INSTABILITIES AND PATTERN FORMATION IN SIMPLE ECOSYSTEM MODELS

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Introduction

Models of chemical and biological processes in the pelagic as well as in the benthic part of the Wadden Sea are very complex and highly nonlinear. As known for a long time nonlinearities can give rise to sudden changes in the behaviour of a system (GUCKENHEIMER & HOLMES, 2002; OTT, 1997). Such changes are caused by instabilities which can occur if environmental parameters cross certain threshold values (bifurcations). From an ecological point of view such instabilities may endanger the ecosystem since the new state of the ecosystem after the bifurcation can be characterised by different properties, i. e. a different composition of the species community. Moreover, nonlinear systems can exhibit different states for a given set of parameters. This phenomenon is called multistability. If several different states coexist then it crucially depends on the initial conditions which of these states is finally realised.

The aim of our studies is to analyse the stability properties of simplified models for particular processes in the pelagial and in benthos. Our main goal is twofold: On the one hand we try to identify threshold values for the parameters which correspond to *instabilities* leading to a new kind of system behaviour. On the other hand our studies shall contribute to the understanding of the underlying mechanisms of possible instabilities in ecosystems. In particular we study models for food chains in the pelagic system and a minimal model for the interaction of nutrient and bacteria in the sediment. The first model class in the pelagial consists of ordinary differential equations, that means we assume a well mixed system. Therefore, the transitions from one behaviour to another one are always assumed to be homogeneous in space. In the sediment we have to deal with partial differential equations, thus the investigation is focussed on the interaction of biological growth processes and physical transport processes. In this part of the work we are mainly interested in the formation of spatially inhomogeneous distributions of nutrients and microorganisms depending on depth in the sediment. Before we present the results of our analysis of models describing key processes in the pelagic and in the benthic system, we give a short survey of the transitions which may occur in ecological systems. Furthermore, we introduce some of the methods we have developed to study transition phenomena in different systems.

Qualitative analysis of nonlinear dynamical systems

The time evolution of natural systems is characterized by a large variety of different long-term behaviours. In general the dynamics can be stationary, periodic, quasiperiodic or chaotic. If environmental parameters (such as nutrient input, temperature) are varied, sudden discontinuous transitions in the long-term behaviour can occur. These transitions, which are called bifurcations, can happen when a system's parameter crosses a certain threshold value. Bifurcations are related to an instability of a certain long-term behaviour and leads to another one. Depending on the nature of the transitions one can distinguish between different types of bifurcations. Our investigation of different simple models describing key processes in the pelagic as well as in the benthic system reveals only a few bifurcations. Therefore, we discuss only those bifurcation situations needed to understand the dynamics of the models considered here.

In our models we are only interested in regular behaviour, i. e. stationary states and periodic motions and their corresponding bifurcations. This means that we consider equilibrium states for food chains or periodic changes in the abundances of chemical substances and organisms. Equilibrium states are in general computed by setting the derivatives in the differential equations to zero and solving a nonlinear equation system. For periodic motions one has to use a specific technique, the Poincaré map, for computation. To find out threshold phenomena for a system one has to look at the stability of the equilibrium state or periodic solution with respect to small perturbations. If all perturbations die out after some time, the state of the system is stable and called attractor. If there is at least one perturbation which leads to another state, this state is unstable and called repellor or saddle. Mathematically this can be checked by computing the eigenvalues of the corresponding Jacobian matrix. The signs of the eigenvalues determine the stability properties. Since the eigenvalues smoothly depend on the parameters of the system, the variation of the parameters can lead to changes in the signs of the eigenvalues. These changes indicate the bifurcations we are looking for.

Let us discuss the relevant bifurcation situations for our food chain models in detail. First of all there can be a transition from one stationary state to another one. Such a situation can occur if a new steady state (or more precisely two steady states, one stable and one unstable) arises. This happens in a *turning point* and corresponds to a crossing of the imaginary axis for one real eigenvalue. In biological terms this could mean, that before the bifurcation there is only one stable state, where the organisms are extinct, after the bifurcation there exists a stable state in which all population densities have a certain nonzero value.

Another situation is the exchange of stability of two different steady states corresponding to two different abundances of species. This could be a transition from one composition of an ecosystem to another one. Mathematically this again corresponds to a change in sign for one real eigenvalue and is called *transcritical bifurcation*.

The *Hopf bifurcation* of a stable steady state is reflected by a transition between stationary and periodic behaviour in the long-term limit. In this situation a pair of complex conjugate eigenvalues of the Jacobian crosses the imaginary axis. If the system was in a stable steady state before the bifurcation, the steady state loses it's stability at the bifurcation point. As a result a stable or unstable limit cycle emerges or vanishes in the Hopf bifurcation. Biologically speaking this would correspond to a transition from stationary abundances to periodic ones.

In the minimal sediment model which will be discussed in detail below we find the bifurcations mentioned above in the case when we neglect the transport through the sediment and concentrate on the local dynamics between nutrients and microorganisms. Without transport we find a homogeneous distribution of nutrients and microorganisms in space. To study pattern formation processes it is common to first look for the transition from homogeneous distributions to inhomogeneous ones. In spatially extended systems there are several possibilities of how patterns can arise. In our minimal sediment model we focus on the interplay of nonlinear reactions (growth processes of the microorganisms) and diffusion. We can show that inhomogeneous distributions can emerge due to the diffusion instability. There are two main conditions which have to be fulfilled for the instability to occur: Firstly, the growth of microorganisms should have an autocatalytic character and, secondly, nutrients and microorganisms should have very different diffusion coefficients. In such a situation inhomogeneous distributions of nutrients and microorganisms can occur without any external forcing.

Analytical search for bifurcations

To locate the bifurcations of a given system in parameter

space is one of the main tasks of qualitative analysis. Whereas several software packages for convenient computation of bifurcations exist these are only capable of calculating bifurcations as a function of up to two parameters. However, we are interested in the whole parameter space. Therefore, we have implemented an analytical approach yielding the bifurcation as a function of all system parameters. Direct analytical computation of the eigenvalues is only possible for small systems with a number of variables, say i. e. interacting species, up to N=4. However, the knowledge of all eigenvalues is not always necessary for bifurcation detection, thus we developed a method based on the determinant of the Jacobian. The determinant of the Jacobian can act as a test function for some of the bifurcations mentioned above. Checking for a vanishing determinant is in general much easier than the factorisation of the Jacobian characteristic polynomial and is possible for systems of any size. The method we use is based on resultants (GUCKENHEIMER *et al*., 1997). The basic idea of this method is that the symmetry of the eigenvalues may be used to split the characteristic polynomial of the Jacobian matrix into two coupled polynomials. The method we developed to study food chains and other ecological models is not only applicable to Hopf bifurcation points, but it is much more general and may also be used to compute other interesting bifurcation situations, like real Hopf, Takens-Bogdanov, Gavrilov-Guckenheimer and double Hopf bifurcations (GROSS & FEUDEL, 2003).

On the impact of interaction functions on food chain stability (with W. Ebenhöh)

Since the pioneering work of LOTKA (1925) and VOLTERRA (1926) many models of ecological food chains have been proposed (see DEANGELIS, 1992). In a constant environment most model systems approach a steady state in which the species coexist in equilibrium. But when environmental parameters are varied, bifurcations like the ones explained above can be expected to occur in almost all food chain models (EDWARDS & BRINDLEY, 1996; GRAGNANI *et al*., 1998; BUSENBERG *et al*., 1990; BOER *et al*., 1998).

A central assumption of ecosystem modelling is that the interaction of species or functional groups can be adequately described by simple mathematical equations. For instance, in a food chain model one will generally assume the rate of predation to be some simple function (e. g. Lotka-Volterra, Holling, Ivlev) of the densities of prey and predator. However, in nature the interaction of species is more complex. Because of adaptation the interaction functions will not only depend on the current state, but also on the history of the system. Even if adaptation processes can be ignored we cannot expect to find a single interaction which will obey any mathematical function exactly. It is therefore commonly assumed that the behaviour of the system does not depend strongly on the exact functional form of the interaction. If this is true minor inaccuracies in the interaction functions will not alter the model dynamics qualitatively. Here, we present a simple, but very general food chain model. We investigate the dynamics of this model without assuming any specific functional form of predator-prey interaction. In this way the impact of different forms of interaction on the dynamics can be seen most clearly.

A general food chain model

To study the stability properties of food chains as important parts of ecosystem models we formulate a conceptual food chain model. The aim of this model is to describe a general food chain with as few parameters as possible. General, easily interpretable parameters are preferred over specific ones for which interpretation can be complicated. The main advantage of the model is that its stability can be analysed without having to specify the interaction functions in any way. We are most interested in such bifurcations in which the initial loss of steady state stability occurs.

We consider a food chain consisting of N active trophic levels. Depending on the system under consideration a level of the food chain may describe one species or a functional group of similar species. Likewise, we use X_n to denote the biomass density or the abundance in level n. The species on level n are assumed to prey solely on species on the immediately lower level n-1. Furthermore, we assume that the biomass loss due to predation in level n-1 is proportional to X_n whereas it is some function G_{n-1} of X_{n-1}. Only a fraction η_n of the biomass flow is converted to predator biomass. Taking these factors into account we obtain a set of N ordinary differential equations (ODEs)

$$dX_n/dt=\eta_n G_{n-1}(X_{n-1})X_n-G_n(X_n)X_{n+1} \qquad n=1\ldots N.$$

In these equations two additional variables X_0 and X_{N+1} appear. The abundance of the nutrient X_0 should be given in terms of an algebraic equation, which we assume to depend only on X_1. By doing so we assume that the dynamics of the nutrient is sufficiently fast. However, this restriction could be easily lifted by setting $X_0=1$ and considering X_1 as the nutrient.

The variable X_{N+1} may be interpreted as the abundance of a super predator. In reality the super predator may be an actual predator of even higher trophic level. Likewise, it may be used to describe any other cause of biomass loss in the top predator population, like natural mortality, disease or cannibalism. We do not model the super predator dynamics explicitly but assume that it inflicts a linear mortality (linear closure) on the top predator

$$G_N(X_N)X_{N+1} \square X_N.$$

Our model contains N interaction functions $G_0 \ldots G_{N-1}$. We will not restrict these functions to any specific functional form, but demand that they are smooth and positive for positive X_n. In this case the model has at least one positive steady state $X_1^*,\ldots, X_N^*$. We define the normalized abundances by

$$x_n:=X_n/X_n^* \qquad n=1\ldots N.$$

Furthermore we define normalized interaction functions

$$g_n(x_n):=G_n(X_n)/G_n(X_n^*)=G_n(X_n^*x_n)/G_n(X_n^*)\} \qquad n=0\ldots N\text{-}1.$$

After normalization we end up with a general food chain model in the form

$$dx_n/dt=\alpha_n(g_{n-1}(x_{n-1})x_n-g_n(x_n)x_{n+1}) \quad n=1\ldots N,$$

where the parameters α depend on the interaction functions in the steady state. The sensitivity of the predator with respect to the abundance of prey is described by

$$\gamma_n:= \partial g_n(x_n)/\partial x_n \mid x=x^*,$$

whereas the sensitivity of the lowest trophic level with respect to nutrient supply is given by

$$h:=-(\partial x_0/\partial x_1)(\partial g_0(x_0)/\partial x_0)g_0(x_0) \mid x=x^*.$$

In order to compare food chains of different length it is desirable to make the number of parameters independent of the length of the food chain. We achieve this by making two more assumptions. First, an alometric slowing-down is observed in most food chains. That is, the dynamics on every level of the food chain is r times as fast as the dynamics on the immediately lower level. We model this quite universal behaviour by assuming

$$\alpha_n=r^{n-1} \qquad n=1...N, \text{ with } 0 < r \leq 1.$$

In the given normalization interactions between similar species should produce similar values of γ_n. Therefore the values of $\gamma_1 \ldots \gamma_{N-1}$ may be assumed to be identical. We define

$$\Gamma := \gamma_1 = \ldots = \gamma_{N-1}$$

Using these definitions general food chains of arbitrary length can be studied in terms of the parameters r, h and Γ.

Of our assumptions about the values of $\gamma_1 \ldots \gamma_{N-1}$ is clearly the strongest one. However, this assumption is only needed to avoid having too many parameters, which would make presentation of the results difficult. Our conclusions will not depend strongly on the assumption. In the general case we would have different $\gamma_1 \ldots \gamma_{N-1}$. The analysis outlined below can be applied to each of these individually.

Bifurcations of general food chains

This general model is well suited to analyse the primary loss of stability of the steady state. The point in which this loss of stability occurs (and the system's natural mode of existence breaks down) will in general be a Hopf bifurcation.

We have studied the bifurcation structure of two-, three- and up to six-level food chains. The results are presented in bifurcation diagrams in the three-dimensional parameter space spanned by the parameters r, h and Γ. Every point in the three dimensional space of the diagram corresponds to a food chain with specific parameter values. Most of these food chains exhibit qualitatively similar dynamics, whereas food chains with qualitatively different dynamics are separated by bifurcations.

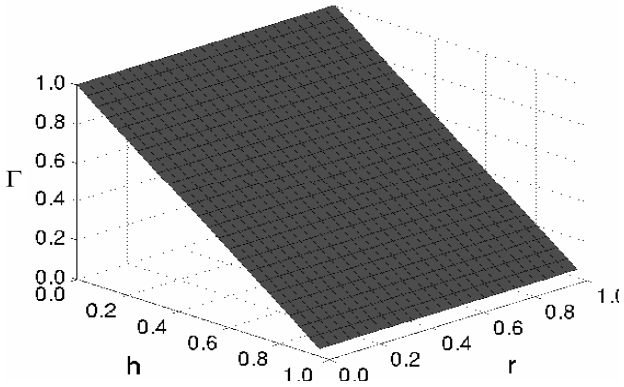

Fig. 1. Bifurcation diagram of the di-trophic food chain with linear closure. The Hopf bifurcation (grey surface) divides volumes of different dynamics. The steady state is stable above the surface.

In case of the di-trophic food chain (Fig. 1) there is only one bifurcation affecting the stability of the steady state. This is a Hopf bifurcation which is shown in the diagram as a grey surface. The bifurcation surface divides the parameter space into two volumes. All parameter combinations found in the top volume correspond to food chains in which the normalized steady state is stable. If we move through the diagram by varying parameter values, the steady state will remain stable until the Hopf bifurcation surface is crossed. It will then become unstable and will remain so in the entire lower volume. Since the stability of the steady state is lost, the system will now approach some other attractor. This new attractor will probably be a limit cycle. However the exact nature and the bifurcations of this attractor cannot be determined with the chosen degree of generality.

The bifurcation diagrams of a food chain of length four is shown in Fig. 2. This diagram contains even more bifurcation surfaces. In fact, the number of Hopf bifurcations equals the food chain length divided by two (rounded down). A transcritical bifurcation is additionally present in all food chains of odd length. Like in the case of shorter food chains, the normalized steady state is only stable above all surfaces. In any case the steady state can be stabilised by making the predators sufficiently sensitive to prey density (high Γ). Likewise, high values of h (which will usually occur in oligotrophic systems) have a stabilizing effect.

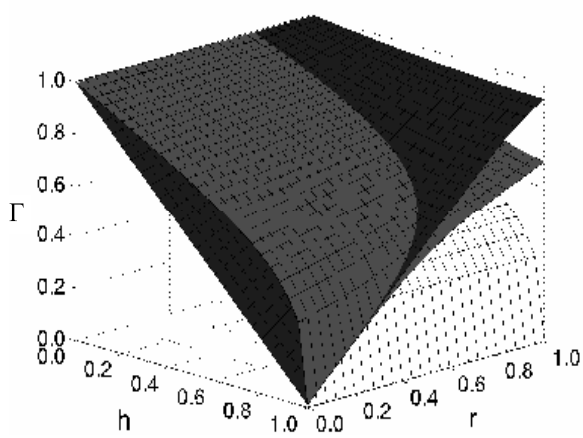

Fig. 2. Bifurcation diagram of the four-trophic food chain. The steady state stability is lost by crossing one of the two Hopf bifurcation surfaces.

However, unlike Γ setting h=1 is not always sufficient to stabilise the steady state. The stabilising effect of h is more pronounced if r is small, i. e. if separation of predator and prey timescales is large. Generally, similar timescales ($r \approx 1$) lead to instability.

Functional forms of interaction functions

The investigation of specific models has revealed that there are some features which almost all models share. For instance, it was first realized by ROSENZWEIG (1971) that increasing supply of nutrients or prey tends to destabilize simple food chains models. This “Paradox of Enrichment” is widely believed to occur in simple models independently of the exact shape of the interaction function. However, in nature the Paradox of Enrichment has rarely been verified (MORIN & LAWLER, 1995). The destabilizing effect of enrichment has been observed in some experiments (LUCKINBILL, 1974; TILMAN & WEDIN, 1991). However, in other experiments enrichment had no effect (CAULEY & MURDOCH, 1990), or even stabilised food chain dynamics (KIRK, 1998).

In the previous section we have shown that high Γ is always beneficial. This is reasonable since high Γ indicates that the predators are very sensitive to the abundance of their prey. The stabilizing effect of increased sensitivity to prey density is very general and can be expected to be found in almost all ecosystems. For instance, SAUNDERS & BAZIN (1974) derived a condition that guarantees stability of a steady state in a simple chemostat model. This condition may be written as $\Gamma>1$. It is therefore reasonable to use Γ to measure the *interactive stability*, i. e. the stability of the predator-prey interaction induced by the predator's sensitivity to prey density. We have studied the dependence of Γ for different interaction functions and present here the results for the well-known Holling type II function and another function which looks similar in shape (see Fig. 3) but exhibits different stability properties. Whereas Γ is decreasing for increasing χ ($\chi := X^*/K$ with K half saturation constant), the second interaction function shows much more complex behaviour. For Holling type II functions we obtain the result that enrichment has always a destabilizing effect on the food chain. However, although the interaction functions G(X) are similar in shape the stability functions $\Gamma(\chi)$ differ dramatically. For our newly

proposed interaction function we find a large interval in which $\Gamma(\chi)$ increases with increasing χ. In this interval enrichment has a stabilizing effect.

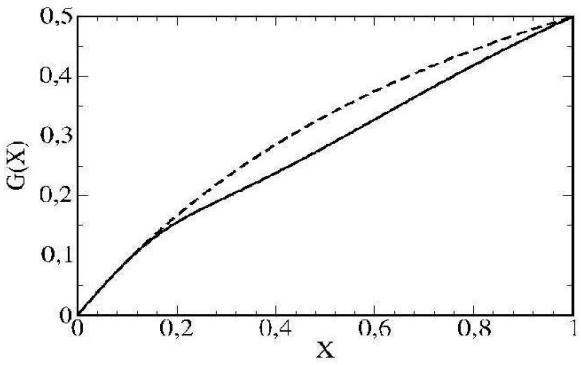

Fig. 3. A proposed interaction function (solid line) in comparison with the Holling type II function (dashed line). It is hard to decide which function is better suited to describe predator-prey interaction in any given system.

In general we find that all commonly used interaction functions behave in a similar way. The stability of equilibria decreases monotonously as prey density is increased. However, our general food chain model shows that the Paradox of Enrichment will not occur in any food chain model. Although we find a Paradox of Enrichment for all commonly used interaction functions, but even minor modifications in the functional form may introduce new types of behaviour. In general, it is true that very low prey concentrations will to some extend have a stabilising effect while very high prey concentrations may be destabilising. In the intermediate region we may have intervals in which enrichment is stabilising as well as intervals in which enrichment is destabilising. Here, the actual behaviour depends strongly on the exact form of the interaction function.

Complex ecosystem models are used to make prediction on the future behaviour of natural systems. Since stability is crucial for the survival of an ecosystem, realistic ecosystem models should be built to mimic the stability properties of the natural systems as closely as possible. Therefore, the most realistic functions should be used. In order to find these functions attempts should be made to measure interaction functions in experiments.

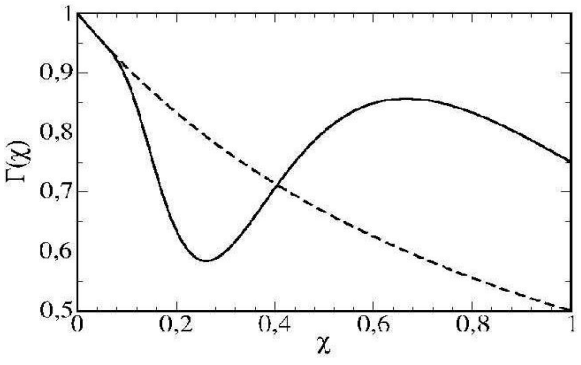

Fig. 4. Comparison of the stability functions corresponding to the proposed interaction function (solid line) and Holling type II (dashed line). The plot reveals the qualitative differences of the stability functions.

Diffusion-Induced pattern formation in a minimal sediment model

The degradation of chemical substances in sediment is proceeded by a complex network of interacting populations of microorganisms (VANCAPPELLEN & WANG, 1996; HUNTER *et al*., 1997). To study the emergence of spatial patterns in the sediment, we restrict ourselves to one bacteria population and analyse a part of the relevant processes. In particular we focus on the interaction between degradation and transport processes in a model, we refer to as the *minimal sediment model* or *MS-model*.

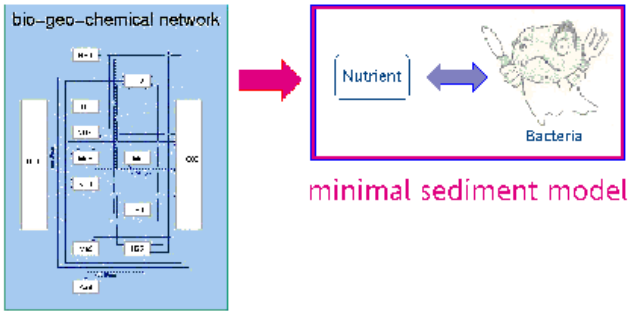

Fig. 5. Instead of the complex network of bio-geo-chemical interactions, we consider a minimal sediment model.

Pattern formation phenomena in reaction-diffusion systems of similar kind to that used for the MS-model have been a central issue to modellers since the fundamental paper of TURING (1952). He showed, that due to the effects of diffusion homogeneous distributions in chemical systems can loose their stability with respect to perturbations. This phenomenon, referred to as *Turing-instability,* was proven to be significant for certain chemical reactions, which were considered as important examples for a group of systems showing complex dynamics (NICOLIS & PRIGOGINE, 1977; NICOLIS, 1995). In the last years also other processes were analysed with regard to their influence on pattern formation: In particular, the research focuses on advection (ROVINSKY *et al*., 1994; KUZNETSOV *et al*., 1997; SATNOIANU *et al*., 1998; SATNOIANU *et al*., 2001) and non-normal diffusion (HENRY & WEARNE, 2002).

In ecological sciences it was found that pattern formation phenomena can be observed in predator-prey systems, which are interacting with transport processes. Several models show Turing instabilities (MURRAY, 1993; KUANG & BERETTA, 1998; ALONSO *et al*., 2002) or other complex dynamics, which destabilises homogeneous distributions (KLAUSMEIER, 1999).

Since profiles of chemicals and/or microorganisms found in natural systems can also show complex structures (MUDRYK *et al*., 2000), we present the MS-model as a very simple system, which shows pattern formation phenomena.

The minimal sediment model

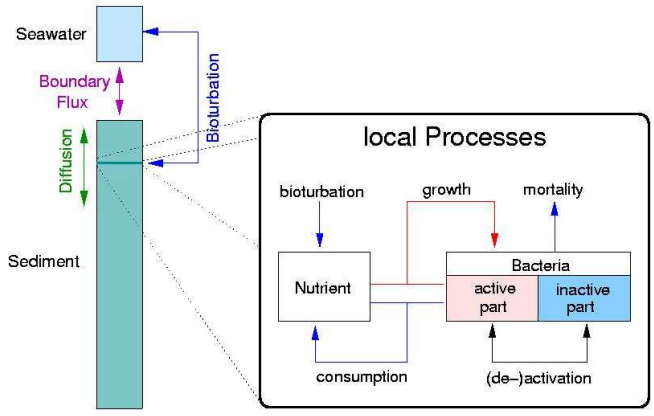

Fig. 6. In the minimal sediment model we consider spatial and local processes.

We employ the MS-model on a vertical one-dimensional domain considering the processes shown in Fig. 6. Thus, the

temporal changes of the population of microorganisms and its nutrient are governed by the partial differential equations:

$$\frac{\partial X}{\partial t} = \underbrace{\frac{X}{X+K}XY}_{\text{degradation}} - \underbrace{mX}_{\text{mortality}} + \underbrace{D_X \frac{\partial^2 X}{\partial z^2}}_{\text{diffusion}}$$

$$\frac{\partial Y}{\partial t} = \underbrace{\Phi \exp(-az)\left(Y_0 - Y\right)}_{\text{bioturbation}} - \underbrace{\frac{X}{X+K}XY}_{\text{degradation}} + \underbrace{D_Y \frac{\partial^2 Y}{\partial z^2}}_{\text{diffusion}}$$

The (dimensionless) balance equations for the variables X (bacteria) and Y (nutrient) consist of the contributions stemming from different processes: Degradation, bio-turbation, loss of bacteria and diffusion. We use the dimensionless parameters: m = 'mortality' rate of bacteria, K = half saturation constant, Y_0 = concentration of nutrient in the seawater, D_X and D_Y = diffusion coefficients of X and Y, respectively. The space coordinate is z, time is denoted by t.

Additional to the equations boundary conditions have to be specified. We generally employ no-flux conditions at the boundaries, except at the upper one, at which we allow for a flux of nutrient into the system.

The dynamics of the local model

In a first step we study the dynamical properties of the local model. To this end we neglect the effects of diffusion and set a=0 in the bioturbation term, so that it is independent of the spatial variable z. Since the local model is proposed to be valid in some inner point of the domain, boundary conditions are neglected.

The dynamics of the spatial model

The spatial model is given by the complete equations. To study the system we firstly consider a simple case, in which the bioturbation is spatially constant and diffusion fluxes occur. Also, boundary fluxes shall be neglected. This case is very similar to the local one and (if we restrain to continuous profiles) we will obtain analogous equilibrium states: Constant profiles taking the values of E0, E1 or E2 over the entire domain are the only (continuous) steady states. The result, that E0 is always and E2 is under certain presumptions an attracting state, can be expanded to this spatial case.

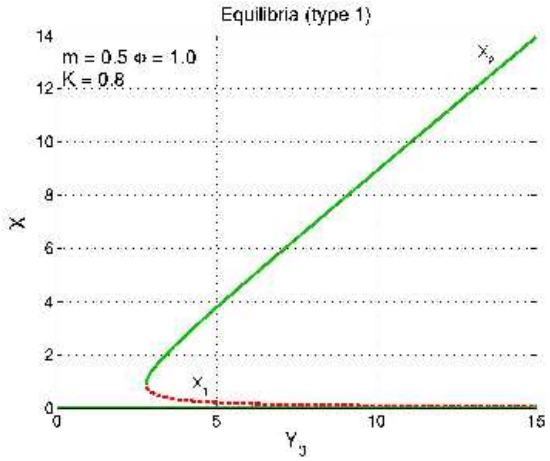

Fig. 7a. Location of equilibria [solid lines = attractors, dashed lines = repellors and saddle nodes]; diagram of type 1: E2 is always an attractor.

We find, that there always exist a trivial equilibrium state E0 = $(0,Y_0)$ at which the bacteria are extinct. Depending on the parametrisation, this steady state can be accompanied by a pair of non-trivial equilibria E1=(X_1,Y_1) and E2=(X_2,Y_2) with $0<X_1<X_2$ and $Y_2<Y_1<Y_2$. E1 is always a saddle, whereas E2 is either an attractor or a repellor. In the latter case, the stability characteristics of E2 can be changed by parameter variation: A sufficiently high increase of Y_0, for instance, will have the result that E2 will turn into an attractor. When changing its characteristics, E2 traverses a subcritical Hopf bifurcation and an unstable periodic orbit emerges (see Figs. 7a and b).

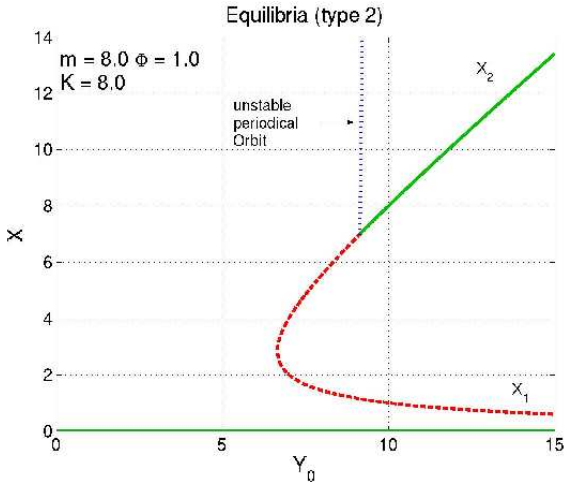

Fig. 7b. Location of equilibria [solid lines = attractors, dashed lines = repellors and saddles, dotted line = periodic points]; diagram of type 2: E2 changes from repellor to attractor, an unstable orbit of periodical points emerges.

Surprisingly, the latter is not necessarily true, if effects of diffusion come into play. In Fig. 8 we plotted the temporal behaviour of a spatial model, in which we included diffusion and took into account, that the effect of bioturbation is decreasing with increasing depth. The first time steps show a diffusion-free profile, corresponding to the E2-equilibrium (due to the non-constant bioturbation the values change slightly with depth). At time step 4 we added a very small perturbation. We observe that the perturbed profile does not return to the monotonous state, but forms a spatially oscillating pattern, instead.

The time series in Fig. 8 shows a cosinoid oscillation with wavenumber 3/2 in the long run. We typically obtain such patterns in the MS-model (cosinoid distributions with small wavenumbers), but also other time series occurred, showing stable profiles, in which one or more cosinus periods are extinct and a constant zero-profile appears (on this spatial interval), instead.

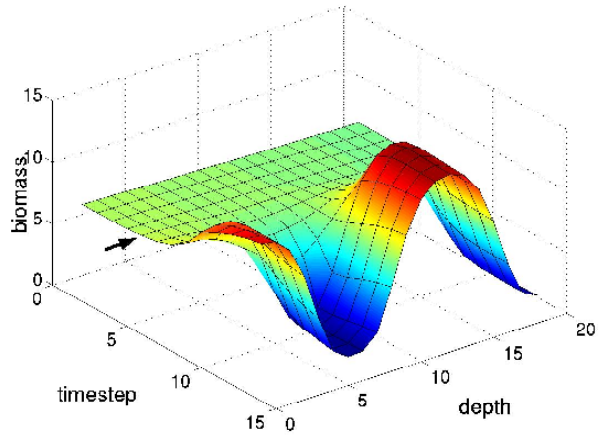

Fig. 8. Profiles of the MS-model in a time series. The diffusion-free profile looses stability, when a perturbation is added (see arrow at time step).

To summarise the appearance of different spatial equilibrium states, we show their locations (at a certain depth - we chose

the first discretisation box) in a bifurcation diagram. Figs. 9a and b show two different bifurcation diagrams: One for a case with constant bioturbation (Fig. 9a), another one for a decreasing bioturbation term (Fig. 9b). In both cases all boundary fluxes are neglected (if nutrient flows into the system from the top, the bifurcation diagram is similar to that of Fig. 9b).

Both diagrams show that at values of Dy compared to Dx the diffusion-free profile is the only non-trivial equilibrium. When this profile passes a bifurcation (characterised by wavenumber n), it becomes sensitive to oscillating perturbations of this wavenumber. Consequently, the diffusion-free distribution loses stability, when passing the first bifurcation. So a natural system, which would have similar behaviour as the MS-model (at these parameter ranges), will never produce a diffusion-free profile, since natural systems are always affected by noise.

Numerical experiments showed that instead of the diffusion-free distribution spatially oscillating patterns become attracting (compare Fig. 8). For certain parameter sets we found that it is possible that there is a coexistence of several attracting equilibria, characterised by oscillating patterns (e. g. 3/2+ and 2+ states). In this case it depends on the form of the added perturbation then, to which pattern the system will converge to.

We could show that applying a non-constant bioturbation (or a boundary-flux of nutrient), the bifurcations split up (see Fig. 9b). In this case the diffusion-free profile loses stability when passing through the first turning point, and we can observe attracting equilibria again, which show almost the same oscillating structures as those found for case 1.

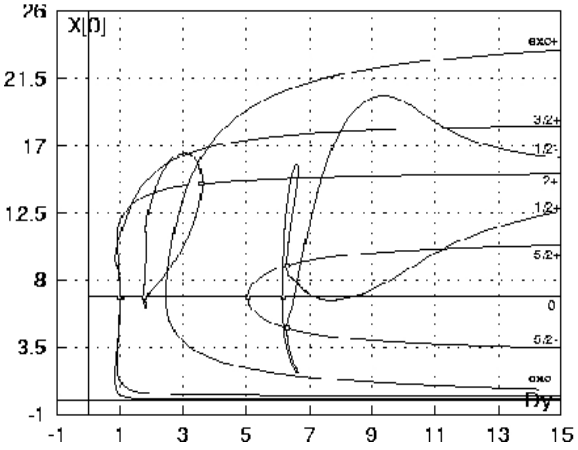

Fig. 9a. Bifurcation diagram (case 1: constant influence of bioturbation). Squares symbolise bifurcations. The branches are labelled due to the wavenumbers of the main mode of their profiles.

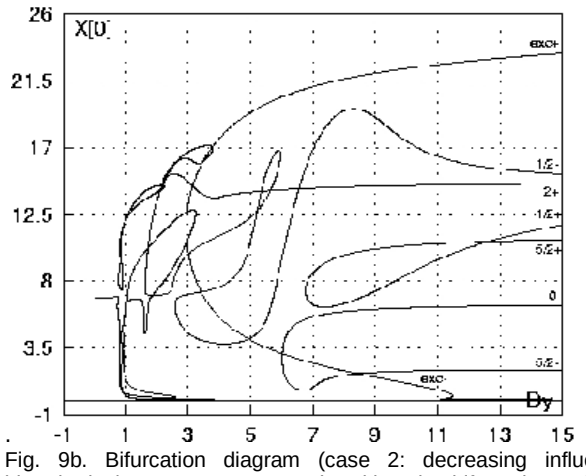

Fig. 9b. Bifurcation diagram (case 2: decreasing influence of bioturbation). Due to symmetry breaking the bifurcation points split up.

By analysing the MS-model, we found that, neglecting diffusion-terms, diffusion-free profiles are the only non-trivial equilibria. When diffusion comes into play, this property can change under certain conditions: In that cases the diffusion-free profile loses its stability and due to a diffusion instability spatial oscillating patterns become attracting instead.

The preconditions for such phenomena of pattern formation can be summarised as follows:

(1) The diffusion of nutrient is high in comparison to that of bacteria. Considering the different sizes of bacteria and nutrients and taking into account that bacteria tend to stick to the sediment matrix, this condition is reasonable.
(2) The growth of bacteria is autocatalytic. This special feature follows from the activation mechanism in the MS-model.
(3) The input of nutrient into the system is high in comparison to the loss of bacteria. This condition relates to the general finding that pattern formation only appears in open systems and requires an input of energy.

Under such conditions the emergence of inhomogeneous spatial patterns takes place without any external forcing.

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REDUCTION OF A COMPLEX BIOGEOCHEMICAL MODEL WITH NEURAL NETWORK AND CLUSTERING TECHNIQUES

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Introduction

In the context of global change, mathematical models of biogeochemical cycles can support the understanding of complex processes controlling the emission of greenhouse gases. In this work a special focus is laid on nitrous oxide, estimated to contribute to global warming to an amount of about 6% (IPCC, 2001).Even though N_2O outflux from coastal and shelf sediments is found to be about one third of the total global emissions (SEITZINGER & KROEZE, 1998), the formation of N_2O is often not incorporated in standard model approaches (e. g. WANG & VAN CAPPELLEN, 1996, SOETAERT *et al*., 1996; HUNTER *et al*., 1998; RINN *et al*., 1999). In part, this gap derives from the scarcity of available datasets preventing an adequate parameterisation of process-oriented modelling frames.

In this study we nonetheless adopt a newly built integrated and mechanistic modelling framework as proposed by (WIRTZ, 2003). Albeit using a relatively large data-set for validation, many process parameters of this model cannot be directly evaluated. The model furthermore requires a set of boundary conditions which characterize a local site and are therefore hardly applicable on a global scale. Both characteristics lead to two key problems in environmental modelling:

1. Can meaningful predictions be made at large model uncertainty?
2. Does a complex and intrinsically uncertain model allow for being up-scaled to larger scales?

In this study we present an approach which simultaneously addresses the issue of up-scaling and model uncertainty using data mining techniques such as neural network-based techniques like the Self-Organizing Map (SOM) (KOHONEN, 2001).

One of our guiding hypothesis is that a reduced-form representation can be proposed if the full account of the uncertainty ranges of all model processes is known. The existence of such a reduced representation is supported by nonlinear data analysis where, for example, a neural network trained with an empirical, high-dimensional dataset of sediment biochemistry (KROPP & KLENKE, 1997) revealed a limited number of distinct system states. We suggest that a similar reducibility should be inherent to the high-dimensional output of a complex biogeochemistry model.

Yet, such a behaviour has never been expressed in strict quantitative terms. Whereas this can be addressed with the SOM algorithm, the low dimensional state maps representing a well trained SOM often do not allow direct interpretation. A further clustering of the SOM results as suggested by VESANTO & ALHONIEMI (2000) improve this aspect, but it does not provide a suitable verbal, graphical or quantitative representation. Thus, the discussion of key mechanisms ruling the system behaviour as well as the coupling to a larger scale modelling frame require further transformation of clustering results for which we suggest the form of a simple transition graph.

Model description

The biogeochemical model used in this work is also described by Wirtz (this volume). It builds upon a synthesis of standard approaches such as those of HUNTER (1998), WANG & VAN CAPPELLEN (1996) and SOETAERT *et al*. (1996), extended into various directions.

Four arrays of biogeochemical reactions are accounted for: degradation of several classes of particulate organic carbon (POC), oxidation of dissolved organic carbon (DOC) organised in different groups of higher and lower molecular weight, re-oxidation of reduced substances and mineral precipitation. Major chemical products are CO_2, mineralised nutrients and methane.

Many improvements were made particularly to enhance the applicability of the model to near-shore sediments characterised by temporally and spatially variable conditions. Besides an overall temperature dependence these are the microbial control of nearly the entire kinetics, the adaptation and competition processes of microorganisms and an array of additional transport mechanisms for chemical or biological species either in the dissolved or particulate phase.

The transport part combines, e. g., non-local exchange between the water column and deeper sediment, trapping of particulate species in the upper sediment matrix or the adhesion behaviour of bacteria. To keep computational loads low, we used a one-dimensional setup in our analysis. N_2O formation is calculated on the basis of a detailed module for the cycling of different nitrogen species.

Data generation under uncertainty

The variation of model-parameter values in physically meaningful ranges constitutes a simple but effective means to reflect parameter uncertainty. Until now, the data amount produced by parameter variations has mainly been used to assess model sensitivities which, in turn, may improve the understanding of the simulated system in general or prepare subsequent stages of model reduction in future studies (KÖHLER & WIRTZ, 2002; WIRTZ, 2001).

In this study, parameter variations do not only reflect underlying uncertainties but also enable the generation of an arbitrary large dataset needed by the following stages of nonlinear analysis. Since we simultaneously varied 62 parameters, a Monte-Carlo algorithm based on two different distribution functions was used. If minimal and maximal range values differed by more than one order of magnitude, a log-normal distribution was applied, whereas random parameter values for smaller ranges were distributed equally.

To compromise between the availability of computer power and the demand resulting from a high-dimensional parameter space, 1000 variations were performed. The varied parameters can be categorized by the following basic groups: