}(t_i))}(\ \cdots\ )\right) \text{ for } i = 0, \ldots, q-2 \tag{9.7}$$

This extension necessitates a restriction to the operator $K_i(a, b)$, see Definition 9.2. If certain stages i are omitted, K_i has to be identical for each stage: $K_i(a, b) = K(a, b)$ for all $i = 0, \ldots, Q$.

Note, ν is not necessarily invertible. Before estimating Equations (9.4) all possible stages of control are estimated. This may lead to set of possible stages of control which are not taken into account during the estimation of the simulation trajectories based on the optimum control solution. However, the numerical effort is not increased in that case because numerical effort is linear in time and number of stages.

If $\vec{U}$, $\vec{u}$, $\vec{X}$ or $\vec{x}$ are continuous, the problem is transformed into one with finite dimensions by approximating on a discrete grid in state or policy space, see Bellman & Dreyfus (1962, Chapter IV). The interpolation error can be controlled by comparing the interpolated results of the performance criterion with the exact value of the performance criterion using the same control function.

The performance of the procedure can be improved if an appropriate definition of the boundary of the state and policy space is defined. If the state space boundaries are violated, which may occur for distinct control vectors, these control vectors can be treated separately:

Algorithm 9.3 (Treatment of Boundary Violation) *If the calculation of Equation (9.1) to a given control vector $\vec{U}(t_i)$ violates the boundaries of state space, the following two cases are tested:*

The state $\vec{x}(t_{i+1}), \vec{X}(t_{i+1})$

1. *describes a physiologically impossible constellation of state variables: the control vector $\vec{u}(t_i), \vec{U}(t_i)$ is marked as illegal. Further trajectories to this area of state space will be excluded from policy space,*

2. *is physiologically possible, but outside of interpolation of state space: extrapolation will be used to estimate Equation (9.3).*

`dp_proc_recalc()` — Evaluation procedure estimating state functions Ξ, ξ

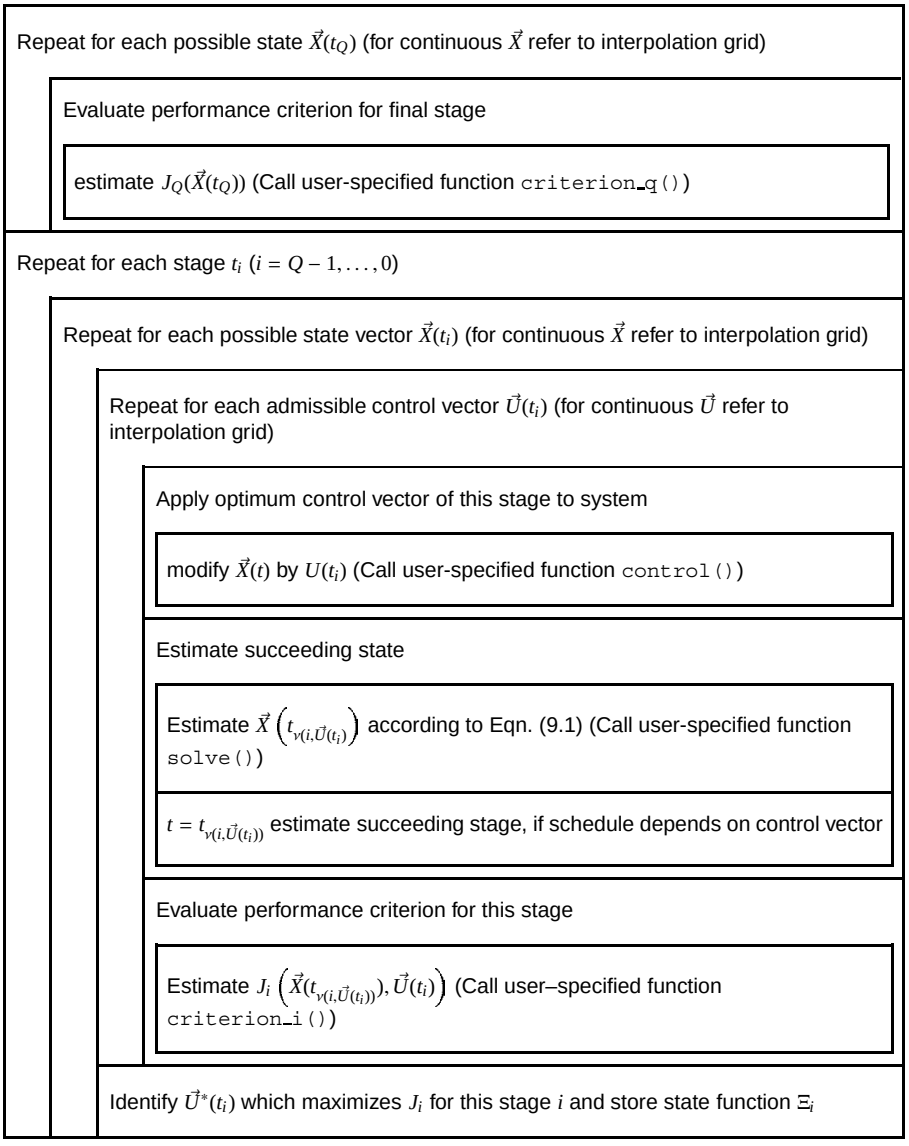

Fig. 9.1 Structure of HDP evaluation procedure. The estimation of Ξ_i or ξ_i for $i = 0, \ldots, Q$ is performed in two steps: the calculation of J_Q in the final stage and then backwards to the initial stage. After calling this procedure `dp_proc_recalc()` the calculated and stored state functions are used to derive an optimum control solution to any possible initial condition, see `dp_solve()`. Remark: Initialization steps are omitted.

9.2.3 Program Library

Though DP solutions may depend on the specific problem (Bellman & Dreyfus, 1962), generic code was developed that is applicable to a general dynamic system, which can be written in the notation of Definition 9.1 and which can be hierarchically structured according to Definition 9.4: the Library for Hierarchical Dynamic Programming [1] (LibHDP), (Seppelt, 2001). Figure 9.1 and 9.2 display a Nassi–Schneiderman diagram for the core Algorithm 9.2 of HDP:

- Procedure `dp_proc_recalc()`: estimation of state functions Ξ_i, ξ_i, cf. Figure 9.1;
- Procedure `dp_solve()`: estimation of the optimum control solution based on the state function, cf. Figure 9.2.

Note, the recursive call of the optimum control problem solver for the local problem in the procedure `dp_solve` introduces the hierarchical concept. Recursive calls terminate because the evaluation procedure `dp_proc_recalc` has to be called only once in the algorithm, see Figure 9.2.

The following sub-libraries and numerical procedures are embedded:

- high order numerical solution of ODE systems with automatic step-size control, based on the Runge–Kutta formulae DOPRI5 and DOPRI8, see Hairer *et al.* (1980);
- *n*-dimensional interpolation in state and policy space using linear and constant interpolation functions;
- generation of interpolation grids in state and policy space (time-dependent, not equally distributed);
- treatment of boundaries of state and policy space according to Algorithm 9.3.

The implementation of the numerical solution of an optimum control problem with this library requires the following steps:

1. Definition of hierarchical dynamic system and hierarchical Q/q-stage processes with model functions $\vec{\varphi}_{\Delta t}(\vec{x}, \vec{u})$ and $\vec{\Phi}_{\Delta T}(\vec{X}, \vec{U})$, procedure `solve()`. In the case of embedded ordinary differential equation systems, the sub-libraries DOPRI5 or DOPRI8 can be called.
2. A procedure `control()` must be defined, which modifies the state vector $\vec{X}$ according to a given control vector $\vec{U}$.

[1] See p. 279 for availability of software.

`dp_solve()` — HDP optimum control problem solver

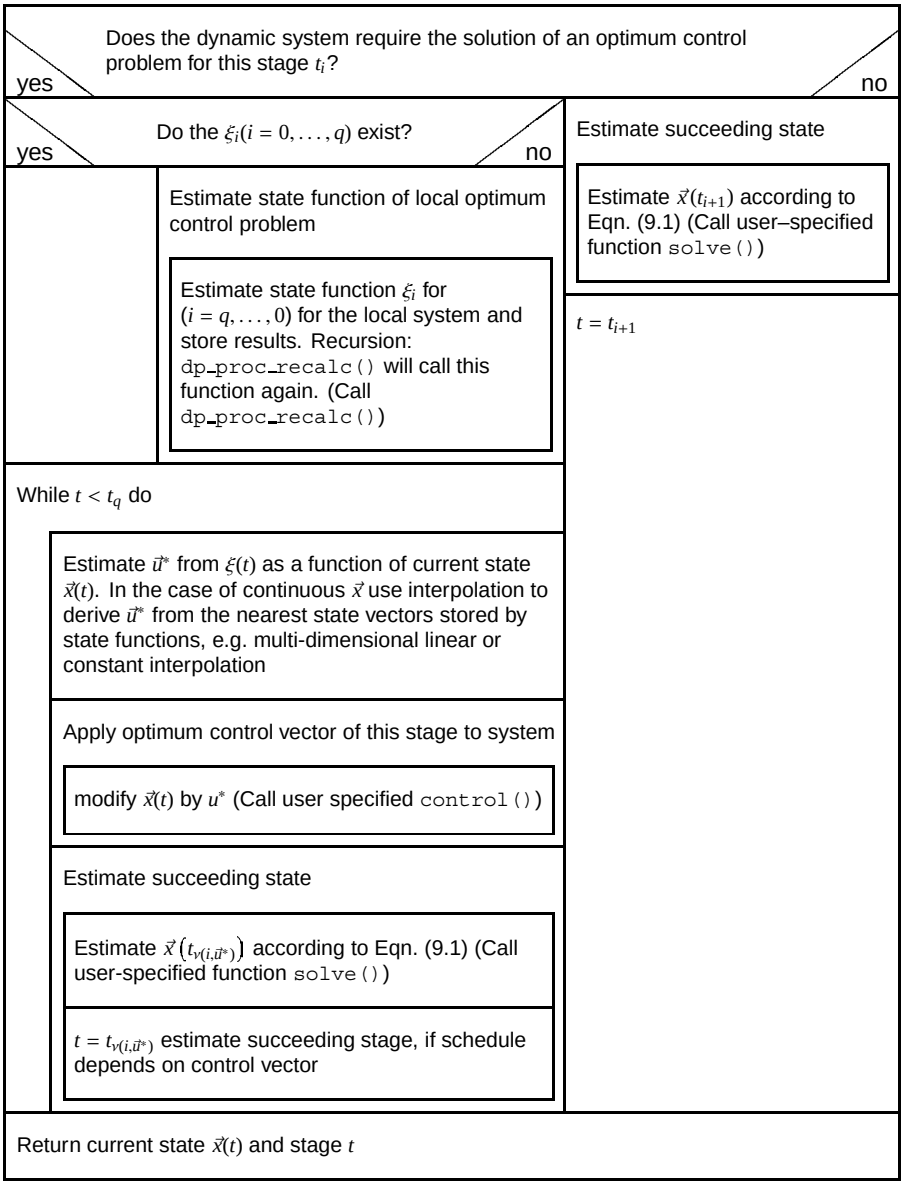

Fig. 9.2 Structure of HDP optimum control problem solver `dp_solve()`. The function is the optimum control problem solver, either as a final solution of a given optimum control problem or as a local part of a structured HDP problem

3. Set up performance criterion $J[\vec{X}, \vec{U}]$ with Markoff property. According to Equation (9.2) this means J_i ($i = 0, \ldots, q-1$) and J_q are set up separately. J_Q is defined by procedure `criterion_Q()` and `criterion_i()` defines J_i for ($i = 1, \ldots, Q-1$). The operator $K(a, b)$ is specified by an identifier when calling the procedure `dp_proc_recalc()`.

4. Set up main code. This is supported by several library functions which can be used

   – to set up the interpolation grid,

   – to run the DP or HDP procedure, which recursively estimates Equation (9.4),

   – to calculate an optimum control solution to a given initial state, and

   – to apply a given control vector to the dynamic system.

9.2.4 Concluding Remarks

However the described developments of HDP are initiated by the identified mathematical heterogeneity of environmental simulation models, applications of HDP for technical systems were studied and compared to genetic programming algorithms in Chouikha (1999). The optimum control procedure was used to set up an optimum control system model by a hybrid Petri net. The comparison to genetic algorithms shows that DP/HDP procedures are less efficient, if it is not possible to re-use precalculated solutions in further steps of optimization, see Chouikha (1999, p. 157).

The proposed framework for optimum control and the HDP procedure can be used as a general concept applicable to a large class of environmental models. Mathematical heterogeneous systems can be treated within HDP. To apply HDP it is not necessary to know any derivatives of the system to state or control vectors. The possibility of iteratively excluding control vectors which lead to physiologically impossible stages is an important feature, especially for ecological systems which may be calibrated only for a distinct subset of system space.

On the other hand, the "dilemma of dimensionality" is an intrinsic property of the underlying DP procedure. It offers approaches to this problem with special respect to environmental models. But this problem cannot be eliminated completely. In the following Chapters 10 and 11 the concept is used to solve several problems of identification of optimum management strategies in agroecosystems.

9.3 OPTIMIZATION AND SPATIALLY EXPLICIT MODELS

Introduction Optimization in spatially explicit models differs entirely from the task of optimum control theory and defines a new class of optimization problems. Two

main topics are responsible for this difference. First, the vector of control variables $\vec{u}$ to be determined is in this case a map of vectors. Without loss of generality we focus on raster-based spatially explicit models. The observed region is denoted by a set of discrete grid points $R = \{(i, j) \mid n_i < i < N_i; m_j < j < M_j\}$. A grid cell of the map is denoted by $\vec{z} = (i, j)$.

Second, the formulation of a scalar performance criterion has to map the space of control and state variables to a scalar value. As state and control variables depend on time and space, a performance criterion for spatially explicit optimization problems is given by double integral in space and time, see Equation (8.1).

9.3.1 Computational Effort

The number of control variables to be determined is increased by the size of the investigation site $|R|$. Assume the control vector is defined by two variables: a discrete variable u_1 with n_1 different attributes and a continuous variable $u_2 \in [a, b]$. In terms of a combinatorial analysis of complexity we can assume that an appropriate discretization of u_2 into, for instance, n_2 discrete values can be given. The combinatorial effort of identifying a optimum control map $\vec{u}(\vec{z})$ for all $\vec{z} \in R$ is given by the term $|R|^{n_1 n_2}$. Complexity increases more than exponentially.

Against this background it is obvious that solutions of optimization problems in spatially explicit models require an appropriate methodology as well as some general simplifications. In general, we do not aim at the aggregation or simplification of the model itself, cf. Figure 8.2. In the following the structure of the general spatial performance is analyzed to find a simplification of the problem.

9.3.2 Local and Global Performance Criteria

A spatially explicit ecological model offers a fascinating functionality in the assessment of ecosystem functions. The ability of accessing any state variable at any location in the investigation site is a function that makes spatially explicit models distinct from all others. Imagine, for instance, that one is able to trace the concentration of a specific substance at the mouth $\vec{z}_0$ of a watershed: $x_i(\vec{z}_0)$. An optimization problem can easily be written in the form: identify the management patterns for maintaining the value of $x_i(\vec{z}_0)$ below a defined constraint or minimize this value, while locating a maximum area of certain habitats.

The difficulties inherent in this optimization problem are obvious. The identification of an optimum location of the habitat is a large combinatorial problem with a single restriction based on the assessment of the single value $x_i(\vec{z}_0)$. A problem like this is denoted as *global optimization* problem.

Task 9.1 (global problem) *Find maps* $u_1^*, u_2^*, \ldots$ *which maximize* $J \rightarrow \max$ *according to Equation (8.1).*

It is difficult to solve a problem like this, with a complexity increasing more than exponentially, from scratch, that means without any knowledge of approximate patterns of the solution.

To simplify the problem we can make use of the fact that spatially explicit models are set up by a repeated application of the same model to different spatial units (either so-called ecotopes, elementary landscapes, or raster cells, see Sections 3.3.1 to 3.3.3). This implies that the state of the variable x_i at location $\vec{z}_0$ is a result of the value of x_i of all cells $\vec{z} \in R$. Some cells may contribute more, some may contribute less, to the final result of $x_i(\vec{z}_0)$ and the relationship between $x_i(\vec{z}), \vec{z} \in R$ and $x_i(\vec{z}_0)$ is highly likely to be nonlinear.

The basic idea that follows from this is to define a local performance criterion in each grid cell. This is structurally a different way, because it aims to map the regional goal function onto the processes in a grid cell. The basic idea is to set up characteristic functions, which are part of the performance criterion and are spatially dependent, as part of the goal function. This approach is comparable with a functional decomposition of the landscape using a spatially explicit simulation model, compare (Cornwell *et al.*, 2001).

A general equation that summarizes the calculation of goal functions for each grid cell is

$$A_i(\vec{z}) = \int_0^{t_{end}} \vec{\lambda}^T \begin{pmatrix} \vec{x}(t,\vec{z}) \\ \vec{u}(t,\vec{z}) \end{pmatrix} dt \quad i = 1, 2, \ldots, k \tag{9.8}$$

A_i are maps that hold local scalar values estimated from calculating the weighted sum of state and control variables and aggregate this to a scalar value by integration over time.

The derived maps may then be estimated by calculating

$$J[\vec{x}, \vec{u}] = \int_R \sum_{i=1}^{k} A_i(\vec{z})\, d\vec{z} \tag{9.9}$$

Integration over the investigation site R aggregates the map variables A_i to a scalar spatial goal function J. Based on this one can formulate a local optimization problem:

Task 9.2 (Localized Problem) *For each cell $z \in R$ estimate $A_i(\vec{z})$ $(i = 1, 2, \ldots, k)$. Based on these characteristic functions maximize $J(z) \rightarrow \max$ according to Equation (9.9).*

Note that spatially explicit optimization is simplified to the estimation of maxima of a reduced set of characteristic functions $A(\vec{z})[\vec{x}, \vec{u}]$ that can be evaluated independently for each cell $\vec{z} \in R$.

Obviously the solutions from Task 9.2 are different from those of Task 9.1. The goal function of Task 9.1 neglects any neighborhood relationships in the control variable

maps. The question is, how large are the differences in the solutions, or do these solutions have more in common than one would expect? The next section will show that the numerical effort for the estimation of solutions for Task 9.2 is orders of magnitudes lower compared to Task 9.1.

How is this achieved? The second basic idea related to the solution of the localized problem is that reducing the global performance criterion to a localized problem for each grid cell allows us to neglect the spatial explicitness of the control variables. We can assume constant maps of control variables $u_i(\vec{z}) = u_i$ for all $\vec{z} \in R$. Searching through all possible combinations of control is reduced by applying the control input homogeneously to the entire study area.

Up to this point we have assembled all the important issues that allow us to solve optimization problems on spatially explicit models. Figure 9.3 summarizes the concept that is derived from this distinction of local and global optimization tasks and performance criteria, including important additional steps of solution analysis.

The first step in this concept is to perform a grid search to identify the characteristic functions $A_i(\vec{z})$ that define the spatial performance criterion.

9.3.3 Grid Search Strategy on Local Problem

The first step is to solve Task 9.2. The implementations described in the following makes use of the ability of the landscape model formulated within the framework of the spatial modeling environment to deal with spatially distributed information and to perform mathematical operations on maps, cf. Sections 1.5.5 and 3.3.3. The characteristic functions $A_i(\vec{z})$ of the local goal function are formulated as maps that are calculated using the spatially explicit model.

The solution of Task 9.1 performs a grid search through the entire control space assuming a homogeneous control variable $\vec{u}(\vec{z})$ for each cell. A series of maps for different combinations of control variables is generated and fed into the spatially explicit model. Maximizing $J(\vec{z})$ for every grid cell depending on the precalculated maps of the goal functions $A_i(\vec{z})$ solves the optimization problem. The result is a set of control variables that optimize the local performance criterion.

The computational effort can be estimated from this. In terms of a combinatorial problem for an optimization based on the local optimization task, kn_1n_2 runs of the spatial explicit model are required, using n_1 and n_2 as examples for a set of control variables u_1 and u_2, see above.

The resulting maps of optimum control variables are then fed into a spatial simulation again that is used to calculate the global performance criterion, cf. Equation (8.1).

9.3.4 Disturbing a Solution: Monte Carlo Simulation

The results from the local optimization approach can be tested by running a Monte Carlo simulation based on the optimum control variable maps. This Monte Carlo

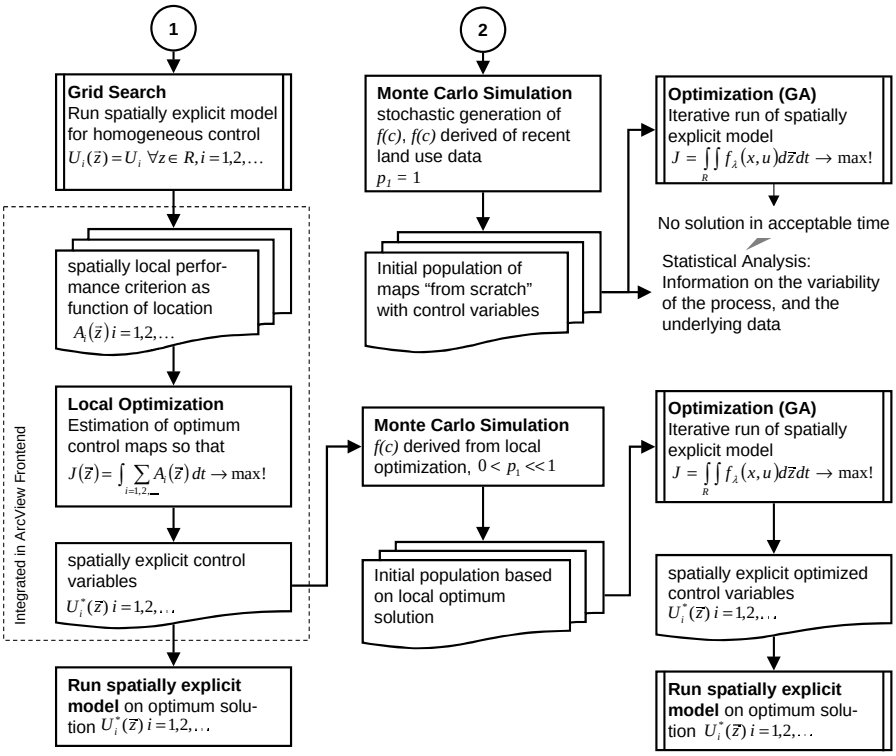

Fig. 9.3 Framework for the estimation of the spatial optimum concept for optimization of land use patterns and related control variables.

simulation *disturbs* the optimum solution stochastically and gives an estimate of how close the local solution is to the unknown optimum.

The set up of a Monte Carlo simulation depends on what is known about the distribution of the parameter to be varied. If the variable is continuous, a continuous distribution with a mean and a variance must be defined. *Disturbance* in this context means that the mean value is set equal to the derived local optimum value and a variance value is defined that specifies the range of variation.

If the variables are discrete or categorical, the disturbance of a solution is a two-stage stochastic process. Let $Z_1(\vec{z}) \in [0,1]$ be a random variable. A new value for the considered control variable u_1 is generated randomly if $Z_1(\vec{z}) < p_1$ for cell $\vec{z}$. This is done by a stochastic variable Z_2 such that $P\left(Z_2(\vec{z}) = u_2(\vec{z}) \,|\, Z_1(\vec{z}) < p_1\right) = f(u_2)$.

For every cell $\vec{z}$ the stochastically generated variable u_2 follows a distribution which is defined by a density function f. The density function f is constant for the entire region and may be generated by a stochastic process, started before generating the stochastic map. Or, it may be derived from the distribution of a known pattern, for

instance the optimum solution. With this set up three different types of Monte Carlo simulations can be distinguished:

- $p_1 = 1$, f generated stochastically: patterns are generated *from scratch*, without any knowledge about a possible spatial pattern;
- $p_1 = 1$, f derived from known patterns such as historic data or optimum local solutions: patterns are based on *reallocations*.
- $p_1 = 0.01x$ and $f(C)$ derived from optimum solution: patterns are disturbances of optimum solutions by a certain percentage x.

9.3.5 Genetic Algorithm Solving the Global Problem

As we have seen in the previous sections the global optimization problem cannot be solved in terms of a combinatorial optimization problem. The application of iterative procedures, which are usually based on gradient search algorithms, may be inappropriate since in many cases the derivative can be estimated neither analytically nor numerically. This is because of the complexity of the ecosystem model and the combination of discrete and continuous control variables.

Genetic algorithms offer a solution to the optimization problem based on the global performance criteria. The first step of GA is to define a representation of the control variables of the optimization problem to a genome. Based on the idea of "survival of the fittest" a stochastically generated first population of a distinct number of individuals runs through an evolutionary process. GA determines which individuals of a population should survive, which should reproduce, and which should die. New individuals are created based on the operations of cross over, mutation, and gene migration.

Application of GA to an optimization problem requires three steps

1. Definition of a representation
2. Definition of the genetic operators
3. Definition of the goal function

The goal function for the problem in hand is given by Equation (8.1). Common libraries support the second step. We used a C++ Library of Genetic Algorithm Components (GALib), see Wall (1996). The first step, the representation of the control variable $\vec{u}(\vec{z})$ of the spatially explicit model to a genome is defined as follows

- Each controllable cell $z \in R$ defines a single gene g_k, $k = 1, \ldots, |R|$. The genome has the length $|R|$.
- The location of the gene in the 1-dimensional array genome string is identified with the location of the cell in the grid map $k \longmapsto \vec{z} = (i, j) \in R$.

- Discrete control variables are an attribute of a cell or gene. Continuous control variables need to be approximated by a discrete value to be coded by GA. The control variables are therefore defined by an allele set $L = (u_1, u_2, \ldots)$ for each gene.

Before starting the genetic algorithm an initial population has to be generated, usually performed by cloning a given individual. We used different populations derived from the three stage stochastic process used for the Monte Carlo analysis. The initial population therefore is based on a stochastic variation of a local optimum land use and fertilizer pattern parameterized by the probability p_1.

The global optimization problem can be solved by basing it on the GALib library. For each generation the algorithm creates an entirely new population of individuals by selecting from the previous population, then mating to produce the new offspring for the new population. Each new individual of the population requires a run of the entire spatially explicit simulation model. The "survival of fittest" strategy is implemented by evaluating the goal function. This process continues until the stopping criteria are met (determined by the terminator).

Figure 9.3 summarizes the methodological concept described in a flowchart. Two main branches are used: Branch 1 starts with the estimation of characteristic function maps, which are the basis for local optimization; Branch 2 shows how to work on the optimization problem without any knowledge of an appropriate initial guess of the solution.

9.3.6 Toolbox for Spatially Explicit Optimization

Structure The framework described above is implemented in the Toolbox for Spatially Explicit Optimization[2] (TSEO). Parts of this toolbox interact with the spatial modeling environment, other parts support analysis of the results within the geographic information system ArcVIEW. The toolbox is structured in three parts:

1. A geographic information system that is used for visualization of the results and offers a graphical front end for the most important functions of the concept.
2. A spatial explicit dynamic system, that is capable of simulating environmental processes on a raster-based data structure.
3. Several programs that set up the toolbox for spatially explicit optimization of dynamic systems. These programs offer the functionality summarized in Figure 9.3. The TSEO command-line interface supports a simple access to the programs of the toolbox.

Exchange of data and maps between these three parts is performed within a database structure using ArcVIEW ASCII raster map format. Spatially explicit simulation

[2] See p. 279 for availability of software.

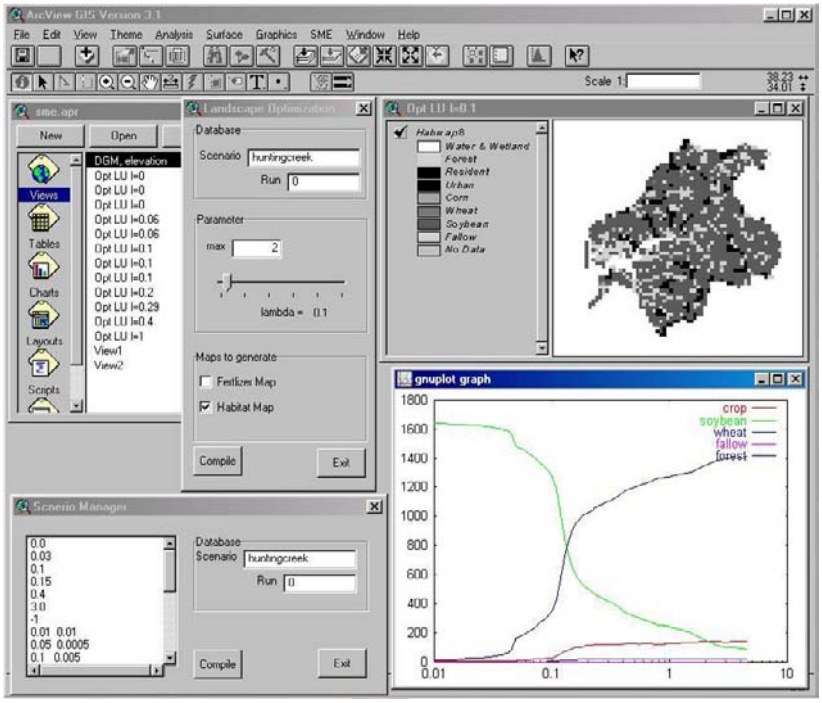

Fig. 9.4 Screen shot of ArcVIEW front end with the local optimization project.

models that are capable of reading and writing the model output in this format are therefore applicable in the toolbox.

Graphical Front end ArcVIEW These concepts require the minimal computational effort so the steps of local optimization and solution analysis are embedded in the GIS front end ArcVIEW and the results are presented as a simple visualization. Figure 9.4 shows a screen copy of the ArcVIEW display with a parameter study of the land use distribution in the Hunting Creek watershed.

Spatially Explicit Simulation Model TSEO assumes a predefined spatially explicit model using a raster-based data structure for the spatial information to be used in the optimization process.

The desired performance criterion is rarely part of the simulation model. Because of this, for application of the optimization toolbox, the simulation model has to be modified to support the optimization toolbox with required information. This information relates to the performance criterion to be maximized. Variables used in the performance criterion are not usually part of the model, as these variables often calculate aggregated indicators of the model system, such as integrals or sums of state

variables. Or, these indicators reflect on boundary conditions or contraints, which are to be met during simulation time. In terms of variables introduced above, within a user code part of the model variables like $A_i(\vec{z})$ are to be calculated, cf. Equation (9.8). At the end of the simulation these maps have to be written to the database.

Functions of Toolbox The toolbox supports the main functions of the concept. These are the grid search in local problem, the identification of optimum maps based on grid search, a Monte Carlo analysis, and the global optimization with genetic algorithms.

The following documentation refers to the implementation using the spatial modeling environment for spatial modeling, cf. Sections 1.5.5 and 3.3.3. If a different modeling environment is used, the steps of initialization and run control of the model system have to be adapted.

Starting from a previously compiled simulation model, the first step is to initialize a database that stores optimization results as well as intermediate information. This is performed by the declariation of all SME parameters like the name of the project, the scenario and the path to the database. The command `tseo init` initialises the database structure according to the current settings of project, model, scenario.

A solution of the localized optimization problem (Task 9.2) is estimated by first running a grid search of the (simplified) space of control variables, started by the command `tseo grid`.

The information obtained from the grid search — these are the maps $A_i(\vec{z})$ — is intermediately stored in the database. Solutions of the localized optimization problem can be calculated depending on parameters of the performance criterion, usually denoted by a weighting scheme $\vec{\lambda} = (\lambda_1, \ldots, \lambda_n)$. For a solution of Task 9.2 values for these weights are to be specified

```
tseo local [<lambda_1> [...] | loop]
```

This instruction stores maps of optimum control variables $\vec{u}^*(\vec{z})$ into the database that specify the spatially explicit optimum solution for the given vector of weights of the performance criterion. Running the spatially explicit model (see next step) uses this map to study the simulation changes according to the obtained solution.

An analysis function supported at this step of the framework is the analysis of the solutions depending on variation of a certain weight λ_i. The `loop`-tag in the command line is used to start a sensitivity analysis. The weight λ_i which is not specified in the command line and replaced by the `loop`-tag is changed according to the information by a parameter file. The results of this scenario analysis are graphically displayed using the command `tseo plot`.

A Monte Carlo analysis is started by using the command `tseo mc <prob>`. Monte Carlo analysis starts from the previously calculated optimum maps of the control variables. The control variable maps are used and randomly modified by the probability

given by <prob>. The program started needs to be aborted manually using CTRL-C key, as Monte Carlo analysis is implemented by an endless loop.

A solution of the global optimization Task 9.1 is calculated using genetic algorithms. To estimate an initial population optimum maps are identified for a certain vector of weights (compare tseo local-instruction). From the optimum maps of control variables an initial population for GA is stochastically generated by a random modification of the probability given by <prob>. The statement for global optimization is therefore

```
tseo global [<lambda_1> [...]] <prob>
```

Note, this is a very time consuming task. One may trace the protocol file to assess convergence success. The command may be aborted by CTRL-C.

If maps of control variables were previously calculated (either by local optimization or by global optimization) these maps are now fed into the model and a spatial optimization is performed using the command tseo run.

Several other functions are available for database management, edititing of configuration, and import/export of data. For additional information the reader is referred to the technical documentation of the toolbox (Seppelt, 2003).

9.4 SUMMARY

The first step of identifying a general or generic notation for optimization of optimum control problems with mathematically heterogeneous models was identified as the core problem of applying environmental models in optimization. The formulation of the task needs to cope with the hybrid structure of an environmental model.

This chapter showed, that general tools for solving environmental management problems can be developed by combining different tools of numerical mathematics and by making use of some general properties of environmental systems for instance their hierarchical structure. In the following chapters we will now study applications of these concepts.

10

Optimum Agroecosystem Management: Temporal Patterns

10.1 INTRODUCTION

In this chapter applications of the agroecosystem model, summarized in Chapter 2, to optimum control theory are presented. The applications consider optimum fertilizer application, pest control, and crop rotation schemes as a dynamic control problem with different time scales. All forcing functions defined in Chapter 2 are used as control variables and are fed into optimization procedures. Several solutions are presented for a German investigation site. Different assessment scenarios of production schemes are compared with the tool of optimization.

Management of agricultural regions is a good exercise of environmental management. Farmers are directly influencing ecological systems and are mutually dependent on these systems. Therefore the question of optimizing management strategies arises. Optimum control theory offers the connection between simulation models, evaluation of the environmental system states, and anthropogenic management.

Estimation of optimum management strategies of agroecosystems in terms of optimum control theory requires:

- formulation of an appropriate and probably complex spatially explicit simulation model for an agricultural region with the incorporation of farmers management; and
- definition of a performance criterion (and — as needed — constraints) which assesses the observed variables and assigns a set of state variables to values

identified with "good" or "bad" environmental states, whatever this means in the considered context.

The first item has been presented in Chapter 2 and 3. The second item was discussed at a theoretical level in Chapter 8. Considering agroecological processes the task is to define an appropriate performance criterion based on the state and control variables of the model in Section 2.7. The overall goal is the estimation of optimum management schemes with respect to ecology and economy (Seppelt, 1999).

10.2 ASSESSING THE STATE OF AN AGROECOSYSTEM

10.2.1 External Cost and Non-measurable Variables

The chosen example of an agroecosystem model is typical for environmental modeling. It shows the solution of two important problems in ecosystem management: the determination of long term strategies with the use of the temporarily structured models and regionalized management optimization.

As shown in Chapter 8 performance criteria have to integrate economic and ecological issues. Economic issues are, for instance, prices for yield, farmers' income, and prices for fertilizer, farmers' expenses — the first to be maximized, the latter to be minimized. Further economic issues may focus on taxation of fertilizer, reduction of fertilizer input, or to fulfill restrictions on fertilizer application in terms of constraints.

The nutrient content in soil or the infestation of pests are examples for the ecological part of the assessment. Whereas the former economic assessment could be defined by a monetary unit, it is difficult to identify units for ecological variables. Ecological and economic issues are difficult to compare.

Considering the issue of the openness of ecological systems in the agroecosystem model, external costs are the loss of nutrients out of the rooting zone, the loss of pesticides (either by volatilization, runoff or leaching).

Examples for unmeasurable variables in the agroecosystem are the amount of nitrogen leached out of the plant-accessible root zone. Nutrient outflow into ground water or the population of a pest, like the sugar beet cyst nematode, are very difficult to measure.

10.2.2 Performance Criteria

Referring to the generic agroecosystem model (see Section 2.7) the state variables crop yield W_C, plant available nitrogen content N, pesticide in soil C_S are used to assess the state of the system. Additionally the control variables applied fertilizer F, applied pesticide A, and planted crop α are considered. All state and control variables are time-dependent. For this reason an aggregation, in mathematical terms an integration or accumulation of the variables, is required to obtain a single scalar

Table 10.1 Overview of the considered scenarios and their performance criteria with the assessed variables and the weights λ_i. Weights are set to zero in Equation (10.1) for variables which are not assessed in a performance criterion, denoted by the missing •. Constraints are understood as constraint for the entire region, e.g. for all $\vec{z} \in G$. All goal functions are quantified by monetary unit per area [€/ha].

Scenario		Assessed variables in Equation (10.1)					Additional constraints
		W_C	N	C_S	F	A	
J_1	"economic"	•			•	•	
J_2	"taxes"	•			•		
J_3	"ecologic"	•	•	•	•	•	
J_4	"N-limit"	•	•				$N(T) < N_{max}$
J_5	"F-limit"	•			•		$\sum F(t_i) < F_{max}$
Weight		λ_W	λ_N	λ_C	λ_F	λ_A	

value. Referring to the general performance criterion defined in Equation (8.2) the following performance criterion J can be defined:

$$\begin{aligned} J[W_C, N, C_S, A, F, \alpha] \quad = \quad & \lambda_W(\alpha(t,\vec{z})) \int_R W_C(t_{end}, \alpha(t_{end},\vec{z}),\vec{z})\, d\vec{z} \\ & - \int_R \int_0^{t_{end}} \lambda_F F(t,\vec{z}) + \lambda_A A(t,\vec{z})\, dt\, d\vec{z} \\ & - \int_R \int_0^{t_{end}} \lambda_N k_l N(t,\vec{z}) + \lambda_C k_l C_S(t)\, dt\, d\vec{z} \end{aligned} \tag{10.1}$$

Note, an integration is performed in time as well as in space. If a non-regionalized or not spatially explicit model is considered the integration in space of the investigation site given by R can be dropped.

The performance criterion in Equation (10.1) additionally incorporated some parts of the simulation model: the terms $k_l N$ as well as $k_l C_S$ integrate the amounts of transported matter our of the rooting zone, assuming a linear flow k_l.

10.2.3 Weighting Schemes

With the weights λ_i the different state and control variables are aggregated to a scalar performance criterion. Setting up values for the weights requires answers to the above stated problems of comparing economic and ecological variables, openness and the use of measurable and non-measurable variables. Different sets of λ values define different assessment scenarios and with this different perspectives to optimality.

Table 10.2 Weights in performance criterion for different crop growth models.

Crop	Sugar beet	Spring barley	Oats	Winter wheat	Winter-barley	Field beans	Oil radish	
Abbr. (α)	sub	spb	oa	ww	wb	fb	or	
Crop-dependent parameters of performance criteria								
λ_W (J_2)	17.1	18.4	19.2	18.5	18.5	—	—	[J/kg]
(all other)	0.4	0.32	0.28	0.08	0.07	0	0	[€/kg]
λ_N (J_3)	15.5	10.5	9.5	10.5	10.5	—	—	[€/kg-N]
F_{max} (J_5)	136	124	81	124	158	—	—	[kg-N/ha]
Vegetation period								
Sowing in	April	April	April	Nov.	Oct.	May	May	
Day of year	91	91	91	284	264	121	121	[d]
t_{end}	188	137	122	280	300	150	120	[d]

λ values for the different criteria

- can be derived from market prices (“economic” criterion);
- may be modified by taxation of fertilizer (“taxes” criterion);
- are estimated by internalization of external effects. This makes use of the approach of an assessment relative to non-disturbance (Nilsson & Bergström, 1995) (“ecologic” criterion);
- can be supported by constraints like limitation of total fertilizer input (“F-limit” criterion) or of nutrient content in soil at harvest time (“N-limit” criterion).

Table 10.1 summarizes these performance criteria. Obviously not all criteria are based on measurable variables. It is necessary to study the results of these different optimization criteria.

As these market prices depend on the crop planted, the weighting scheme of the performance criterion changes as a function of the control variable α (planted crop). Table 10.2 lists all weights that are derived from market prices of energetic balances.

10.3 AGRICULTURAL OPTIMUM CONTROL PROBLEM

10.3.1 Optimization Task

We are now able to formulate a general optimum control problem based upon the knowledge of the agricultural process summarized in a simulation model:

Task 10.1 *Based on the agroecological model in Section 2.7 estimate a function of optimum fertilizer input $F^*(t, \vec{z})$, of pesticide application $A^*(t, \vec{z})$ and a sequence $\alpha^*(t_i, \vec{z})$ of planted crop, so that a performance criterion J is maximized.*

Note that

- Fertilization and pesticide application are discrete events. It follows that not only the amounts but also the time of optimum application must be estimated.
- The spatial dependency of fertilizer, pesticide application and model parameters complicate the problem tremendously.
- With the specification of the control variable planted crop α, a set of model parameters and also the model structure is changed during simulation.

Temporal patterns of this task are studied in detail in this chapter. Chapter 11 studies the resulting spatial patterns of the optimization task.

10.3.2 Hierarchical Structure of the Problem

The underlying procedures for solving the numerical optimization problems are derived from the dynamic programming approach, introduced in Section 9.2. The algorithm is appropriate for the given problem, as it can cope with the hybrid system with discrete and dynamic properties. However, to reduce computational effort a hierarchical structure of the problem is recommended. The hierarchical structure for this problem can be derived from the different temporal scales used in the model.

The optimum control problem is at first structured using the hierarchy in time, which is defined by the process dynamics. One can distinguish between fast processes like crop growth, pesticide dynamics, fertilization, and pesticide application and slow processes like population dynamics and crop rotation design. Additionally, control variables may be continuous and discrete.

The problem can be structured in the framework of a hierarchical control model. In a first step a *local optimum control problem* is solved, with the optimization of fertilizer input in a vegetation period for each crop. These solutions are stored as a function of initial values and crop identifiers. In the second step, the *global optimum control problem* is solved and an optimum crop rotation is estimated where every crop receives its optimum fertilizing scheme. In this step the performance criterion makes use of the performance criterion of the local problem.

$$\widehat{J}_n[N, J] = \sum_{i=1}^{Q} J_n[W_C, N, F, A, C_S] - \Lambda_N \int_R \int_0^{t_{end}} k_l N(t, \vec{z})\, dt\, d\vec{z} \qquad (10.2)$$

The solution of this global task makes intensive use of the previously stored local solutions which reduces computational effort and couples a discrete and continuous optimum control solution.

Table 10.3 Comparison of optimal fertilizing strategies from different performance criteria and crops. The last column shows literature values of expected yield and recommended fertilizer (Niesel-Lessenthin, 1988). Total amounts of applied fertilizer from J_3 printed in italics are used as F_{max} values for J_5. All values in kg/ha. Symbols are: $W_C(t_{end})$ harvest biomass, N_{tot} total amount of nitrogen leached from root zone during vegetation period, F_{tot} total amount of fertilizer applied (optimized).

		J_1 "econ."	J_2 "taxes"	J_3 "ecolog."	J_4 "$N(t_{end})$– limit."	J_5 "F_{max}– limit."	Reference values
Sugar beet	$W_C(t_{end})$	18000	13700	13000	17400	12100	13000–26000
	N_{tot}	62	47	21	50	26	
	F_{tot}	305	228	*136*	236	128	140–210
Winter wheat	$W_C(t_{end})$	10400	9600	9000	10100	8400	7600–14400
	N_{tot}	67	28	23	35	24	
	F_{tot}	208	138	*121*	160	113	100–210
Winter barley	$W_C(t_{end})$	13600	12800	11200	12300	11300	7600–14400
	N_{tot}	67	53	39	48	44	
	F_{tot}	290	192	*158*	179	147	100–210
Spring barley	$W_C(t_{end})$	15000	14000	10000	13000	9600	6400–11200
	N_{tot}	36	25	11	22	13	
	F_{tot}	294	202	*124*	178	118	100–170
Oats	$W_C(t_{end})$	10300	9400	5600	9000	6100	6400–12400
	N_{tot}	33	21	8	19	9	
	F_{tot}	241	142	*81*	130	75	80–170

10.4 SHORT-TERM SOLUTIONS: MANAGING A VEGETATION PERIOD

10.4.1 Optimum Fertilizing Schemes

The estimation of optimum fertilizing schemes to different performance criteria (see Table 10.1) are derived first. Table 10.3 contains the results of total fertilizer application, harvest biomass, and leached nitrogen for different crops. Literature values are added for comparison (Niesel-Lessenthin, 1988). Optimum fertilizing schemes from "economic" lead to a maximum consumption of fertilizer with a high amount of nitrogen loss. A reduction of fertilizer input can be achieved with governmental restrictions. With the use of "taxed" fertilizer (J_2) or the limitation of harvest nitrogen pool $N(t) < N_{min} = 45$ kg/ha (J_4), total fertilizer input is reduced by 30%. This leads to a reduction of nitrogen loss in the same range, while yield reduction is less than 15%.

Introducing external costs into assessment (J_3) results in the lowest values of leached nitrogen after vegetation period: less than 60% of the results of J_1. This fertiliz-

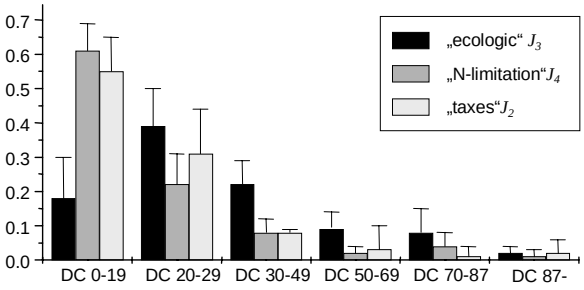

Fig. 10.1 Distribution of optimum fertilizer amounts of grains in the main development stages for different performance criteria. Standard deviation is calculated based on fertilization schemes applied to different grains (winter sheat, winter barley, oata, spring barley).

ing scheme incorporates a notable reduction of yield: 25% less than the results of "economic" assessment.

These calculations use a unmeasurable variable for assessment, due to the nonzero weight λ_N. One can ask for an assessment based on these results using measurable state variables. This problem is solved using J_5 for assessment. This limits the maximum amount of applied fertilizer to $F_{max} = \sum F_i^*$ using the optimum fertilizing schemes F^* calculated on the basis of the "ecological" assessment with J_3.

On a closer examination the optimum function $F^*(t)$ explains the time dependence of the fertilizer application. For a comparison of the fertilizing schemes the results of the grain-models are taken for detailed study. A comparable time scale can be defined using the stages of development denoted by the development code, see Section 6.2.1 and (Zadoks *et al.*, 1974). Figure 10.1 summarizes the distribution of fertilizer (results of optimum control assessed by J_1, J_3, J_4 in the development stages normalized by the total amount). This figure explains why the solution of J_3 attains a 60% reduction of fertilizer and nitrogen loss with a considerable smaller reduction of yield. Fertilizer is applied only in the main stages of growth which are DC30 to DC49, see (Zadoks *et al.*, 1974). The solutions derived by other scenarios (J_2, J_4) of assessment lead to optimum fertilizing schemes, which set up a sufficient amount of fertilizer at the beginning of the vegetation period. Obviously, this increases the amount of nitrogen loss.

10.4.2 Optimum Pesticide Application Timing

Figure 10.2 shows the results of optimum pesticide application schemes to the performance criterion of Equation (10.1). The parameter of variation is the initial pest infestation $P(0)$ and the time, denoted by main development stages. All figures show the relative distribution of application amounts $A^*(t)$ with respect to the maximum application amount of a whole vegetation period and the entire spectrum of initial

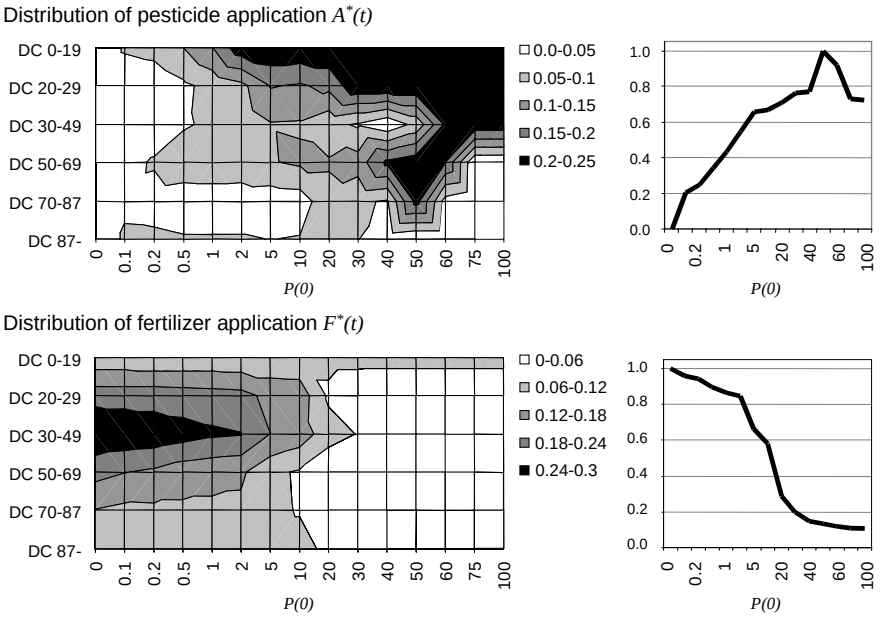

Fig. 10.2 Distribution of pesticide and fertilizer application for control of pest population P in a vegetation period using criterion J_3 ("ecologic") for assessment.

pest infestations. The left figures show the distribution function as a density plot and allow an analysis of time dependence. The right figures show the accumulated application amount of fertilizer and pesticide as a function of initial pest population relative to the maximum amount applied.

The distribution of the fertilizer schemes is shown in the lower figures. For low initial pest infestation one can identify the results described in the former paragraph. Above a critical level of investigation the fertilization scheme changes completely. No fertilizer is applied at the stages after DC20 and the total amount of applied fertilizer is less than 20% of the normal amount.

The reason for this optimum fertilizing scheme is that fertilization is not decisive for the outcome of yield. Yield is controlled only by pest control throughout pesticide application.

Optimum pesticide application schemes appears as follows:

- The pest population is controlled at the earliest stages with an optimum amount, slightly above the critical dose to get response in the pest population. The pest population shows a high growth rate. To achieve a maximum effect in pest control with a minimum amount of pesticide getting washed into the upper soil layer, an early application date is important.

- For moderate pest populations below the critical level two or three application events can control the pest population. If more application days are necessary, continuous but small applications of pesticide are optimal. This reduces pesticide runoff into the upper soil layer.
- Above the critical level of initial pest infestation, the pesticide application is decisive for the yield amount. The amount of applied pesticide reaches a maximum. For the control of the pest population an application during the entire vegetation period becomes necessary.
- With a further increase of the initial pest population it becomes impossible to maintain a sufficient amount of yield. Optimum application amounts are reduced for a limitation of pesticide runoff.

10.5 LONG-TERM SOLUTIONS: MANAGING CROP ROTATIONS

Fertilization and crop rotation design are the selected variables for the estimation of long-term strategies. Figure 10.3 shows an example of a complete solution of the optimum control problem: An optimum crop rotation (based on $\widehat{J}_3$) with locally optimum fertilized crops (continuation of J_3). The figure shows a typical crop rotation of the farming systems in the investigation site: A sequence of sugar beet and winter wheat/barley with a period length of two to three years. For detailed analysis the continuation of the local performance criteria J_1 "economic", J_3 "ecologic" and J_4 "N-limitation" are chosen.

10.5.1 Nutrient Balance

An important question in the assessment of the nutrient circulation is, whether the nutrient balance can be equalized observing a vegetation period or a crop rotation. The weight Λ_N in Equation (10.2) incorporates the amount of nitrogen loss into the assessment of the crop rotation. One can include or exclude the local assessment of nitrogen loss with the choice of the local performance criterion. Table 10.4 summarizes the results of a seven year crop rotation with all possible scenarios.

Only if the local assessment does not restrict the application of fertilizer (like J_1), can a global assessment of $N(t)$ reduce the amount of nitrogen loss. If a considerable reduction of fertilizer is achieved in the vegetation period, the resulting amount of leaching nitrogen cannot be reduced any more, even if $N(t)$ is used in the global performance criterion.

10.5.2 Pest Control

An important part of a long-term stable agricultural yield in this investigation site is the control of the sugar beet cyst nematode *H. schachtii*. Control of this pest can be

Table 10.4 Total amount of nitrogen leached after a 7 year crop rotation for long-term performance criteria. The calculation of the average and standard deviation values was carried out with respect to different initial populations $P_1(t_0)$.

	$\widehat{J}_1$	$\widehat{J}_3$	$\widehat{J}_4$	
$\Lambda_N = 0$	650 (±40)	190 (±45)	275 (±35)	[kg/ha]
$\Lambda_N > 0$	450 (±45)	180 (±10)	275 (±32)	[kg/ha]

carried out by designing the optimum crop rotation schemes. In the given example it is the population of *H. schachtii* which effects the yield of sugar beet, the most important, most valuable crop. After planting of sugar beets the planting of a non-host crop can reduce the population of nematodes in a crop rotation. For this reason, the optimum crop rotation solution in Figure 10.3 consists of a two to three year crop rotation of sugar beet, with intermediate planting of wheat. Crops like oil radish or field beans may decrease the population of nematodes more efficiently — these crops are catch crops, which enable *H. schachtii* to hatch but disable the larvae before they become fertile, see (Schmidt *et al.*, 1993). On the other hand, these crops do not have a positive effect on farmers' income.

A general property of all these solutions of the optimum control problem is displayed in Figure 10.4. The optimum solution consists of two most rapid approaches to a local and a global optimum path. The local optimum state of nitrogen content in soil is a content of 50 kg/ha or less is reached within the first vegetation period with its optimum fertilizing scheme. All further fertilizing schemes start and end with an average nitrogen content of approximately 50 kg/ha. This demonstrates that the assumption for assessment of Section 10.2 is plausible. The global optimum control path is reached after three vegetation periods. This path is characterized by an interval of 80 to 200 eggs and juveniles in 100 g soil of *H. schachtii*. Figure 10.4 shows three different initial conditions ($P_1(t_0) = 10, 100, 1000$ e. + j./100g). Note, the optimal solution leaves this path, if the assessment stops at the end of the simulation interval.

10.6 DISCUSSION

It is well-known that ecological systems are complex and hierarchical systems. As a consequence ecological simulation models tend to be complex. Because of this, the analysis of human impact on ecosystems using simulation models in terms of scenario analysis is limited.

This chapter has shown that a systematic search throughout the policy space of environmental impact can be provided by the application of numerical optimum control theory to environmental models. The approach links ecological process models with the human impact in a clear manner, distinguishing between state, control, and assessment variables and models.

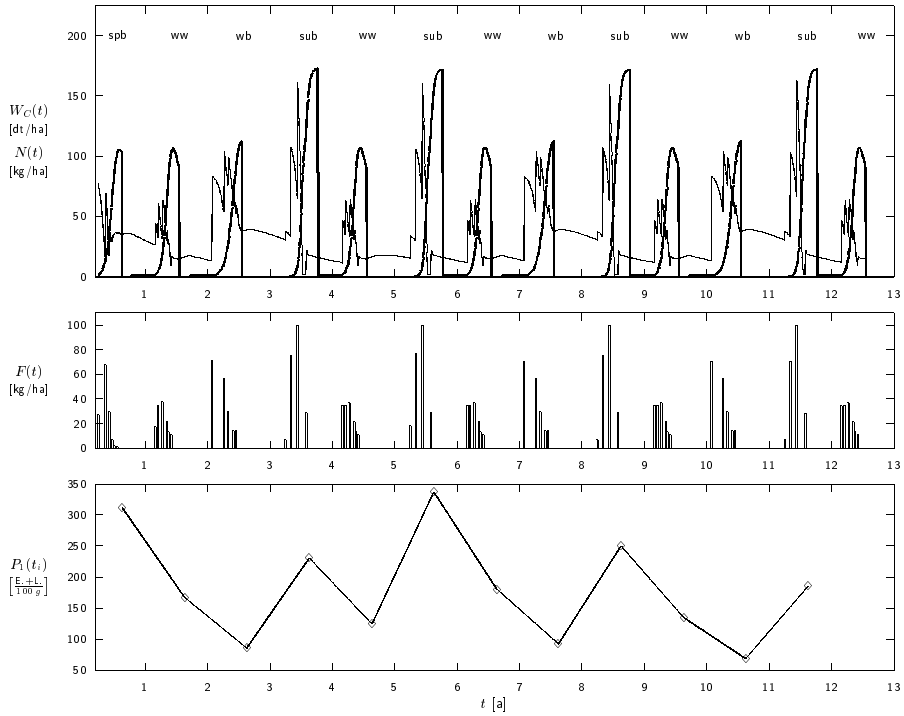

Fig. 10.3 Optimum crop rotation of t_{end} = 13 years with optimum fertilizing schemes (horizontal axis shows t in years). State variables: biomass $W_C(t)$ (thick line) Nitrogen content in soil $N(t)$ (thin line upper plot), and Population of *H. schachtii* $P_1(t_i)$. Control variables: fertilizer $F(t_i)$ (center plot) and planted crop ($\alpha(t_i)$) notation in upper plot. Initial values: N_0 = 50 kg/ha, $P_1(t_0)$ = 500 eggs and juveniles per 100 g soil.

Problems and perspectives of this approach in ecological system science are presented. The main difficulties of this approach, which give hints to further research needs, are

- to model a performance criterion or indicator, which evaluates all important disciplinary aspects of environmental processes,
- to find an appropriate level of model aggregation, and
- to apply a suitable procedure of numerical optimum control.

The analysis of different performance criteria and the related optimum solution is comparable to the standard approach of scenario analysis is. A very interesting outcome of the case studies is to study and compare different views of optimality by modification of the performance criterion. It allows the comparison of different policy strategies of farm management. The proposed framework permits the analysis of different indicators of environmental assessment and can answer the question whether environmental variables are aggregated in a suitable way. Facing this, it may also

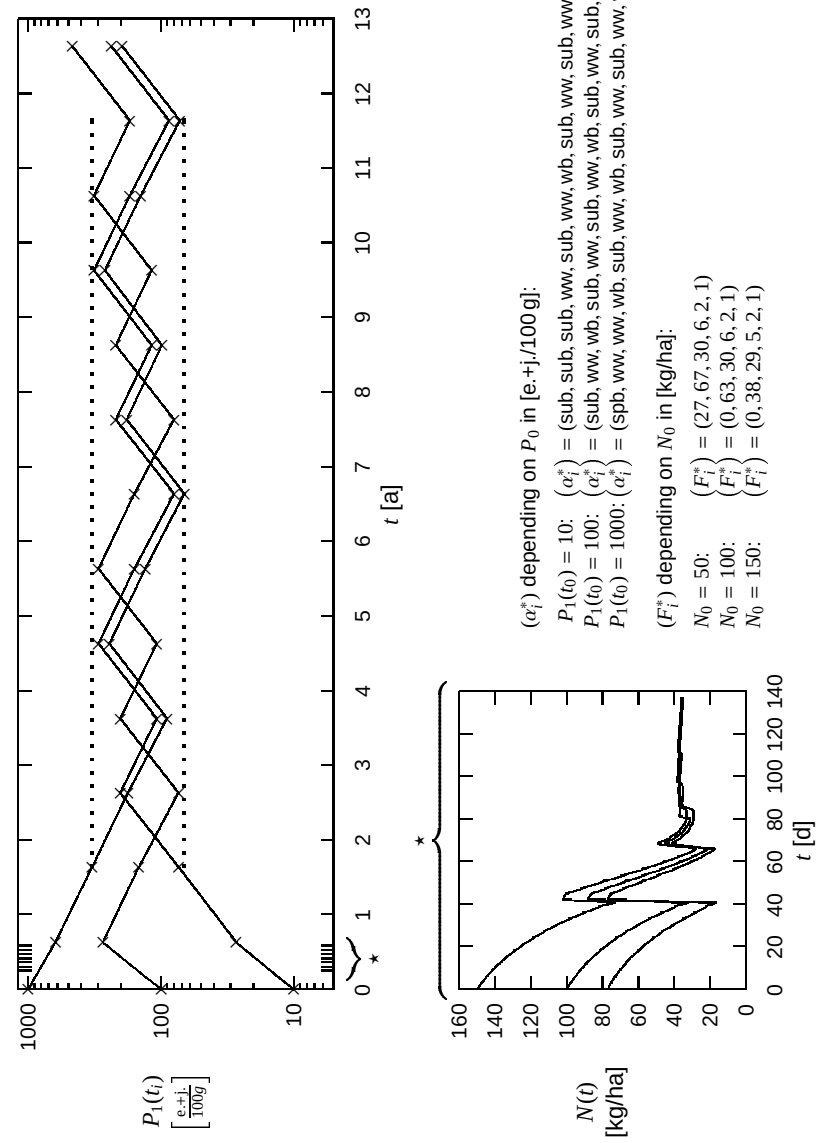

Fig. 10.4 Quantitative characterization of the most rapid iterated approach to an optimum path of soil nitrogen content (lower left, first vegetation period) and population of nematodes (upper).

give an answer to the question of how to incorporate externalities into the process assessment.

Overall, the choice of a simulation model on an appropriate level of aggregation is decisive for the success of the approach. A more complex model may be more realistic. On the other hand, this may lead to problems of computational effort or of assessing the process in an appropriate way.

The proposed framework for optimum control and the dynamic programming procedure with a hierarchical structure of different time scales comes out as a general concept applicable to a large class of environmental models. Mathematically heterogeneous systems like ecosystem models can be treated. On the other hand, the "dilemma of dimensionality" is an intrinsic property of the underlying procedure. Approaches to this problem with special respect to environmental models are presented. However, this problem cannot be eliminated completely. Further research should focus on robust procedures of optimum control of mathematically heterogeneous models with fewer prerequisites on the underlying model.

11

Optimum Agroecosystem Management: Spatial Patterns

11.1 INTRODUCTION

This chapter extends the results obtained to a spatial dimension. The focus is on the spatially explicit estimation of optimum fertilizer input and crop rotation schemes as a dynamic control problem on different time scales. Besides solution of the optimum control problems, this chapter focuses on the regionalization of the optimum control problem. The task is solved by the identification of homogeneous units in the observed region by a geographic information system. These maps are set up by a vector database. The second innovative topic, which enables a regionalized solution of the optimum control problem, is the estimation of families of optimum solutions parameterized by spatial properties. Technical problems concern efficient database access, which is solved within the GIS Arc/INFO, ArcVIEW. The proposed methodology supports the process of decision support in precision farming, cf. (Seppelt, 2000).

11.1.1 Site-specific Agroecological Modeling

An estimation of management strategies in agricultural landscapes needs to incorporate the spatial variability of soil into decision systems. The technology of *precision farming* (or, variable rate technology, site-specific farming) proposes solutions to this question (Lu *et al.*, 1997). Precision farming can be represented as incorporating four main areas of management: spatially referenced data collection, data analysis, decision making, and variable rate treatment (Usery *et al.*, 1995). Technical solutions exist for the steps "data collection" and "variable rate technology" (Lu *et al.*,

1997). A question still under discussion is how to derive management strategies from observed field properties. Strickland *et al.* (1998) emphasize the enhancement of environmental stewardship through accurate and precise application of chemicals and fertilizer to reduce leaching and runoff. However, the step "decision support" is still under discussion. Lu *et al.* describe simulation models as a tool to compare different management scenarios. A methodological concept for the estimation of management schemes is still under discussion.

11.1.2 Aims, Scope and Region

The aim is to estimate improved farm management strategies on a regional scale. We focus on the "Neuenkirchen" investigation site, described in Section 2.2.1 on page 40. The case study is performed on a sub-watershed "Ohebach" of the Neuenkirchen catchment site, see Section 2.3.1. The entire investigation site with its several layers of information is displayed in Figure 3.9 on page 86. The solution of the problem will be based only on publicly accessible databases. In the precision farming context, this means no GPS-based measured yield maps are used for model input. Map data is derived from the digital soil map (scale 1:5000). The data documents the soil properties of the watershed with several parameters. The soil can be characterized as homogeneous with minor small-scale variations. A 1–2 m layer of loess is topped by colluvial sediments depnding on the slope (Orthic to Gleyic Luvisols), see Section 2.3.1, p. 40 and (McVoy *et al.*, 1995) for details. The average field size is 30 ha. The typical crop rotation in the region consist of several cereals and fallow land with the main crop being sugar beets.

Figure 11.1 shows the underlying data set and the pedological homogeneous units with the field capacity. The whole area is mainly homogeneous: the average field capacity is 202 mm and the standard deviation is 58 mm. Pedological units with a field capacity below the average, which are the more permeable units, cover an area of 19 ha which is 20% of the entire observation site. Application of precision farming approaches to a homogeneous region like this shows the capability of the developed methodology: aiming at an optimum spatially explicit management it is an *experimentum crucis*.

11.2 OPTIMUM CONTROL IN REGIONALIZED MODELS

11.2.1 Agroecological Simulation Model

In analogy to the foregoing chapter, the agroecological model summarized in Section 2.7 is used in optimum control procedures. For detailed analysis of the regionalized problem, the processes considered are:

- crop growth of different crops (sugar beet, winter wheat, winter barley, spring barley, oats, field beans and oil radish);

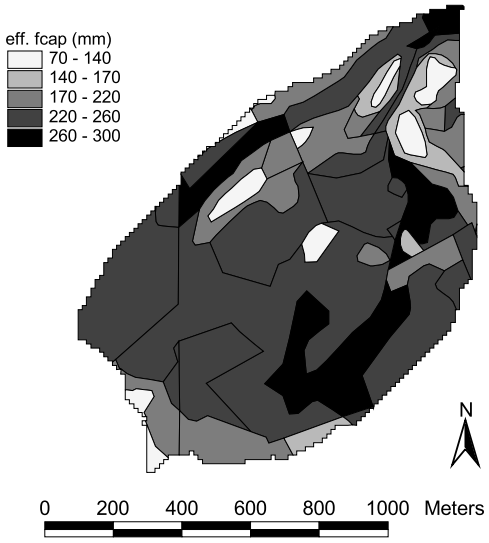

Fig. 11.1 Database for spatial referenced optimization of crop rotation and fertilizer application: map of effective field capacity in the root zone of the catchment area "Ohebach".

- nutrient cycle (mineralization, N_2 fixation, N uptake by crop, etc.);
- population dynamics of the sugar beet cyst nematode *H. schachtii*.

The main processes that are neglected are the environmental fate of xenobiotica as well as growth of weed. The vector of state variables can be written as: $\vec{x}(t,\vec{z}) = \left(W_C(t,\vec{z}), N(t,\vec{z}), P_1(t,\vec{z})\right)^T$. The control variables are fertilizer input $F(t)$ and crop rotation $(\alpha(t_i))_{i=1,2,\ldots}$ with $\alpha(t_i) \in \{$ *sugar beet, winter barley, winter wheat, summer barley, field beans, oil radish, fallow* $\}$. Note, the vector $\vec{z}$ introduces the spatial dependency of state and control vector. The model is applied to the investigation site using the method of regionalization, see Definition 3.2 and the explanations of this example in Section 3.3.1.

Without loss of generality the initial nitrogen content $N_0(\vec{z})$ as well as the initial population of *H. schachtii* is equal for all locations of the investigation site $\vec{z} \in R$. A second simplification is that k_l, the percolation velocity of solute nitrogen in the root zone, is the only model parameter that depends on spatial referenced parameters: $c(\vec{z}) = k_l(\vec{z})$. However, this does not affect the generality of the following concept.

Based on these considerations the general model equation can be written as

$$\begin{aligned} \vec{x}(t,\vec{z}) &= M_{\Delta t}\left(\vec{x}_0, \vec{u}(\vec{z}), \vec{c}(\vec{z})\right) \\ \begin{pmatrix} W_C(t,\vec{z}) \\ N(t,\vec{z}) \\ P_1(t,\vec{z}) \end{pmatrix} &= M_{\Delta t}\left(\begin{pmatrix} W_C(t_0) \\ N(t_0) \\ P_1(t_0) \end{pmatrix}, \begin{pmatrix} F(t,\vec{z}) \\ \alpha(t,\vec{z}) \end{pmatrix}, k_l(\vec{z})\right) \end{aligned} \qquad (11.1)$$

11.2.2 Optimization Task

The performance criterion used for setting up the spatially referenced optimization problem follows Equation (10.1). The variables C_S and A are not considered in this task. Note the integration over the investigated region R is very important in calculating a scalar value from the regionalized model.

The general Task 8.2 defined in Chapter 8 on page 169 is specified as follows for the problem in hand:

Task 11.1 *Calculate an optimum spatially referenced fertilizer scheme* $F^*(t, \vec{z})$ *and crop rotation* $\alpha^*(t, \vec{z})$ *so that the model Equation (11.1) is solved and the spatial performance criterion, Equation (10.1), is maximized for all* $\vec{z} \in R$.

If this task is to be solved by numerical algorithms, the crucial point is the quantification "for all $\vec{z} \in R$". Precision farming approaches state that a grid of 15 to 30 meters (Sadler *et al.*, 1998) is necessary for the identification of soil properties. Consider an area of 16 km^2, like the investigation site "Neuenkirchen". This would lead to a grid of at least $N_1 = |R| = 4500$ points. Secondly, a vector data set and the regionalization using the ecotope concept leads to a set of more than 3000 units, see Figure 3.9. This is an enormous computational effort, if that grid is used for an estimation of management strategies by optimum control theory. It must be drastically decreased by appropriate methodology and intelligent database management.

11.3 CONCEPT OF OPTIMUM SPATIAL CONTROL

One has to remember that dynamic programming can be used to calculate a *set* or *family* of optimum solutions. Developing the concept of hierarchical dynamic programming (HDP) (see Section 9.2) made use of storing these solutions as a function of the initial condition $\vec{u}^*[\vec{x}_0]$. The basic idea for a regional optimization which follows from this, is to estimate a set or a family of optimum control solutions depending on initial conditions *and* different spatial parameters $\vec{u}^*[\vec{x}_0, \vec{z}]$. The important steps to make the concept of HDP available for a regionalized model, are:

- to associate the *model parameters* $\vec{c}$ to a map that specifies the regionalization of the model: the ecotope map S_{hom}, and
- to associate the *control variable* $\vec{u}$ to a map that defines the spatial scale on which the system can be managed. Let us denote this map by S_{field}, assuming that we want to estimate optimum spatially localized agricultural management on the field scale.

However S_{hom} is set up by different layers of spatial information, for example maps with different soil parameters, S_{soil}. These parameters may be used for a parameterization of the family of optimum control solutions derived by DP/HDP.

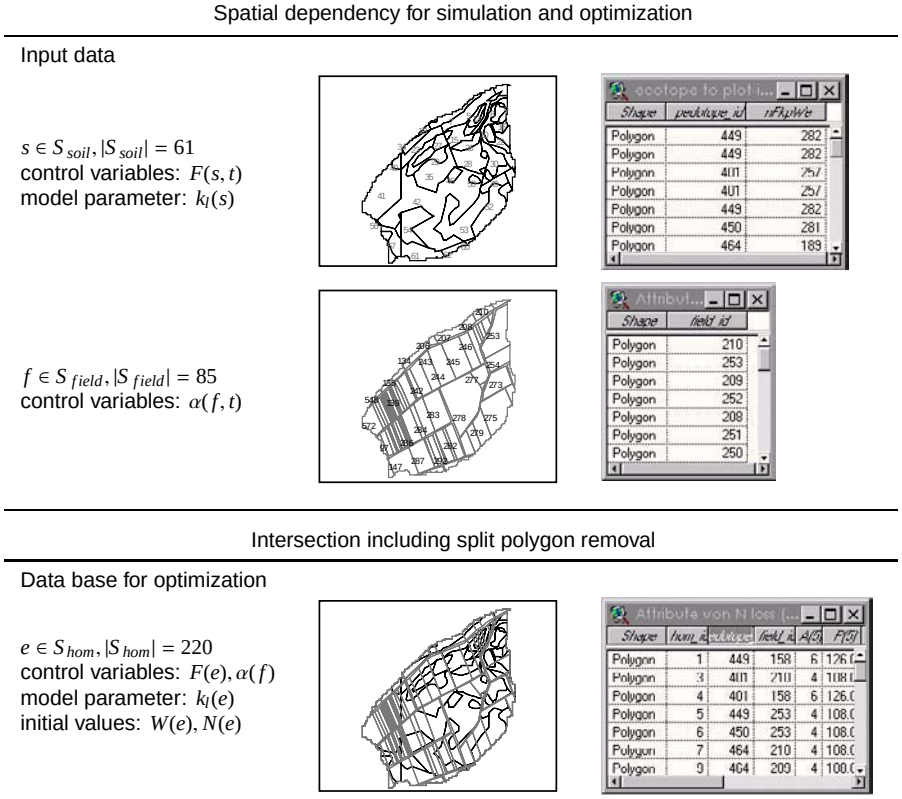

Fig. 11.2 Database concept in GIS: the underlying data sets consist of geometric information, a decomposition of the region by irregular polygons (left column) and the associated attribute tables for soil properties and field identifiers (mid column). Dependencies on the simulation model and the optimum control problems are noted in the right column. Associations between units of the input maps are derived from the intersection map, shown in the bottom row.

Using vector based maps each map S is a tessellation of $s \in S$ polygons, see Section 3.3.1. One or more attributes g_i are associated to each polygon $s \in S$. The spatial dependence can be denoted by $g_i(s)$ as $s \in S$ denotes a homogeneous area with respect to g. Two maps are used here for a solution of Task 11.1:

- The digital soil map (1:5000) S_{soil} with the attribute "field capacity" $g_1(s)$ in [mm] and "rooting depth" $g_2(s)$ [cm] ($s \in S_{soil}$). The model parameter leaching rate $c(s) = k_L(s)$ is set up by these soil-properties.
- The land use map S_{field} with the field borders. Each field $s \in S_{field}$ is identified by a unique number $g_3(s) \in \mathbb{N}$, $s \in S_{field}$.

Based on this data structure one can access the soil map, the field map and the ecotope map by unique identifiers stored in the GIS atabase. Figure 11.2 shows this technique:

Input data consists of the geometric information and the associated database with soil properties and field identifiers. The right column summarizes which model variables depend on this spatial information. Simulation and optimization is based on the intersected maps shown in the last row. In the observed region the intersection map consists of $N_2 = |S_{hom}| = 315$ homogeneous units. For each of these units a simulation is performed and all results are aggregated and visualized by the GIS. Note that the database table of the ecotope-map includes all identifiers for the access of the soil, field and ecotope map, as well as the modeling results, see Figure 11.2 middle of last row.

The calculation of intersection polygons leads to geometric units called *silver polygons* (Breunig, 1996) with an area less than $100\,m^2$ in this case, but with large length or extent. For instance, silver polygons appear along linear strictures like pathways or ditches. These shapes appear, for instance if two polygons show an approximately parallel but not identical border. These polygons are deleted or joined to larger shapes manually after visual control. This reduces the element of S_{hom} from $N_2 = 315$ to $N_2 = 220$.

Technical aspects of the model integration are summarized as follows: Data preprocessing is performed using GIS Arc/INFO. Model integration and optimization is done using ArcVIEW Desktop GIS.

- Based on the maps generated within Arc/INFO, a list of identifiers is derived from which the associations between S_i $(i = 1, 2, \ldots)$ can be retrieved.

- For each simulation/optimization run, a master script file generates an appropriate parameter file for the model using the parameters derived from the database by their identifiers and a prototype parameter file. The step depends on the considered regionalization solution, see next section.

- The optimization procedure of iterated dynamic programming checks, whether it is necessary to start an optimization process, or if a previously calculated or optimum control function can be used. This is done by comparing the pedotope identifier with all previously calculated solutions.

- Simulation results files are rearranged and provided with the necessary identifiers for visualization in GIS.

A regionalization is performed based on this data set of optimum solutions and the identifier given in the ecotope map S_{hom}. Efficiency increases with an increase of access to pre-calculated results with equal pedological properties, e.g. equal $g_1(s), g_2(s)$.

The basic innovation of this approach is a careful separation between spatial area with distinct properties. A simulation and optimization is only performed for regions with new or distinct properties. This distinguishes this solution from all grid-based modeling approaches.

11.4 OPTIMIZATION AND SIMULATION EXPERIMENTS

11.4.1 Types of Spatial Solutions

The results of the study are understood in terms of a simulation experiment. The experiment is separated into three steps of regionalization

1. Regional scale: Assumption of a homogeneous region.
2. Field scale: Calculation of optimum management strategies for each field, using the properties of the pedological unit, that covers the largest part of the field.
3. Below field scale: Calculating an optimum crop rotation for a field together with optimum fertilizing strategy for each pedological unit.

The first step in the simulation experiment is taken as a reference solution. This pure simulation run uses coarse information. All optimization results in the following steps should improve yield, diminish nitrogen loss or decrease fertilizer input. The last step, can be understood as precision farming simulation experiment. It should improve ecological conditions of the observed area.

Solution 11.1 (Regional Reference Solution) *Let $p \in S_{soil}$ denote that pedological unit, which covers the largest area of the observation site R. A solution of Task 11.1 is derived as follows:*

1. *Optimization: Calculate $\vec{u}^*$ so that*

$$\begin{array}{rcl} \vec{x}(t) & = & M_t\left(\vec{x}_0, \vec{u}^*, \vec{c}(p)\right) \\ J[\vec{x}, \vec{u}^*] & \geq & J[\vec{x}, \vec{u}] \end{array} \quad \text{for all } t \in [0, T], \vec{u} \in U \tag{11.2}$$

2. *and perform a regional simulation using $\vec{x}(e,t) = M_t\left(\vec{x}_0, \vec{u}^*, \vec{c}(e)\right)$ for all $e \in S_{hom}$.*

Step 1 has to be run once, and step 2 $N_2 = 220$ times. The results of this optimization solution fall into line with the results in discussed in Section 10.5 and the observed management of the region (McVoy *et al.*, 1995). The crop rotation $\alpha(t_i) =$ (*sugar beet, wheat, barley, sugar beet, wheat, barley, sugar beet*) is calculated with a total fertilizer amount of 1503 kg/ha. As nitrogen dynamics are calculated for each pedological unit, the amount nitrogen loss vary from 459 kg/ha to 650 kg/ha with an average of 477 kg/ha.

Solution 11.2 (Optimum Plot Management) *A solution of Task 11.1 is estimated for each field $f \in S_{field}$.*

1. *Let $p_f \in S_{hom}$ identify that pedological unit, which covers the large area of the field f*

$$\max_{e \in S_{hom}, e \subseteq f} \text{area}(e) = \text{area}(p_f).$$

Calculate $\vec{u}^*(p)$ so that

$$\begin{array}{rcl} \dot{\vec{x}}(p_f, t) & = & M_t\left(\vec{x}_0, \vec{u}^*(p_f), \vec{c}(p_f)\right) \\ J[\vec{x}(p_f), \vec{u}^*(p_f)] & \geq & J[\vec{x}(p_f), \vec{u}(p_f)] \end{array} \quad \textit{for all } t \in [0, T], \vec{u}(p_f) \in U \tag{11.3}$$

2. *The regional simulation is performed for each ecotope $e \in S_{hom}$ using*

$$\dot{\vec{x}}(t, e) = M_t\left(\vec{x}_0, \vec{u}^*(p_f), \vec{c}(e)\right) \quad \textit{with } e \subseteq f.$$

Step 1 has to be run $N_3 = |S_{soil}| = 52$ times, and step 2 $N_2 = 220$ times. In comparison to the first "reference" solution, the total amount of applied fertilizer slightly decreases to 1464 kg/ha and nitrogen loss increases to 485 kg/ha. The average assessment of all estimated optimum management strategies is improved by 4%.

A spatial application of optimum control theory to the smallest homogeneous area, as requested in the introducing section, needs a more precise definition of spatial dependency with the control variables: fertilization depends on pedological units, crop rotation scheme depends on the field.

Solution 11.3 (Precision Farming) *Calculate $\vec{u}^*(e, f)$, so that*

$$\begin{array}{rcl} \dot{\vec{x}}(e, t) & = & M_t\left(\vec{x}_0, \vec{u}^*(e, f), \vec{c}(e)\right) \\ J[\vec{x}(e), \vec{u}^*(e, f)] & \geq & J[\vec{x}(e), \vec{u}(e, f)] \end{array} \quad \textit{with } t \in [0, T], \vec{u}(e, f) \in U \tag{11.4}$$

for all $e \in S_{hom}$ and all $f \in S_{field}$, with the specification

$$\vec{u}(e, f) = \begin{pmatrix} F(e) \\ \alpha(f) \end{pmatrix}$$

$\vec{u}$ depends with the first element on each ecotope. For a given f it is $u_2(f) = \alpha(e) =$ constant for all $e \subseteq f$ that intersect the field f.

For detailed analysis, the underlying algorithm of this solution is summarized in Figure 11.3. The main loop estimates solutions for all fields $f_i \in S_{field}$ in the following way. All homogeneous units of the field f_i are collected in a list S' and sorted with the largest (area) ecotope first. The first step of optimization determines the optimum fertilizer scheme and an optimum crop rotation. Soil-dependent optimum fertilizer schemes using this crop rotation are estimated in all other steps. Every time a new optimum control solution is requested, the database be questioned for a pre-calculated solution to equal soil properties.

The calculation effort of this solution is estimated as follows: optimization procedures are started for each $p \in S_{soil}$. The effort of calculating optimum fertilizing schemes

Regionalized HDP — Regionalized Hierarchical Optimum Control

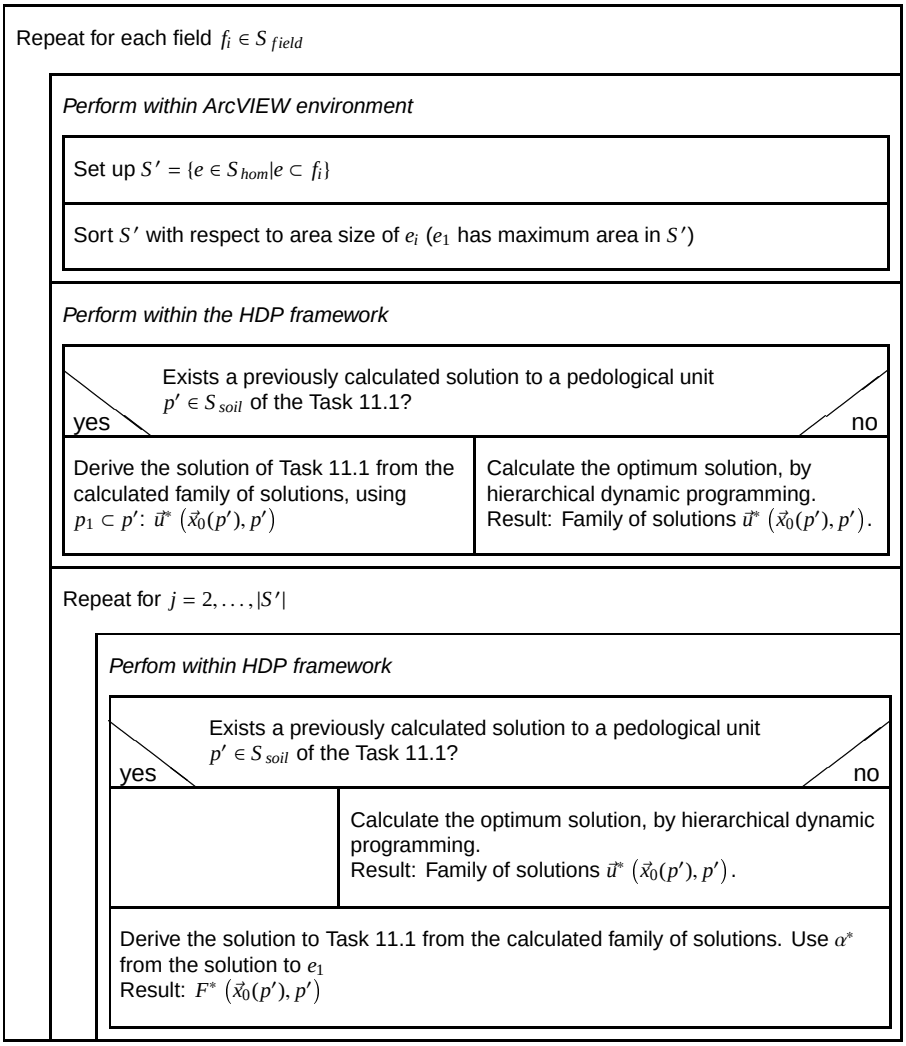

Fig. 11.3 Flowchart of calculation procedure for regionalized optimum control Solution 11.3. The entire algorithm is implemented in script files started from the GIS ArcVIEW. The headline printed in *italic* denotes the environment the following steps are derived from; hierarchical dynamic programming, or GIS ArcVIEW.

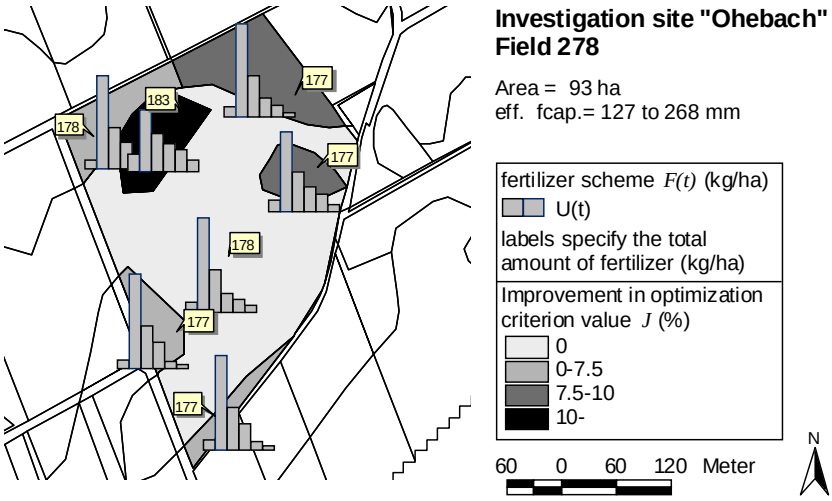

Fig. 11.4 Zoom into "Field 278" of investigation site "Ohebach". The 93 ha field is set up by 7 pedological units. The total amount of fertilizer applied is labeled.

for each $e \in S_{hom}$ is equal to the estimation of simulation results. Therefore the effort of this solution is equal to that of Solution 11.2. Results from this solution improve the performance criterion results by 1% compared to Solution 11.2. The total amount of fertilizer applied (1464 kg/ha) and nitrogen loss (490 kg/ha) does not differ very much from the previous results.

11.4.2 Results

The results obtained cannot be discussed using average values of the whole area. The calculation of averages or total amounts neglects any spatial variability. Therefore, more precise analysis of the achieved results needs inspection of the spatial distribution of fertilization, nitrogen loss, and crop rotation design.

For an analysis of nitrogen applications we focus on a single vegetation period of one crop (winter wheat) on a given field. Figure 11.4 shows the intensive investigation "Field 278" of the "Ohebach" region. The field consists of seven homogeneous pedological units with an effective field capacity of 127 up to 268 mm.

The grey shading shows that management can be improved by precision farming (Solution 11.3) up to 10% in comparison to the Solution 11.2. This is performed by an optimum allocation of fertilizer to the stages of crop development, qualitatively displayed with the bar charts.

In Figure 11.5 nitrogen loss is mapped for the whole area as a result from Solution 11.2 (right) and Solution 11.2 (left). Pedological units with low nitrogen retention

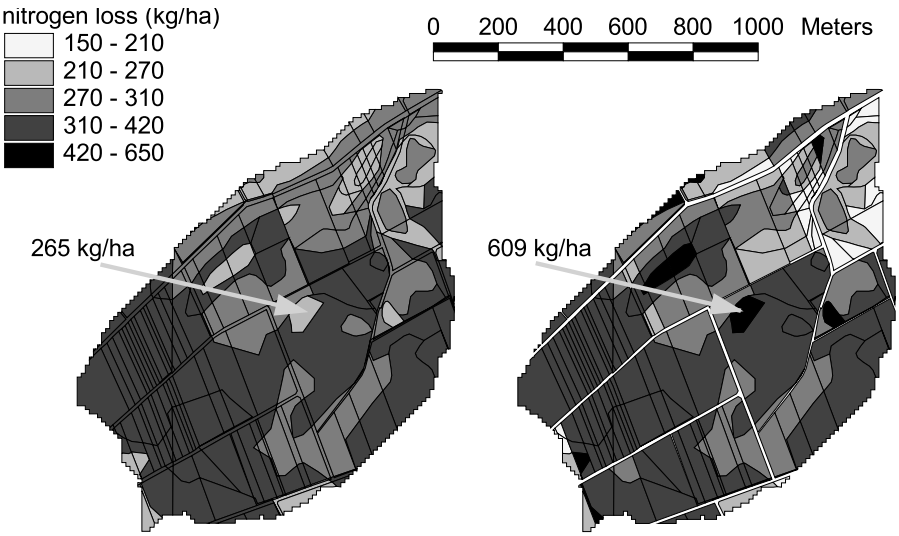

Fig. 11.5 Amounts of nitrogen loss in Solution 11.3 (left) and Solution 11.2 (right) in a 7-year crop rotation. High amounts of nitrogen loss can be found (see arrows), if local areas with low field capacity are fertilized equal to the neighboring areas.

potential are identified and optimum fertilizer application schemes are adapted. For instance, nitrogen loss can be decreased from 609 kg/ha to 265 kg/ha at a pedological unit: the "hot spot" of "Field 278" shown in Figure 11.4.

Figure 11.6 completes these results. The whole observation region "Ohebach" is shown, with the results of year three to seven of the optimum crop rotation from the precision farming Solution 11.3. The upper part of the figure shows the population density of *H. schachtii* and the lower part shows the planted crop. Note that different optimum crop rotations are estimated for minimization of nitrogen loss and pest control. Exemplary two crop rotations are noted for fields A and B below the maps. Fallow crops are used as catch crops for *H. schachtii*, see (Schmidt *et al.*, 1993). Moreover, less nutrient demanding crops are planted in the more permeable regions of the investigation site (north-western part).

11.5 DISCUSSION

Precision farming aims at incorporating local spatial variability into agricultural management. The application of optimum control theory connects spatial properties with agroecological simulation models and questions of management assessment. The results can only be discussed properly with their spatial attributes. Regional aver-

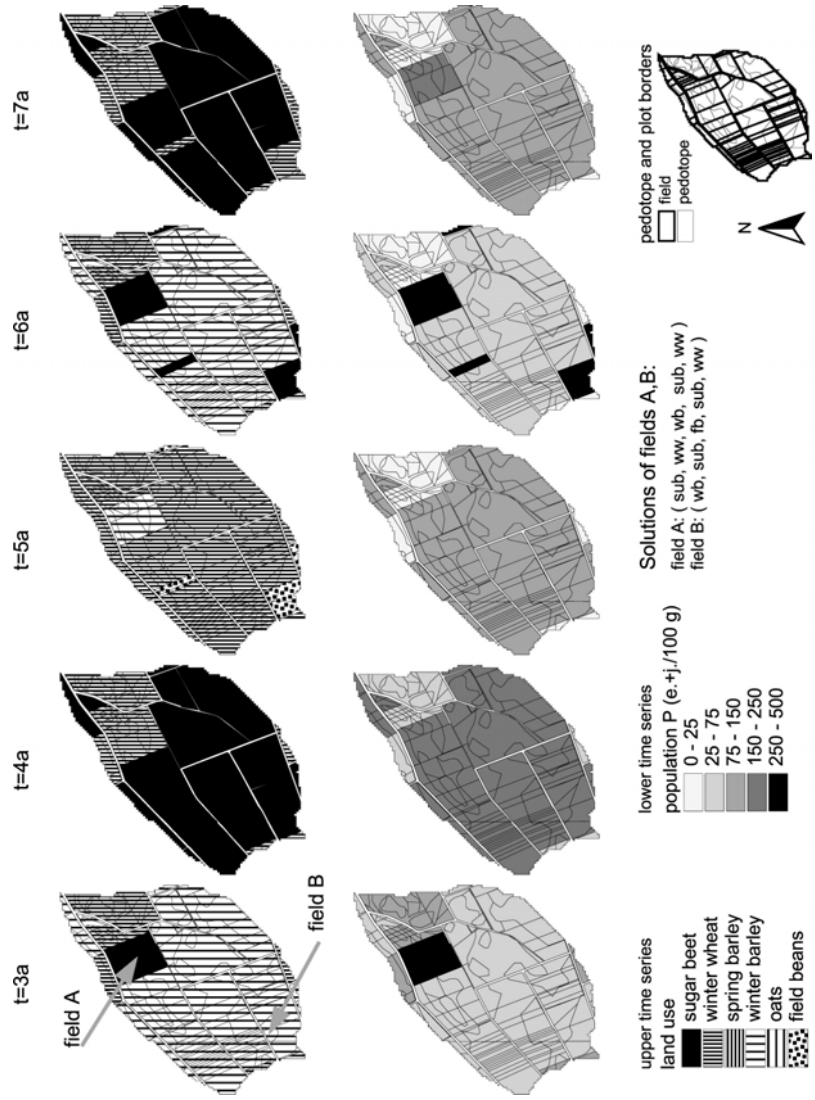

Fig. 11.6 Regional optimum crop rotation in investigation site "Ohebach". Optimum crop rotation including precision farming solution of optimum fertilizer input. For detailed study, two crop rotation solutions are noted below the maps.

ages show no improvement by precision farming (Solution 11.3) in comparison to the reference Solution 11.1.

The most interesting results in the context of precision farming are that the fertilizer scheme is not the only factor that should be estimated and applied for each pedological unit. There is also a spatial dependence in the allocation of the optimum crop rotation.

The proposed methodological framework offers a theoretical base for the application of optimum control for spatial problems in agroecological modeling. GIS comes out as a framework, which enables agroecological simulation models to be coupled with spatial databases. GIS-functions and robust optimization procedures decrease the numerical effort, so that there are no differences between the calculation effort of the standard optimization Solution 11.2 and the precision farming Solution 11.3.

Overall, the case study shows that agroecological process models with regionalized parameter fields integrated in numerical optimum control procedures may support the decision process in precision farming systems.

The proposed methodology can be used for further development, which may focus on

- the integration of more detailed agroecological process models, including models for solute transport in soil, with specifications from pedo transfer functions, which uses more attributes from soil and yield maps.
- the stepwise integration of information. This means, starting from the past (and known) climatic parameters and conditions and the current state of fields we can estimate the optimum management strategy for the rest of the vegetation period. A typical problem to be solved within the framework of dynamic programming, as these solutions do not need any further numerical effort.

12

Changing Landscapes: Optimum Landscape Patterns

12.1 INTRODUCTION

Spatially explicit ecosystem models allow water and matter dynamics in a landscape to be calculated as functions of spatial localization of habitat structures and matter input, see Section 3.3.3. The operation of several ecosystem services as a function of different management schemes for a mainly agricultural region is studied in this chapter. Optimization tasks are formulated for this purpose.

Section 3.3.3 gave a short summary of the investigation area. Figure 3.14 (p. 92) presented a map of the region. The focus is on the Hunting Creek Watershed which is located entirely within Calvert County in Maryland, USA. The 78 km^2 study area belongs to the drainage basin of the Patuxent river (2356 km^2) which is one of the major tributaries of Chesapeake Bay. Main land uses of the watershed are forest and agricultural habitats. Rapid population growth, development and change in land use and land cover have become obvious features of the landscape.

The application of the spatially explicit model follows a hierarchical concept. Most of the investigations are made for the Hunting Creek watershed model 200 m grid, the focal level. A smaller sub-watershed is chosen to test certain functions of the framework developed, cf. Section 9.3. Finally the results are transferred to the Patuxent landscape model with a 1 km grid and compared on different spatial scales, see Figure 12.1.

The task is to calculate optimum land use maps and fertilizer application maps. The framework for optimization of spatially explicit models discussed in Section 9.3.6 is used for numerical optimization using this generic landscape model. The results are

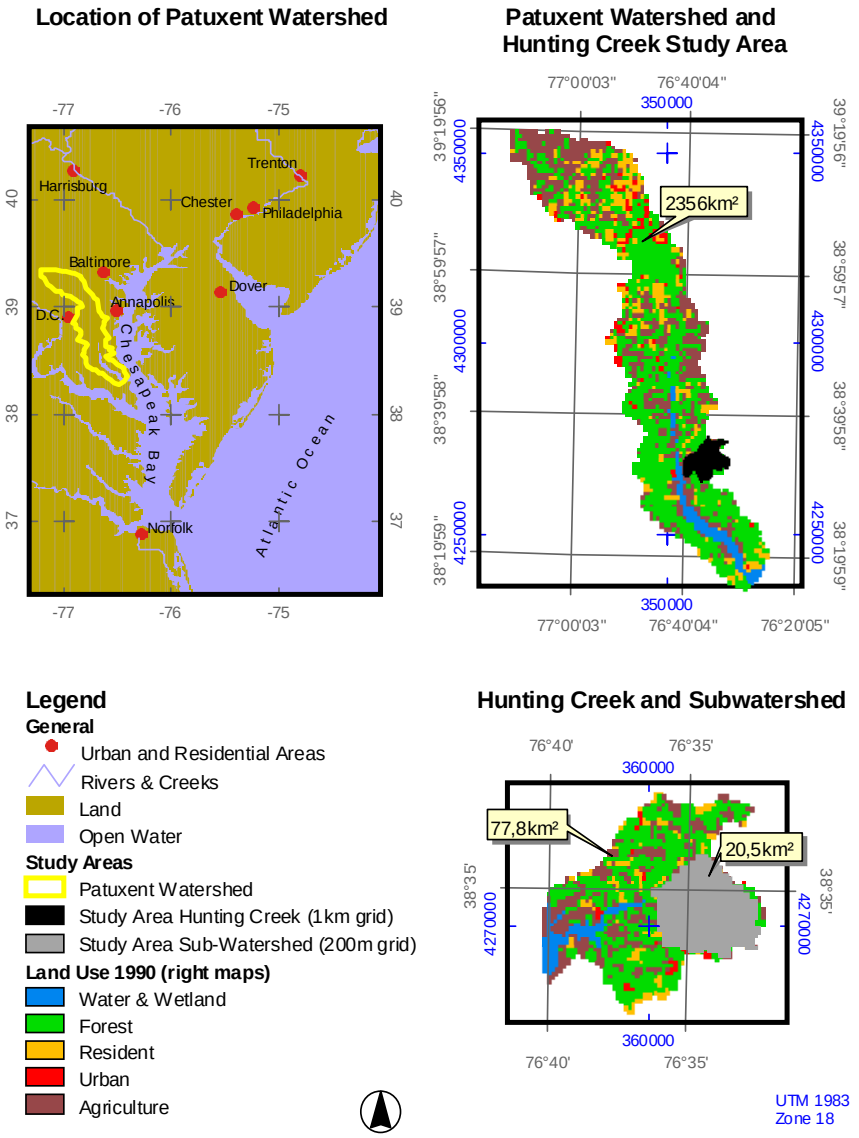

Fig. 12.1 Location of Patuxent river within the catchment of the Chesapeake Bay region and the hierarchical structure of the three study areas.

tested within the tool set using Monte Carlo simulation, which is based on different stochastic generators for the independent control variables. Gradient free optimization procedures (Genetic Algorithms) are used to verify the simplifying assumptions. The results are studied with respect to varying climatic conditions. Additionally, spatially explicit comparisons of the resulting spatial patterns are performed and the

results are compared with recent land use in the investigation area, cf. (Seppelt & Voinov, 2002).

12.2 PERFORMANCE CRITERIA FOR SPATIALLY EXPLICIT LANDSCAPE OPTIMIZATION

12.2.1 Economic–Ecologic Assessment

The observed region is denoted by a set of discrete grid points $\vec{z} \in R$. Seven different land use types are considered: soybeans, winter wheat, corn, fallow, forest, cities and rural areas. $c(\vec{z})$ denotes the land use (or habitat type) in cell $\vec{z}$. Controllable cells are $L = \{soybeans, winter\ wheat, corn, fallow, forest\}$. $R_c = \{\vec{z} \in R \mid c(\vec{z}) \in L\}$ denotes the grid points with controllable cells $c(\vec{z}) \in L$.

Without loss of generality focus is on the estimation of the total required amount of fertilizer, similar to the problems discussed in Chapter 10. In this case we need to set up a spatially explicit performance criterion. Our goal is to find out what is the optimum land use pattern and what should be the spatially explicit strategy of fertilizer application to reduce nutrient outflow from the watershed and increase yield? For a definition of a performance criterion one has to take into account crop yield, fertilizer application and nutrient outflow.

- The first variable of the economic part of the performance criterion is the harvest biomass $H(c, \vec{z})$ in [kg/m^2] is the yield of crop c (if any) harvested from cell $\vec{z}$.
- The second economic variable $F(\vec{z}, t)$ in [kg/m^2] is related to the cost of agricultural production and considers the amount of fertilizers applied at cell $\vec{z}$ for the habitat type $c(\vec{z})$ at time t. As time of fertilization is a crucial parameter for reduction of nitrogen leached, we use results of optimum fertilizer timing derived from the optimum control solution in Section 10.4. These are in accordance with the best management practice recommendations for the temporal allocation of the total fertilizer amount of the investigation sites.
- Ecological aspects are taken into account by the variable nutrient outflow out of a grid cell with horizontal flows of surface and subsurface water: $N(\vec{z})$ in [kg/m^2]. This can be interpreted as overconsumption of retention capability of the ecosystem, an eutrophication.

The first two factors are easier to compare if we operate in terms of prices. The economic yield $Y(\vec{z})$ of an agricultural site $\vec{z}$— farmers' income — can be calculated as the difference of market price for the harvested biomass of crop minus the production costs given by the cost of fertilizers applied. The revenue from the yield over the whole study area is

$$A = \int_R p_H(c) H(c, \vec{z})\, d\vec{z} \tag{12.1}$$

where $p_H(c)$ is the current market price of crop c. The price of fertilizers applied is then

$$B = p_F \int_R \int_0^{t_{end}} F(\vec{z}, t)\, dt\, d\vec{z}, \tag{12.2}$$

where p_F is the unit price of nitrogen fertilizer. Obviously A is to be maximized while B is to be minimized, which means that $Y = A - B$ is to be maximized. Y denotes the *economic* part of the goal function.

There are different ways of modeling the *ecological* part of the performance criterion. One possibility is to take into account the total amount of nutrients generated by all the cells in the study area,

$$C = \int_R \int_0^{t_{end}} N\left(\vec{z}, t\right)\ dt\, d\vec{z} \tag{12.3}$$

This is the distributed nutrient leaching. More realistic, and comparable to measurements of gauging stations, is to consider the amount of nitrogen in the outlet cell of the watershed $\vec{z}_0$. This case takes into account the compensation mechanisms of uptake along the pathways of nitrogen while it travels across the watershed and estimates the actual water quality in the river estuary:

$$C = \int_0^{t_{end}} N(\vec{z}_0, t)\, dt \tag{12.4}$$

In both cases C is to be minimized. The crucial problem is to integrate the *ecological* part C and the *economic part* Y to a scalar goal function. For this purpose C is to be expressed in units that can be compared with the monetary measure that we derived in Y. Without going into any further details at this point, let us simply assume a weighting coefficient λ, and formulate the goal function as

$$J = Y - \lambda C \tag{12.5}$$

The optimization task is:

Task 12.1 *Based on the spatially explicit landscape model described in Section 3.3.3 identify maps of optimum land use c^* and the related optimum fertilizer application amounts F^* which maximize $J \rightarrow \max$ according to Equation (12.5).*

This task is an example for a global optimization problem in spatially explicit models (Task 12.1) as introduced in Section 9.3. Numerical solution of this task requires a enormous computational effort.

12.2.2 Localization of Optimization Problem

A second approach is to derive a local performance criterion in each grid cell that allows a local optimization problem to be formulated as defined by Task 9.2. Let us analyze how the performance criterion from Equation (12.5) may be reformulated in this context: The goal function is defined for every grid cell $\vec{z}$, as a function of $\vec{z}$. The economic yield Y can simply be assessed on a grid scale level by

$$Y(\vec{z}) = p_H(c)H(c,\vec{z}) - p_F \int_0^{t_{end}} F(\vec{z},t)\, dt \tag{12.6}$$

The amount of nitrogen leaving the watershed can be approximated by estimating the net amount of nitrogen loss from every grid cell.

$$C(\vec{z}) = \int_0^{t_{end}} N(\vec{z},t)\, dt \tag{12.7}$$

This is the amount of nitrogen leaching produced locally and that can possibly be transported to the watershed mouth. $Y(\vec{z})$ and $C(\vec{z})$ are now calculated for a specific cell. They do not incorporate integration over the entire study area. Based on this the local goal function for every cell is then:

$$J(\vec{z}) = Y(\vec{z}) - \lambda_N C(\vec{z}) \tag{12.8}$$

The optimization problem is now reduced to the optimization of land use and fertilizer application for every grid cell. This approach neglects any neighborhood effects and can be written in terms of a local optimization task. The general localized performance criterion in Equation (9.8) in Section 9.3.2 (p. 184) can be applied by setting

$$\left.\begin{array}{rcl} A_1(\vec{z}) & = & Y(\vec{z}) \\ A_2(\vec{z}) & = & \lambda_N C(\vec{z}) \end{array}\right\} \tag{12.9}$$

Task 12.2 *Based on the spatially explicit landscape model described in Section 3.3.3 estimate $c^*(\vec{z}) \in L$ and $F^*(\vec{z})$ for each cell $\vec{z} \in R_c$, which maximize: $J\left(\vec{z}\right) \rightarrow \max$ according to Equation (12.8) using the definition in Equation (12.9) and Equation (9.8).*

We have to study the relationship of the global and the local solutions of the optimum control problem. Task 12.2 formulates a worst case scenario. Considering the nutrient outflow the goal function from Task 12.1 takes into account the capability of the retention function of an ecosystem, which models the through flow of nutrients more precisely. The goal function of Task 12.2 on the other hand performs a worst case upper estimate of the net nutrient outflow. In this contribution we will study the methodological framework in more theoretical detail. Finally we should be aware of getting multiple solutions to the problem.

12.2.3 Multi-criteria Assessment of Ecosystem Functions

For a more general analysis, more environmental factors are taken into account. The following ecosystem functions can be quantified by state variables, or derived from a set of state variables assumed in the ecosystem model:

- Basic ecosystem productivity given by the total rate of net primary production $NPP(\vec{z})$ [kg/m^2]. This also indirectly represents the retention capability of nutrients (nitrogen) and the uptake of greenhouse gas CO_2, and has been identified as an important indicator of overall ecosystem services provided by a land use type (Costanza *et al.*, 1997).
- Nutrient outflow out of a grid cell with horizontal flows of surface and subsurface water: $N(\vec{z})$ [kg/m^2]. This can be interpreted as overconsumption of retention capability of the ecosystem, eutrophication, see above.
- The amount of surface water baseflow in the streams: $Q_B(\vec{z})$ [m^3/d] calculated as the total of the 50% of the minimal daily flow values. This identifies how land use change affects the hydrologic conditions in the area. In most cases lower baseflow is associated with increased vulnerability to drought and peak flooding, which makes it an important characteristic of the landscape and the health of associated ecosystems.

For these ecosystem functions the simulation model dynamically calculates the required state variables. We may further expand the number of functions that are taken into account in the performance criterion. For example, it would make perfect sense to include the value of land used for recreation or for housing, in which case agricultural or forested habitat will become residential. However, methodologically it will be the same and we do not want to make the calculations any more complex at this time.

A performance criterion aggregates state variables, which represent the considered ecosystem functions. For optimization purposes we need to define the performance criterion, which aggregates the three ecological variables listed above and the economic variables into a scalar function. However these variables are not compatible in terms of units. To match the units among the different elements in the performance criterion, we introduce a *vector* of weighting factors $\vec{\lambda}$. N has to be minimized, while all other variables are to be maximized. This leads to the following performance criterion:

$$\begin{aligned} J(\vec{z}) &= Y(\vec{z}) + \lambda_{QB} Q_B(\vec{z}) + \lambda_{NPP} NPP(\vec{z}) - \lambda_N N(\vec{z}) \\ &= Y(\vec{z}) + \left(\lambda_{QB}, \lambda_{NPP}, -\lambda_N\right) \cdot \begin{pmatrix} Q_B(\vec{z}) \\ NPP(\vec{z}) \\ N(\vec{z}) \end{pmatrix} = Y(\vec{z}) + \vec{\lambda}^T \cdot \vec{x}(\vec{z}) \end{aligned} \tag{12.10}$$

Compared to the performance criterion in Equation (12.8) we now have a vector of weights $\vec{\lambda} = \left(\lambda_N, \lambda_{QB}, \lambda_{NPP}\right)^T$. The specification of J is a multi-dimensional

problem. Our other problem is that the performance criterion is formulated in terms of global landscape conditions: we are concerned with the water quality and quantity at the outlet of the drainage area, we are considering the total NPP of the area and the total profits from the agricultural crops. However, to apply the localized spatial optimization algorithm, we need to formulate these goals in term of local variables that can be traced for each individual cell. As we will see below this may not be always possible.

The local performance criterion is quite identical to the global one for the economic part and for NPP. Both these variables are additive, therefore if we maximize NPP or agricultural profits for each individual cell, we will be also maximizing the total profit and total NPP from the watershed. Accounting for water quality and quantity is not that straightforward, since these variables are not additive and undergo much change and transformation on their way between the localized (individual cell) and the drainage point of the watershed. Yet, for now we will assume that the water quality can be described globally by the water quality in each cell and, similarly, that the baseflow at the drainage point (calculated as the total of the 50% of the minimal daily flows) is related to the total of the less-than-average surface water stages in cells.

In the following we will analyze how the optimization results are influenced by the different weighting of the ecosystem functions in the performance criterion. Essentially the weights in this formulation are the dollar values that we assign to the different ecosystem functions.

12.2.4 Numerical Effort

A simulation period of 551 days is considered. It covers the growth periods of all crops, starting with soybeans and ending with the harvest of winter wheat. Before planting and after harvesting a crop, fallow is assumed to be the land use type of the cell. 20 minutes processor time is required for one simulation run of the entire model on a Sparc Ultra 10 Workstation. It is evident that a simple search through the entire control space of Task 12.1 is not practicable.

Tasks 12.1 and 12.2 can be classified as a combinatorial optimization problem. Referring to Section 9.3.1 a precise estimation of the computation effort can be given. We are to sort through all the possible combinations of six available land use types over the study area. Assuming a homogeneous land use and discrete stages of possible total fertilizer input, for say six stages $F \in \{0, 25, 50, 75, 100, 150\,\mathrm{kg/ha}\}$, Task 12.2 leads to $I_2 < |F|\ |L| = 36$ combinations. Considering that no fertilization takes place for $c \in \{forest, fallow\}$ we get $I_2 = 26$ combinations.

The number of possible combinations for Task 12.1 depends on the size of the study area $I_1 = |F|^{|L|\,|R_c|}$. For example, for the Hunting Creek watershed, which is represented by $|R_c| = 1681$ controllable cells of 200 m^2, there are $I_1 = 3.2 \cdot 10^{64}$ different land use patterns. For a smaller sub-watershed that covers 25% of the total area and $|R_c| = 483$ controllable cells there are still $I_1 = 4.7 \cdot 10^{53}$ possible land use patterns.

12.3 VALIDATION OF CONCEPT: RESULTS FOR HUNTING CREEK WATERSHED

12.3.1 Local Optimization

We focus on the methodological aspects of the proposed framework first using the performance criterion in Equation (12.8) to maximize farmers' income against nitrogen loss of the watershed. The results in terms of landscape ecological issues will be briefly described in the following section. The solution of Task 12.1 performs a grid search through the entire control space assuming homogeneous land use and identical fertilizer amounts for each cell. A series of maps for different combinations of crops and fertilizer application rates are generated and stored. Maximizing $J(\vec{z})$ for every grid cell, depending on the pre-calculated maps of the goal functions $Y(\vec{z})$ and $C(\vec{z})$, solves the optimization problem. The result is a pair of land use and fertilizer maps that optimize the local performance criterion. This pair is then fed into a spatial simulation that is used to calculate the global performance criterion, cf. Equation (12.5).

We start the analysis of the results with Branch 1 in the flow chart of Figure 9.3. Homogeneous control variables for each possible land use type and a certain fertilizer amount are set up: $c(\vec{z}) = c_0 \in L,\ F(\vec{z}) = F_0$ for all $\vec{z} \in R_c$. Running simulations within SME for all possible combinations in the step "grid search", we derive maps $Y(\vec{z})$ and $C(\vec{z})$ which are used to estimate the local optimum solution.

The estimation of local optimum land use maps does not require any computational effort. It sorts through all possible combinations in the maps $Y(\vec{z}), C(\vec{z})$. This easily allows parameter studies for the weighting parameter λ_N. Figure 12.2 shows the results of a parameter study for the Hunting Creek watershed in an aggregated way: the number of different land use types is plotted as a function of λ_N. Figure 12.3 shows 3 maps of optimum land use derived from this parameter study: optimum land use patterns are displayed for the λ_N values 0.0 (upper left), 0.1 (upper right), and 5.0 (lower left).

- A zero value of λ_N leads to a pathologic solution: the optimum solution is to plant the most valuable crop in the entire study area. Only villages, urban area and open water remains the same (non-controllable cells).

- An increase of λ_N introduces forest into the land use pattern. The more nutrient outflow is "punished" by an increase of λ , the higher is the fraction of forest in the study area.

- With an increase of λ_N agricultural cells change to crops with a better nutrient up-take/yield-efficiency. This depends on the market prices of the crop.

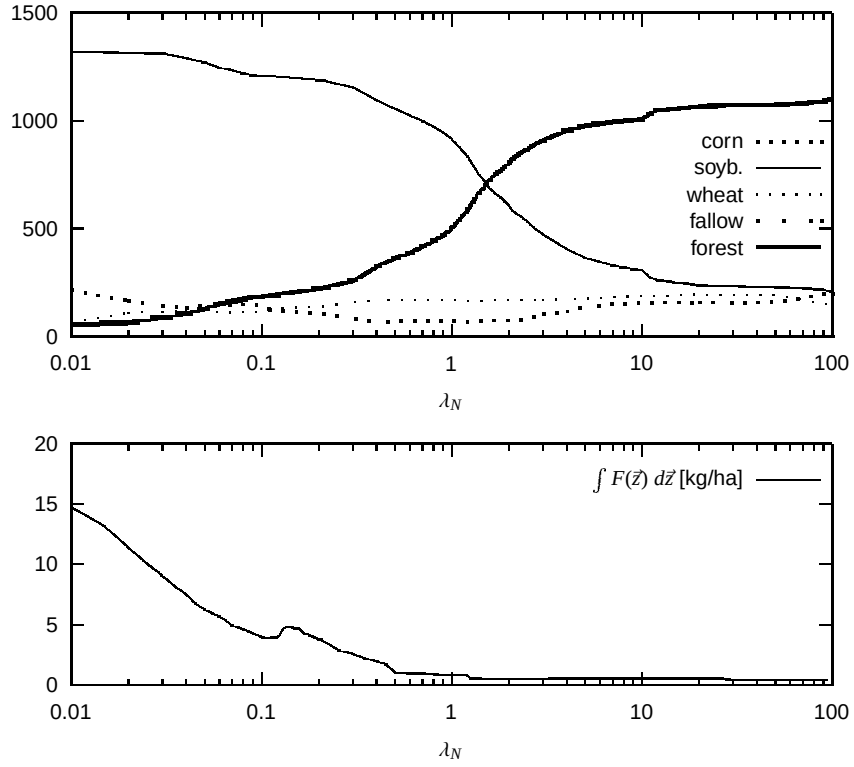

Fig. 12.2 Results of parameter study of optimum land use maps. The number of forest, fallow, soybean, corn and wheat cells in the Hunting Creek watershed are plotted against λ_N.

12.3.2 Monte Carlo Simulations

An analysis of these results can be performed by a Monte Carlo simulation. Figure 9.3 shows Monte Carlo simulations in two boxes in the mid column:

- Monte Carlo simulation "from scratch" correspond to the first box of Branch 2, compare first item in section above. It performs an analysis of the variability of the entire process and sets up an initial population for the genetic programming algorithm.
- The step after local optimization, which corresponds to the reallocation $p_1 = 1$ or the *disturbance* of an optimum solution $p_1 < 1$, item 2 and 3 of previous section.

For the given problem of land use and fertilization optimization, the algorithm can be described mathematically by a two-stage stochastic process. Let $Z_1(\vec{z}) \in [0, 1]$ be a random variable. A new land use is generated randomly if $Z_1(z) < p_1$ for cell

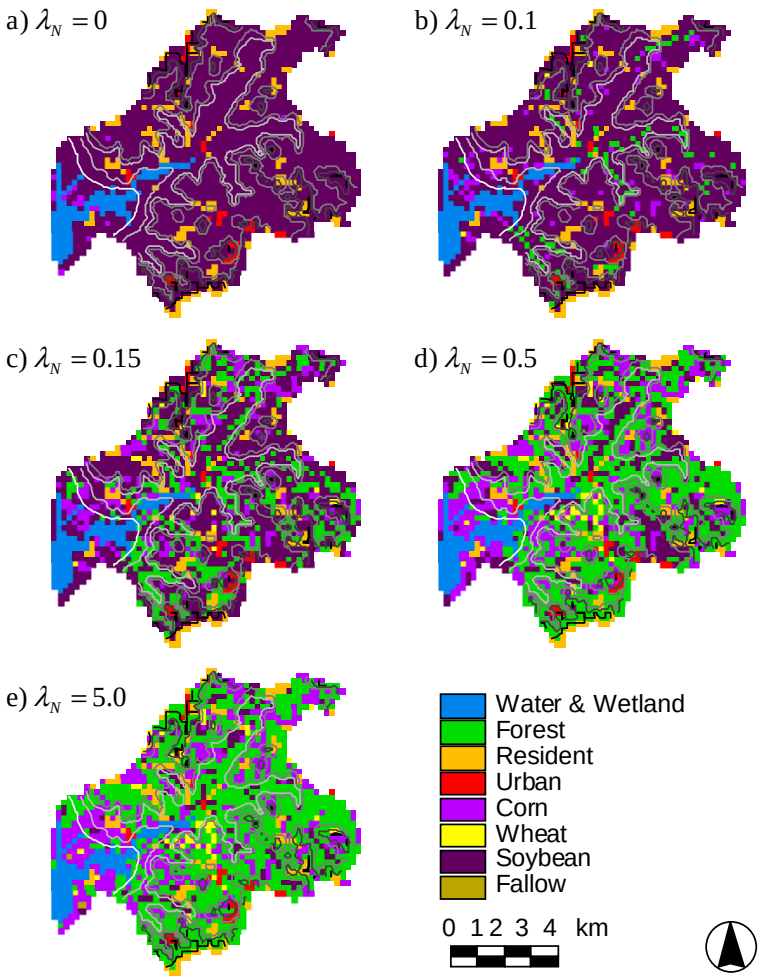

Fig. 12.3 Optimum land use maps derived for optimization using the weighting $\lambda_N = 0$ (a), $\lambda_N = 0.1$ (b), $\lambda_N = 0.13$ (c), $\lambda_N = 0.5$ (d), and $\lambda_N = 5.0$ (e). Lower areas near rivers and creeks can be identified by the contour lines.

$\vec{z}$. This is done by a stochastic variable $Z_2 \in \{corn, soybeans, wheat, fallow, forest\}$ such that $P\left(Z_2(\vec{z}) = c(\vec{z}) \,|\, Z_1(\vec{z}) < p_1\right) = f(c)$.

For every cell $\vec{z}$ the stochastically generated land use c follows a distribution which is defined by a density function $f(c)$. The density function $f(c)$ is constant for the entire region and may be generated by a stochastic process, started before generating the stochastic land use map. Otherwise it may be derived from the distribution of a known land use pattern, for instance the optimum solution, cmp. Section 9.3.4.

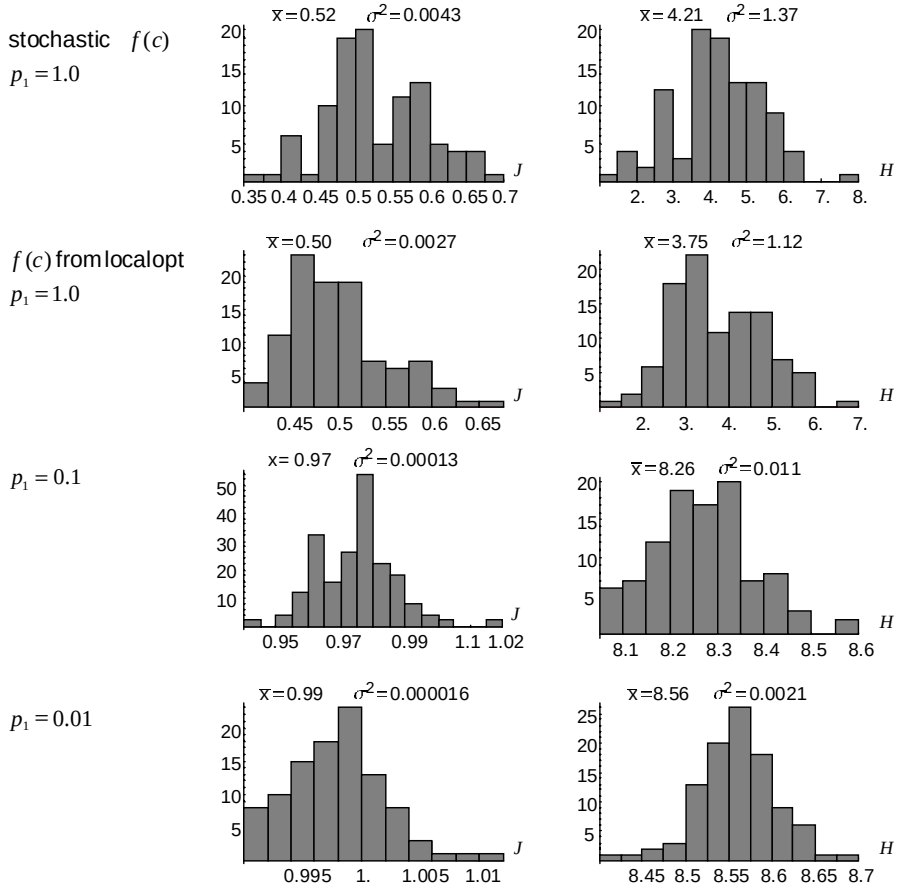

Fig. 12.4 Resulting distribution of goal function values (left column) and total harvest biomass (right column) of Monte Carlo simulations for different stochastic processes (rows).

Figure 12.4 summarizes the results of several Monte Carlo runs. Using the smaller sub-watershed (see Figure 12.1) allows to generate more realizations. The first column in Figure 12.4 shows histograms of the global goal function results according to Equation (12.5). The goal function values are normalized by the goal function value derived by the local optimization. Values below unity denote simulation runs where the global goal function returns values below the local optimization. Values above unity denote that the local solution was improved. The second column shows the histogram of the yield in the study area in US-\$/m^2 for comparison.

Row one can be identified as Monte Carlo simulation from scratch: the distribution of land use types $f(c)$, the land use type, and the fertilizer amount for each grid cell are randomly generated. The second row derived $f(c)$ from the local optimization distribution. Rows three and four of Figure 12.4 disturb the local optimization land use

Table 12.1 Correlation analysis of local optimization solution with underlying spatial data.

	Porosity	Infiltration rate	Field capacity	Percolation rate	Hydrologic conductivity	Elevation	Aspect	Slope	$c(\vec{z})$
$\lambda_N = 0.0$									
$c(\vec{z})$ corr.	0.046	-0.28	0.2	-0.44	-0.34	-0.20	0.071*	0.052	1.0
sign.	0.057	0.25	0.42	0.073	0.16	0.42	0.003	0.031	
$F(\vec{z})$ corr.	-0.027	0.045	-0.035	0.11†	0.2†	-0.075†	-0.044	-0.049*	0.18†
sign.	0.27	0.067	0.15	0.0	0.0	0.002	0.069	0.044	0.0
$\lambda_N = 0.1$									
$c(\vec{z})$ corr.	0.13†	-0.16†	0.13†	-0.18†	-0.2†	0.11†	-0.001	0.028	1.0
sign.	0.0	0.0	0.0	0.0	0.0	0.0	0.97	0.25	
$F(\vec{z})$ corr.	0.10†	-0.14	0.087†	-0.95†	-0.15†	-0.001	-0.031	-0.036	0.19†
sign.	0.0	0.0	0.0	0.0	0.0	0.98	0.21	0.146	0.0
$\lambda_N = 0.2$									
$c(\vec{z})$ corr.	0.25†	-0.33†	0.26†	-0.32†	-0.58†	0.089†	-0.60*	-0.67†	1.0
sign.	0.0	0.0	0.0	0.0	0.0	0.0	0.014	0.006	
$F(\vec{z})$ corr.	0.17†	-0.21†	0.17†	-0.21†	-0.23†	0.021	-0.003	-0.08†	0.37†
sign.	0.0	0.0	0.0	0.0	0.0	0.39	0.89	0.001	0.0
$\lambda_N = 1.0$									
$c(\vec{z})$ corr.	0.41†	-0.47†	0.41†	-0.47†	-0.38†	-0.011	-0.046	-0.041	1.0
sign.	0.0	0.0	0.0	0.0	0.0	0.67	0.061	0.089	
$F(\vec{z})$ corr.	0.16†	0.016†	0.14†	0.17†	-0.09†	-0.08†	0.017	-0.01	0.21†
sign.	0.0	0.0	0.0	0.0	0.0	0.001	0.49	0.69	0.0

† significant correlation according 2-sided significance level 0.01 (Spearman–Rho)
* significant correlation according 2-sided significance level 0.05 (Spearman–Rho)

pattern with the probability $p_1 = 0.1$ and $p_1 = 0.01$. Obviously, stochastic generation of land use patterns has limitations for identifying a map, which is optimum in terms of the performance criterion. From the last two rows of Figure 12.4 it can be shown, that an increase in the probability p_1 immediately leads to solutions which are far from the solution derived from local optimization. The local optimization approach seems to be very close to a global optimum. However, there are land use patterns which are "better" in terms of the global optimization. Are these land use patterns the ones that take into account the neighborhood relationships of the control variables?

12.3.3 Statistical Analysis

What are the driving parameters for the optimum solutions? The question can be answered by a simple bivariate correlation analysis based on the resulting land use and fertilizer maps and the spatial input data of the model. Table 12.1 summarizes the results of 4 correlation analysis studies of the optimum solutions to the set of weights $\lambda_N = 0.0,\ 0.1,\ 0.2$ and 1.0. However, the sample size is high (1690) we

used non-parametric correlation according to Spearman–Rho (Davis, 1984), because normal distribution of the resulting parameters cannot be assumed. Input data maps are the soil map and the elevation map. Parameters of the soil map are porosity [m^3 pore space per m^3 sediment], infiltration rate [m/day], field capacity [m pore space per m sediment], percolation rate [m/day], horizontal hydraulic conductivity [1/day]. From the elevation map the aspects and slope are derived using GIS functions.

Setting $\lambda_N = 0.0$ neglects any ecological issues of agricultural production and fertilization. The optimum solution is a land use map with the most valuable crop and a high fertilizer amount. The correlation analysis shows that hardly any the important parameters for nutrient transport in soil are responsible for the land use map. One more general result is that the fertilizer application always correlates with the habitat type: each crop gets its specific optimum amount of fertilizer.

An increase of the λ value shows significant correlation to the parameters of the soil map. For $\lambda = 1.0$ land use $c^*(\vec{z})$ and fertilization $F^*(\vec{z})$ show significant correlation with all parameters of the soil map. Weak correlations are also identified to the parameters of the elevation map, especially to aspect and slope. This shows that spatial relationships (to neighborhood cells) find their interpretation in the locally optimum solution from the spatially explicit model. Note, due to the large sample size, a small sample set is sufficient for a significant correlation. In general all correlation values are low. However, statistical analysis gave a validation of the derived results.

12.3.4 Genetic Algorithms

The only way to answer the question on the importance of neighborhood relationships in the control variable maps is to set up an optimization procedure that uses Equation (12.8) for assessment. As we have seen from the results of the Monte Carlo simulation, the application of GA based on an initial population from scratch will fail, because the variability of a population from scratch is much too broad. GA needs too many iterations to converge to the solution we derived by the local optimization approach, compare to Figure 9.3 upper right.

The smaller sub-watershed of the Hunting Creek is once again used for a detailed study of this behavior. Figure 12.5 displays the convergence process of a GA run from scratch and the GA run from local optimum (smaller graph). It takes 300 generations (4500 simulation runs) to achieve 80% of the goal function value. For this reason the local optimum solution is used for the generation of the initial population, see Figure 9.3 (lower part, mid column).

From the former results we can generate certain rules for the parameterization: too large variations in the initial population take us away from the optimum. We set $p_1 = 0.01$ for the stochastic generation of the initial population. This has to be assured within each step when generating a new population: mutation probability should be much smaller than p_1, cross-over probability should be equal to zero. To enable modifications in the population we set migration probability to a high value (0.9). The graph in Figure 12.5.b shows the results of the GA run started from the

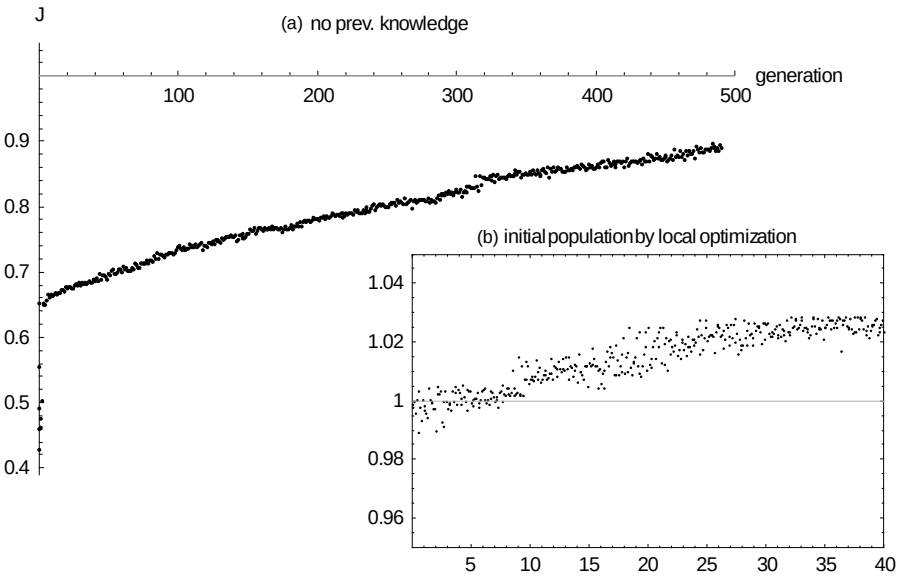

Fig. 12.5 Development of global performance criteria values during Genetic programming process. (a) the GA process "from scratch". (b) the GA process started from a local optimum solution with a stochastically "disturbed" of "mutated" population.

local optimum solution. The GA process clearly separates from the initial population and improves the optimum solution by 2%.

What are the changes compared to the local optimum solution? Two maps are compiled to show the differences in each grid cell based on the best generation of GA set up by 15 individuals. Figure 12.6 shows the results. The map in Figure 12.6.a shows the average fertilizer difference. The map in Figure 12.6.b presents the modified land use cells.

Only a small number of cells are changed: 43 out of 513 cells (8%). The distribution of land use types remained the same. The global optimization by GA performed a *reallocation* of habitats. We expected a couple of solutions, which can improve the local solution. A complex problem like this might have multiple solutions. This would have led to various examples (of habitat and fertilization maps) which change different cells compared to the initial solution from the local optimization. However, the map b) shows that nearly all of the individuals in the best generation modified the same grid cells. Most of the modified cells belong the class where more than 13 out of 16 individual changed the cell in the same way.

It is difficult to derive an explanation as to why these are the crucial cells by statistical approaches, however that would allow further improvement of spatial optimization. The broad spectrum of spatial input data and the very complex network of dynamic and spatial process in the simulation model, mean that no significant correlation can be identified. Using principle component analysis is not possible to reduce state space

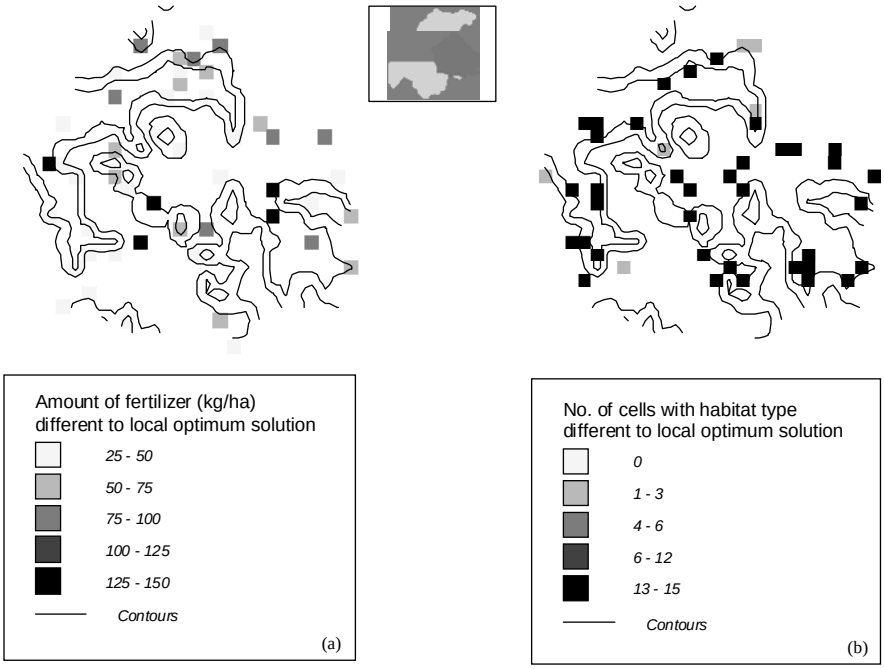

Fig. 12.6 Analysis of GA results. The maps show the difference from one generation (15 individuals) of the GA to the local optimum maps for the sub-watershed: a) fertilizer amounts. b) this map counts how many individuals of the population have a different land use type than the local optimum solution. The small map in the center displays the extent and location of the sub-watershed within the Hunting Creek watershed.

for analysis. A possible approach is to perform a bivariate correlation of $c(\vec{z}_0)$ and $F(\vec{z}_0)$ to the neighborhood cells, (north-east, north,..., south-west $c(\vec{z}_0)$). Two topics make us expect illusory correlations: first, analysis of the entire region, using every grid cell (and its neighbors) as a repetition just gives a general answer, which is mainly driven by a global aspect of the global slope of the catchment. Second, the landscape model uses linkages between cells which are not direct neighbors for the hydrological sub-module (Voinov *et al.*, 1999).

12.4 RESULTS OF MULTI-CRITERIA OPTIMIZATION

12.4.1 General Results for Optimum Land Use Patterns

In the first analysis the optimization results can be investigated using the habitat distribution of the entire investigation area. If we use only one dimension of the vector of weights $\vec{\lambda}$ in the performance criterion, these results can be summarized as

follows: neglecting all ecological concerns and focusing on economic profits only, $\vec{\lambda} = 0$, the optimum land use, is to plant soybean (70%) and corn (30%). The entire study area changes to agricultural use only. Introducing ecological aspects in the performance criterion makes forest an optimum habitat. In detail:

- Focusing on NPP, forest (70%) and corn (30%) become the dominant land use;
- Prioritizing N-output, a distribution of land use assuming 70% forest and 12% soybean and 12% corn is most efficient;
- Considering baseflow Q_B most important, one would expect forest to cover most of the area, since it seems to be the kind of habitat that is most favorable to increase water retention, cf. for example (Pattanayak & Kramer, 2001). However, optimization results show fallow dominating the landscape, which is quite suspicious.

Two questions result from this preliminary analysis:

1. How do these results change if scenarios of assessment are combined, e.g. if the weights of ecosystem function values given by λ are modified?
2. Which regions are effected by a change of land use and how is this related to the current data for land use distribution in the study area?

The second step in analysis of the results is the estimation of optimum land use distributions as a function of different weighting schemes. This requires a broad range of optimization runs with varied $\vec{\lambda}$ values. This can be performed without much computational effort due to the separation of local and global optimization methodologies.

A graphical representation of the habitat distribution as a function of the multi-dimensional weighting space $\vec{\lambda}$ is hardly possible. Nevertheless, Figures 12.7 and 12.8 give an idea about how the changes in the optimum land use distribution in the Hunting Creek area are driven by different weighting schemes. Figure 12.7 shows how optimization results of habitat distributions change with a variation of the weights λ_N (plot a), λ_{QB} (plot b) and λ_{NPP} (plot c). All three figures support the above mentioned general conclusion, that forest becomes an important part of the landscape, if ecological issues are taken into account in the performance criterion. Depending on the ecosystem function stressed by the weighting in the multi-dimensional performance criterion, for the remaining area different habitat types are chosen. Focusing on net primary production, corn is an important habitat. Corn and wheat are chosen, if nutrient outflow is considered in the goal function.

Note that for the *x*-axis a logarithmic scale is chosen. We get different results of optimum land use distribution changing λ_N and λ_{QB} within 5 orders of magnitude. Whereas the optimized land use distribution changes with a variation of λ_{NPP} in the interval $\lambda_N = 1, \ldots, 10$. These results can be interpreted as a sensitivity analysis of

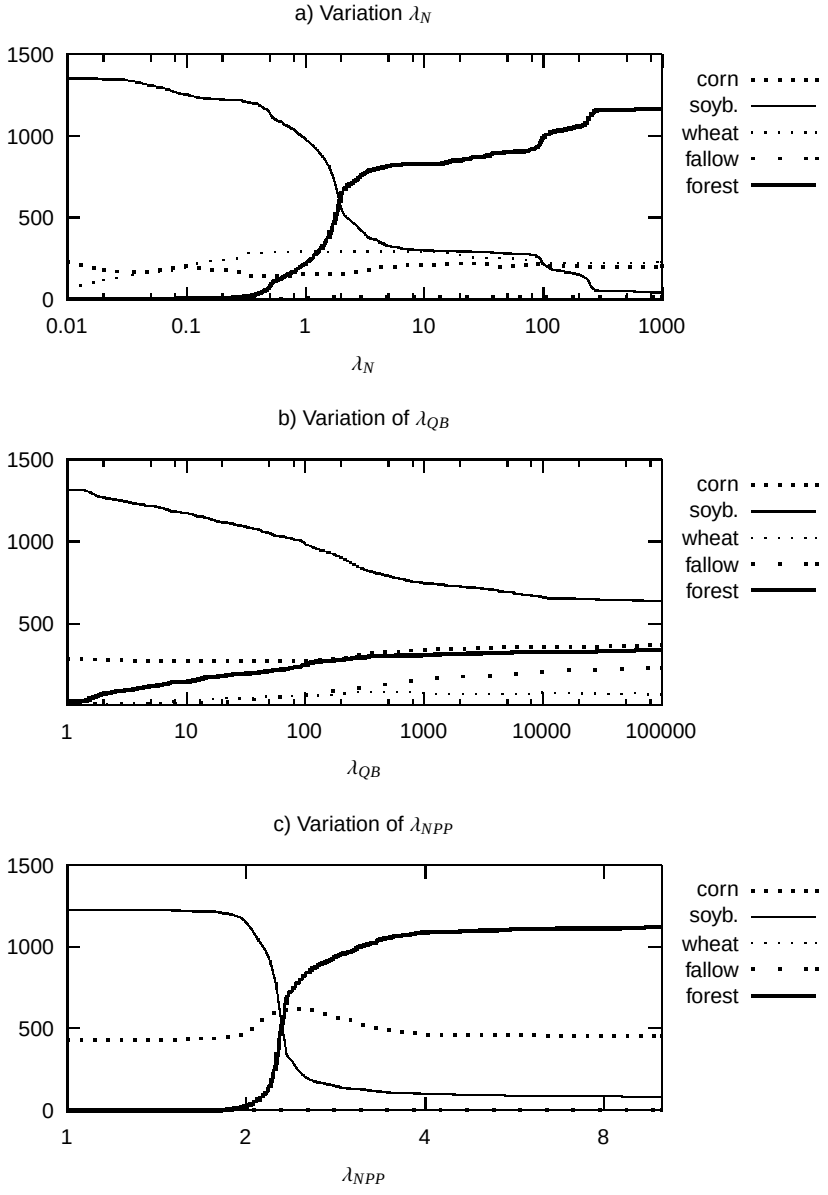

Fig. 12.7 Optimum land use distribution as a function of weighting coefficients λ_N, λ_{QB} and λ_{NPP}. Plot a) shows the response of the optimum land use distribution to a variation of λ_N ($\lambda_{QB} = \lambda_{NPP} = 0$), c) the response to λ_{QB} ($\lambda_N = \lambda_{NPP} = 0$) and the lower plot c) to λ_{NPP} ($\lambda_N = \lambda_{QB} = 0$).

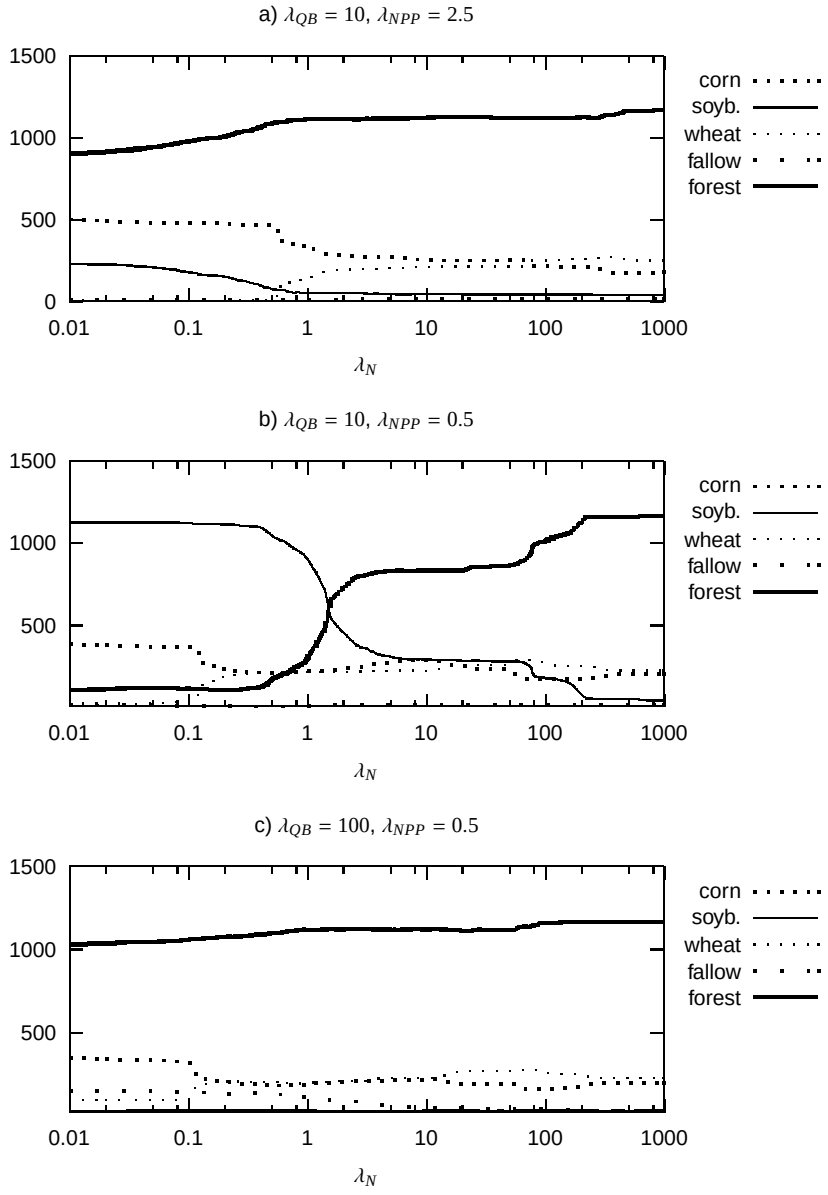

Fig. 12.8 Optimum land use distribution as a function of weighting coefficient λ_N.

a parameterized multi-criteria analysis. This provides a basis to choose weighting scenarios for more detailed studies.

Figure 12.8 shows three similar graphs. For selected values of λ_{NPP} and λ_{QB} the land use distribution is plotted as a function of λ_N. Forest is an important habitat in the landscape covering more than 50%, if net primary production or baseflow is considered in the performance criterion. Also fallow may be an optimal land use, if baseflow is stressed and nutrient outflow is neglected.

Based on the general behavior of the model derived from the sensitivity analysis in Figure 12.7, one could hardly infer the plots presented in Figure 12.8. The general conclusion is that, although the performance criterion is simple and linear, there are essentially nonlinear changes in the optimal landscape patterns. We know from former work that these patterns are caused by a highly complex network of spatially distributed parameters and processes in the underlying simulation model.

12.4.2 Scenarios of Optimized Land Use Patterns

Next six weighting schemes of $\vec{\lambda}$ are selected for more detailed analysis. Table 12.2 lists the selected values for the weighting vector $\vec{\lambda}$ in the upper part. Note, with the exception of Scenario 2, all economic elements of the weighting vector are set according to recent prices for crops and prices of fertilizer. This means that optimization of ecosystem functions can be interpreted in economic values. In Scenario 2 $Y(\vec{z})$ is neglected, i.e. set to zero. With this scenario a closer look is taken at the interrelationship between the three ecosystem functions in the optimization results with respect to the attributes of the study area, e.g. soil properties, elevation, etc.

Table 12.2 summarizes the optimization results in an aggregated way, listing habitat distribution and the total amount of fertilizer applied in each of the 6 optimization solutions. For comparison, recent land use (1990) shows 70% forest and 30% agricultural habitats for all controllable cells, that is open water, rural and urban areas are neglected in the comparison.

These optimized habitat maps and optimal fertilizer maps are now fed into the Hunting Creek model and full spatially explicit simulations on these so-called optimization scenarios are run. Results can be then analyzed with respect to spatial properties as well as with respect to the overall performance measures, such as total nutrient outflow from the entire watershed.

In addition we can compare the results with some of the information available from other published sources, cf. for instance the ECOTOX database (Jørgensen *et al.*, 2000). It was encouraging to find that most of the results of our simulation, like NPP, have the same order of magnitude as reported in literature, cf. Table 12.2 lower part.

Surface water and nutrient concentration in the basin outlet cell are important aggregated indicators for numerous spatial hydrologic processes and for the nutrient cycle. The drainage cell connects to the Patuxent river, which then drains into Chesapeake

Bay. To analyze the nutrient balance three scenarios are chosen for Figure 12.9: Scenario 1, 2 and 4. These scenarios cover the range of variation for all scenarios. The figures display the last year of simulation from July to June, $t \in [186, 551]$.

In the upper plot, Figure 12.9.a, the surface water level is displayed. The resulting simulations based on optimization Scenarios 1 and 4 show water levels twice as high as the result from Scenario 2. Considering the chosen weight, cf. Table 12.2 this result is somewhat contradictory to the optimization goal. A higher value for λ_{QB} should result in a higher baseflow, which should result in a higher average water level and lower peaks of the surface water level in the outlet cell.

One may hypothesize that it is most likely that by maximizing the amount of surface water in each cell, actually the baseflow is decreased, since more water on the surface means more water available for immediate runoff, higher evaporation, and as a result less water in saturated layer, that feeds the stream network during dry periods. The performance criterion can be modified to make it better represent the baseflow in the

Table 12.2 Definition of weighting scheme $\vec{\lambda}$ for optimization Scenarios 1 to 6 (upper part of table) and aggregated optimization results of the control variables land use and fertilizer input. Last column shows recent distribution of agricultural and forest area and literature values for selected state variables of performance criterion.

	Scen. 1	Scen. 2	Scen. 3	Scen. 4	Scen. 5	Scen. 6	Unit	Remarks
Specification of performance criterion								
λ_Y	p_H, p_F	0	p_H, p_F	p_H, p_F	p_H, p_F	p_H, p_F		λ_Y[a]
λ_N	0.05	0.01	1.5	0.0	50.0	0		
λ_{NPP}	0.0	0.5	0.5	0.0	2.5	2.5		
λ_{QB}	0.0	100	10	100000	1000	0		
Resulting control variables								
Percentage of land use $H(\vec{z})$								
Corn	10.5	21.1	13.7	22.4	13.3	37.8	%	
Soybean	79.2	1.8	36.8	38.6	1.9	12.8	%	
Wheat	9.9	5.7	13.2	4.4	14.2	0.1	%	
Fallow	0.1	9.1	0.8	14.2	0.3	0	%	70.9 %[b]
Forest	0.2	60.5	35.5	20.5	66.9	49.5	%	29.1 %[c]
Applied fertilizer								
$\sum F(\vec{z})$	5.58	2.14	2.79	2.61	0.65	4.62	g/m^2	
Resulting state variables								
$\sum NPP$	148	635	442	265	699	667	g/m^2/y	650[d]
$\sum N(\vec{z}_0)$	2.05	0.84	0.91	2.24	0.37	0.69	g/m^2	

[a] λ_Y denotes the prices for fertilizer and harvest biomass defining $Y(\vec{z}) = p_H H(\vec{z}) + p_F F(\vec{z})$.
[b] Total agricultural area, Hunting Creek, 1990
[c] Forest Area Hunting Creek 1990
[d] cf. (Jørgensen *et al.*, 2000, Table 2-202)

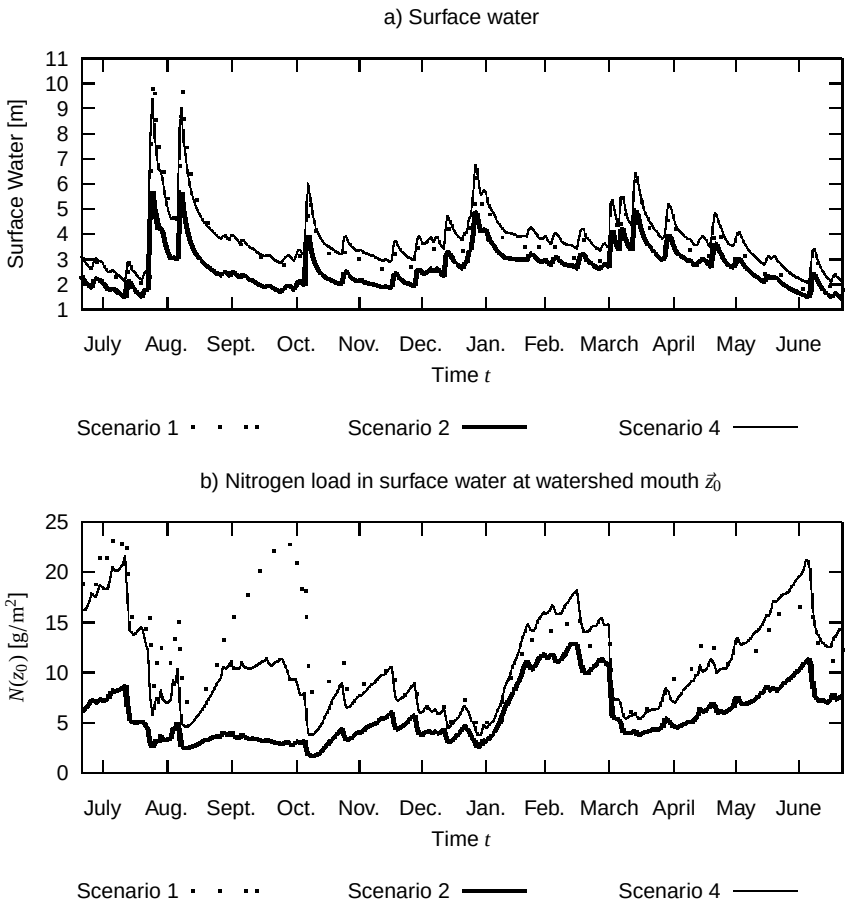

Fig. 12.9 Time series of surface water level (plot a) and nitrogen load (plot b) both taken at the watershed outlet cell $\vec{z}_0$. Results from the Scenarios 1, 2 and 4 display the overall variation of all six scenarios.

stream. Instead of surface water in the cells, of infiltrated water is calculated. In Equation (12.10) Q_B is replaced by the accumulated amount of infiltrated water, the weighting coefficient is denoted by λ_I.

In this optimization one obtains a displacement of corn by forest in the landscape (Figure 12.10), but further on, with even higher weights attached to the baseflow, one finds that it is fallow that displaces soy beans, not forest. Even though the infiltration coefficient per se is three times higher for forests than for fallow, apparently now the infiltration capacity starts to play the most important role. The amount of water infiltrated depends not only upon the infiltration rate, but also on the amount of pore space in the unsaturated zone, that can take water in, in the infiltration process. For

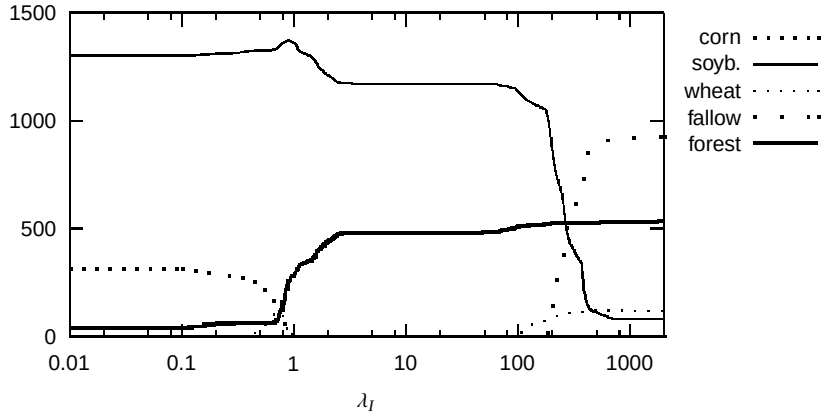

Fig. 12.10 Optimum land use distribution as a function of weighting coefficient λ_I of the performance criterion adding yield and accumulated infiltrated water.

fallow, evaporation from the unsaturated layer is assumed to be ten times higher than in forests. As a result one gets more infiltration capacity in fallow, and, hence, more water infiltrated.

If baseflow is calculated globally one still achieves the highest results for mostly forested landscapes. The final conclusion from this is that optimization for baseflow is *not achieved* with the chosen methodology of *local* optimization, e.g. simplifying the spatially explicit problem. There seems to be no good way to express baseflow (a global feature) in terms of some local variables and processes. Processes that show high spatial interaction are hard to treat with this local optimization methodology. Performance criteria and optimization algorithms need to be formulated on a global or at least regional scale.

On the other hand, minimization of nutrient outflow is achieved by local optimization. Figure 12.9.b displays the time series of the nitrogen load in the outlet cell. Scenario 1, which almost neglects any ecological aspects, results in higher nutrient concentration. Scenario 2 and Scenario 4 result in lower nitrogen concentrations. Note that this is an outcome of spatial allocation of land use type only, the climatic conditions (most importantly precipitation and atmospheric N input) as well as fertilizer application are constant, cf. Table 12.2.

These two results may sound contradictory, since nutrient flow is strongly related to hydrology. Apparently nutrient flow is more spatially buffered and has less spatial variability, so the local performance criterion captures the effects that play the most important role globally.

Figure 12.11 gives an overview of the 1990 land use in the Hunting Creek region. The watershed area is shared between urban, rural, open water, forest and agriculture habitats. No distinction for different crops is made in that map. Figure 12.11 also offers detailed maps of a small region near the creek. These areas near rivers and creeks were identified as crucial in terms of optimization for the nutrient balance in the

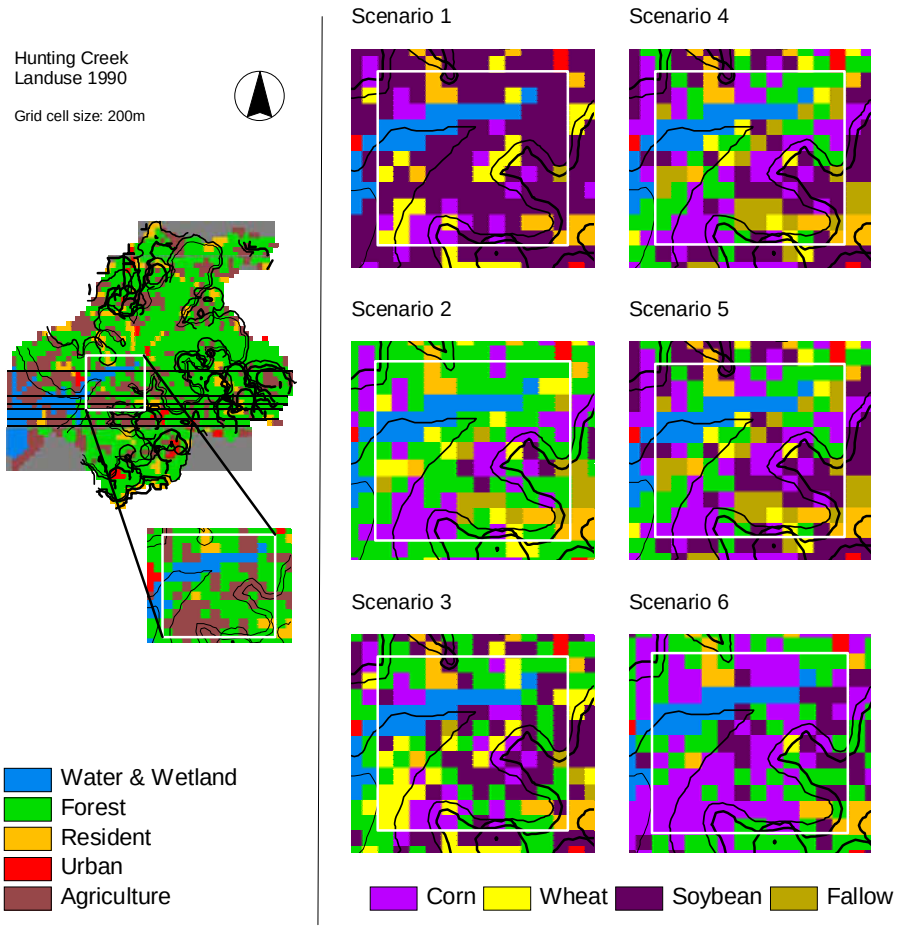

Fig. 12.11 Resulting land use patterns of the six optimization scenarios.

region. These pattern are clearly endogenous as these are derived from the processes coded in the model together with the application of the model in the optimization task, cf. Section 3.1.3.

The map from Scenario 1 shows that neglecting ecosystem functions and ecological impacts of agricultural production results in an optimum with agricultural habitat occupying the entire study area. All other weightings result in more heterogeneous optimal landscape patterns. Two issues should be noted. First, cells selected for agricultural production show similar patterns independent of the chosen weighting scheme. Only the crop variety planted depends on the ecosystem function(s) chosen in the performance criterion. Second, the cells allocated for agricultural production seem to be the same, perhaps shifted by some grid cells, as in the current land use for agriculture in Hunting Creek. One may derive the hypothesis that the history

of agricultural production in Hunting Creek developed towards a somewhat optimal landscape. The question is raised how one can compare the recent land use with the results derived from the optimization procedure.

12.5 CLIMATIC VARIABILITY AND OPTIMUM LAND USE PATTERNS

All results up to this point are based solely on climatic conditions of two years 1990/91. An important question is, how do optimum land use pattern depend on climatic variation? Does the methodology respond sensitively to changing precipitation or radiation?

These questions can be answered either by a sensitivity analysis in the related parameters or by application of the methodology to several consecutive years. Based on the Hunting Creek model an optimization study was performed calculating optimized land use and fertilizer maps. We focus on the problem of optimizing land use patterns with respect to nitrogen outflow and economic yield as introduced in Section 12.2.1.

Figure 12.12 displays the land use distributions (plot a) and the optimum fertilizer amounts (plot c) as a function of the weighting coefficient λ_N for the eleven years 1985 to 1995. The variation through the years is quantified by the derived plots of standard deviation of land use (plot b) and fertilization (plot d).

From these results one can derive, that approximately 10% of the controllable cells depend on the climatic situation of the considered year. Additionally, standard deviations vary as a function of λ_N. Second, standard deviation for the fertilizer amounts is below 50 kg/ha. Extreme scenarios, like very small and very large values of λ_N lead to higher standard deviation values for the optimum fertilizer amounts.

12.6 MULTI-SCALE ANALYSIS OF LANDSCAPE PATTERNS

The comparison of landscapes required the comparison of habitat patterns. Two approaches of pattern comparison come to mind, if one considers grid-based maps with discrete attributes. The coarsest approach is to compare the distribution of habitats in the entire area. This neglects any spatial patterns. The finest approach is to compare cell by cell, or pixel by pixel and to count the number of matches. This may be much too strict as patterns may appear transposed, rotated or slightly shifted in any two maps. We would still call these landscapes similar if we were visually comparing them. What we need is a distance measure, which allows a merger of both approaches. There are different procedures of multi-scale map comparison in development using different methodologies, for example fuzzy logic as presented by Hagen (2003).

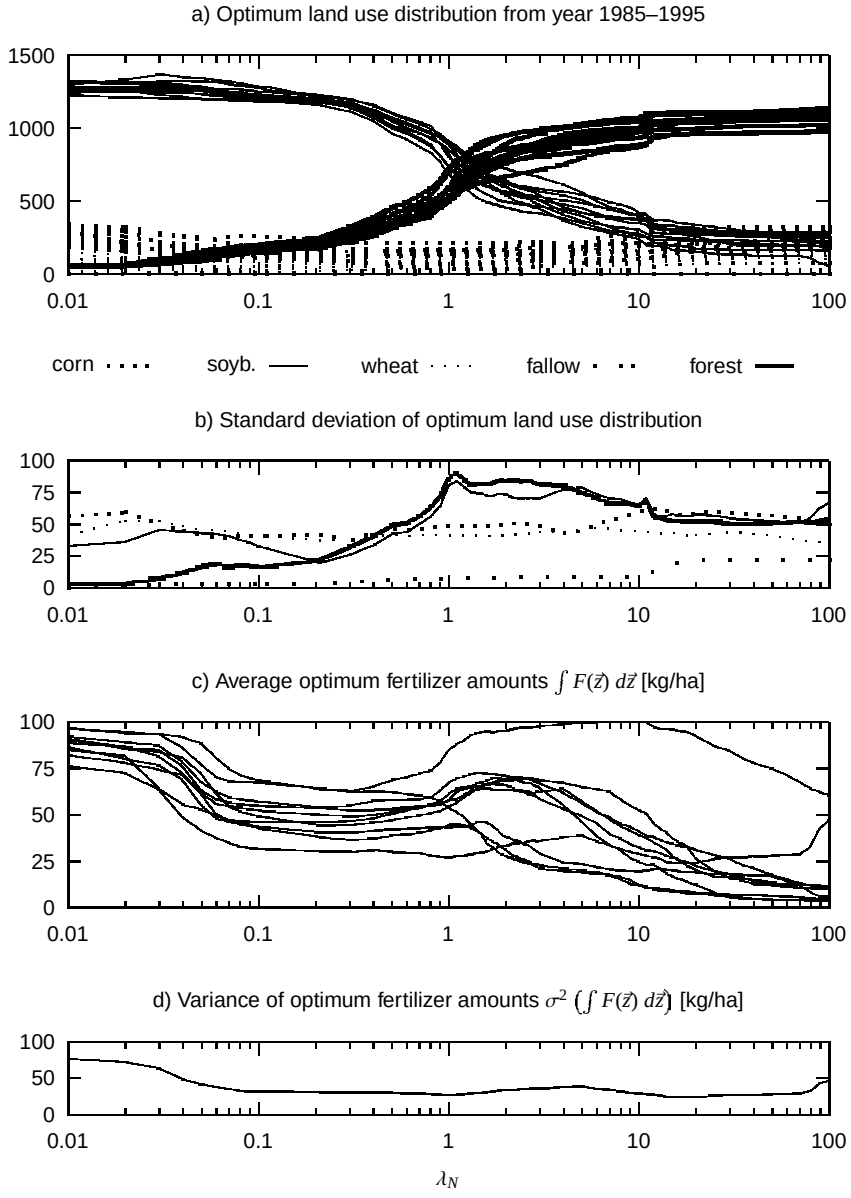

Fig. 12.12 Results of optimum land use pattern to climatic variation. Optimization results base on the simulation in the consecutive year 1985 to 1995. Plot a) and b) display the habitat distribution for the 11 runs (a) and the derived variance. Plot c) and d) analogously plot the average fertilizer amount.

12.6.1 Distance Measure of Discrete Maps

Habitat maps show discrete attributes, for instance soybean (1), corn (2), urban (3) etc., which may be summarized by an integer attribute $H(\vec{z}) \in \{1, 2, \ldots\} = S$. The number of attributes of classes — here habitat types — is given by $|S|$. The attribute of a certain grid cell $\vec{z}$ is denoted by $H(\vec{z})$.

The basic idea for the comparison of two habitat maps H_1 and H_2 goes back to the multi-scale approach from Costanza (1989) supported by some analytical considerations. Using a moving window with the edge length $w \geq 1$ the number of cells in the window, belonging to a certain class, i is compared for each habitat map H_1 and H_2. Let us denote this moving window at cell $\vec{z} \in R$ and the width and length $w \geq 1$ by $U_w(\vec{z})$.

Let $g_i(H \cap U_w(\vec{z}))$ denote the number of cells with the attribute i in a window $U_w(\vec{z})$ at location $\vec{z}$ on map H. Then

$$\rho_w(H_1, H_2) = \frac{1}{2}\frac{1}{\text{size}(R)}\frac{1}{\text{size}(H_1 \cap U_w(\vec{z}))}\sum_{\vec{z}\in R}\sum_{i=1}^{|S|}\left|g_i(H_1 \cap U_w(\vec{z})) - g_i(H_2 \cap U_w(\vec{z}))\right|$$

defines a function which measures the distance between map H_1 and map H_2 using a moving window of size w^2. The function size$(\cdot)$ denotes the size of considered map in the argument given in numbers of grid cells.

Function ρ_w is very intuitive and has all the essential features of a distance measure:

1. $\rho_w(H, H) = 0$ for an arbitrary $w \geq 1$: the distance between two identical maps is zero.

2. If $\rho_w(H_1, H_2)$ is divided by size(R) the function is normalized to unity for entirely different maps: $\rho_w(H_1, H_2) = 1$ for each $w \geq 1$ if and only if $H_1(\vec{z}) \neq H_2(\vec{z})$ for all $\vec{z} \in R$.

   Setting the maximum value of ρ_w equal to unity is an arbitrary definition. Neglecting this normalization is a reasonable choice, too. This might allow us to compare maps with different shapes. However, using the normalized value, the following properties of ρ_w become valid.

3. $\rho_1(H_1, H_2)$ denotes the difference between H_1 and H_2 in grid cell scale. This means $1 - \rho_1$ is the fraction of cells which are identical.

4. Let L define the maximum diameter of the study area or the given map H: $L = \max \text{diam}(H)$. The diameter is given by length of the largest of all possible cross-sections of a map. Then $\rho_\infty(H_1, H_2) = \rho_L(H_1, H_2)$ denotes the distance if the moving window covers the entire study area R. In that case the distribution of attributes in the maps H_1 and H_2 is compared. That means that $1 - \rho_\infty$ denotes the fraction of attributes with an equal distribution in both maps.

For an overall assessment of the map distance $\rho(H_1, H_2) = \frac{1}{L}\int_0^L \rho_w(H_1, H_1)dw$ may be calculated. The upper limit of integration is given by the maximum diameter of the study area. A second integrative measure derived from ρ_w is $\rho_0(H_1, H_2) = \min_{w=1,\ldots,L} \rho_w(H_1 H_2)$ together with the w_0 value, for which ρ_w equals its minimum. These two values indicate the similarity or distance of two maps H_1 and H_2 as well as the scale or distance at which most patterns fit.

Additionally, one can prove that ρ, ρ_∞, ρ_0 and ρ_1 are distance measures in a mathematical sense. It holds true, that

(i) $\rho(A, A) = 0$ (ii) $\rho(A, B) \neq 0 \Leftrightarrow A \neq B$ (iii) $\rho(A, C) \leq \rho(A, B) + \rho(B, C)$

12.6.2 "Correlation"-analysis of Landscape Patterns

This approach of map comparison is now applied to the results of the landscape optimization Scenarios 1 to 6. Similar to correlation analysis, Table 12.3 displays the ρ_0 values and the window sizes w_0, for which ρ_w is minimal.

This clearly shows that habitat maps from Scenarios 1 are different from all other habitat maps in terms of their similarity to other maps ($\rho_0 > 0.65$). Compared to Scenarios 2 to 6 this scenario is characterized by very low values for ecosystem functions. However, minimum values of ρ_w are reached for $w = 3, \ldots, 9$. To explain this one should recall that non-controllable cells presenting urban, open water and rural areas are also taken into account for map comparison. In this case spatial patterns of these cells dominate the map comparison values.

All other comparisons lead to smaller ρ_0 values. In these cases the w_0 value is a good indicator of what may be causing this similarity. If w_0 is close to the study area size $L = 58$, similarity is mainly caused by the agricultural habitat distribution over the entire study area. Smaller values of w_0, e.g. for comparisons of Scenarios 2 vs. 9, 3 vs. 8 and 6 vs. 9, show that certain more local landscape patterns cause similarity. Comparing these results with weighting schemes of $\vec{\lambda}$ in Table 12.2 we arrive at a surprising result: the $\vec{\lambda}$ vectors for these scenarios are not close to each other in the 3-dimensional weighting space. This again makes clear that the underlying processes incorporated into the spatially explicit simulation model are highly nonlinear with respect to dynamics and to spatial dynamics of material fluxes.

With the map distance measure developed one can answer the question raised in the previous section. How similar is the recent land use compared to the maps resulting from the optimization procedure? Table 12.3 shows map distance measures for the recent land use and the maps resulting from the optimization scenarios. Note that in this application of the distance measure only the habitat types for forest, agriculture, open water, urban and rural are taken into account to match the categories on the underlying data set of the 1990 land use map.

As expected the optimized map from Scenarios 1 is different from the 1990 land use map ($\rho = 0.59$). However, some similarities are identified for a 3-cell-wide moving

Table 12.3 Map comparison of optimum habitat maps H for the Scenarios 1 to 6 and comparison with recent land use. The table displays the ρ_0 values of two optimized habitat maps H_i and H_j ($i = 1, \ldots, 6$; $j = 1, \ldots, i$) and the associated w_0 values. The table is to be read like a correlation matrix, see text.

	1990 land use	1	2	3	4	5
1	0.59 (3)					
2	0.1 (9)	0.72 (7)				
3	0.31 (5)	0.35 (9)	0.38 (27)			
4	0.46 (6)	0.37 (52)	0.41 (9)	0.26 (24)		
5	0.04 (15)	0.66 (5)	0.14 (38)	0.32 (6)	0.54 (9)	
6	0.17 (7)	0.65 (3)	0.19 (57)	0.34 (33)	0.41 (9)	0.27 (56)

window. Results from Scenarios 3 and 4 seem to be closer to the 1990 land use map. The maps resulting from the optimal Scenarios 2 to 4 are almost identical to the 1990 map. The similarity is caused by similar patterns at the scale of 5 to 7-cell-wide windows. This proves the hypothesis from the previous section: the resulting maps from the optimization are similar to the recent land use map. Note that this holds only for a distinction between aggregated agricultural and forest cells as this is the level of detail the data land use map offers.

12.6.3 Optimization Results on Differing Scales

The methodological framework presented can easily be transfered to different regions without any increase of computational effort as long as is it possible to apply the local optimization approach. This was performed for the entire Patuxent watershed, a region 2359 km^2 in size. The spatial data set for a spatially explicit application of the generic landscape model (see Section 3.3.3) in this case is set up by a grid cells of 1km^2 size, see Figure 12.1. Additionally the results of optimum habitat distribution are displayed for the small sub-watershed within the Hunting Creek catchment.

We focus on the problem of optimizing land use patterns with respect to nitrogen outflow and economic yield, see Section 12.2.1. Figure 12.13 displays the results of land use distribution of the study areas Hunting Creek (b) and Patuxent (a) as well as the smaller sub-watershed (c). Figure (b) is equal to Figure 12.2. Note, relative land use distributions are plotted as both areas have different numbers of controllable cells R_c: sub-watershed $|R_c| = 485$, Hunting Creek $|R_c| = 1652$, and Patuxent $|R_c| = 2133$.

The striking result of this multi-scale analysis of optimization results with three embedded study areas and two different granularities (cells sizes) is, that the resulting function of land use distribution are very similar. The calculation of the correlations coefficients for Patuxent and Hunting Creek leads to an overall correlation of $r^2 = 0.87$. Calculating correlation coefficients for land use habitats separately lead to: corn $r^2 = 0.61$, wheat $r^2 = 0.89$, soybean $r^2 = 0.94$ and forest $r^2 = 0.97$. These

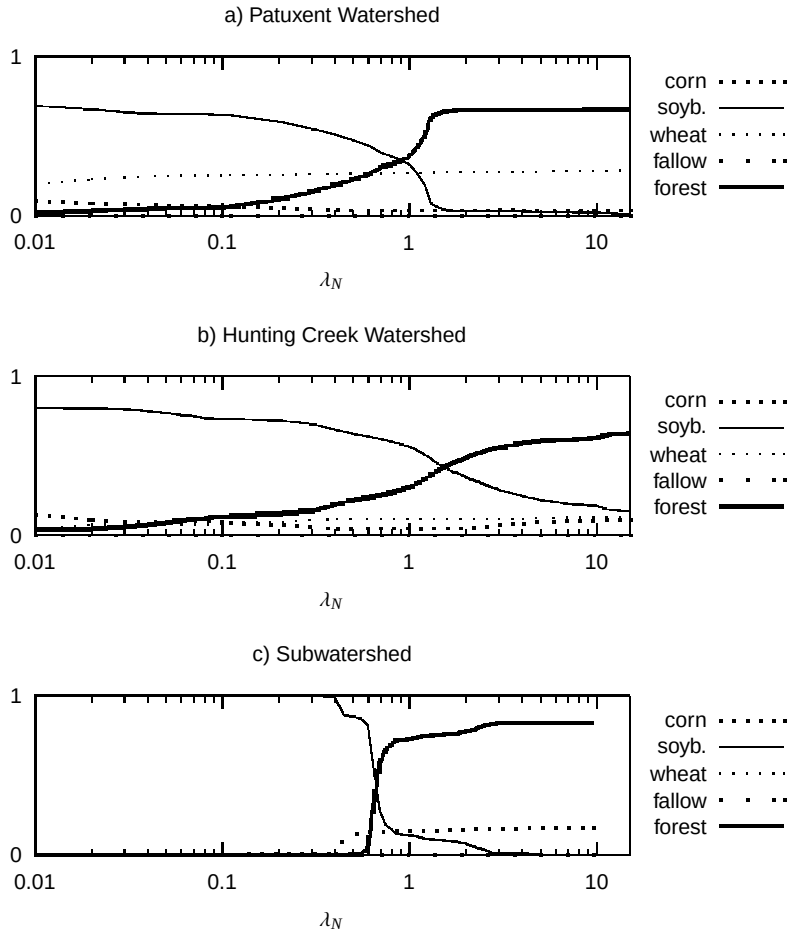

Fig. 12.13 Comparison of optimum land use distribution optimizing economic yield against nutrient loss for Patuxent study area (a), Hunting Creek watershed (b) and the sub-watershed (c) based on climate data from 1990/91.

values aggregate the results too much, as no spatial patterns are taken into account. However, one can state that the endogenous pattern derived and identified from the Hunting Creek study appears in the Patuxent Landscape Model, too. Second, exogenous pattern such as different soil type results in slightly different optimum habitat. For instance wheat is a more frequently chosen habitat for Patuxent than it is for Hunting Creek. Figure 12.14 display three different optimum habitat maps of the Patuxent watershed for selected values of λ_N.

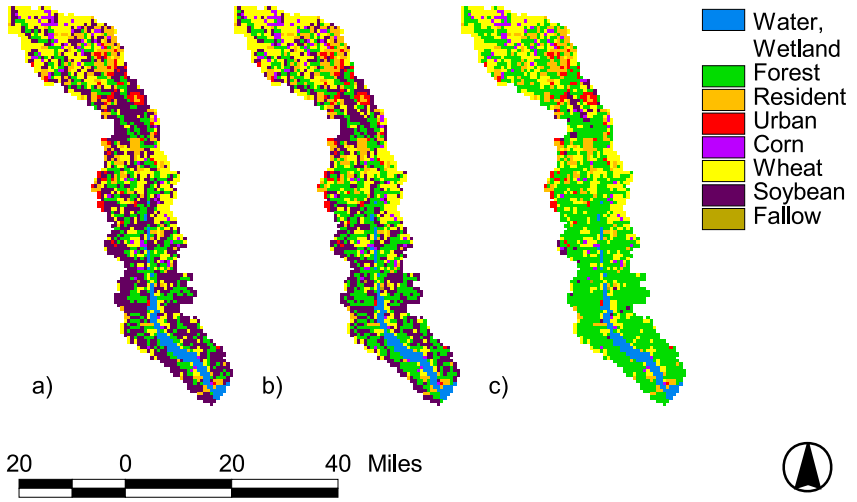

Fig. 12.14 Local optimum land use maps for Patuxent watershed using $\lambda_N = 0.5$ (a), $\lambda_N = 1.0$ (b) and $\lambda_N = 10.0$ (c).

12.7 SUMMARY AND OUTLOOK

12.7.1 Methodological Aspects

Building upon the background of the spatial modeling environment the application of the proposed framework presented in Section 9.3.6 is capable of answering different questions of landscape management. Run-time solutions for optimization problems can be derived (for example in the ArcVIEW front end) if it is possible to set up a local optimization criterion and if a global solution is not required. In this case the computational effort does not significantly depend on the size of study area. On the other hand, the use of GA for global optimization offers the ability of parallelization in the optimization process. In summary, this framework seems to be applicable to a large class of problems in landscape ecology. It enables integration of simulation models and environmental management.

The only simplification, which was introduced to derive a solution to this very complex optimization task, was to assume a weak dependency of the single parameters of the control variable maps upon the neighborhood. This allows a characteristic function to be set up for each grid cell of the model. We focus on simple goal functions that assess the state of a certain grid cell only. The core question which lies behind this consideration of neighborhood relationships of the control variable map is, how strong is the synergistic effect of land use change for a given watershed? It is an exciting question to be investigated in the framework of optimization, see for example (M üller, 1998; Wolfert *et al.*, 2002).

As the modeling and optimization approach presented incorporates aspects of topology and connectivity of cells, statistical analysis applied to multi-dimensional spatially explicit models is limited. The methodology of map comparison presented extends analysis of multivariate statistics. With the use of landscape pattern comparison we are able to show how much optimization results differ in terms of local patterns for global (whole watershed) land use distribution. Additionally, invariant patterns can be identified and the spatial scale of the invariant patterns can be quantified. invariant property

12.7.2 Optimization Results as Multi-stage Decision Process

There are several major results of this study. First, on a global scale the optimization problem is based on a multi-dimensional performance criterion and leads to optimum land use patterns, which support certain ecosystem functions. These patterns can be studied as a function of weighting coefficients in the performance criterion. Second, with an adequate map comparison methodology one can show that certain patterns are invariant to different weightings of ecosystem functions in the performance criterion. invariant property

One may summarize these results qualitatively in the following way, which may be interpreted as a multi-stage decision-making process.

1. If only economic considerations are taken into account in the performance criterion, cells that are optimal for agricultural production are identified;
2. If ecosystem functions are considered (one of $\lambda_{NPP}, \lambda_{QB}, \lambda_N > 0$) less fertile sites and cells crucial for the regional nutrient balance are identified;
3. Depending on particular weighting schemes for $\lambda_{NPP}, \lambda_{QB}, \lambda_N$ a certain combination of fertile and less fertile cells are allocated for agriculture;
4. The remaining cells are allocated for forest habitats.

12.7.3 Application of Results

Comparison to Real World Data These studies may be viewed as model experiments of spatial change in land use allocation in the landscape. In this context it is interesting to see that some optimized habitat maps are fairly close to maps of the existing landscape. We can conclude that in some sense the existing landscape in the Hunting Creek watershed is optimal, at least in terms of some of the assessment scenarios.

Second, an important result that advocates an application to more realistic spatially explicit management problems is the variation of the optimization results under changing climatic conditions. This suggest an application of the concept in the framework of climate change scenarios for different investigation sites. A possible concept would

be to use stochastically generated climatic conditions driven by an increase of mean temperature and precipitation together with a spatially explicit population dynamic model for different vegetation types.

Experiments on a Landscape Scale It is difficult to design, implement and perform experiments that allow the results obtained in these studies to be tested. This is neither a disadvantage nor should this impede an implementation of the derived management strategies to a landscape. First, models enable us to do investigations and simulations studies as presented in this chapter, because they allow to be studied results without effecting a real world landscape. Second, real world landscape management problems show a larger spectrum of constraints.

One has to keep in mind this fact when studying publications on experiments on this landscape ecological issue. Li *et al.* (2002), for example, derived that only 10% of the nutrient reduction is caused by spatial configuration of habitats. On the other hand, Kuusemets & Mander (2002) performed an experimental analysis on nutrient flow management in a 378 ha watershed in Estonia and advocate establishment of buffer zones at the banks of the stream, that would remove 2000 to 2640 kg nitrogen a year. Naiman and Décamps (1997) as well as Malard *et al.* (2002) state more qualitatively that riparian zones play an essential role in water and landscape planning and in restoration of aquatic systems. The spatial arrangement of surface-subsurface exchange patches affects heterogeneity in stream nutrient concentration, surface water temperature and colonization of dry reaches by invertebrates.

This is in accordance with the results of the landscape optimization results studied in this chapter, albeit, only a limited view of the mentioned aspects of the field experiments were considered in the landscape model. One important result can be derived from these considerations. An application of landscape management patterns and scenarios to real world management problems can be supported by the consideration of real boundary conditions in the optimization task.

12.7.4 Patterns and Processes

Several results were obtained in the studies that offer a deep insight in the relationship of landscape pattern and the spatially explicit processes responsible. First, important areas with high retention capabilities — buffer zones — were identified and fertilizer maps were set up depending on soil properties. This shows that optimization methods even in complex simulation models can be a useful tool for a systematic analysis of management strategies of ecosystem use.

Second, the results speak in favor of the statement that the developed methodology gives robust optimization solutions based on complex ecosystem models. They extend the previous analysis for multi-dimensional performance criteria and show how to identify important regions or groups of cells, which support certain ecosystem functions.

Third, the results are likely to be scale invariant. Typical patterns of optimum land use distributions as a function of a weighting coefficient of the performance criterion are similar for the three embedded study areas as well as for landscape models regionalized using a different granularity.

Fourth, the results show superposition of endogenous and exogenous patterns. It is difficult to identify which are mostly caused by endogenous processes and which patterns are caused by external driving forces. The statistical analysis (Section 12.3.3) could prove that not all patterns are caused by site conditions. The concept of map comparison helps to identify similarities in the resulting patterns. However a relationship to determining processes is hardly possible. These questions can only be answered by a more detailed analysis of the underlying model together with different parameterizations of the performance criterion. The processes model, which is embedded in the optimization framework, builds the connection of patterns and processes.

12.7.5 Outlook

The approach may be extended by the integration of the neighborhood of a given grid cell $U_w(\vec{z})$ with $w > 1$. The proposed framework is capable of dealing with goal functions defined on all $\vec{z} \in U_w(\vec{z}_0)$. This allows the assessment of habitat structures in the goal functions. Habitat suitability of certain species determined by patch configuration may be assessed with this extension.

Besides this, some methodological requirements could be derived. In these studies we identified processes that could not be handled within the localized optimization methodology. Two directions for further research can be derived from those results. First, criteria should be defined that characterize sub-models with their appropriate spatial optimization strategy. Second, methodology for global or at least regional scale spatial optimization must be developed or improved.

Finally, possible extensions to this concept are to integrate economic models into the landscape model to achieve a more detailed description of the anthropogenic processes. There are models of urban growth, and modeling interrelations with economic models, as suggested by Irwin & Geoghegan (2001).

13

Conclusions, Perspectives and Research Demands

13.1 RETROSPECTION

It is difficult to distill a few important topics from an entire book which itself is a distillation of numerous publications. A few general statements, however, should be given at the end to answer the questions about what we have learned from this text.

First of all, I have tried to clarify, that modeling is not a mystery, nor an art, it is a science. Fundamental statistics as well as criteria from scientific theory should be applied to assess performance of simulation models. It is a general rule that environmental models should be based on physical processes and derived from first principles wherever possible. We learned that the scale of interest, the focal level, often defines the mathematical structure, and that nonlinearities are introduced by implementing processes from different spatial and temporal scales to the focal level. Nonlinearities are a result of moving across scales during the modeling process. These are first answers to some of the questions Wu & Hobbs (2002) raised in their overview paper.

Additional recommendations for environmental modeling are to understand models as a toolbox, to assure reusability of models or sub-models, and to aim at integration of present models, because modeling from scratch is rarely appropriate for solving and assessing environmental problems. Firstly, because the resource time is limited because financial support may be limited and secondly because data availability on the considered process may be insufficient. By applying spatially explicit models to a real landscape (either by the use of highly aggregated partial differential equations or by using integrated model systems) we have achieved a methodological link between functioning of ecosystems and landscape patterns. Based on this, endogenous

patterns could be separated from exogenous patterns. And, in any real world landscape endogenous and exogenous patterns are superimposed. Assessing landscape patterns by simply applying landscape metrics may be insufficient. This has been identified as research a demand in environmental science and landscape ecology by several authors (Turner *et al.*, 2001; Opdam *et al.*, 2002). By the use of physically based spatially explicit models we are able to study ecological flows in landscape mosaics. We may relate landscape metrics to ecological processes and may identify causes, processes and consequences of land use and land cover change, see again (Wu & Hobbs, 2002). This can be a first step for further theoretical studies in landscape ecology as demanded by Bastian (2001). Simulation models undoubtedly play an important part in environmental science as these enable us to move the focus from qualitative analysis of ecological issues to quantitative research.

13.2 CONCLUSIONS

Finally, in their idiosyncratic synthesis of recent research demands in landscape ecology Wu & Hobbs identify the need of integration of human activities into landscape ecology as well as the optimization of landscape patterns as important research topics in the coming decades (Wu & Hobbs, 2002). These issues have been discussed in detail throughout the third part of this text.

Scenario analysis is a common tool for model analysis and for assessing different development pathways. But scenario analysis is limited, if model complexity growth, the number of driving forces increase and spatially dependency is introduced. Applications of environmental models in terms of optimum control theory are a very promising branch of ecological system theory.

This methodology offers a link between anthroposphere and biosphere processes. It introduces economics into ecological modeling and is therefore an important part of ecological economics. If the performance criterion is defined following these considerations of ecological economics, which introduce costs for ecosystem services or ecosystem damage, we can study human impact on the environment by economic considerations. This may increase awareness of ecosystems functions and provide us with information on the environmental costs of our impact (Costanza, 2000; Costanza *et al.*, 1997; Scheffer *et al.*, 2000). This is possible because economic considerations always aim at maximizing yield, which is in accordance to the optimization approach.

A second important analogy in nature of the optimization approach is that nature does not waste available energy. Using the evolutionary concept of maximizing information and function by using a minimum of free energy, is a second valuable approach for the optimization concept (Jørgensen *et al.*, 1998; M üller, 1998).

Applications of optimization and optimum control enable us to study dependencies of the driving forces of a system to environmental outcomes. Of course, the computational effort is tremendous. However a considerable spectrum of possible application of control theory to environmental model is presented in this book. Anyway, one

should not forget the increasing power of computers in the future. This is why optimization using environmental models should find its way into the application of decision support systems for environmental management.

13.3 PERSPECTIVES

Heterogeneity has been a point of discussion throughout this text. One reason for this diversity in environmental models is that models come from a multitude of different origins, see Part I. This pluralism of approaches make environmental modeling a fascinating and very promising branch of science. We need this pluralism to solve recent environmental problems in an acceptable time. It is neither understandable by decision makers nor helpful for the environment to spent much time on model development, testing and verifying before offering possible solutions. Increasing population growth will intensify human impact on nature. Resources will be withdrawn from the environment more quickly and time for suggesting alternative strategies for a sustainable use of environmental resource, let it be water, food or space, will be reduced.

Environmental modeling research should therefore concentrate on the modularity, reusability and transferability of models. It is not appropriate to start modeling from scratch, even if "modeling is also fun" (Pahl-Wostl, 1995). One should aim at viewing environmental models as a toolbox. This can be supported by mathematics in all related environmental scientific disciplines like biology, ecology, landscape ecology etc. Mathematics can act as a common language. My wish is, that this text supports environmental research with a methodological foundation and is a stimulus for new ideas, exciting approaches and further applications of integrating applied mathematics to environmental sciences.

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Web Resources

Additional resources to the material of this book may be obtained from the URL `http://www.wiley-vch.de/books/info/3-527-30732-X/`.

Animation and Video Files are available from the above noted URL, which illustrate the spatially explicit simulations discussed in Chapters 3 and 6, see Figures 3.3 (p. 77), 3.7 (p. 82), 3.8 (p. 84), and 6.8 (p. 134).

Software and Libraries The following software tools and numerical libraries are currently available free of charge to educational and non-profit organizations from the above mentioned URL.

- The development platform for hybrid low level Petri nets (hPEN), see Section 5.3 (p. 115);
- The library for hierarchical dynamic programming (LibHDB), see Section 9.2.3 (p. 180);
- The toolbox for spatially explicit optimization (TSEO), see Section 9.3.6 (p. 188).

Any publications of work based upon experiments that use the above mentioned software must include a suitable acknowledgment.

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Parts of Chapters 2, 8 through 12 are reprinted from (Seppelt, 1999; Seppelt, 2000; Seppelt, 2001; Seppelt & Voinov, 2002) with permission from Elsevier, Ltd.

Results in this contributions were obtained using the GAlib genetic algorithm package, written by Matthew Wall at the Massachusetts Institute of Technology (Wall, 1996).

Quotations

Introduction, page xvii Charles Lutwidge Dodgson (1832 – 1898) better known as Lewis Carroll: *Alice's Adventures in Wonderland*.

Part I, page 1 Augusta Ada Byron (1815 – 1852), was a woman ahead of her time. For the next hundred years she would be known as the daughter of Lord Byron the poet. Only in this century would she become known as the first "computer programmer". This is her comment on the Analytical Engine designed (but never built) by Charles Babbage.

Part II, page 97 Alan Alexander Milne (1882 – 1956). Chapter 6 of *Winnie–the–pooh* . . . in which Eeyore has a birthday and gets two presents.

Part III, page 157 Berthold Brecht (1898 – 1956): *Three Penny Opera*, 1931 Berlin, Schiffbauerdamm: Aye, make yourself a plan // They need you at the top! // Then make yourself a second plan // Then let the whole thing drop.

Index