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Biogeochemical Models in the Environmental Sciences

The Dynamical System Paradigm and the Role of Simulation Modeling

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Abstract: Dynamical systems are *the* paradigm for the representation of complex systems. The fixed encoding in a closed set of equations, however, contrasts with the openness of biogeochemical systems. Parameter identification is a major problem in biogeochemical systems and calibration of parameters converts models into 'fitting machines'. Openness, self-modification, and historicity of biogeochemical systems make non-trivial predictions of future outcomes impossible. Notwithstanding, simulation models serve as instruments of synthesis and have heuristic value to challenge existing data and theories. The modeling process itself, as a learning and communication process, can be a mode of coping with different types of complexity.

Keywords: *models in biogeochemistry*, *dynamical system*, *simulation model*, *self-modifying system*, *complexity*.

1. Introduction

System metaphors pervade ecology and the environmental sciences. System metaphors are characterized by a set of basic attributes, *i.e.* interacting parts, organization, collective behavior, and whole system functionality (Paton 1993). Machine and circuit are concepts associated with system metaphors. The circuit concept of ecosystems accounts for fluxes of matter and energy in arbitrarily defined ecosystems (developed *e.g.* by Odum 1983). The machine metaphor (Haken 1993) stands for the regular input-output behavior of determinate machines that follow clockwork mechanisms. Systems theory has transferred the system metaphor into a set of formal and theoretical methods. Although systems theory originated in information theory and cybernetics, its formal approaches claim universal and interdisciplinary validity (Lilienfeld 1978).

Environmental sciences regard their object of study as complex natural systems. Different concepts of complexity can be distinguished, first, descriptive complexity, second, ontological complexity, third, complex (non-linear) dynamical systems, and fourth, an emerging 'complexity paradigm' replacing the classic, simplifying paradigm (Emmeche 1997). The notion of ontological complexity is questioned by some researchers, which maintain that complexity has to be conceived as a relation between representation and a represented system (Hauhs & Lange 1996). Complexity thus is a function of the chosen description; systems that can not be described by a single theory or discipline are regarded as complex (Kornwachs & Lucadou 1984). Accordingly, the number of different, non-equivalent descriptions of a certain system has been equated with the degree of complexity of the system (Casti 1986).

Dynamical systems have become *the* formal paradigm in the 'discovery of complexity' across a range of disciplines: Dynamical systems as universal paradigm propelled the diffusion of complexity concepts in the empirical sciences and have become the leading paradigm for both conceptual and numerical models of complex phenomena. Encoding in a dynamical system is regarded as an adequate way of coping with the (descriptive) complexity of natural systems, allowing for better system understanding and the simulation and prediction of system 'behavior'. Consequently, in the environmental sciences ecosystems are treated, modeled and simulated as (if they were) dynamical systems (see *e.g.* Bossel 1997, Richter 1994).

Models play an outstanding role in the study, management, and utilization of complex natural systems. Models can be differentiated according to the degree of process description, which ranges from indicators to empirical, functional approaches and to mechanistic (stochastic to deterministic) physically based models (Bork & Rohdenburg 1987, Hoosbeek & Bryant 1992). Accordingly, three types of models can be distinguished (Bossel 1992): First, behavior-descriptive models, *e.g.* the growth-and-yield tables of forestry. These so-called empirical, functional, and predictive black box models dominate ‘utilization technology’ in forestry, agriculture, and the management of water resources (Hauhs *et al*. 1998). Second, elementary-structure models that elucidate determined basic processes. Due to the aggregate description, the parameters of these models lack empirically measurable counterparts and have to be fitted. The Lotka-Volterra equations are an example for this approach (Richter 1985). Third, mechanistic ‘real-structure’ models that make use of supposedly ‘real’ empirical parameters. Simulation models in the environmental sciences are elementary- to real-structure models, depending on model purpose (*e.g.* research models vs. management models; Huwe & van der Ploeg 1992).

In this paper we focus on mechanistic dynamical models, which simulate biogeochemical processes in ecosystems on a variety of scales. The field of biogeochemical models encompasses models for the behavior and cycling of water and elements, ecotoxicological models, and global change models.

Biogeochemical models as scientific products may be regarded from the perspective of prediction or the perspective of understanding, following a debate on the aims of science (Toulmin 1981). As predictive instruments, they are used to simulate the behavior of complex systems and to compute scenarios of system behavior under varying external conditions. Examples are the effect of different fertilizer regimes on nutrient losses to the aquatic system, the behavior of newly created pesticides or the effect of climate change on the terrestrial carbon cycle. On a societal level, models fulfil important roles as management models, as decision support models and in risk assessment studies on different spatial and temporal scales. Dynamical simulation modeling was inspired by and in turn nourished the hope that the environmental sciences would open a way towards environmental engineering (see *e.g.* Patten 1994, and the title of the conference proceedings edited by Dubois [1981]). The goal was to enable an ecosystem engineer to manipulate natural systems according to societal aims.

In the following, the paradigm of dynamical systems will be characterized, with particular reference to the notions of state and time. We will show how the dynamical system paradigm is adapted in the modeling procedure prevailing in the environmental sciences and we will cast a light on a number of problems arising in the course of the modeling procedure. The paradigm of self-modifying systems is presented as an alternative to the essentialist dynamical system paradigm. Making reference to the two opposing paradigms, fundamental limitations of the dynamical systems approach in the environmental sciences are discussed. Emphasis is on ‘noise’ and on the internal production of variables, which can not be accounted for in dynamical systems. In our opinion, dynamical models are not suited for the prediction of the future behavior of natural systems. While dynamical models (as products) may play a role as heuristic tools, the modeling process itself can be a way of coping with descriptive and communicative complexity.

2. The dynamical system as a paradigm

The increasing interest in middle-number systems along with the ‘discovery of complexity’ in mathematics, physics and the biological sciences (Hedrich 1994) has found its formal counterpart in the paradigm of complex dynamical systems. Originally a mathematical formalism, it has inspired research in the empirical sciences and has found widespread adoption in ecology and the environmental sciences. "A dynamical system is one whose state changes with time (*t*)" (Arrowsmith & Place 1994, p. 1, first sentence). The generic system diagram for any continuous dynamical system is shown in Fig. 1.

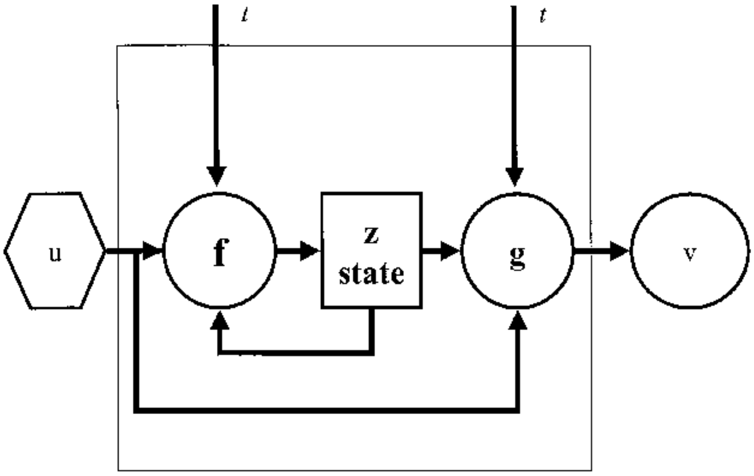

Figure 1: Generic system diagram for a continuous dynamical system: The general form of the state equations describing the system is: ¶z/¶*t* = f (z, u, *t*) and v = g (z, u, *t*); z is the state vector, u the vector of environmental inputs, v the vector of system outputs, *t* the (external parameter) time, f the (vector) state function and g the (vector) output function (adapted from Bossel 1997).

The notion of an abstract system state lies at the heart of dynamical systems: The abstract state is the entirety of all states of a system at a given time. The states of a system are represented by the state variables, which contain all the information relevant to the present of a particular process. The possible states of the system are delimited by an abstract phase space, which has a fixed number of degrees of freedom. The degrees of freedom are defined by the state variables of the system. The system state moves along trajectories in the phase space. In an exo-perspective on the dynamical system, the system collapses to a closed system (Kampis 1994): The system and its boundaries are defined externally and analytically, closing the system towards its environment except for the vector of environmental input (external variables). The encoding in a dynamical system as a formal set is invariable (first order system). This implies a syntactic conception of information, as pragmatic information would not only change the state but also the structure of the system (Kornwachs & Lucadou 1984). Fitting into a concept of formal computation (as opposed to *e.g.* informal, biological and physical concepts; Emmeche 1994), the system is regarded as a processor of syntactic information, which processes incoming signals according to fixed rules, excluding 'noise' from the dynamical system.

The temporal dynamics of the system, *i.e.* the transition from state to state, comes about as the state variables are updated by a transition function. The transition function is a causal-determinate function for a determinate system: If the state of a dynamical system at a certain time is known, the state for any other point in time can be computed. Accordingly, the same transition function can be applied for every interval. Its effect is reversible as the effect of time can always be 'undone' by the application of the time evolution function. In this exo-physical concept of time-invariance (Kampis 1994), time is scalar, invariant, reversible and universal. The underlying notion of time is parameter time (Drieschner 1996), derived from absolute Newtonian time, which has the following characteristics (Mittelstaedt 1980, p. 15): Both its topological structure (temporal sequence) and its metric structure (parameter time) are equal. Time has no relationship to objects external to it, while any process refers to the same absolute, universal time (external time).

At the outset of dynamical system building, the set for the encoding of the system is needed. The material object under study is not the system, because every material object contains an unlimited number of variables and, therefore, of possible systems. The system is a list of variables (Ashby 1976, p. 40). The task of the modeler is to vary the list of variables until the system becomes determinate: a determinate machine is one whose behavior can be encompassed in a list of variables that is logically and mathematically workable (Lilienfeld 1978, p. 37). The basic question is which variables are necessary in order to express a given domain of phenomena (Kampis 1992a). Modeling is thus faced with a frame problem (Paton 1996); *i.e.* the question how reading frames or frames of description should look like (Kampis 1992a).

Notwithstanding the frame problem, an essentialist notion underlies the dynamical system paradigm: It is assumed that the modeler can discern the essential properties of the represented system. Modelers pretend to isolate "… the essential (behaviorally relevant) system structure, *i.e.* the identification of essential state variables, their feedbacks, and critical parameters" (Bossel 1992, p. 264). In this view, the dynamical system retains the essence of the represented system, *i.e.* that which remains the 'nature' of the system throughout its change from potentiality to actuality. Abstract state and system structure stand for this essence.

3. Ecosystems as dynamical biogeochemical systems?

Ecosystems are constituted from two perspectives (O'Neill *et al.* 1986, p. 8-13): First, there is the population-community approach, which views ecosystems as networks of interacting populations and in which the environment is regarded as context. Secondly, there is the process-functional approach that focuses on matter and energy fluxes, regarding ecosystems (and compartments) as bio-physico-chemical reactors (see *e.g.* "the soil as a reactor" by Richter 1986). Here the function is considered more important than the biotic entities performing it. The circuit and the machine metaphor have been formalized to deal with the biogeochemical perspective on ecosystems.

Biogeochemical models, the focus of this paper, deal with a range of spatiotemporal scales. At one extreme, inputs and outputs of total landscape units (catchments, watersheds) are measured and modeled. At the other extreme, processes such as decomposition or the nitrogen cycle are studied at the point scale. Models for (agro-)ecosystem management and environmental risk assessment deal *e.g.* with the dynamics of organic matter (Powlson 1996), the loss of (excess) nutrients such as nitrogen (*e.g.* de Willigen 1991, de Willigen & Neetson 1985, Engel 1993, Frissel & van Veen 1981, Groot *et al*. 1991, van Veen 1994) and phosphorous (*e.g.* Cassell *et al*. 1998), and with the dynamics of organic contaminants such as pesticides (*e.g.* Calvet 1995, Richter *et al*. 1996, Walker 1995) and other xenobiotics (Behrendt 1999).

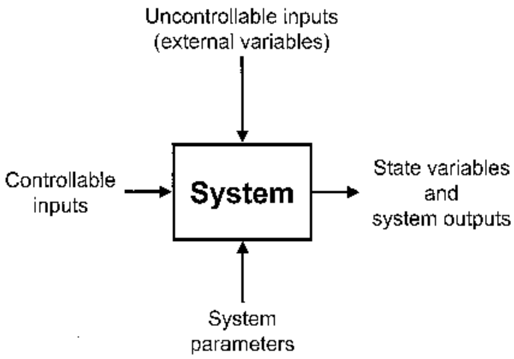

Figure 2: Characteristics of dynamical systems in the environmental sciences. The system describes the transformation of inputs into outputs and system states under the influence of external driving variables and system parameters (adapted from Berg & Kuhlmann 1993, pp. 4-5 and Gnauck 1995).

Mechanistic biogeochemical models are encoded as dynamical systems, which are developed in an iterative procedure consisting of the following steps (adapted from Joergensen 1991 and 1995):

- Definition of problem and bounding of the problem in time, space and subsystems
- Development of model structure
- Sensitivity analysis
- Calibration
- 'Validation' (conceptual validity)
- Application as scientific or predictive tool
- Validation of prognoses (operational validation)

In the course of model structure development, a conceptual model and mathematical formulations of the processes are developed. For the representation of ecosystems as dynamical systems the problem of system identification, *i.e.* the identification of state variables, system structure, and the characteristics of the components, as well as the problem of parameter identification have to be addressed (Richter 1994). The system structure, which connects the elements of the system, is invariable (first-order system). The number of degrees of freedom (variables) is given by the respective system structure. System state and system output of these determinate systems (Fig. 2) is a function of parameter time and of the

- initial values of the variables;
- parameters of the system;
- boundary conditions, *i.e.* the external variables or driving factors;
- temporal transition function of the state variables as a function of parameters and boundary conditions.

Characteristic limitations of this modeling procedure are investigated in the following.

3.1 System structure and processes

Modelers face a basic problem. There are neither theories that allow the construction of models from first principles nor theories that relate observations across different scales (Hauhs *et al.* 1996). Process descriptions that have been obtained on different but mostly small scales in field and laboratory studies, become the point of departure for model construction: From the variety of process descriptions, the modeler chooses the 'relevant' processes to represent a determined domain of phenomena, without disposing of *a priori* criteria of relevance nor *a posteriori* criteria to test the selection. Thus, modelers tend to base their choice on what from their background of experience seems important, *i.e.* on prior experience and intuition (Hornung 1996), putting together what seems relevant to them. Presumably there is an optimal level of model complexity (Wissel 1989, p. 3), *i.e.* a point where the degree of model complexity – measured *e.g.* by the number of state variables – matches data resolution and quality, leading to maximal knowledge gain about the modeled system (Joergensen 1992, p. 87). However, whether such a point exists indeed and how it is to be found in practice is far from clear. In modeling practice the idea prevails that accounting for more processes leads to more realistic model structures and hence to more accurate models. Environmental systems are regarded as complex, thus "increased complexity in models is interpreted as evidence of closer approximation to reality" (Oreskes, in press). The tendency of putting together as many processes (with their respective parameters) as possible has been termed 'naive modeling' by Hauhs *et al*. (1996). It entails the unrestricted increase of degrees of freedom and frequently leads to non-identifiability of model parameters and overparameterization (see below).

3.2 Parameters

In ecology, parameters are coefficients regarded as constant for a specific (eco-)system (Joergensen 1991, p. 67), although in principle no measurable aspect can be considered constant over the observed temporal scales in ecosystems (Hauhs 1992) due to manifold feedbacks. Although the application of parameters as constants is unrealistic, the dynamical system approach calls for determined parameter values. Many parameters depend upon internal and external variables and are computed as parameter functions, considered constant for a specific system. For example, hydraulic conductivity depends upon water content in a supposedly reproducible way.

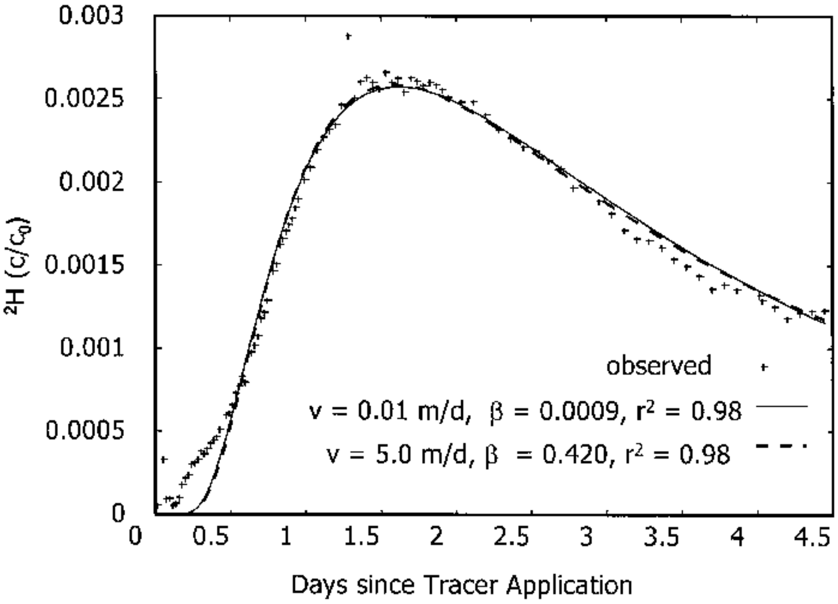

Figure 3: Breakthrough curve for a Deuterium tracer experiment, together with two different best fits to parameterize a model on soil water movement. The model visualizes the soil as a column containing mobile and immobile fractions of water; ß is the ratio of water contents of the two fractions and v convection velocity. The two (!) degrees of freedom are already too much for a unique solution (from Lange 1998).

Spatial structure is a focal issue in the environmental sciences (De Boer 1992, Jarvis 1995, O'Neill *et al.* 1989, Risser & Box 1987, Wiens 1989), as in ecosystems processes in a hierarchy of spatial scales interact shaping a highly heterogeneous medium. The interaction of scale and structure is even more problematic than the non-linearity of the processes. Due to the spatial heterogeneity of ecosystems on all scales, spatial structure is unknowable at any scales of real interest (Beven 1996). In terrestrial ecosystems, virtually all parameters like the conductance parameters or temperature are spatially distributed. Typical examples are hydraulic conductivities or temperature. For modeling purposes, a spatially distributed parameter function has to be computed, which is an arbitrarily distributed continuos-valued function. It is neither constrained by theory (*e.g.* first principles) nor by *a priori* fixation and it is only loosely restricted by measurement due to variability. The parameter function thus offers enough degrees of freedom to be fitted to any data set, as demonstrated by Fig. 3. Fitted parameters may allow for adequate reproduction of data, though saying little about the 'correct' value of the parameter and leaving the issue of parameter identifiability open (Hornung 1996). Non-identifiability of parameters is a major shortcoming of environmental models.

3.3 Variables and degrees of freedom

In a dynamical system, the variables are defined in advance, staking out the phase space of the system. Ecosystems are (stochastic) systems with an infinite number of variables and hence an infinite-dimensional phase space (Lange 1998). To represent a domain of phenomena, the 'relevant' variables have to be chosen for the dynamical system. However, there are only subjective criteria of which set of variables is necessary, which set is sufficient, and which parts of a set are superfluous to represent a certain domain. Table 1 describes the different organic matter pools and their parameterization for a specific site used in three simulation models of nitrogen dynamics. The choice of number, size, and kinetic coefficients of the organic pools is "obviously arbitrary" (Richter & Benbi 1996).

3.4 Initialization

In the initialization step, initial values are attributed to the state variables of the system, making the initial state of the system explicit. Due to ecosystem heterogeneity and measurement problems, the actual initial value of a variable can not be assessed. Thus initial values are approximated or chosen arbitrarily, assuming that the system has a short memory and is not sensitive to initial conditions.

Table 1: Characteristics of the different organic matter pools distinguished in three simulation models for agricultural nitrogen dynamics. Parameterization is for a specific site in Denmark (adapted from Vereecken et al. 1991).

Model	Pool	C/N ratio	% of organic C	Half life time
SWATNIT	Litter	8	8-1	693 d
	Manure	10	+/- 1	693 d
	Humus	12	92 – 99	189 y
DAISY	Biomass Pool 1	6	0.28	693 d
	Biomass Pool 2	10	0.04	49.5 d
	Soil Organic Pool 1	11	+/- 80	515 y
	Soil Organic Pool 2	11	+/- 20	10 y
AMINO	Humus	16	99.2	50 y
	Fraction 2	12	< 0.5	77 d
	Fraction 3	58	<0.5	3 y
	Fraction 4	76	0.5	130 d
	Fraction 5	76	<0.5	37 d
	Fraction 6	24	<0.5	65 d
	Fraction 7	24	<0.5	590 d

3.5 Boundary conditions and external driving variables

Ecosystems are open systems that do not sustain a boundary of their own. Thus, ecosystems and their boundaries are defined arbitrarily, *i.e.* any biotic-abiotic system of interaction can be envisaged as an ecosystem. The choice of boundaries and boundary conditions determines external variables and internal system variables. However, in the practice of field investigation, the precise location of even the analytically defined boundaries is unknown and the assessment of boundary conditions remains vague (Hoffmann 1997).

Ecosystem boundaries are usually chosen in such a way that physical factors, *e.g.* weather and climate, become external variables of the system. The external driving variables are assumed to be independent of the respective ecosystem, *i.e.* there is no feedback. They presumably propel the ecosystem which, encoded as a dynamical system, reacts to the external variables in a determinate way.

Future weather and climate conditions can not be known *a priori*, therefore in practice, weather records from the past are used to compute short-term behavior (Addiscott 1993). However, past weather records may be unrepresentative of the full range of natural driving forces (Konikow & Bredehoeft 1992). Particularly when driving forces themselves are subject to major changes (*e.g.* global climate change) the ‘information content’ of weather records is invalidated.

3.6 Calibration

Calibration is the attempt to find the best accordance between computed and observed data by the variation of some selected parameters (Joergensen 1992, p. 68). However, due to the non-identifiability of parameters and to overparameterization, calibration is a ‘fitting exercise’. Therefore, it is an open question whether it assures predictive capacity and whether it contributes to understanding (see below).

4. Selforganization and self-modifying systems

Dynamical systems theory has inspired the paradigmatic shift from external organization to self-organization in the empirical sciences (Kratky & Wallner 1990). In ecology and ecosystem theory, the paradigm of self-organization is gaining influence (*e.g.* Kauffman 1993, Müller 1997). Self-organization can be envisaged as an irreversible process leading to complex structures of the system through the cooperative action of subsystems. Several concepts of self-organization have emerged, *e.g.* cybernetics, autopoiesis (Maturana & Varela 1980), molecular self-organization (Eigen & Schuster 1979), and synergetics (Haken 1990). In most of these concepts, self-organization is viewed as a cyclic, recursive process from an exo-perspective. For example an autopoietic machine is defined as "a machine organized as a network of processes of production of components that produces the components which realize the network of processes that produced them" (Maturana & Varela 1980, p. 78). Cyclic self-organization in which components produce identical or essentially similar components can in principle be represented by non-linear dynamical systems. In contrast to this cyclic conception, *original* self-organization can be visualized by a spiral shifting away from its original position in an adaptive evolutionary process. Original self-organization can be represented by the notion of self-modifying component systems, in which the focus is on incessant (self-)modification. Component systems have the following properties (Kampis 1992b):

- The set of the different types of the components of the system is open-ended.
- The system produces and destroys its own components during its typical activities.

Due to the production, destruction, and *de novo* interaction of components, these systems constantly produce new variables, leading to internal novelty. Sources of internal novelty may be the following (Kampis 1994):

- Neglected or ‘frozen’ lower level variables
- New interactions with the environment
- New contexts
- Change of material properties

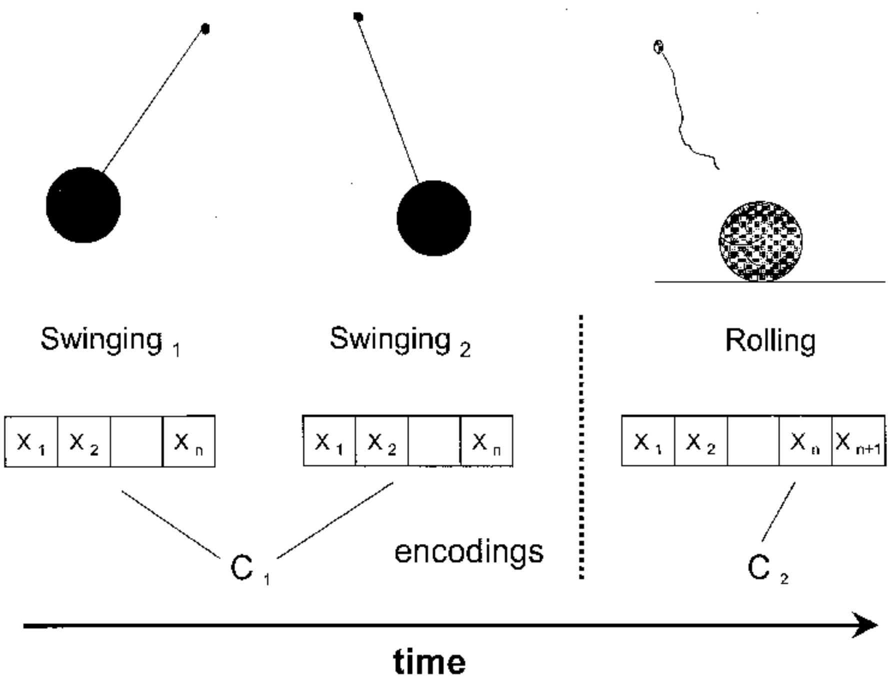

Figure 4: Encoding of a dynamical system, taking the pendulum as an example. The set of variables (= encoding) on the left side represents the swinging of the pendulum. However, this encoding is not able to

account for new variables of motion that keep coming up in the course of time (see the right sight of the figure). New variables thus invalidate old encodings and the system becomes unpredictable (adapted from Kampis 1994).

Take a pendulum as an example (Fig. 4): It is encoded as a ‘typical’ pendulum swinging back and forth, yet in the course of time new variables of motion keep coming up. Adepts of real-structure models claim that such a model "would be able to predict what would happen if the pendulum were stopped" (Bossel 1992). The prediction is only possible though, if the potentiality of a stoppage is incorporated *a priori* into the encoding, *i.e.* if it is accounted for in the reading frame. However, systems pick up information on-line and there is an unlimited supply of things we do not take into account in a given model (Kampis 1992a), so that it is impossible to map all the relevant properties of the components in advance. Newly produced variables are definable only *a posteriori*.

The validity of the respective set determines the validity of the prediction of system behavior. The encoding of the system in a determined frame of description as in the case of dynamical systems cannot account for the complexity of temporal production of variables (Kampis 1994), which successively invalidates the set. The time frame is crucial here: While in the short run (as indicated by system times, see below) a given set may predict system behavior with a certain degree of accuracy, in the long run self-modifying systems become unpredictable. The encoded abstract system state is outdated by the production of internal novelty. As component systems are self-referential, an external point of reference is lost. The system becomes an endo-system to which an external observer has no access. On large scales, the exo-models thus break down.

The notion of time in self-organizing systems is fairly different from time in dynamical systems. External parameter time is replaced by the concept of endo-time or system time. System time is linked to the period of time a system takes before reproducing (Kümmerer 1996). Hierarchy theory assumes that natural systems can be described in the framework of a nested, constitutive hierarchy (Ahl & Allen 1996, O’Neill *et al*. 1986, Müller 1992). The different levels of organization correspond to different temporal scale levels and to different system times. Accordingly, system times vary from minutes/days (*e.g.* chemical reactions in soil; molecular level) to months/years (*e.g.* population dynamics; nutrient cycles) and decades/centuries (*e.g.* ecosystems, landscapes, global system) (Ulrich 1993). Symmetry breaking in self-organizing systems (Prigogine *et al*. 1969) entails irreversibility and the notion of structurally determined systems that depend upon their history.

The paradigm of self-modifying systems is non-classical, as these systems are:

- Non-determined: In open systems ‘properties’, ‘states’ and ‘objects’ are definable only *a posteriori*.
- Non-local: Objects are context- and time-dependent, are globally dissolved and thus only (*a posteriori* and) globally definable.
- Non-predictable: Internal novelty can not be handled externally, as the advent of new variables invalidates the encoding.

Table 2 contrasts the two paradigms, the exo-physical, essentialist paradigm with its notion of reversibility and the paradigm of self-organization, represented by the endo-physical concept of self-modifying systems. Within the essentialist paradigm, properties and states stand for the identity of the system and can be defined *a priori*. Causality is transparent, the ontologically conceived complexity of the system is invariable and the system is computable as properties, states and transition functions are well defined. In ecological modeling, a strong notion of essentialism is represented by the ‘base model’, which accounts for the complete input-output behavior of a real ecosystem and which is valid for all frames (Zeigler 1976).

Table 2: The classical, reversible, essentialist paradigm of dynamical systems versus self-modification as a model of original self-organization (compiled from Kampis 1994 and Paslack 1991).

	Essentialism (Reversibility)	**Self-modification (Irreversibility)**
Being-Becoming	Properties States	Relations Confluences (potentiality)
Objects	Objects locally and *a priori* definable	Objects globally and *a posteriori* definable (Objects context- and time dependent)
Causality	Transparent Strong	Opaque Weak

	Linear	Non-linear; circular
System	Dynamical systems Analytically defined Given hierarchy Closed	Growing systems Realistically defined Self-created hierarchy Open
Complexity	Constant	Variable
Environment	Environment structures system External regulation (external drivers)	Systems structure environment Internal regulation
Time	Scalar, universal parameter time (exo-time)	System time (endo-time)
Dynamics/ Development	Reversible trajectories Continuity Regularity	Irreversible Process Bifurcation Singularity
Computability	Computable	Non-computable (Set not definable in advance)

Theoretical ecologists take different positions with regard to the base model concept. While valid real-structure models are supposed to be achievable in principle (Bossel 1992, Nielsen 1992) others doubt that such representations can be achieved even for simple real ecosystems (Wissel 1989, pp. 1-7); Joergensen (1992) acknowledges that such a base model can never be fully *known*, because of the complexity of the system and the impossibility to *observe* all states. In this view, complexity is ontologically conceived and the impossibility of condensing the essence of an ecosystem into a dynamical system is attributed to practical observational and computational (and not principal) limitations.

In the paradigm of self-modification, ‘properties’ must be envisioned in a relational way as they depend on a changing material context. The notion of a system state has to be abandoned, as states require variables as expressions of the properties of the system. The identity and the definition of the system’s components is context and time-dependent and "is only revealed at the end of a process, when all confluences and relations are already known in retrospect" (Kampis 1994).

Modern natural science is based on an exo-physical conception, in which the material system under study is regarded as a sender and the observer as a receiver, collecting the signals emitted by the object. This exo-physical concept collides with the endo-physical notion of self-modifying systems, which pick up and create information on-line and for which limited internal accessibility of information is an ontologically conceived factor (Kampis 1994). In such systems, definitions become temporally changeable due to self-modification; thus, the classical concept of computability where everything has to be defined in advance ceases to work.

5. Dynamical systems as analytical tool for ‘noisy’ ecosystems?

Systems theory claims to be an interdisciplinary, universal theory, which allows for privileged access to complex phenomena (Lilienfeld 1978). Dynamical systems as formal, paradigmatic representation of complex systems play an outstanding role in a proclaimed ‘structural scientific revolution’ driven by the ‘discovery of complexity’ (see *e.g.* the title of Hedrich 1994). In the empirical sciences, the theory of dynamical systems is important regarding both the diffusion of complexity concepts and its application in natural system modeling. The mathematical theory describes the possible behavior of natural systems, only if these systems are adequately represented by systems of partial differential equations. Dynamical systems can only show the behavior prescribed by the mathematical theory, and no other behavior (Hedrich 1994, p. 30).

The theory of dynamical systems and its application in empirical sciences, like ecology and the environmental sciences, strives to fit the conception of modern natural science as laboratory science (Hoyningen-Huene 1989). In the laboratory, closed systems are constructed in which if-conditions or antecedents are prepared to produce observable effects or consequences. The corresponding notion of causality is interventionist (Janich 1992) in that intervention in a specific, controlled setting makes causal relationships appear. According to Vico’s ‘*verum factum*’ principle, truth and understanding are attributed only to systems prepared or created by humans (Hösle 1990). Following Hacking (1992), parts of our environment have to be remade laboriously into a ‘quasi-laboratory’ to reproduce laboratory phenomena. The dynamical systems approach makes use of process descriptions and of parameters established under laboratory conditions, it aims at the exclusion of ‘noise’ and tries to achieve a high degree of closure. Thus, the theory of dynamical systems attempts to work with the laboratory model and has indeed been applied successfully to allopoietic, technical systems.

Dynamical systems are *the* paradigm in the environmental sciences, both as a conceptual background and as the formal base of simulation modeling (Joergensen 1992, Richter 1994, Richter *et al*. 1996) although the transferability of system analysis and the paradigm of dynamical systems to ecosystems has been questioned in general already two decades ago (Müller 1979). For the following reasons, we consider the dynamical system paradigm inadequate for the representation of ecosystems.

Dynamical systems omit the openness constitutive of ecosystems. Closed dynamical systems run counter to the heterogeneity of ecosystems and to the practical and theoretical limitations imposed on the observation of ecosystems. We agree with the work of Oreskes *et al.* (1994) who show that ecosystem openness and the formal closeness of dynamical systems collide in three respects: First, dynamical systems require input parameters that are incompletely known (*e.g.* the distributed parameters). Secondly, they are based on continuum theory that entails a loss of information on structure and processes on finer scales (Oreskes, in press); *e.g.*, the Darcian velocity used for the differential equations is different from the actual velocity at the pore scale. Continuum is a hypothetical idealization, disregarding the discreteness of ecological entities (Breckling 1992). Thirdly, Oreskes *et al* (1994) show that they recur to additional inferences and assumptions (*e.g.* kinetic effects are usually neglected), making use of auxiliary hypotheses until the dynamical system and the corresponding simulation model fit the data. Several system structures may produce the same results; *i.e.* model results are underdetermined by the data.

A dynamical system is an abstraction in which the system is separated from its environment or background. The background is regarded as noise that is eliminated in the abstraction step as only well-defined inputs (the input vector) reach the system. Thus, the system and its input and output vector become a conceptually closed system. The notion of noise is based on a noise/non-noise difference in conjunction with the system/environment difference introduced by information theory and system analysis. Yet in ecology, there are no grounds on which noise (background) and system (abstraction from the background) could be distinguished. Ecosystems and order in ecosystems may actually be the result of ‘noise’ – thus, "noise is music to the ecologist" (Valsangiacomo 1998, p. 270). In system analysis what started out as an *ecological system* becomes a mere *system* losing its ecological trait: For ecological issues are issues in which an system-environment-*context* is structured due to the development of selective behavior of the system towards its environment. The ecological view of a system-environment-*context* implies unity (of the system-environment difference) despite difference (of system and environment) or even unity due to difference (Luhmann 1990, pp. 21f.).

The differences introduced to abstract a certain system from its context prevent re-unification and unity of context and environment. For example, reintegration of the population-community difference by the process-function difference is impossible. Correspondingly, ecosystem theory has not come up with a single example of successful reconstruction or prediction of both aspects of a given system (Lange 1998).

In dynamical systems, a *fixed* number of variables are contained. However, the assumption of a fixed number of degrees of freedom collides with the constant come and go of organisms and the generic innovation and extinction in ecosystems along time, resulting in the production of internal novelty, the change of system structure, and the creation and extinction of new variables. In our view, ecosystems have to be regarded as self-modifying component systems, for which the *a priori* definition of variables is impossible. Internal novelty and constant drift of ecosystems and their components is not ‘noise’, but it is essential for the structural coupling of an open system to its environment (Maturana & Varela 1987) and for the structuring of the system-environment context, both in the past and the future. Separation of system and context can at best give a static, momentary view of a frozen system ‘state’. Dynamical system modeling of future states assumes that the abstract state and the external parameter time account for a determinate temporal transition. However, self-modifying systems do not transit from one state with determined properties to another determinate state, but are in an incessant process of original self-organization, in which relations are continually established and lost and states are superseded by confluences. No dynamical system can account for this internal novelty and the peculiar system times of system components. For short time frames, dynamical system descriptions may retain validity. In the long run, however, the dynamical system as a reading frame becomes outdated (Kampis 1994).

The notion of reversibility underlying the dynamical system paradigm implies that any moment in time is equal and that past states can be computed from present states. The history of the system is supposed to be contained in the system structure and specific parameters. Such systems are trivial machines that are synthetically determined, analytically determinable, predictable, and independent of history, *i.e.* there is an operator relating input to output (Foerster 1998). However, the failure of simulation models is attributed precisely to the ignorance of the historical character of systems and of system memory (Lange 1998). It has been hypothesized that sequences in complex systems show non-trivial long-range correlations, entailing a considerable memory effect (Ebeling *et al*. 1995, pp. 48-50). 'Historicity' denotes the dependence of the present 'state' of a system upon its history. The notion of historicity corresponds to the notion of non-trivial machines, in which the historical record of operations influences present operations. Non-trivial machines are unpredictable and in most cases not analytically determinable (Foerster 1998). On top of that, self-modifying systems are not even synthetically determined. Temporal dynamics of self-modifying systems are characterized by symmetry breaking, irreversibility, non-linearity, bifurcations, and evolution. From (the discovery of) complexity a path is leading to history (Longo 1994).

5.1 Validation, validity and future scenarios

The conventional notion of validation distinguishes between 'operational validation' and 'conceptual validity' (Rykiel 1996). According to that view, conceptual validity tests the internal logic of a model and says little about the predictive capacities of the model. Operational validation pretends to be an "objective test on how well the model outputs fit the data" (Joergensen 1991, pp. 68f.). Operational validation thus does not imply that the internal structure of the model corresponds to actual processes, but would be the demonstration that a model possesses a satisfactory range of accuracy consistent with the intended application of the model.

However, the conventional notion fails for practical and principal reasons. Generally accepted standards for testing and validating ecosystem models are nonexistent. In contrast, current practice is characterized by vague, subjective claims that model predictions show 'acceptable' agreement with data (Kirchner *et al*. 1996). Validation procedures commonly consist in comparing modeled and measured data or the outputs of different models for the same set of input data. Biogeochemical models for agroecosystems have been validated this way, showing considerable deviation when different model outputs are compared to each other and to measured data (*e.g.* de Willigen 1991, de Willigen & Neetson 1985, Diekkrüger 1992). Aside from these practical limitations, there are more fundamental shortcomings of the validation procedures in the earth sciences that are discussed by Rastetter (1996). The basal impossibility of the verification and validation of (closed) models of (open) natural systems has been demonstrated by Oreskes *et al*. (1994).

Measured data used for model calibration and validation do not cover the range of potential conditions of system and external variables, particularly as data usually belong to short-term data sets. Accordingly, model validity is restricted to the range of conditions represented by the respective data set. When this range is surpassed, the predictive capacity of the model is in doubt and can only be confirmed *a posteriori*; *i.e.* there is no prediction.

The calibration step, in which models with a large number of non-identifiable parameters (overparameterization) are fitted to measured data, assures that models can be adapted to a given data set, irrespective of the internal structure of the model. Not only are models underdetermined by data (Oreskes *et al*. 1994), they can even become immune to data (Hauhs *et al*. 1996): eventual lack of predictive power is attributed to the 'intrinsic complexity' of the system under study, leading at best to a readjustment of the model (*e.g.* by the re-calibration of parameters or the addition of further processes). The role of simulation models as predictive tools in the environmental sciences and as instruments of decision support has been harshly criticized for the lack of validity and validation. Mac Lane (1988) speaks of the construction of massive imaginary future scenarios to provide predictions that cannot be verified by checking against objective facts. To him models are speculation without empirical check. Funtowicz and Ravetz (1992) criticize the absence of effective tests for demonstrating what sort of correspondence, if any, there is between models and reality. To them models are devoid of certainty, quality, and reality and are to be regarded as a post-modern phenomenon. In the absence of testing, models may take on an aura of reality in the minds of their *users* (Philip 1991) – a particular precarious point if models are employed as risk assessment tools.

5.2 A role for dynamical simulation models in the environmental sciences?

We claim that mechanistic simulation models of ecosystems are not suitable for predictive purposes, as they are not able to produce non-trivial predictions of future outcomes (Hauhs *et al*. 1996). While the mathematical behavior of the formal dynamical system is computable, the 'behavior' of the natural system is not. Existing data sets or empirically recognized patterns in natural systems may be reproduced by models, but this is not prediction. Non-predictability partly owes to the self-modifying character of ecosystems that cannot be represented by any dynamical system. To embrace the complexity of natural systems (Kay & Schneider 1995) means to abandon the idea of predictability.

The implications for ecological risk assessment are profound. Unpredictability of natural systems notwithstanding, there are still calls to improve the predictability of biogeochemical system behavior as part of a strategy to reduce global risks, *e.g.* to decrease the risk of nitrate leaching to the groundwater (WBGU 1999, p. 323). Nevertheless, there is growing awareness that true predictability cannot be achieved. For example, Richter (1994) states that, after repeated application, a faster decomposition of a newly produced pesticide may be explained by the adaptive evolution of the microorganisms, but it can not be predicted. The intrinsic unpredictability of ecosystems suggests following the precautionary principle in risk assessment (Westra 1997), instead of succumbing to the ecosystem engineering fallacy.

However, if dynamical simulation models are not suited for predictive purposes, what role is left to them in the environmental sciences?

We agree with Nancy Cartwright's statement that models are "a work of fiction" and that "some properties ascribed to objects in the model will be genuine properties of the object modeled, but others will be merely properties of convenience" (Cartwright 1983, p. 153). In terms of general modeling theory, the model consists of a set of attributes representing a part of the original and a set of abundant attributes without correspondence to attributes of the original (Stachowiak 1983, p. 119).

Despite not being a 'real' thing, "a model may resonate with nature" (Oreskes *et al*. 1994) and thus has heuristic value, particular to guide further study. Corresponding to the heuristic function, Joergensen (1995) claims that models can be employed to reveal ecosystem properties and to examine different ecological theories. Models can be asked scientific questions about properties. According to Joergensen (1994), examples for ecosystem properties found by the use of models as synthesizing tools are the significance of indirect effects, the existence of a hierarchy, and the 'soft' character of ecosystems. However, we agree with Oreskes *et al*. (1994) who regard models as "most useful when they are used to challenge existing formulations rather than to validate or verify them". Models, as 'sets of hypotheses', may reveal deficiencies in hypotheses and the way biogeochemical systems are observed. Moreover, models frequently identify lacunae in observations and places where data are missing (Yaalon 1994).

As an instrument of synthesis (Rastetter 1996), models are invaluable. They are a good way to summarize an individual research project (Yaalon 1994) and they are capable of holding together multidisciplinary knowledge and perspectives on complex systems (Patten 1994).

While models as a product may have heuristic value, we would like to emphasize also the role of the modeling process: "[…] one of the most valuable benefits of modeling is the process itself. These benefits accrue only to participants and seem unrelated to the character of the model produced" (Patten 1994). Model building is a subjective procedure, in which every step requires judgment and decisions, making model development 'half science, half art' and a matter of experience (Hoffmann 1997, Hornung 1996). Thus modeling is a learning process in which modelers are forced to make explicit their notions about the modeled system and in which they learn how the analytically isolated components of a system can be 'glued' (Paton 1997). As modeling mostly takes place in groups, modeling and the synthesis of knowledge has to be envisaged as a dynamic communication process, in which criteria of relevance, the meaning of terms, the underlying concepts and theories, and so forth are negotiated. Model making may thus become a catalyst of interdisciplinary communication.

In the assessment of environmental risks, however, an exclusively scientific modeling process is not sufficient, as technical-scientific approaches to 'post-normal' risks are unsatisfactory (Rosa 1998) and as the predictive capacity and operational validity of models (*e.g.* for scenario computation) is in doubt. The post-normal science approach (Funtowicz & Ravetz 1991, 1992, 1993) takes account of the stakes and values involved in environmental decision making. Following a 'post-normal' agenda, model development and model validation for risk assessment should become a trans-scientific (communication) task, in which "extended peer communities" participate and in which non-equivalent descriptions of complex systems are made explicit, negotiated, and synthesized. In current modeling practice, however, models are highly opaque and can rarely be penetrated even by other scientists (Oreskes, personal communication). As objects of communication, models still are closed systems and black boxes.

6. Conclusion

The dynamical system paradigm remains within the limits of an exo-physically conceived systems theory which is based on conceptually closed systems and which claims that essential, systemic properties arise from the particular configuration of system components. To achieve closure of dynamical systems, the structure and processes of biogeochemical systems are idealized or simplified, disregarding spatial and temporal variability. Criteria for the identification of essential components, processes, and parameters and for their adequate combination in dynamical systems are lacking. Thus, the choice of 'relevant' processes and parameters and the fabrication of system structure are highly subjective. Owing to the impossibility of model validation, models run the risk of losing contact to the empirical 'reality' they refer to.

In biogeochemical systems, the interplay of biological components with their geochemical environment play a crucial role in the processing of chemical substances. As to this interaction, the paradigm of dynamical systems represents only a halfway discovery of complexity. In our view, the closed encoding of ecosystems as dynamical systems runs counter to the self-modifying character of ecosystems as a result of their singular history in a singular context. As nonstationary systems (self-modification) in a nonstationary context (history), 'complex natural systems' are unpredictable.

While in the environmental sciences a representationalistic notion of dynamical system models as the product of scientific endeavor prevails, we emphasize the importance of the modeling process. Modeling can be a way of coping with different types of complexity: the complexity of integrating and synthesizing (reductionist) statements and of gluing analytically isolated components; the descriptive complexity that allows for numerous, non-equivalent system descriptions, depending upon standpoint; the communicative complexity, both inter- and trans-scientific, arising from nonequivalent descriptions of complex systems. Modeling can be a means of reduction of complexity as it is realizing *one* arrangement (or agreement) amongst innumerous contingent arrangements.

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