Dynamics of Autocatalytic Reaction Networks

Replication with Translation

Diplomarbeit

zur Erlangung
des akademischen Grades

Magister rerum naturalium

Institut für theoretische Chemie
Formal- und Naturwissenschaftliche Fakultät der
Universität Wien

vorgelegt von
Robert Happel
Wien, 1994

für meine Eltern

An dieser Stelle möchte ich mich ganz herzlich bei allen bedanken, die zum Gelingen dieser Arbeit beigetragen haben.

Zuallererst bei Herrn Prof. Dr. Peter Schuster für die Aufnahme am Institut für theoretische Chemie und für seine Vorlesungen, die in mir das Interesse an diesem Fachgebiet weckten.

Dr. Peter Stadler verdanke ich einen ersten Einblick in die Welt der Wissenschaft und die Beteiligung an vielen wissenschaftlichen Arbeiten.

Besonderen Dank schulde ich meinem Kollegen Mag. Robert Hecht, der mit unermüdlicher Geduld als "Retter in der Not" zur Stelle war, wann immer ich nicht mehr weiter wußte.

Auch alle andern Kolleginnen und Kollegen waren stets hilfsbereit und sorgten für ein angenehmes Arbeitsklima.

Meinen Eltern und meiner Großmutter danke ich für die moralische und die finanzielle Unterstützung während all der vielen Jahre.

Meiner Heike danke ich für Alles ...
... und der Mutzi für das viele Schnurren.

Zusammenfassung

Das Verhalten von autokatalytischen Reaktionsnetzwerken unter Einbeziehung der Translation als intermediären Schritt wurde mit analytischen und numerischen Methoden untersucht.

Ein allgemeines chemisches Modell wurde erstellt, und die daraus hervorgehenden kinetischen Differntialgleichungen untersucht. Als Spezialfälle wurden ein mutualistisches, aus dem Hypercyclusmodell von Eigen und Schuster abgeleitetes Modell mit geschlossener cyclischer Katalyse und ein auf wechselseitiger Konkurrenz nach dem Muster von Schlögl aufgebautes Modell herangezogen.

Das dynamische Verhalten im Limit langer Zeiten wurde für drei unterschiedliche Randbedingungen untersucht, nämlich im Evolutionsreaktor, im gerührten Durchlußreaktor und in einem gegenüber Materieaustausch abgeschlossenem Reaktionsgefäß.

Für das mutualistische Model wurden die Bedingungen für das Auftreten von Grenzcyclen untersucht. Außerdem wurde chaotisches Verhalten im selben Gebiet des Parameterraumes für die Selektionsmatix wie im reinen Replikatorfall festgestellt.

Weiters wurde der Einfluß von Mutationen sowohl auf den Replikationsteil, als auch auf den Translationsteil untersucht, und critische Werte für das Auftreten von Bifurkationen ermittelt.

Darüberhinaus konnte ein interessantes Verhalten bei der Einbeziehung von Diffusion in die kinetischen Gleichungen festgestellt werden. Im mutualistischen System kommt es bei Grenzcyclen zunächst zur Ausbildung einer räumlich homogenen, aber zeitlich periodischen Lösung, die aber bei Erhöhung der Diffusionskoeffizienten der Substrate auch räumlich inhomogen wird, bis sie schießlich in eine räumlich inhomogene, aber zeitich stationäre Lösung übergeht.

Abstract

The behavior of a class of autocatalytic reaction-networks with translation as intermediate step was investigated.

A general chemical model was derived, and the corresponding kinetic differential equations were studied by both analytical and numerical methods. Some special cases were considered: a mutualistic model, which was derived from the hypercycle-model by Eigen and Schuster, and a competitive one, based on competition and closely related to the Schlögl model.

Three different boundary conditions were used to describe the long time behavior of the dynamical systems: the evolution-reactor, the continuously stirred tank-reactor, and finally a closed system that admits only exchange of energy.

Conditions for the existence of limit cycles were derived for the mutualistic system. A strange attractor exists in the same region of the parameter-space as in the pure replicator case without intermediates.

The influence of mutation was considered both to the replication-part and the translation-part, and some critical values for the occurrence of bifurcations were obtained.

Furthermore, the system displayed some interesting features with the introduction of diffusion. When starting with a limit cycle in the mutualistic system, a spatial homogeneous but cyclic solution was obtained for small diffusion constants of the substrate. Increase in the diffusion-constants of the substrates yields spatially inhomogeneous patterns. Further increase of the diffusion constants tends to spatially inhomogeneous but stationary solutions.

Contents

1 Introduction

1.1 Evolution

Very detailed knowledge of biological and biochemical processes governing the reproduction of cells has been accumulated in the last decades. With this knowledge, it became possible to ask questions concerning the physical nature of life itself in a very detailed and precise way. Among many others, this comprises questions about the uniqueness of the genetic code, about the optimality of enzymatic action as well as the origin of life itself.

It is a well established fact that conditions on Earth in the beginning (that is in the first hundreds of millions of years after its formation) would not have admitted the existence of complicated bio-polymers [78, 44]. This raises the question of emergence and evolution of these bio-polymers and the intricate systems of interactions between them.

The logic of evolution may be condensed into the following statements [14]:

- natural selection is a consequence of self-reproduction under conditions far from thermodynamic equilibrium.
- Variation is due to imprecise reproduction or other modifications involved in the reproduction process.
- Evolution is the result of variation and natural selection under conditions far from thermodynamic equilibrium.

Charles Darwin was the first to stress this interplay of selection and variation as the principle of evolution. To recognize the importance of advantages or disadvantage, however slight, of individuals over others as the fundamental driving force of selection seems to be one of the principal archievments of Darwin's work [10].

1.2 Self-Organization

"The self organization of matter associated with the origin of life must have started from random events in a sense of non-existing of fundamental

organization." [12]. In his famous paper, which stimulated much research in this field, Manfred Eigen sets out the development of a theory about self organization. He addresses the question of self organizing matter into replicating 'individuals'.

Glansdorff and Prigogine [29] created a thermodynamic theory of open systems in the vicinity of a steady state and presented tools which enable the quantitative treatment of this question. It follows that a system consisting of *information carriers* organizing themselves in the above meaning, must fulfill the following properties:

- The system must be open and far from internal equilibrium.
- The net formation rate of individual information carriers must be positive in the absence of (unspecific) growth restrictions. Furthermore the spontaneous formation of information carriers will be neglected.

A computer model of molecular evolution has been developed by Walter Fontana, Wolfgang Schnabl and Peter Schuster where evolutionary optimization and adaptation has been studied. The object of interest are strings with length ν of symbols out of an alphabet of κ characters. Usual $\kappa = 4$ or $\kappa = 2$ associated with DNA (RNA)-sequences containing all four bases G, C, A, T (U) or just two corresponding pairs (G, C or A, T(U)) respectively. These sequences form exclusively either faithful or erroneous copying of sequences already present [24] or with additional insertion- and deletion-steps [23], and decompose according to a first order rate law.

Different computer models of self organization to this one mentioned above has been established. Fontana set up a (stochastic) dynamical system in which the objects are discrete symbolic maps, such that map j applied to map i yields map k [22].

Well established models of natural selection in the contexts of genetics, sociobiology, prebiotic chemistry, immunology and ecology exhibit similar behavior.

1.3 Adaptation and Evolution

No population can grow forever at a constant rate. This fact, first forcefully articulated by Malthus [39], represented one of the starting points of Darwin's thinking. An excess productivity can be sustained for a few generations at most; uncontrolled growth quickly reaches the limits of natural resources. Some individuals are better adapted than others to the resulting selection pressure. Their offspring will be more numerous. The driving force of selection is therefore competition, both within and between species.

1.4 Types of Interaction

The analysis of the interaction between two species can be quite complicated, involving the effects of exterior and interior parameters. As a first approximation, however, one may distinguish (apart from the case of zero interaction) three basic situations.

- *Competition*: Two species are rivals in the exploitation of a common resource. The more there is of one species, the worse for the other one. Because of the importance of competition as a limiting factor in evolution, such situations have attracted considerable attention.

- *Symbiosis*: This is the reverse situation: both species benefit from each other. The more there is of one species, the better for the other one. Such *mutualistic* relationships have been treated by Eigen and Schuster [15, 16, 17] In particular, there are good reasons to think that also living cells of the type occurring in higher organisms are the outcome of a symbiosis between more primitive organisms.

- *Host-parasite relationship*: The situation, here, is asymmetrical. The parasites benefit from the host but they do it no good. Examples are e.g. various viruses.

2 Methods

2.1 Ordinary Differential Equations

2.1.1 Canonical Forms for Linear Operators

Let $T : E \to E$ be an operator. Its characteristic polynomial can be written as

$$p(t) = \prod_{k=1}^{r} (t - \lambda_k)^{n_k}$$

where λ_k are the r distinct eigenvalues and n_k are their multiplicities. Clearly $n_1 + n_2 + \ldots + n_r = \dim E$. The *generalised eigenspace of T belonging to λ_k* is defined as

$$E(T, \lambda_k) = \ker(T - \lambda_k)^{n_k} \subset E$$

Proposition 2.1 (Primary decomposition theorem) *Let T be an operator on a complex vector space E. Then E is the direct sum of the generalised eigenspaces of T. The dimension of the eigenspaces equals the multiplicity of the corresponding eigenvalue.*

We say an operator A is *semisimple* iff its complexification is diagonalizable. It is *nilpotent* if there is an $n \in N$ such that $A^n = 0$.

Proposition 2.2 *For any operator $T \in L(\mathbb{R}^n)$ there is an unique operator S and N on $\mathbb{R}^n$ such that $T = S + N$, $SN = NS$, where S is semisimple and N is nilpotent.*

The semisimple part S itself may be decomposed into a part S_R corresponding to real eigenvalues and a part S_C corresponding to complex conjugate pairs of eigenvalues. By an appropiate change in coordinates S_R may be rewritten in diagonal form and S_C then consists of 2×2 blocks of the form

$$C_i = \begin{pmatrix} a & -b \\ b & a \end{pmatrix}$$

where a and b are real This representation for S is called (real) canonical form. If we allow for complex entries S is diagonalizable as a whole; instead

of the matrices A_i we have the pair of complex eigenvalues of A_i in the diagonal.

An *elementary nilpotent block* is a matrix of the form

$$N_1 = \begin{pmatrix} 0 & & & & \\ 1 & . & & & \\ & . & . & & \\ & & . & . & \\ & & & . & . \\ & & & 1 & 0 \end{pmatrix}$$

Proposition 2.3 *Let N be a nilpotent operator on a real vector space E. Then E has a basis such that N is represented by a matrix of the form $N = diag(N_1, \ldots, N_r)$ in which N_k is an elementary nilpotent block and the size of N_k is a nonincreasing function of k. The number r of blocks is equal to* dim ker$A$. *Two nilpotent operators of the same vectorspace are similar iff they have the same canonical form N.*

Let us now consider an operator of the form $T = \lambda\ E + N$ where E is the unit operator and N is nilpotent. If we choose the basis such that the matrix N is a nilpotent canonical form, we find the matrix representation of T to be $N + \lambda\ E$. This matrix has block diagonal form with identical blocks of the form

$$\begin{pmatrix} \lambda & & & & \\ 1 & . & & & \\ & . & . & & \\ & & . & . & \\ & & & . & . \\ & & & 1 & \lambda \end{pmatrix}$$

which are called *elementary* JORDAN *blocks*. The number of such blocks is

$$r = \dim\ \ker(T - \lambda)$$

and their size is $\frac{m}{r}$, where m is the dimension of the vector space. If λ is complex the elementary blocks may be rewritten in real form for a *pair* of

conjugate eigenvalues.

$$\begin{pmatrix} D & & & & \\ E_2 & . & & & \\ & . & . & & \\ & & . & . & \\ & & & . & . \\ & & & E_2 & D \end{pmatrix}$$

$$D = \begin{pmatrix} a & -b \\ b & a \end{pmatrix} \quad \text{and} \quad E_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Proposition 2.4 *The canonical form for an arbitrary operator T may now be written as the direct sum of matrices of the above form. It is Therefore a block diagonal matrix consisting Jordan blocks corresponding to the eigenvalues λ_k of T. Each block has size n_k and is made up of dim* $\ker(T - \lambda_k)$ *elementary Jordan blocks.*

2.1.2 Linear ODEs with Constant Coefficients

Let $T : E \to E$ be a linear operator . Its *exponential* is defined as

$$\exp T = \sum_{k=1}^{\infty} \frac{T^k}{k!}.$$

This series converges for all $T \in L(E)$. If $Q = PTP^{-1}$ then the exponential of Q is given by

$$\exp Q = P \cdot \exp T \cdot P^{-1}$$

and if x is a real eigenvector of T belonging to λ, then x is also eigenvector to $\exp T$belonging to e^{λ}.

Let us now consider the solutions of the homogeneous linear system

$$\dot{x} = A \cdot x$$

Proposition 2.5 *Let A be an operator on $\mathbb{R}^n$. Then the* initial value problem $\dot{x} = A \cdot x \quad , \quad x(0) = x_0 \in \mathbb{R}^n$ *has the unique solution.*

$$x(t) = \exp(t \cdot A) \cdot x_0$$

The exponential of an elementary n-dimensional Jordan block B may be readily calculated: with

$$\exp(t \cdot B) = e^{\lambda t} \cdot \begin{pmatrix} 1 & & & & & \\ t & 1 & & & & \\ p_2 & t & 1 & & & \\ . & . & . & . & & \\ . & . & . & . & . & \\ p_{n-1} & p_{n-2} & . & . & t & 1 \end{pmatrix}$$

In coordinates we may write down the solutions of the initial value problem as

$$x_j(t) = e^{\lambda t} \sum_{k=1}^{j-1} \frac{t^k}{k!} x^0_{j-k};$$

where x^0_i denotes the coordinates of x_0.

If λ is complex we identify $\mathbb{C}^m$ and $\mathbb{R}^{2m}$ by the correspondence

$$(x_1 + \imath y_1, x_2 + \imath y_2, \ldots, x_m + \imath y_m) = (x_1, y_1, x_2, y_2, \ldots, x_m, y_m)$$

The solution is formally the same as above, but with the complex vector z instead of the real vector x. With $z^0_i = x^0_i + \imath\, y^0_i$ we obtain the solution in real variables:

$$x_i(t) = e^{at} \sum_{k=0}^{j-1} \frac{t^k}{k!} \left[x^0_{j-k} \cos bt - y^0_{j-k} \sin bt \right]$$

$$y_i(t) = e^{at} \sum_{k=0}^{j-1} \frac{t^k}{k!} \left[y^0_{j-k} \cos bt - x^0_{j-k} \sin bt \right]$$

where $\lambda = a + \imath\, b$.

Proposition 2.6 *Every trajectory of $\dot{x} = Ax$ tends to 0 for $t \longrightarrow \infty$, iff every eigenvalue of A has negative real part.*

Definition 2.1 *Let $(a, b) \subset \mathbb{R}$ be an open interval, $U \subseteq \mathbb{R}^n$ a region. A map $\Phi : U \times (a, b) \longrightarrow \mathbb{R}^n$ is called the* **flow**, *if $\Phi(\Phi(x, t_1), t_2) = \Phi(x, t_1 + t_2)$ holds.*

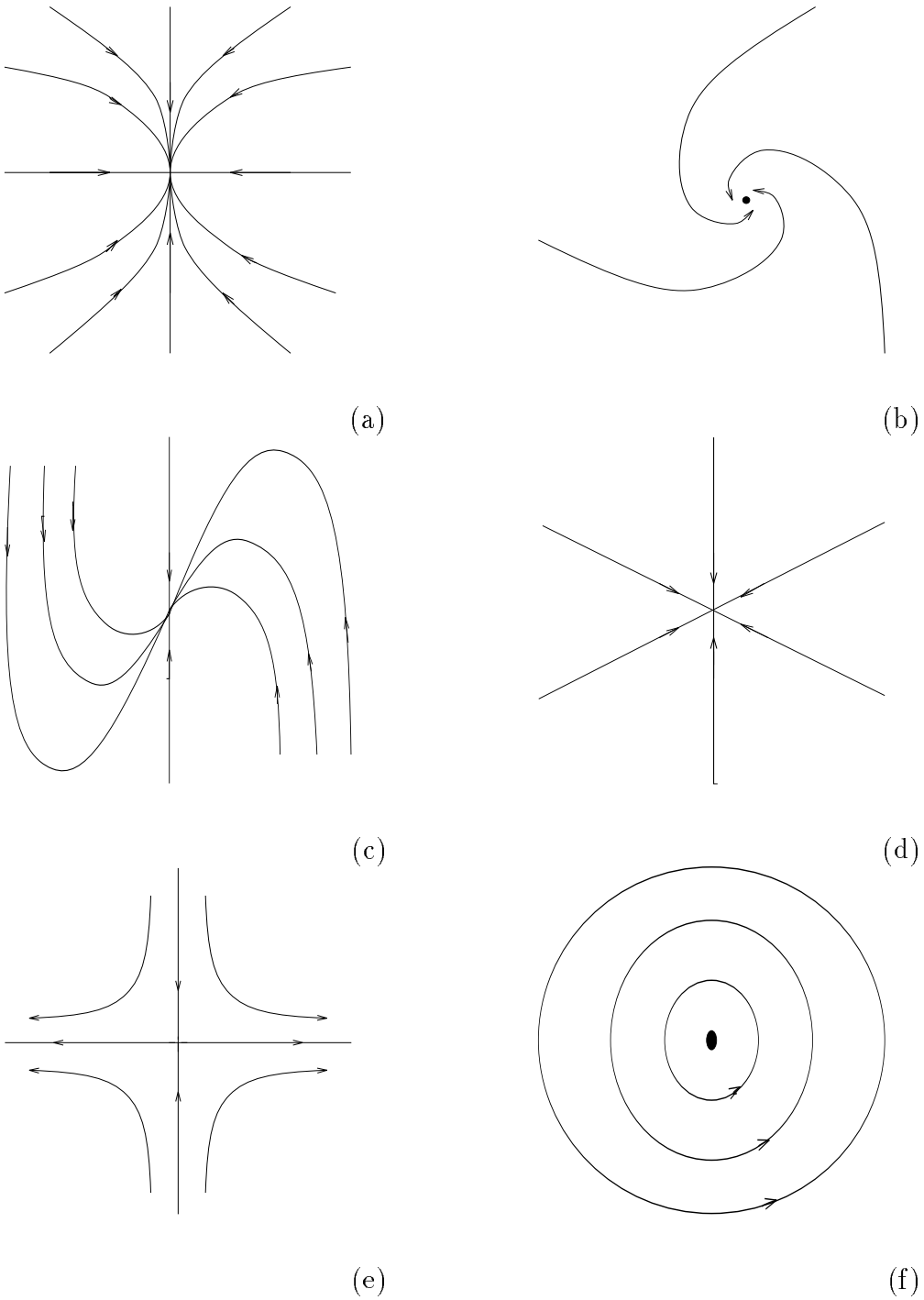

Figure 1: Phase portraits a the two-dimensional ODE: Stable fixed points: (a)-(d); Structurally stable: (a),(b),(e);

The linear *flow* exp (tA) induced by the linear operator A is a *contraction* iff the real parts of all eigenvalues of A are negative, i.e. if $|\exp(tA)x|$ decays exponentially. If all eigenvalues have positive real parts this quantity grows exponentially and the flow is called an *expansion*. If all eigenvalues of A are nonzero the flow is called *regular*, and if the real parts of all eigenvalues are nonzero we have a *hyperbolic flow*. If the flow is hyperbolic it is just the direct sum of a contraction and an expansion.

We remember that when A is semisimple, the operator and thus also the differential equation breaks down into a number of uncoupled equations of dimensions one ore two. The classification of the one-dimensional flows is straight forward. A qualitative summary of the two-dimensional case is given in fig. 1 and a quantitative one in terms of trace and determinant of A in fig.2.

2.1.3 Routh-Hurwitz Conditions

The Routh-Hurwitz criteria [41] are just stated without proof, which can be found in [26]

We define the Hurwitz matrix H associated with the polynomial

$$p_n = a_n x^n + a_{n-1} x^{n-1} + \ldots + a_1 x + a0$$

as the $n \times n$ matrix

$$H = \begin{pmatrix} a_{n-1} & a_{n-3} & a_{n-5} & \ldots & 0 \\ a_n & a_{n-2} & a_{n-4} & \ldots & 0 \\ 0 & a_{n-1} & a_{n-3} & \ldots & 0 \\ 0 & a_n & a_{n-2} & \ldots & 0 \\ 0 & 0 & a_{n-1} & \ldots & 0 \\ \vdots & \vdots & \vdots & \ldots & 0 \\ 0 & 0 & 0 & \ldots & a_0 \end{pmatrix}.$$

The leading principal minors of the matrix are $\Delta_i = |H_{(i+i,\ldots,n)}|$; then if $a_n > 0$, all roots of p_n have negative real part iff all of the following inequalities hold:

$$\Delta_1 > 0, \quad \Delta_2 > 0, \quad \Delta_3 > 0, \quad \ldots \quad \Delta_n > 0.$$

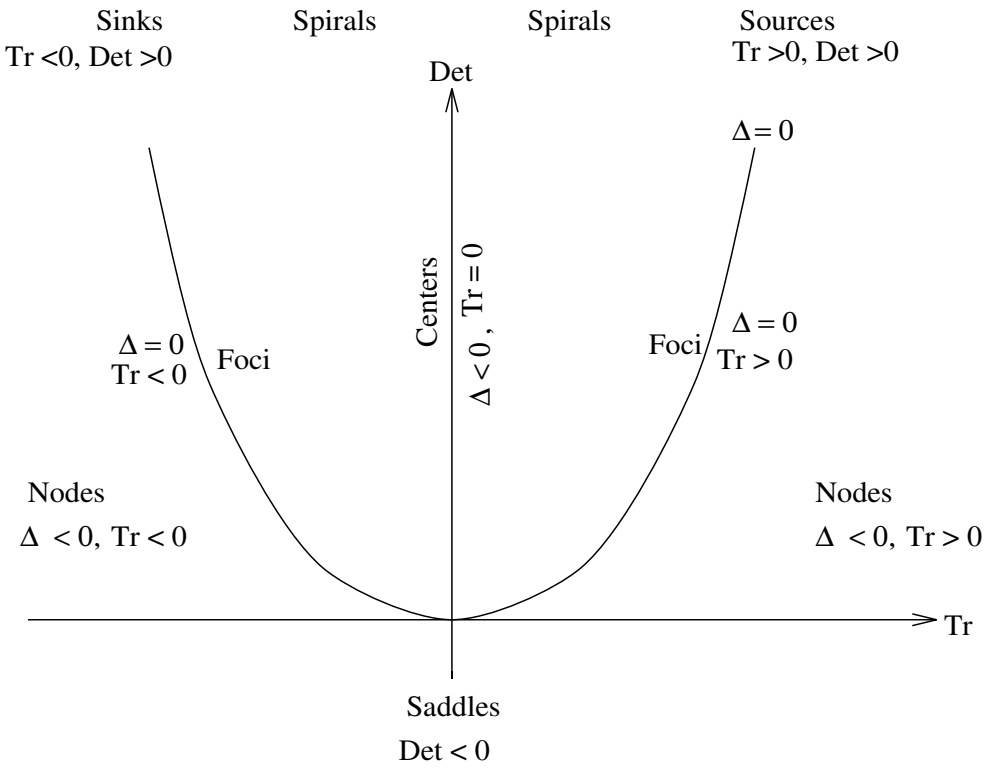

Figure 2: Classification of the two-dimensional linear ODE $\dot{x} = Ax$ in terms of the invariant quantities $\Delta = \det A$ and $\mathrm{Tr}\ A$.

As an illustrative example, we take the case $n = 4$; then the following inequalities have to be fulfilled:

$$|a_3| > 0, \quad \begin{vmatrix} a_3 & a_1 \\ a_4 & a_2 \end{vmatrix} > 0, \quad \begin{vmatrix} a_3 & a_1 & 0 \\ a_4 & a_2 & a_0 \\ 0 & a_3 & a_1 \end{vmatrix} > 0, \quad \begin{vmatrix} a_3 & a_1 & 0 & 0 \\ a_4 & a_2 & a_0 & 0 \\ 0 & a_3 & a_1 & 0 \\ 0 & a_4 & a_2 & a_0 \end{vmatrix} > 0$$

writing out these determinants, we get

$$\begin{aligned} a_3 &> 0 \\ a_2a_3 - a_1a_4 &> 0 \\ a_1a_2a_3 - a_1^2a_4 - a_3^2a_0 &> 0 \\ a0(a_1a_2a_3 - a_1^2a_4 - a_3^2a_0) &> 0 \end{aligned}$$

From the last two inequalities, for a_0 corresponds with the determinant of the matrix, we get the condition for purely imaginary roots of the characteristic polynomial. If $a_0 > 0$ only three inequalities is are responsible for the existence of bifurcations.

As the coefficients of the characteristic polynomial of a matrix are invariant under a similarity transformation of the matrix, the left hand sides of the Routh-Hurwitz -conditions are invariant under that transformation too.

2.1.4 Nonlinear Dynamical Systems

A dynamical system is a way of describing the passage in time of all points in a given *state space* S. Mathematically this space S will be an Euclidian space or an open subset of an Euclidian space.

Definition 2.2 *A* dynamical system *is a C^1 map $S \times \mathbb{R} \longrightarrow S$. If we have $\phi_t(x) = \phi(x_j; t)$, the map $\phi_t : S \longrightarrow S$ satisfies*

- *$\phi_0 : S \longrightarrow$ is the identity;*
- *The composition $\phi_t \circ \phi_s = \phi_{s+t}$ for all s,t in $\mathbb{R}$.*

Definition 2.3 *Let E be an Euclidean vector space; $W \subseteq E$ and f: $W \longrightarrow E$ a continuous map. A solution of the (nonlinear) differential equation*

$$\dot{x} = f(x)$$

is a differentiable function $u : J \longrightarrow W$ defined on some interval $J \subseteq \mathbb{R}$ such that for all $t \in J$ holds

$$\dot{u}(t) = f\left(u(t)\right).$$

So we repeat some fundamental theorems concerning existence, uniqueness and continuity of solutions for ODEs of the above form.

Proposition 2.7 (Existence and Uniqueness) *Let $f \in C^1(W)$ and $x_0 \in W$. Then there is some open interval $J \subseteq R$ and a* unique solution

$$x : J \longrightarrow E \qquad \textit{satisfying} \qquad x(0) = x_0.$$

Proposition 2.8 (Continuity of Solutions) *Let $f \in C^1(W)$ and $y(t)$ be a solution of $\dot{x} = f(x)$ defined on a closed interval$[t_0,t_1]$ with$y(t_0) = y_0$. There is a neighborhood $U \subset E$ of y_0 and a constant k such that if $z_0 \in U$, then there is a unique solution $z(t)$ also defined on $[t_0,t_1]$ with $z(t_0) = z_0$; and z satisfies*

$$|y(t) - z(t)| \leq k|y_0 - z_0|e^{k(t-t_0)}$$

Proposition 2.9 *Every dynamical system on an Euclidean vectorspace gives rise to a differential equation:*

$$\dot{x} = \frac{\partial}{\partial t}\phi_t\Big|_{t=0}(x)$$

and conversely every autonmous differntial equation $\dot{x} = f(x)$ arising from a C^1-map defines a dynamical system: $\phi(t,x) = u(t)$ is the solution of the initial value problem with $u(0) = x$ and $\dot{x} = f(x)$.

2.2 Limit Sets

It is not possible in general to calculate the solution curves $u(t)$ explicitly. In fact we don't have to know the exact solutions for the investigation subjects to this thesis. But we ought to know where a trajectory comes from, where it goes to, i.e. the *asymptotic behavior* of a given trajectory.

Definition 2.4 *A invariant set G for a flow ϕ_t is a subset $G \subseteq E$ such that*

$$\phi_t(x) \in G \quad for \quad x \in G \quad \forall \quad t \in I\!R.$$

The most simple examples are fixed points $\bar{x}$, i.e. $(f(\bar{x}) = 0)$.

Definition 2.5 *$\bar{x}$ is called a* **fixed point** *(or rest point or equilibrium) of a system of differential equations $\dot{x} = F(x)$, if $F(\bar{x}) = 0$.*

We divide the subspaces spanned by the generalized eigenvectors $\xi_1, \ldots, \xi_r$ into three classes:

- $E_s = \text{span}\{\xi_1^s, \ldots, \xi_r^s\}$ is called the **stable eigenspace**.It is spanned by the generalized eigenvectors with eigenvalues with negative real part.
- $E_u = \text{span}\{\xi_1^u, \ldots, \xi_r^u\}$ is called the **unstable eigenspace**.It is spanned by the generalized eigenvectors with eigenvalues with positive real part.
- $E_c = \text{span}\{\xi_1^c, \ldots, \xi_r^c\}$ is called the **center eigenspace**.It is spanned by the generalized eigenvectors belonging to eigenvalues with vanishing real part.

Definition 2.6 *A point $p \in W$ is called* nonwandering for the flow ϕ_t *if, for any neighborhood U of p, there exist arbitrarily large T such that $\phi_t(U) \cap U \neq \emptyset$.*

A nonwandering point lies on or near orbits which come back within a specified distance of themselves. Fixed points and periodic orbits are thus nonwandering. The set of all nonwandering points is closed. Note that all invariant sets consist of nonwandering points.

Definition 2.7 *The ω-limit of x, denoted by $\omega(x)$, is the set of all points p which have the following property: there are points $\phi_{t_1}(x)$, $\phi_{t_2}(x)$, ... on the orbit of x and such that $\phi_{t_i}(x) \longrightarrow p$ as $t_i \longrightarrow \infty$. Correspondingly the α-limit $\alpha(x)$ with all points q for which such a sequence exists for $t_i \longrightarrow -\infty$.*

Definition 2.8 *A closed invariant set $A \subset E$ is called an* attracting set *if there is some neighborhood of A such that $\phi_t(x) \in U$ for all $t \geq 0$ and $\phi_t(x) \longrightarrow A$ as $t \longrightarrow \infty$ for all $x \in U$. The set $\bigcup_{t \geq 0} \phi_t(U)$ is the* domain of attraction *of A.*

There is an analogous definition for *repelling sets.*

Domains of attraction of disjoint attracting sets are necessarily nonintersecting and seperated by the stable manifolds of non-attracting sets.

A fixed point $\bar{x}$ is *stable* if for every neighborhood V of $\bar{x}$ in U there is a neighborhood $V_1 \subset V$ such that every solution $x(x_0, t)$ with $x_0 \in V_1$ is defined and lies in V for all $t > 0$. If, in addition, V_1 can be choosen such

that $x(x_0,t) \longrightarrow \bar{x}$ as $t \longrightarrow \infty$ then $\bar{x}$ is said to be *asymptotically stable*. Asymptotically stable fixed points are called to be *sinks*. A fixed point is called a *source* if there is a neighborhood U of $\bar{x}$ such that for every $y_0 \in U|$ $\bar{x}$ there is a $T > 0$ such that $y(y_o,T) \notin U$.

We close this section with a working definition of an *attractor* as given by Guckenheimer and Holmes [30].

Definition 2.9 *The closed set* Λ *is* indecomposable *if for every pair of points* x, y *in* Λ *and for all* $\epsilon > 0$ *there are points* $X = x_0,x_1,\ldots,x_n = y$ *and* $t_1,\ldots,t_n \geq 1$ *such that*

$$dist(\phi_{t_i}(x_i - 1), x_i) < \epsilon$$

Definition 2.10 *An* attractor *is an indecomposable closed invariant set* Λ *with the property that, given* $\epsilon > 0$, *there is a set* U *of positive Lebesgue measure in the* ϵ*-neighborhood of* Λ *such that* $x \in U$ *implies that the* ω*-limit of* X *is contained in* Λ *and the forward orbit of* x *is contained in* U.

There are different types of attractors for dynamical systems: An equilibrium is by far the most simple case. Fixed points will often be treated by analytical methods in this work. Limit sets consisting of equilibria and orbits connecting them are important in the models discussed here, although the are not structurally stable. Limit cycles and continua of periodic orbits are in generally very difficult to treat analytically, whereas *strange attractors* do not allow for extensive analytical treatment.

2.3 Linearisation of Vector Fields

Suppose we know a fixed point $\bar{x}$ of the differential equation $\dot{x} = f(x)$ and we wish to know the behavior of the dynamical system in a neighborhood of this point. We answer this question by studying the linear system

$$\dot{\xi} = [\partial f(\bar{x})]\cdot\xi,$$

where $(\partial f(\bar{x}))_{ij} = [\partial f_i/\partial x_j]$ at the position of the fixed point $\bar{x}$. $\partial f(\bar{x})$ is called the *Jacobian* (matrix) of the vector field f.

Proposition 2.10 (Hartman-Grobman) *If $\partial f(\bar{x})$ is hyperbolic then there is a homeomorphism h defined on some neighborhood U of $\bar{x}$ in E locally taking orbits of the nonlinear flow ϕ_t of $\dot{x} = f(x)$ to those of the linear flow $\exp t\partial f(\bar{x})$. The homeomorphism h preserves the sense of the orbits and can also be chosen to preserve parametrization by time.*

Definition 2.11 *The set $W^s_{loc}(\bar{x})$ ($W^u_{loc}(\bar{x})$) defined below is called the local stable (unstable) manifold of $\bar{x}$.*

$$\begin{aligned} W^s_{loc}(\bar{x}) &= \{x \in U | \phi_t(x) \to \bar{x} \text{ as } t \to \infty, \text{and } \phi_t(x) \in U \ \forall t \geq 0\} \\ W^u_{loc}(\bar{x}) &= \{x \in U | \phi_t(x) \to \bar{x} \text{ as } t \to -\infty, \text{and } \phi_t(x) \in U \ \forall t \leq 0\} \end{aligned}$$

Proposition 2.11 (Stable Manifold Theorem) *Suppose that $\dot{x} = f(x)$ has a hyperbolic equilibrium $\bar{x}$. Then there exist local stable and unstable manifolds of the same dimensions n_s and n_u as the eigenspaces E^s and E^u of the linearized system and tangent to them at $\bar{x}$. The local stable and unstable manifolds are as smooth as the vector field f.*

Let $\bar{x}$ be a hyperbolic equilibrium of $\dot{x} = f(x)$. If $W^u_{loc} = \emptyset$ then $\bar{x}$ is a sink. If $W^s_{loc} = \emptyset$ the fixed point is a source, otherwise it is a *saddle point.* (For nonhyperbolic flows we will define a saddle as homoeomorph to a hyperbolic saddle.) There is method to determine whether a fixed point is stable which does not depend on the hyperbolicity of the flow:

Proposition 2.12 (Ljapunov) *Let $\bar{x}$ be a fixed point for $\dot{x} = f(x)$ and $v : W \to I\!R$ be a differentiable function defined on some neighborhood $W \subseteq U$ of $\bar{x}$ such that:*

- $v(\bar{x}) = 0$ *and* $v(x) > 0$ *if* $x \neq \bar{x}$,
- $\dot{v}(x) \leq 0$ *in* $W \setminus \{\bar{x}\}$.

  Then $\bar{x}$ is stable. Moreover, if
- $\dot{v}(x) < 0$ *in* $W \setminus \{\bar{x}\}$

then $\bar{x}$ is asymptotically stable.

A stable fixed point is said to be globally stable if all trajectories tend towards it for $t \to \infty$.

A second class of limit sets – besides fixed points – consists of certain unions of equilibria and trajectories connecting them. If distinct fixed points are connected we have a *heteroclinic orbit*, if a fixed point is connected to itself we have a *homoclinic orbit*. Both are sets of nonwandering points.

2.4 Structural Stability

Definition 2.12 *Let $f \in C^m(E)$, $m \in \mathbb{N}$ and $\epsilon > 0$. We say $g \in C^m(E)$ lies in an ϵ-neighborhood of f with respect to a compact set $K \subset E$, if for all $x \in K$ holds*

$$\min\{\|f(x) - g(x)\|, \|\partial(f-g)(x)\|\} < \epsilon.$$

Definition 2.13 *Two vector fields f and g are* topologically equivalent *if there exists a homeomorphism h which takes the orbits $\phi_t^f(x)$ of f to orbits $\phi_t^g(x)$ of g, preserving the senses but not necessarily parametrization by time.*

Definition 2.14 *A vectorfield f is called* structurally stable *if there in an $\epsilon > 0$ such that all C^1 functions g in an ϵ-neighborhood of f are topologically equivalent to f.*

For gradients systems there is an easy to verify sufficient condition for structural stability:

Proposition 2.13 *Gradient systems for which all fixed points are hyperbolic and all intersections of stable and unstable manifolds are transversal, are structurally stable.*

It is an unsolved problem whether the union of all structurally stable flows is generic in arbitrary dimensions. For planar flows on compact manifolds the problem is solved by the following

Proposition 2.14 (Peixoto) *Let M be a compact two-dimensional manifold. (If M has a boundary then assume the flux transverse.) A C^r vector field on M is stucturally stable iff*

- *the number of fixed points and periodic orbits is finite and they are all hyperbolic;*
- *there are no orbits connecting two saddle points;*
- *The set of nonwandering points consists of fixed points and periodic orbits;*

Moreover, if m is orientable, the set of stucturally stable vector fields is generic, i.e. open dense in $C^r(M)$.

It is a nice result that both hyperbolicity and semisimpicity are *generic* properties of linear operators, i.e. semisimple (hyperbolic) operators on E form an open dense subset of $L(E)$. This means that almost all operators have this property and that the slightest perturbation of a nongeneric operator leads to a generic one. That means if we do not know all entries of the matrix A exactly, we may assume any generic property we want to have; it would not make sense to insist on a single special form of A.

On the other hand there may be good reasons for not assuming a particular generic property. If there are natural symmetries in the ODE or if the flow must conserve some quantity, say the energy, then the assumption of a generic property may be a mistake.

2.5 Fractal Sets and Strange Attractors

In an Euclidean Space $\mathbb{R}^n$ a real number determines a *similarity* transformation by

$$\mathcal{S} : x \to r \cdot x.$$

This transformation thus sends a set M to $\mathcal{S}(M)$.

Definition 2.15 *A bounded set M is called* self-similar *with respect to a ratio r and an integer n, when M is the union of n nonoverlapping subsets,*

each of which is congruent to $\mathcal{S}(M)$. (Congruent means identical except for displacement and rotation.) Analogously we call a set M self-similar with respect to an array of ratios $(r_i, i = 1, \ldots, n)$, when M is the union of n subsets each of which is congruent to $\mathcal{S}_{r_i}(M)$. An unbounded set is selfsimilar with respect to a ratio r if $\mathcal{S}(M)$ is congruent to M.

Self-similarity is a usual quality of a class of sets known as *fractals*. These are characterized by rather strange metric properties which can be considered as non-integer dimensions.

Fractal dimensions thus are not topological but *metric* notions. Let H be a metric space. Given a bounded set $M \subset H$ there are many methods of covering it with balls

$$B_\rho(x) = \{y \in H | \text{dist}(x, y) \leq \rho\}$$

of radius ρ. These coverings often involve the notion of a *dimension* in a natural way. For simple examples the values of these dimensions are equal, but for more complex sets their values may differ.

Let H be an n-dimensional Euclidean space. In this case the concept of volume is well defined:

$$\text{vol}(d\text{-dim. ball of radius } \rho) = \gamma(d)\rho^D$$

where $\gamma(d) = \frac{\Gamma(\frac{1}{2})^d}{\Gamma(1+\frac{d}{2})}$ and d is the topological dimension of the balls. Cantor suggested to center a ball $B_\rho(x)$ in each point x of M and to use these balls' union as smoothed out version of M. We will denote this set by $M(\rho)$. The d-dimensional content (i.e. length, area, volume etc.) may be estimated from

$$V(\rho) = \frac{\text{vol}(M(\rho))}{\gamma(n-d)\rho^{n-d}}.$$

However the limit $\lim_{\rho \to 0} V(\rho)$ need not exist. Therefore Minkowski defined upper and lower d-content by the limes superior and the limes inferior respectively. He also discovered that there is a unique number D such that the upper content vanished for $d > D$ and the lower content is infinite for $d < D$ at least for sufficiently smooth sets. Bouligand [5] recognized that D may be

non-integer; he used the value D_- where the lower content becomes infinite as metric dimension.

A different approach was done by Pontrjagin [47]. As before we cover a bounded set M by balls of radius ρ. Let $N(\rho)$ be the smallest number of such balls to cover M. $N(\rho)$ is finite since M is bounded. This leads immediately to

$$D_{PS} = \liminf_{\rho \to 0} \frac{\log N(\rho)}{\log(\frac{1}{\rho})}.$$

The quantity $\log N(\rho)$ was called the ρ-entropy of M by Kolmogorov and Tihomirov [37]. They also studied a modified definition using $C(\rho)$, the largest number of points in M such that their mutual distances exceed 2ρ, instead of $N(\rho)$. They called $\log C(\rho)$ the *capacity* of M and thus the metric dimension based on this quantity is referred to as *capacity dimension* D_C. (As before one might also use $lim\ sup$ in stead of $lim\ inf$; one gets the corresponding "upper" dimensions.)

Let $h(\rho) = \gamma(\rho) \cdot \rho^d$. Hausdorff defined the following measure based on the covering of the set M by balls of radius $\rho_i < \rho$:

$$\mu(\rho) = \inf_{\rho_i < \rho} \sum_i h(\rho_i).$$

The limit

$$\lim_{\rho \to 0} \inf_{\rho_i < \rho} \sum_i h(\rho_i)$$

may be finite, zero or infinite depending on d. In fact there is a unique D, such that this limit vanishes for larger values of d and diverges for smaller ones. This constant D is called the *Hausdorff dimension* of the set M.

The following definition of a *fractal* is due to Mandelbrot [40] :

Definition 2.16 *A set M is called a fractal, if the Hausdorff dimension is strictly larger than the topological dimension of the set M.*

2.6 Ljapunow Exponents

The most common measure for a chaotic attractor is the spectrum of Ljapunov exponents [20]. Let A be an attractor of the differential equation $\dot{x} = f(x)$; and let $x_0 \in A$. How does the difference d_0 between x_0 and

a close neighbor y_0 develop with time? To investigate this we look for a differential equation for $d(t) = y(t) - x(t)$:

$$\dot{d} = \dot{y} - \dot{x} = f(y) - f(x) \approx f(x) + J(x) \cdot d - f(x)$$

where $J(x)$ is the Jacobian matrix of f at the position $x(t)$. Thus the difference d is governed by

$$\dot{d} = J(x(t)) \cdot d.$$

Formally one can integrate this differential equation using the operator

$$\mathcal{L}(t) = \hat{T} \exp[\int_0^t J(x(\tau))d\tau]$$

where the time ordering operator $\hat{T}$ has been introduced because the Jacobian matrices for different times do not commute in general. The solution reads simply

$$d(t) = \mathcal{L}(t) \cdot d(0).$$

Let $\mu_i(t)$ be the eigenvalues of $\mathcal{L}(t)$. The *Ljapunov* exponents are then defined as

$$\lambda_i = \lim_{t\to\infty} \frac{\log \mu_i(t)}{t}.$$

In most cases it is not possible to calculate Ljapunov exponents for the flows of differential equations analytically. An appropriate numerical algorithm has been given by [3], a well tested `FORTRAN` program is also available in the literature [80].

We will not repeat their calculations here but rather give only a sketch of these algorithms. We look at the time evolution of an n-cube with one corner in the origin under the action of $J(x(t))$. This cube shall be spanned by a set of orthonormal vectors $\{e_k\}_1^n$. After some time the cube has been deformed and we are left with a parallelepipede spanned by the vectors $\{e_k(t)\}_1^n$. We denote the content of the subcube which is spanned by the first m of these vectors by $vol_m(t)$. After some time τ the contents $vol_m(\tau)$ are determined. Then the vectors $\{e_k(t)\}_1^n$ are re-orthonormalized by the method of Cram and Schmidt; from $t = \tau$ we start again with a unit cube and let the flow distort it until $t = 2\tau$. The Ljapunov exponents can then be calculated from a sufficiently long time series according to

$$\sum_{i=1}^{m} \lambda_i = \lim_{j\to\infty} \frac{1}{j} \sum_{i=1}^{j} \frac{\log vol_m j(\tau)}{\tau}.$$

For a determination of only the largest Ljapunov exponent one can start with an arbitrary starting vector e and look at its distortion under the action of $J(x(t))$. After a few initial steps it turns into the direction of the largest eigenvalue of the Jacobian, and since it remains locked there, it points always into the direction of the largest eigenvalue of $\mathcal{L}(t)$. Everything one has to do is to renormalize its length in certain timesteps τ to keep it finite. If k_j is the norm of this vector before the $j+1^{st}$ renormalization step, the largest Ljapunov exponent becomes

$$\lambda_1 = \lim_{k\to\infty} \frac{1}{k\cdot\tau} \sum_{j=1}^{k} \log k_j.$$

We remark that the Ljapunov exponents in general depend on the initial condition x_0 on the attractor A. For a rather large class of strange attractors investigated so far however, they are constant values for all points $x \in A$.

The spectrum of the Ljapunov exponents allows one to give a classification of attractors rather easily:

- If all exponents are negative A is a stable fixed point.
- If all exponents but one are negative A is a stable limit-cycle. The zero exponent belongs to the eigen-vector pointing into the direction of the orbit.
- If all exponents are non-positive but two or more are zero we have a quasi-periodic attractor; the zero exponents belong to the tangential directions of A.
- At least one exponent is positive: A is a chaotic attractor.

The Ljapunov exponent explains why chaotic attractors are so difficult to treat: nearby trajectories diverge *exponentially* and, for the attractor A is bounded, are folded back into a neigborhood of their initial values in a very complicated way. Thus long-time predictions of the orbit of a given point are impossible: any rounding error grows exponentially and after some time the whole information on the initial value is lost; it might have been everywhere on A.

Assume that the Ljapunov exponents are ordered such that

$$\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_k \geq 0 > \lambda_{k+1} \geq \ldots \geq \lambda_n.$$

Then the quantity

$$D_L = k - \frac{\sum_{i=1}^{k} \lambda_i}{\lambda_{k+1}}$$

is called the *Ljapunov dimension.*

2.7 Diffusion

There are two principal approaches to diffusion : the *macroscopic* and the *stochastic*; both will - under certain assumptions - lead to the same "law".

In the case of the macroscopic (i.e. thermodynamic) approach, diffusion is the flux of a component that arises from a spatial concentration gradient of this component. The gradient represents the driving force of this process. Assume that the diffusion of component i takes place in a medium which is in excess; then

$$J_{i,diff}(x) = -L_{ii} \left(\nabla \frac{\mu_i}{T} \right)_{T,p}$$

where $J_{i,diff}$ is the flux of the component i due to diffusion at x, μ_i is its chemical potential and L_{ii} is the phenomenological coefficient. For an ideal solution this is equivalent to

$$J_{i,diff}(x) = -D_i \nabla c_i$$

with c_i the concentration of species i and D_i its diffusion coefficient; this is called *Fick's first law of diffusion.*

In a given volume element $\Delta\ V$ with interior Ω and surface $\partial\Omega$, the change of mass over dt in that volume element is

$$\frac{\partial c_i \Delta V}{\partial t} = - \oint_{\partial\Omega} \langle J_i d\vec{o} \rangle$$

with $\vec{o}$ the unit normal on the surface. The negative sign is caused by the fact that the flux is directed outward. With Green's theorem, this yields

$$\frac{\partial c_i \Delta V}{\partial t} = - \int_{\Omega} \nabla J_i dV.$$

Letting $\Delta V \longrightarrow 0$,

$$\frac{\partial c_i}{\partial t} = -\nabla J_i$$

If the diffusion coefficient is space independent, this yields *Fick's second law of diffusion.*

$$\frac{\partial c_i}{\partial t} = D\Delta c_i$$

The other approach to diffusion is to view it as a stochastic process involving individual particles. The microscopic process underlying diffusion in an isotropic medium is a random walk of the diffusing particles. The change of direction and momentum is due to collision with other particles. Under the assumption of several simplifications again the diffusion equation is obtained.

The space in which diffusion takes place is of central importance to the behavior of solutions of reaction diffusion systems. The natural domain for such models is a bounded subspace of $\mathbb{R}$, $\mathbb{R}^2$ or $\mathbb{R}^3$, with boundary conditions that can arise in a physical context. For a closed vessel, these would correspond to homogeneous *Neumann* or *no-flux boundary* conditions.

$$\langle \nabla u, \vec{o} \rangle = 0 \qquad \text{on} \qquad \partial\Omega,$$

where again $\vec{o}$ denotes the unit outer normal. If the walls are permeable to some substances, mixed boundary conditions are appropiate; in the limit of infinite permeability, this yields *Dirichlet boundary conditions.*

$$u = c \qquad \text{on} \qquad \partial\Omega,$$

where c is a function of space, but usually is taken to be constant in subregions of the boundary $\partial\Omega$. *Mixed* boundary conditions are a linear combination of these two,

$$(1-\alpha)\langle \nabla u, \vec{o} \rangle + \alpha(u - c) = 0.$$

For the sake of simplicity only rectangular domains with Neumann boundary conditions are used for this work.

2.7.1 Diffusion as a 'stabilizing process'

Diffusion alone cannot produce any pattern-formation,since the pure diffusion equation $\dot{u} = D\Delta u$ describes a process, which tends to drive to equilibrium

all local perturbations. But in the case of coupling with nonlinear reactions diffusion has a double role : 'on the one hand, it increases the stability of the steady state, but on the other hand, it increases the manifold of perturbations compatible with the macroscopic equations of change. ... if the second effect is dominant, we may expect symmetry breaking instabilities.'[48]

2.7.2 Reaction Diffusion Equations and Symmetry Breaking

In general, the reaction diffusion equation has the form:

$$\dot{u} = D\nabla^2 u + f(u)$$

where $f(u)$ is the reaction part and $D\nabla^2 u = D\Delta u$ is the diffusion part.

If a uniform solution of a reaction diffusion system is unstable due to diffusion, a perturbation of that homogeneous state can be amplified by diffusion and ultimately lead to a new (steady or unsteady) state. But not all perturbation show this property. Especially, a uniform perturbation of a uniform state cannot induce the formation of a nonuniform state.

Those perturbations that can lead to a nonuniform state were termed 'symmetry breaking' [29, 43], because a higher degree of symmetry can be ascribed to the uniform state.

Only in very limited number of cases, exact solutions for reaction diffusion equations are known. One example is the travelling wave solution for the FitzHugh-Nagumo-equation [21].

2.7.3 Approximation of Solutions of Reaction-Diffusion equations

A partial differntial equation $\dot{u} = F(u, u_x, u_{xx})$ an a domain Ω, subject to certain boundary conditions, can be approximated by dividing the domain into elements in which the solution is constant in space; the solutions in adjacent elements are coupled by discrete approximations of the space derivatives. for example the reaction diffusion equation $\dot{u} = f(u) + Du_{xx}$ in $\Omega = [0,1]$ under Neumann boundary conditions, after dividing Ω into m equal elements $e_i =$

$[\frac{i}{m}, \frac{i+1}{m}]$ leads to the system of ordinary differntial equations

$$\begin{aligned} \dot{u}_i &= f(u_i) + m^2 D(u_{i-1} + u_{i+1} - 2u_i) \quad \text{for} i = 2, \ldots, m-1 \\ \dot{u}_1 &= f(u_1) + m^2 D(u_2 - u_1) \\ \dot{u}_m &= f(u_m) + m^2 D(u_{m-1} - u_m). \end{aligned}$$

Here we use

$$\lim_{\Delta x \to \infty} \frac{\Delta}{\delta x} \left(\frac{\Delta}{\delta x} \right) = \frac{\partial^2}{\partial x^2}$$

with $\Delta : \Delta f(x) = f(x + \frac{\Delta x}{2} - f(x - \frac{\Delta x}{2})$. Setting $\Delta x = \frac{1}{m}$, the limit $m \to \infty$ thus yields the continuous formulation. It is obvious that the formulation for $\dot{u}_1$ and $\dot{u}_m$ corresponds to Neumann boundary conditions.

For Dirichlet boundary conditions, the appropiate formulation is

$$\begin{aligned} \dot{u}_1 &= f(u_1) + m^2 D(u_2 + c_0 - 2u_1) \\ \dot{u}_m &= f(u_m) + m^2 D(u_{m-1} + c_1 - 2u_m), \end{aligned}$$

where c_0 and c_1 are the boundary values at $x = 0$ and $x = 1$ respectively. For cyclic boundary conditions,

$$\begin{aligned} \dot{u}_1 &= f(u_1) + m^2 D(u_2 + u_m - 2u_1) \\ \dot{u}_m &= f(u_m) + m^2 D(u_{m-1} + u_1 - 2u_m) \end{aligned}$$

are appropiate.

This approach approximates the reaction diffusion equation as an m-dimensional coupled system of sparsely coupled ordinary differential equations. If there are k components, the k dimensional system of partial differential equations is approximated as a $k \times m$ dimensional system of ordinary differential equations. If the discretization is made infinitely fine the original system is regained; for this reason, partial differential equations can be viewed as infinite dimensional systems of ordinary differential equations.

2.7.4 Diffusion Stability

Just for the sake of completeness we will state the following slightly modified theorem by Berman, Plemmons [4] and Streissler [73].

Theorem 2.1 *Let* $\mathbf{A}$ *be a real* $n \times n$*-matrix with eigenvalues with negative real part except for two zero eigenvalues, let* $\mathbf{D} > 0$ *be a real diagonal* $n \times n$*-matrix with* $d_i \geq 0$ *and at least one* d_i *non-vanishing. Then all the principal minors of* $-\mathbf{A}$ *are nonnegative iff* $-\mathbf{A} + \mathbf{D}$ *is nonsingular for every* $\mathbf{D}$*.*

The proof is analogous to that stated in Streissler [73], so that it will not be repeated here.

3 The Model

3.1 Replicator Networks

If we consider just replication and neglect the translation-part then we get kinetic differential equations that are denoted by the term *Replicator equations* [59, 35]

$$\dot{x}_k = x_k \left(f_k(\mathbf{x}) - \sum_{j=1}^{n} x_j f_j(\mathbf{x}) \right) \quad \text{for} \quad k = 1, \ldots, n$$

where $\mathbf{x} = (x_1, \ldots, x_n)$. This equation describes the selection process. Adding errors while replicating allows to describe evolutionary processes such as mutation or recombination [53, 58, 60, 56], [68] – [72]

Many works have been performed on this subject and on special cases, such as the development of the hyper-cycle [12], [15] – [17]

3.2 Reaction Networks

There are n replicating species in all dynamical systems treated in this work. For each species k=1,...,n X_k represent the genom and T_k denotes the gene-products, necessary for replication (e.g. the DNA (RNA) polymerases). Because it is impossible to deal with all the single steps that are necessary for self-replication, very severe simplifications had to be made.

Every kind of life and in that sense also every kind of replication is bound to metabolism which causes all these systems to be dissipative. So there have to be different kinds of out-flow to compensate for the inflow of raw materials, such as energy or monomers.

We therefore assume the following general scheme for our dynamical system:

$$\begin{aligned} A + X_k + T_l &\xrightarrow{a_{kl}} 2X_k + T_l \\ B + X_k &\xrightarrow{\tau_k} X_k + T_k \\ X_k &\xrightarrow{\varphi_1} P \\ T_k &\xrightarrow{\varphi_2} Q \end{aligned} \tag{1}$$

3.3 Boundary Conditions

In order to have experimentally reproducible conditions of replication there are three kinds of boundary conditions, which lead to somewhat different sets of kinetic differential equations:

1. the **Continuously Stirred Tank Reactor** (**CSTR**).
2. the **Evolution Reactor**.
3. and a closed model with **Regeneration** of the monomers.

3.3.1 CSTR

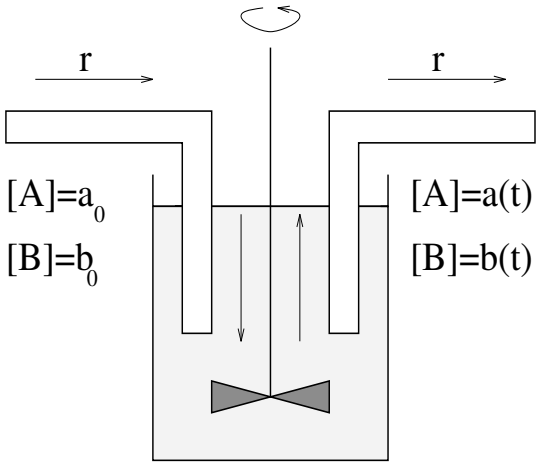

Figure 3: continuously stirred tank reactor

In fig. (3), a schematic view of a continuously stirred tank reactor is given. The flow rate r can be controlled. As shown in [60, 63], the total concentration of the replicating species becomes a_0 for $t \to \infty$.

3.3.2 Evolution Reactor

The evolution reactor, as shown in fig.(4) is a kind of dialysis reactor with walls impermeable to polynucleotides and polypeptides. A flow is provided,

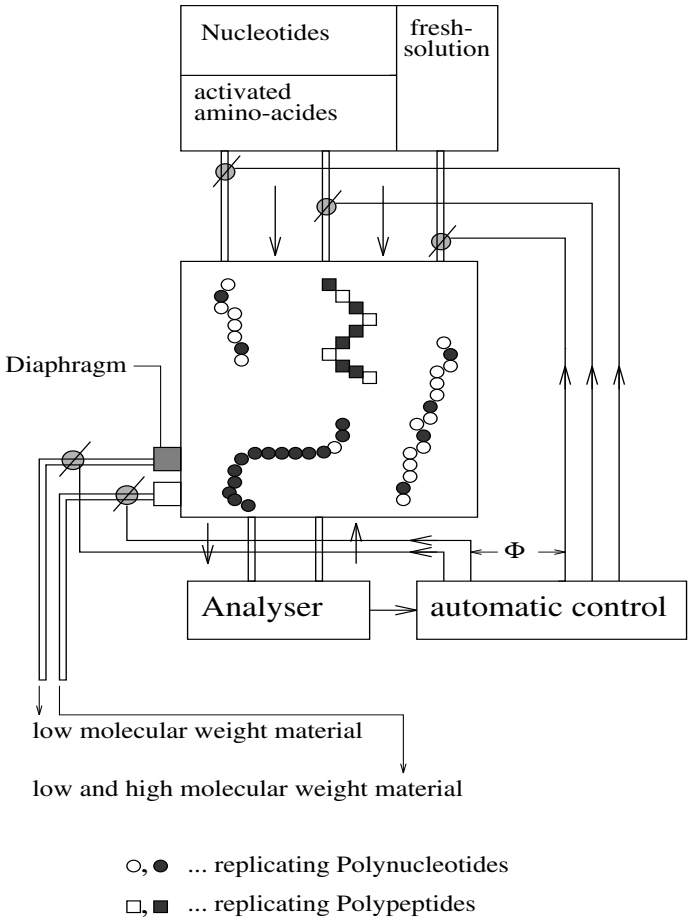

Figure 4: Evolution-reactor with external controlling device.

which keeps a reaction mixture of replicating species (e.g. DNA or RNA molecules or polypeptides) away from equilibrium. Transport of energy rich material from the stock solutions into the reactor is adjusted in such a way that the concentrations of the nucleoside triphosphates (GTP, ATP, CTP and TTP (or UTP)) are in great excess in in the reactor. The polynucleotide concentrations and that of the activated amino-acid molecules together with the polypeptides are controlled separately, so that the result are two concentration simplices. Although this kind of evolution reactor is extremely difficult to realize and therefore very unrealistic, it gives much simplification in the kinetic equations.

3.3.3 Regeneration

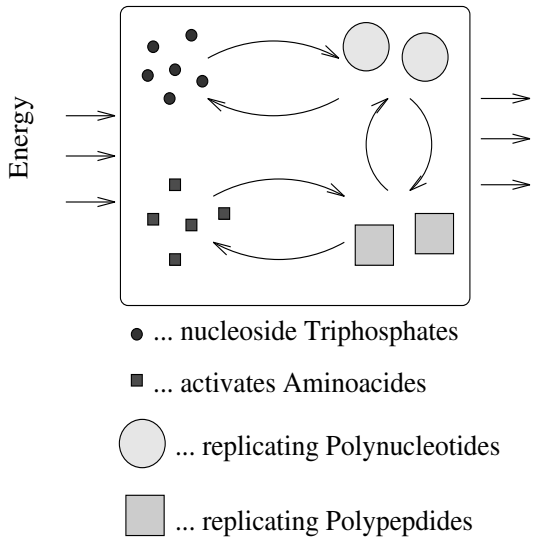

Figure 5: A model for a closed system with regenerating monomers

In this model there is no flux of material into or out of the system. In order to keep the system away from equilibrium, a flow of energy is needed to allow regeneration of the monomers that are produced by degradation of the replicating species. The degradation is considered to be a single step process. Even if this assumption is very non-realistic, this step accounts for degradation and reactivation of the monomers in a sense of overall-kinetics again. Fig. (5) presents a schematic overview of this kind of reaction vessel.

3.4 Kinetic Differential Equations

3.4.1 Constant Organization

Since the primary products are always in great excess, they do not account for the kinetic equations and are written in braces. There is a dilution flux,

such that the total concentration of all replicating species keeps constant.

$$\begin{array}{rcl} (A) + X_k + T_l & \xrightarrow{a_{kl}} & 2X_k + T_l \\ (B) + X_k & \xrightarrow{\tau_k} & X_k + T_k \\ X_k & \xrightarrow{\Phi^x} & \star \\ T_k & \xrightarrow{\Phi^{\sim}} & \star \end{array} \tag{2}$$

The reaction constants a_{kl} form a $n \times n$ matrix $\mathbf{A}$, that is also called the *selection matrix*. This leads to the following differential equations:

$$\begin{array}{rcl} \dot{x}_k & = & x_k \left((\mathbf{A}t)_k - \Phi^x \right) \\ \dot{t}_k & = & x_k \tau_k - t_k \Phi^{\sim} \end{array} \tag{3}$$

and because all species live on their concentration simplices the dimension of the mathematical problem reduces by two.

$$\sum_{k=1}^{n} x_k = 1 \quad \text{and} \quad \sum_{k=1}^{n} t_k = 1 \tag{4}$$

The fluxes are readily calculated

$$\Phi^x = \sum_{i}^{n} x_i \sum_{j}^{n} a_{ij} t_j \quad \text{and} \quad \Phi^{\sim} = \sum_{i}^{n} x_i \tau_i \tag{5}$$

Theorem 3.1 *Suppose the Matrix* $\mathbf{A}$ *is nonsingular, then there is a unique fixed point in int* $\mathcal{S}_n$ *if and only if*

$$\mathbf{B} = \mathbf{A}^{-1} \quad \textit{with components} \quad b_{kl}.$$

Proof:

$$\begin{array}{rcl} \bar{x}_i & = & \dfrac{\displaystyle\sum_{j}^{n} b_{ij}}{\tau_i \displaystyle\sum_{k}^{n} \frac{1}{\tau_k} \sum_{j}^{n} b_{kj}} > 0 \quad \text{and} \\ \\ \bar{t}_i & = & \dfrac{\displaystyle\sum_{j}^{n} b_{ij}}{\displaystyle\sum_{k}^{n} \sum_{j}^{n} b_{kj}} > 0 \end{array} \tag{6}$$

where $\mathbf{B} = \mathbf{A}^{-1}$.

■

3.4.2 CSTR

$$\begin{aligned} A + X_k + T_l &\xrightarrow{a_{kl}} 2X_k + T_l \\ B + X_k &\xrightarrow{\tau_k} X_k + T_k \\ X_k &\xrightarrow{r} \star \\ T_k &\xrightarrow{r} \star \\ A &\xrightarrow{r} \star \\ B &\xrightarrow{r} \star \end{aligned} \tag{7}$$

The kinetic equations read:

$$\begin{aligned} \dot{a} &= -a\sum_{j=1}^{n} x_j(\mathbf{A}t)_k + r(a_0 - a) \\ \dot{b} &= -b\sum_{j=1}^{n} \tau_j x_j + r(b_0 - b) \\ \dot{x}_k &= x_k\left(a(\mathbf{A}t)_j - r\right) \\ \dot{t}_k &= \tau_k b k_i - t_k r \end{aligned} \tag{8}$$

Again the reaction constants a_{kl} form the selection matrix $\mathbf{A}$.

Theorem 3.2 *Suppose the Matrix* $\mathbf{A}$ *is nonsingular, then there at most two equilibria.*

Proof: Let

$$\mathbf{B} = \mathbf{A}^{-1} \quad \text{with components} \quad b_{kl},$$
$$\alpha = \sum_{j=1}^{n} b_k j \quad \text{and} \quad \kappa = \sum_{j=1}^{n} \frac{1}{\tau_j} \sum_{l=1}^{n} a_{jl}.$$

Then the inner equilibria are

$$\bar{x}_k = \frac{r^2}{\bar{a}\bar{b}} \frac{\alpha}{\tau_k} \quad \text{and} \quad \bar{t}_k = \frac{r}{\bar{a}}\alpha \tag{9}$$

and some algebra yields

$$\bar{a} = \frac{\alpha n r}{(b_0 - \bar{b})} \tag{10}$$

$$\bar{b} = \frac{a_0 b_0 n + 2\alpha b_0 \kappa r - \alpha n^2 r \pm n\sqrt{{a_0}^2{b_0}^2 - 2\alpha a_0 b_0 n r - 4\alpha^2 b_0 \kappa r^2 + \alpha^2 n^2 r^2}}{2\left(a_0 n + \alpha\kappa r\right).}$$

So there are a maximum number of two inner rest points, since there are at most two positive real solutions of (10).

■

Since it was not possible to calculate the eigenvalues of the Jacobian of this system for the general case only some special cases with much easier mathematical structure could be solved.

4 Competitive Model

4.1 Competitive Model under Constant Organization

In the competitive model, which is quite similar to the Schloegl model [49], the selection matrix **A** reduces to a diagonal matrix, so that we get the following reactions:

$$\begin{aligned} (A) + X_i + T_i &\xrightarrow{k_i} 2X_i + T_i \\ (B) + X_i &\xrightarrow{\tau_i} X_i + T_i \\ X_i &\xrightarrow{\Phi^x} \star \\ T_i &\xrightarrow{\Phi^\sim} \star \end{aligned} \tag{11}$$

Equation (3) and (4) becomes

$$\begin{aligned} \dot{x}_i &= x_i \left(k_i t_i - \sum_{j=1}^{n} k_j x_j t_j \right) \\ \dot{t}_i &= x_i \tau_i - t_i \sum_{j=1}^{n} x_i \tau_i \end{aligned} \tag{12}$$

From

$$\bar{x}_i = \frac{\bar{\Phi}^x \bar{\Phi}^\sim}{k_i \tau_i} \quad \text{and} \quad \bar{t}_i = \frac{\bar{\Phi}^x}{k_i} \tag{13}$$

we get the inner equilibrium:

$$\bar{\Phi}^x = \frac{1}{\sum_{i=1}^{n} \frac{1}{k_i}} \qquad \text{and} \qquad \bar{\Phi}^\sim = \frac{\sum_{i=1}^{n} \frac{1}{k_i}}{\sum_{j=1}^{n} \frac{1}{k_j \tau_j}} \tag{14}$$

and finally

$$\begin{aligned} \bar{x}_i &= \frac{1}{k_i \tau_i \sum\limits_{j=1}^{n} \frac{1}{k_j \tau_j}} \\ \bar{t}_i &= \frac{1}{k_i \sum\limits_{j=1}^{n} \frac{1}{k_i}}. \end{aligned} \tag{15}$$

4.1.1 Stability Analysis

The Jacobian becomes:

$$\mathbf{J} = \begin{pmatrix} -k_1x_1t_1 & -k_1x_1t_2 & \dots & -k_1x_1t_n & k_1x_1(1-x_1) & -k_1x_1x_2 & \dots & -k_1x_1x_n \\ -k_2x_2t_1 & -k_2x_2t_2 & \dots & -k_2x_2t_n & -k_2x_2x_1 & k_2x_2(1-x_2) & \dots & -k_2x_2x_n \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -k_nx_nt_1 & -k_nx_nt_2 & \dots & -k_nx_nt_n & -k_nx_nx_1 & -k_nx_nx_2 & \dots & k_nx_n(1-x_n) \\ \tau_1(1-t_1) & -\tau_1t_1 & \dots & -\tau_1t_1 & -\tau_1 & 0 & \dots & 0 \\ -\tau_2t_2 & \tau_2(1-t_2) & \dots & -\tau_2t_2 & 0 & -\tau_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\tau_nt_n & -\tau_nt_n & \dots & \tau_n(1-t_n) & 0 & 0 & \dots & -\tau_n \end{pmatrix}$$

Considerably effort was taken to perform a barycentric transformation [35], but since this was not possible, only the special case with equal reaction constants was investigated.

$$k_i = k \qquad \tau_i = \tau$$

At the fixed point

$$\mathcal{P} = (\dots, \frac{1}{n}, \dots) \tag{16}$$

the Jacobian reduces to

$$\mathbf{J} = \begin{pmatrix} -\frac{k}{n^2} & -\frac{k}{n^2} & \dots & -\frac{k}{n^2} & \frac{k}{n}\left(1-\frac{1}{n}\right) & -\frac{k}{n^2} & \dots & -\frac{k}{n^2} \\ -\frac{k}{n^2} & -\frac{k}{n^2} & \dots & -\frac{k}{n^2} & -\frac{k}{n^2} & \frac{k}{n}\left(1-\frac{1}{n}\right) & \dots & -\frac{k}{n^2} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\frac{k}{n^2} & -\frac{k}{n^2} & \dots & -\frac{k}{n^2} & -\frac{k}{n^2} & -\frac{k}{n^2} & \dots & \frac{k}{n}\left(1-\frac{1}{n}\right) \\ \tau\frac{n-1}{n} & -\frac{\tau}{n} & \dots & -\frac{\tau}{n} & -\tau & 0 & \dots & 0 \\ -\frac{\tau}{n} & \tau\frac{n-1}{n} & \dots & -\frac{\tau}{n} & 0 & -\tau & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\frac{\tau}{n} & -\frac{\tau}{n} & \dots & \tau\frac{n-1}{n} & 0 & 0 & \dots & -\tau \end{pmatrix}$$

Fortunately, it is possible to decompose this matrix into four blocks, whose eigenvalues can be readily derived, because they are circulant. So we can bring $\mathbf{J}$ into the nicer looking form of

$$\mathbf{J} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}. \tag{17}$$

The eigenvalues of any circulant matrix **A** can be calculated, for they are simply

$$\lambda_j = \sum_{k=0}^{n-1} a_k z^{kj} j = 0, \ldots, n-1 \ , \tag{18}$$

where the a_k are the entries of the matrix **A** and z is

$$z = e^{\left(\frac{2\pi\imath}{n}\right)} \tag{19}$$

with the following eigenvectors

$$\xi_j = \left(1, z^j, z^{2j}, \ldots, z^{(n-1)j}\right) \tag{20}$$

So it it possible to calculate the eigenvectors and hence the eigenvalues of every matrix, which consists of four (are more) circulant parts of the form (17). in [31] this method is shown more explicitly. The usual "master-equation" becomes the form .

$$\begin{aligned} \mathbf{A} \cdot \xi_j &= \lambda_j \xi_j \\ \xi_j &= (\nu_j, \beta\, \nu_j) \end{aligned} \tag{21}$$

where the ν_j have the form of (20). From (21) some calculations lead straightly to

$$\beta = \frac{\lambda_D - \lambda_A \pm \sqrt{((\lambda_A - \lambda_D)^2 + 4\lambda_B \lambda_C)}}{2\lambda_B} \tag{22}$$

If we manage to get β then it is no more problem to calculate the eigenvalues of the matrix **A**.

$$\begin{aligned} \Lambda_j &= \lambda_A + \beta\lambda_B \\ &= \frac{\lambda_A + \lambda_D \pm \sqrt{((\lambda_A - \lambda_D)^2 + 4\lambda_B \lambda_C)}}{2} \end{aligned} \tag{23}$$

In the case of the competitive model the eigenvalues of the four parts are

$$\lambda_A = \begin{cases} -\frac{k}{n} & : \quad j = 0 \\ 0 & : \quad j \neq 0 \end{cases} \qquad \lambda_B = \begin{cases} 0 & : \quad j = 0 \\ \frac{k}{n} & : \quad j \neq 0 \end{cases}$$

$$\lambda_C = \begin{cases} 0 & : \quad j = 0 \\ \tau & : \quad j \neq 0 \end{cases} \qquad \lambda_D = -\tau \qquad \forall j$$

If equal reaction constants of all species are assumed then all, but the one-dimensional eigenvalues of the competitive model are saddles.

- **j=0** :

$$\Lambda_{0_1} = -\frac{k}{n} \qquad \text{and} \qquad \Lambda_{0_2} = -\tau \tag{24}$$

These eigenvalues,which belong to the eigenvector **1** are the *external* eigenvectors, which do not contribute to the behavior of our dynamical system.

- **j $\neq$0** :

$$\Lambda_j = \frac{-\tau \pm \sqrt{\tau^2 + 4\frac{k}{n}\tau}}{2} \tag{25}$$

Because for j $\neq 0$ the discriminant of (25) is always greater than τ there are always $\frac{(n-1)}{2}$ positive eigenvalues of the Jacobian. Therefore the inner fixed point is always a saddle. Because all sub-simplices are invariant, equation (25) also is also valid for all "inner" fixed points of these sub-simplices . Only the transversal eigenvalues are negative. The only sinks in this system are the one-dimensional equilibria.

So from a given start-point all species,but for the fittest, have to perish and only one species will survive.

4.1.2 Competitive Model with two species

The two species model is the most simple case, where just two species are competing for the provided monomers.

$$\begin{aligned} \dot{x} &= x\left(k_1 t - k_1 x t - k_2(1-x)(1-t)\right) \\ \dot{t} &= \tau_1 x - t\left(\tau_1 x + \tau_2(1-x)\right) \end{aligned} \tag{26}$$

The first derivatives are simply

$$\begin{aligned} a &= \frac{\partial \dot{x}}{\partial x} = x\left(k_2 - t(k_1+k_2)\right) \\ b &= \frac{\partial \dot{x}}{\partial t} = x(k_1+k_2)(1-x) \\ c &= \frac{\partial \dot{t}}{\partial x} = t(\tau_2-\tau_1) + \tau_1 \\ d &= \frac{\partial \dot{t}}{\partial t} = x(\tau_2-\tau_1) - \tau_2 \end{aligned} \tag{27}$$

So we get a 2×2 Jacobian with the characteristic polynomial

$$\lambda^2 - \lambda(a+d) + ad - cb$$

with $a + d = tr\,(\mathbf{A})$ and ad - cb is $\det\,(\mathbf{A})$

$$\lambda_{+,-} = \frac{tr\,(\mathbf{A}) \pm \sqrt{tr^2\,(\mathbf{A}) - 4\det\,(\mathbf{A})}}{2}$$

So at the inner fixed point (6) equation (27) becomes

$$\begin{aligned} a(\bar{x},\bar{t}) &= 0 & b(\bar{x},\bar{t}) &= -\frac{k_1 k_2 (k_1+k_2)\tau_1\tau_2}{(k_1\tau_1 + k_2\tau_2)^2} \\ c(\bar{x},\bar{t}) &= \frac{k_1\tau_1 + k_2\tau_2}{k_1+k_2} & d(\bar{x},\bar{t}) &= -\frac{(k_1+k_2)\tau_1\tau_2}{k_1\tau_1 + k_2\tau_2} \end{aligned} \tag{28}$$

So we finally can compute the eigenvalues for the reduced full system

$$\lambda_{+,-} = \frac{1}{2}\left(-\frac{(k_1+k_2)\,\tau_1\tau_2}{k_1\tau_1 + k_2\tau_2} \pm \sqrt{\frac{(k_1+k_2)^2\,\tau_1^2\tau_2^2}{(k_1\tau_1 + k_2\tau_2)^2} + \frac{4k_1k_2\tau_1\tau_2}{k_1\tau_1 + k_2\tau_2}} \right) \tag{29}$$

For two species the inner fixed point of the competitve model is always is a saddle, because the discriminant is always greater then the left term.

The other equilibria in the corners are sinks. At the fixed point (0 , 0) the eigenvalue becomes ($-k_2$, $-\tau_2$) and at the other fixed point (1 , 1) it is ($-k_1$, $-\tau_1$).

4.1.3 Competitive Model for 3 species

The characteristic polynomial then becomes

$$\frac{\left(\lambda^2\gamma_1 + \lambda\gamma_2 - \gamma_3\right)^2}{\left(k_1\,k_2\,\tau_1\,\tau_2 + k_1\,k_3\,\tau_1\,\tau_3 + k_2\,k_3\,\tau_2\,\tau_3\right)^2} = 0 \tag{30}$$

$$\begin{aligned} \gamma_1 &= k_1\,k_2\,\tau_1\,\tau_2 + k_1\,k_3\,\tau_1\,\tau_3 + k_2\,k_3\,\tau_2\,\tau_3 \\ \gamma_2 &= (k_1\,k_2 + k_1\,k_3 + k_2\,k_3\,)\,\tau_1\,\tau_2\,\tau_3 \\ \gamma_3 &= k_1\,k_2\,k_3\,\tau_1\,\tau_2\,\tau_3 \end{aligned}$$

So it is possible to calculate the eigenvalues of the Jacobian of the inner fixed point, which simply are

$$\lambda_{1,2,\pm} = \frac{-\gamma_2 \pm \sqrt{\gamma_2^2 + 4\,\gamma_1\,\gamma_3}}{2\,\gamma_1} \tag{31}$$

Because the square-root of (31) is always greater then γ_2, there have to be two positive eigenvalues and two negative ones, so that the inner fixed point always has to be a saddle.

The sub-simplices of the three species model is "invariant" to cyclic permutation of the indices so only one fixed point is considered.

- **Fixed Point**

  $$\bar{\mathbf{x}} = \left(\frac{k_3\tau_3}{k_1\tau_1 + k_3\tau_3}, 0, 1 - \frac{k_3\tau_3}{k_1\tau_1 + k_3\tau_3}\right), \bar{\mathbf{t}} = \left(\frac{k_3}{k_1 + k_3}, 0, 1 - \frac{k_3}{k_1 + k_3}\right)$$

  The characteristic polynomial of the Jacobian at this equilibrium becomes

  $$\begin{gathered}(\lambda\,(k_1 + k_3) + k_1k_3)\cdot \\ (\lambda\,(k_1\tau_1 + k_3\tau_3) + k_1\tau_1\tau_3 + k_3\tau_1\tau_3)\cdot \\ (\lambda^2\,(k_1\tau_1 + k_3\tau_3) + \lambda\,(k_1\tau_1\tau_3 + k_3\tau_1\tau_3) - k_1k_3\tau_1\tau_3)\end{gathered} \tag{32}$$

  So the eigenvalues become

  $$\lambda_1 = -\frac{k_1k_3}{k_1 + k_3} \tag{33}$$

  $$\lambda_2 = -\frac{k_1\tau_1\tau_3 + k_3\tau_1\tau_3}{k_1\tau_1 + k_3\tau_3} \tag{34}$$

  $$\lambda_{3,4} = -\frac{(k_1 + k_3)\,\tau_1\tau_3 \pm \sqrt{(k_1\tau_1\tau_3 + k_3\tau_1\tau_3)^2 + 4\,(k_1\tau_1 + k_3\tau_3)\,(k_1k_3\tau_1\tau_3)}}{2\,(k_1\tau_1 + k_3\tau_3)} \tag{35}$$

  Again there is one positive eigenvalue such that this fixed point is a saddle.

- **Fixed Point**

$$\bar{\mathbf{x}} = (1,0,0) \ , \bar{\mathbf{t}} = (1,0,0)$$

Here we have just

$$(\lambda + k_1)^2 \cdot (\lambda + \tau_1)^2 = 0 \tag{36}$$

so that there are only negative eigenvalues

$$\lambda_{1,2} = -k_1 \tag{37}$$

$$\lambda_{3,4} = -\tau_1 \tag{38}$$

All fixed points of this system but for the one-dimensional corners of the simplex, which are sinks, are saddles.

4.1.4 General Eigenvalues of the Competitive Model

Conjecture 4.1 *The characteristic polynomial of the general competitive model (3) is:*

$$\left(\frac{\lambda^2 \sum_{j=1}^{n} \prod_{\substack{i=1 \\ i \neq j}}^{n} k_i \tau_i + \lambda \left(\prod_{j=1}^{n} \tau_j \right) \cdot \sum_{j=1}^{n} \prod_{\substack{i=1 \\ i \neq j}}^{n} k_i - \prod_{i=1}^{n} k_i \tau_i}{\sum_{j=1}^{n} \prod_{\substack{i=1 \\ i \neq j}}^{n} k_i \tau_i} \right)^{n-1} = 0 \tag{39}$$

Some simplifications are possible, because

$$\frac{\prod_{i=1}^{n} k_i \tau_i}{\sum_{j=1}^{n} \prod_{\substack{i=1 \\ i \neq j}}^{n} k_i \tau_i} = \frac{1}{\sum_{j=1}^{n} \frac{1}{k_j \tau_j}}$$

and

$$\frac{\prod_{j=1}^{n} \tau_j \sum_{j=1}^{n} \prod_{\substack{i=1 \\ i \neq j}}^{n} k_i}{\sum_{j=1}^{n} \prod_{\substack{i=1 \\ i \neq j}}^{n} k_i \tau_i} = \frac{\sum_{j=1}^{n} \prod_{\substack{i=1 \\ i \neq j}}^{n} k_i \tau_i}{\prod_{j=1}^{n} k_j \tau_j \sum_{j=1}^{n} \frac{1}{k_j \tau_j}} = \frac{\sum_{j=1}^{n} \frac{1}{k_j}}{\sum_{j=1}^{n} \frac{1}{k_j \tau_j}}.$$

So the characteristic polynomial becomes finally

$$\left(\lambda^2 + \lambda \frac{\sum_{j=1}^{n} \frac{1}{k_j}}{\sum_{j=1}^{n} \frac{1}{k_j \tau_j}} - \frac{1}{\sum_{j=1}^{n} \frac{1}{k_j \tau_j}} \right)^{n-1} = 0 \tag{40}$$

Theorem 4.1 *For the interior rest point there are always positive roots of (39).*

Proof: It is very easy to calculate the eigenvalues of the whole system by solving equation (40).

$$\lambda_{k\pm} = \frac{1}{2} \left(-\frac{\sum_{j=1}^{n} \frac{1}{k_j}}{\sum_{j=1}^{n} \frac{1}{k_j \tau_j}} \pm \sqrt{\left(\frac{\sum_{j=1}^{n} \frac{1}{k_j}}{\sum_{j=1}^{n} \frac{1}{k_j \tau_j}} \right)^2 + \frac{4}{\sum_{j=1}^{n} \frac{1}{k_j \tau_j}}} \right). \tag{41}$$

$$k = 1 \ldots (n-1)$$

But even this quite complicated formula doesn't show anything particularly new. There are $\frac{n}{2}$ positive eigenvalues that cause the interior fixed point (and the interior fixed points of all sub-simplices) to be saddles. ■

If we once more consider equal reaction constants, we can see that the eigenvalues (41) become equal to (25). Additionally, numerical results suggest very strongly that (41) holds.

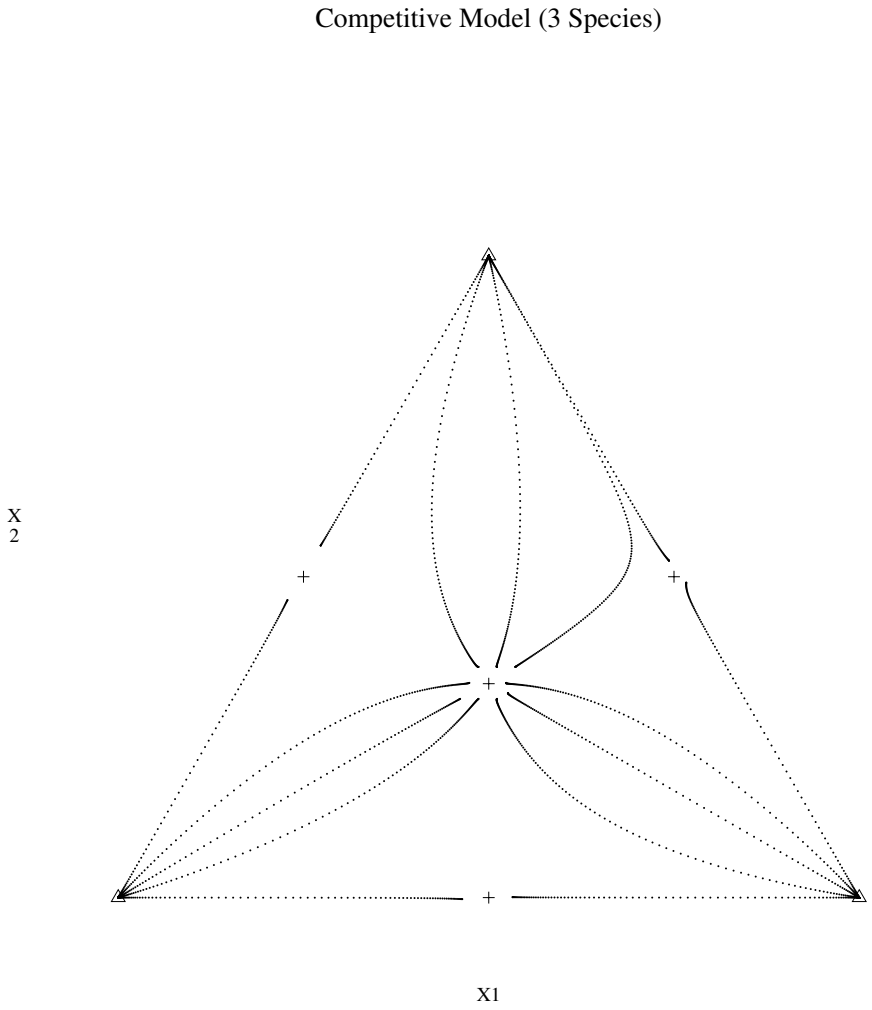

Figure 6: Example for phase portrait of competitive model under constant organization; x-part

4.2 Competitive Model in the CSTR

$$\begin{aligned} A + X_i + T_i &\xrightarrow{k_i} 2X_i + T_i \\ B + X_i &\xrightarrow{\tau_i} X_i + T_i \\ X_i &\xrightarrow{r} \star \\ T_i &\xrightarrow{r} \star \\ A &\xrightarrow{r} \star \\ B &\xrightarrow{r} \star \end{aligned} \tag{42}$$

The kinetic equations read:

$$\begin{aligned} \dot{a} &= -a\sum_{j=1}^{n} k_j x_j t_j + r(a_0 - a) \\ \dot{b} &= -b\sum_{j=1}^{n} \tau_j x_j + r(b_0 - b) \\ \dot{x}_i &= x_i(k_i a t_i - r) \\ \dot{t}_i &= \tau_i b x_i - t_i r \end{aligned} \tag{43}$$

For t $\longrightarrow \infty$ the total concentrations become [63, 60]

$$a + \sum_{i=1}^{n} x_i \longrightarrow a_0 \qquad \text{and} \qquad b + \sum_{i=1}^{n} t_i \longrightarrow b_0 \tag{44}$$

such that

$$\bar{a} = a_0 - \sum_{i=1}^{n} x_i \qquad \text{and} \qquad \bar{b} = b_0 - \sum_{i=1}^{n} t_i \tag{45}$$

There are two inner fixed points with

$$\begin{aligned} \bar{t}_i &= \frac{r}{k_i \bar{a}} \\ \bar{x}_i &= \frac{r^2}{k_i \tau_1 \bar{a} b} \end{aligned} \tag{46}$$

Let

$$\lambda = \sum_{i=1}^{n} \frac{1}{k_i} \quad \text{and} \quad \kappa = \sum_{i=1}^{n} . \frac{1}{k_i \tau_i} \tag{47}$$

Then we get

$$\bar{a}_{1,2} = \frac{1}{2}\left(a_0 \pm \sqrt{a_0^2 - \frac{4r^2\kappa}{\bar{b}}}\right). \tag{48}$$

From (48) we can derive

$$\bar{a} = \frac{r\lambda}{b_0 - \bar{b}} \tag{49}$$

$$\bar{b} = \frac{\kappa r^2}{\bar{a}\,(a_0 - \bar{a})} = \frac{\lambda r - \bar{a} b_0}{\bar{a}} \tag{50}$$

After some algebra, this finally looks like:

$$\bar{a}_{1,2} = \frac{a_0 b_0 + \lambda r \pm \sqrt{(a_0 b_0 - \lambda r)^2 - 4 b_0 \kappa r^2}}{2 b_0} \tag{51}$$

$$\bar{b}_{1,2} = \frac{2 b_0^2 \kappa r}{a_0 b_0 \lambda + 2 b_0 \kappa r - \lambda^2 r \mp \lambda \sqrt{(a_0 b_0 - \lambda r)^2 - 4 b_0 \kappa r^2}} \tag{52}$$

which is equal to

$$\bar{a}_{1,2} = \frac{2r\,(a_0 \lambda + \kappa r)}{a_0 b_0 + \lambda r \mp \sqrt{(a_0 b_0 - \lambda r)^2 - 4 b_0 \kappa r^2}} \tag{53}$$

$$\bar{b}_{1,2} = \frac{a_0 b_0 \lambda + 2 b_0 \kappa r - \lambda^2 r \pm \lambda \sqrt{(a_0 b_0 - \lambda r)^2 - 4 b_0 \kappa r^2}}{2\,(a_0 \lambda + \kappa r)}. \tag{54}$$

So we get for the critical value of the flux-rate r a rather simple expression:

$$r_{crit\pm} = \frac{a_0 b_0}{\lambda \pm 2\sqrt{b_0 \kappa}} \tag{55}$$

Only the solution, where $\lambda > 2\sqrt{b_0 \kappa}$ gives positive values for r. Beyond this bifurcation-point, only the trivial solution can exist.

If all k_i are k and all τ_i are τ in (47) then λ becomes $\frac{n}{k}$ and κ becomes $\frac{n}{k\tau}$, but expression (55) does not depend upon k and we get

$$\hat{r}_{crit\pm} = \frac{2 a_0 b_0}{n \pm 2^{3/2}\sqrt{\frac{n}{tau}}}. \tag{56}$$

So for a given value of r , a_0 , b_0 and τ we can derive a critical value for n.

$$\hat{n}_{crit_{1,2,\pm}} = \frac{2\left(2r + a_0 b_0 \tau \pm 2\sqrt{r^2\,(r + a_0 b_0 tau)}\right)}{r\tau} \tag{57}$$

4.2.1 Stability Analysis

For the stability analysis of the Jacobian matrix of the fixed point for the competitive model under the CSTR it is possible to use the restriction to the simplex (45) in the long time behavior.

So we may reduce the dimension of our problem bye two, since there are two simplices. The remaining two eigenvalues are due to the outflow: $\lambda_{extern,\pm} = -r$.

The Jacobian at the inner equilibrium is then

$$\underline{\mathrm{J}} = \begin{pmatrix} -kxt & -kxt & \dots & kx(1-nx) & 0 & \dots \\ -kxt & -kxt & \dots & 0 & kx(1-nx) & \dots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\ \tau(1-nt) & 0 & \dots & -x\tau - r & -x\tau & \dots \\ 0 & \tau(1-nt) & \dots & -x\tau & -x\tau - r & \dots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \end{pmatrix} \tag{58}$$

$$\lambda_A = \begin{cases} -nkxt & : \quad j = 0 \\ 0 & : \quad j \neq 0 \end{cases} \qquad \lambda_B = kx(1-nx) \qquad \forall j$$

$$\lambda_C = \tau(1-nt) \qquad \lambda_D = \begin{cases} -x\tau - r & : \quad j = 0 \\ -x\tau & : \quad j \neq 0 \end{cases}$$

The eigenvalues are computed by using equations (21)

- $\mathbf{j = 0}$:

$$\Lambda_{0_\pm} = \frac{-nx(kt+\tau) - r \pm \sqrt{\left(nx\left(\tau - kt\right) + r\right)^2 + 4kx(1-nx)(1-nt)}}{2} \tag{59}$$

- $\mathbf{j \neq 0}$:

$$\Lambda_{j_\pm} = \frac{-r \pm \sqrt{r^2 + 4kx(1-nx)(1-nt)}}{2} \tag{60}$$

Again the competitive model in the CSTR. displays the same features as under constant organization: The inner fixed points are saddles.

4.3 Competitive Model with Regeneration

The regeneration model is a closed model that admits no matter-flux, as shown in figure (5), but is similar to the CSTR in it's mathematical structure. Only exchange of energy is possible in order to re-activate the monomers.

The chemical schema looks like

$$\begin{array}{rcl} B + X_i & \xrightarrow{\tau_i} & X_i + T_i \\ A + X_i + T_i & \xrightarrow{k_i} & 2X_i + T_i \\ X_i & \xrightarrow{g_i} & A \\ T_i & \xrightarrow{\gamma_i} & B \end{array} \tag{61}$$

The kinetic equations are

$$\begin{array}{rcl} \dot{a} & = & \sum_{i=1}^{n} x_i \left(g_i - k_i a t_i\right) \\ \dot{b} & = & \sum_{i=1}^{n} \left(\gamma_i t_i - b x_i \tau_i\right) \\ \dot{x}_i & = & x_i \left(k_i a t_i - g_i\right) \\ \dot{t}_i & = & \tau_i b x_i - \gamma_i t_i \end{array} \tag{62}$$

This model is again restricted to the simplices

$$a = 1 - \sum_{j=1}^{n} x_j \qquad \text{and} \qquad b = 1 - \sum_{j=1}^{n} t_j. \tag{63}$$

Because of condition (63) there have to be two zero eigenvalues according to the lack of any flow of matter.

So the dimension of equations (62) can be reduced by two.

$$\begin{array}{rcl} \dot{x}_i & = & x_i \left(k_i (1 - \sum_{j=1}^{n} x_j) t_i - g_i\right) \\ \dot{t}_i & = & \tau_i (1 - \sum_{j=1}^{n} t_j) x_i - \gamma_i t_i \end{array} \tag{64}$$

The fixed points can be calculated by

$$\bar{x}_i = \frac{\gamma_i \bar{t}_i}{\tau_i \bar{b}} = \frac{\gamma_i g_i}{k_i \tau_i \bar{a} \bar{b}} \tag{65}$$

$$\bar{t}_i = \frac{g_i}{k_i \bar{a}} \tag{66}$$

Let

$$\lambda = \sum_{j=1}^{n} \frac{\gamma_j g_j}{\tau_j k_j} \quad \text{and} \quad \kappa = \sum_{j=1}^{n} \frac{g_j}{k_j} \tag{67}$$

Then we get

$$\begin{array}{rcl} \bar{a}^2 \bar{b} - \bar{a} \bar{b} + \lambda & = & 0 \\ \bar{a} \bar{b} - \bar{a} + \kappa & = & 0. \end{array} \tag{68}$$

So it is possible to calculate the equilibria of (64)

$$\begin{aligned} \bar{a}_{\pm} &= \frac{1+\kappa \pm \sqrt{(\kappa-1)^2-4\lambda}}{2} \\ &= \frac{2(\lambda+\kappa)}{1+\kappa \mp \sqrt{(\kappa-1)^2-4\lambda}}, \end{aligned} \tag{69}$$

$$\begin{aligned} \bar{b}_{\pm} &= \frac{1-\kappa \pm \sqrt{(\kappa-1)^2-4\lambda}}{1+\kappa \pm \sqrt{(\kappa-1)^2-4\lambda}} \\ &= \frac{\kappa-\kappa^2+2\lambda \pm \kappa\sqrt{(\kappa-1)^2-4\lambda}}{2(\lambda+\kappa)}. \end{aligned} \tag{70}$$

Here the condition for real roots of (69) is

$$\kappa > 1+2\sqrt{\lambda} \qquad \text{or} \qquad \kappa < 1-2\sqrt{\lambda}. \tag{71}$$

If we consider equal reaction constants $k_i = \alpha$, $\tau_i = \beta$, $g_i = \gamma$ and $\gamma_i = \delta$ so we get the critical values for e.g. α:

$$\alpha_{crit} = \gamma n(1+2\delta\beta \pm 2\sqrt{\delta\beta(1+\delta\beta)}) \tag{72}$$

Also a critical value for n can be derived. Since $n \in \mathbb{N}$ the value n_{crit} is a upper limit.

$$n_{crit} = \frac{\alpha(1+2\beta\delta \pm 2\sqrt{\beta\delta(1+\beta\delta)})}{\gamma} \tag{73}$$

4.3.1 Stability Analysis

Because circulant blocks of the Jacobian are necessary, only equal reaction constants are considered. Here again the bars for the equilibria are omitted because it is much simpler to write. The eigenvalues of the Jacobian at the interior equilibrium are

- **j = 0:**

$$\Lambda_{j=0_{\pm}} = \frac{-nkxt-\gamma \pm \sqrt{((\gamma-nkxt)^2+4kx\tau(1-nx)(1-nt))}}{2} \tag{74}$$

- $\mathbf{j \neq 0}$:

$$\Lambda_{j\neq 0_{\pm}} = \frac{-\gamma \pm \sqrt{\gamma^2 + 4kx\tau(1-nx)(-nt)}}{2} \tag{75}$$

Once more all inner rest points are saddles.

5 Mutualistic Model

5.1 Mutualistic System under Constant Organization

The mutualistic system is coupled cyclic, such that the n-th species helps (indirectly) to replicate the first one. This model is closely related to the hyper-cycle model [61, 62]. All indices are meant to be taken modulo n.

$$\begin{aligned} (A) + X_i + T_{i-1} &\xrightarrow{k_i} 2X_i + T_{i-1} \\ (B) + X_i &\xrightarrow{\tau_i} X_i + T_i \\ X_i &\xrightarrow{\Phi^x} \star \\ T_i &\xrightarrow{\Phi^\sim} \star \end{aligned} \tag{76}$$

Again the kinetic equations may be formulated.

$$\begin{aligned} \dot{x}_i &= x_i \left(k_i t_{i-1} - \sum_i^n k_i x_i t_{i-1} \right) \\ \dot{t}_i &= x_i \tau_i - t_i \sum_i^n x_i t_i \end{aligned} \tag{77}$$

with the inner fixed point:

$$\begin{aligned} \bar{x}_i &= \frac{1}{k_{i+1}\tau_i \sum_j^n \frac{1}{k_{j+1}\tau_j}} \\ \bar{t}_i &= \frac{1}{k_{i+1} \sum_j^n \frac{1}{k_{j+1}}} \end{aligned} \tag{78}$$

5.1.1 Stability Analysis

Again the case with equal reaction constants is considered.

$$k_i = k \qquad \tau_i = \tau$$

Since the Jacobian of this model is almost identical with that of the competitive model only the part B of (17) is given in detail.

$$\mathbf{B} = \begin{pmatrix} -\frac{k}{n^2} & -\frac{k}{n^2} & \dots & \frac{k}{n}\left(1-\frac{1}{n}\right) \\ \frac{k}{n}\left(1-\frac{1}{n}\right) & -\frac{k}{n^2} & \dots & -\frac{k}{n^2} \\ \vdots & \vdots & \ddots & \vdots \\ -\frac{k}{n^2} & -\frac{k}{n^2} & \dots & -\frac{k}{n^2} \end{pmatrix}$$

The eigenvalues of the four circulant parts are then:

$$\lambda_A = \begin{cases} -\frac{k}{n} & : \quad j = 0 \\ 0 & : \quad j \neq 0 \end{cases} \qquad \lambda_B = \begin{cases} 0 & : \quad j = 0 \\ \frac{k}{n} e^{2\pi i j/n} & : \quad j \neq 0 \end{cases}$$

$$\lambda_C = \begin{cases} 0 & : \quad j = 0 \\ \tau & : \quad j \neq 0 \end{cases} \qquad \lambda_D = -\tau \qquad \forall j$$

- **j=0** :

$$\Lambda_{0_1} = -\frac{k}{n} \qquad \text{and} \qquad \Lambda_{0_2} = -\tau \tag{79}$$

  Again $\Lambda_{0_{1,2}}$ are the external eigenvalues.

- **j $\neq$0** :

$$\Lambda_j = \frac{-\tau \pm \sqrt{\tau^2 + 4\frac{k}{n} e^{-2\pi i j/n} \tau}}{2} \tag{80}$$

Bifurcations occur for vanishing real parts of the eigenvalues. Thus the following formula has proved to be useful.

$$\Re(\sqrt{a + \imath\, b}) = \sqrt{\frac{1}{2}\left(a + \sqrt{a^2 + b^2}\right)} \tag{81}$$

So we may apply equation (81) to equation (80), and get

$$\Re(\Lambda_j) = -\tau + \sqrt{\frac{\tau}{2}} \sqrt{\tau + \frac{4k}{n}\cos\varphi + \sqrt{\tau^2 + \frac{8k\tau}{n}\cos\varphi + \frac{16k^2}{n^2}}}. \tag{82}$$

After some algebra a critical value for the occurrence of Hopf-Bifurcations is derived.

$$\left(\frac{k}{\tau}\right)_{crit} = -\frac{1}{n}\frac{\sin^2\left(\frac{2\pi(n-1)j}{n}\right)}{\cos\left(\frac{2\pi(n-1)j}{n}\right)} \tag{83}$$

Only some values of j can fulfill (83).

$$\frac{n}{4} < j < \frac{3n}{4} \qquad \Longrightarrow \qquad n > 2$$

If we consider this condition for various values of n we can see that

- **n = 3 , j = 1** :

$$\left(\frac{\tau}{k}\right)_{crit} = \frac{1}{2}$$

- **n = 4 , j = 2** :

$$\frac{\tau}{k} = 0$$

- **n ≥ 5** :
  There are no more stable fixed points. All solutions will yield limit cycles.

5.1.2 Mutualistic Model for two species

Again the two-species case is investigated at first:

The kinetic equations read

$$\begin{aligned} \dot{x} &= x\left(k_1(1-t) - k_1 x(1-t) - k_2(1-x)t\right) \\ \dot{t} &= \tau_1 x - t\left(\tau_1 x + \tau 2(1-x)\right) \end{aligned} \tag{84}$$

The Jacobian at the inner fixed point becomes

$$\mathbf{J} = \begin{pmatrix} 0 & -\frac{k_1 k_2 (k_1+k_2)\tau_1\tau_2}{(k_1\tau_2+k_2\tau_1)^2} \\ \frac{k_1\tau_2+k_2\tau_1}{k_1+k_2} & -\frac{(k_1+k_2)\tau_1\tau_2}{k_1\tau_2+k_2\tau_1} \end{pmatrix}. \tag{85}$$

The eigenvalues of the inner fixed point then are

$$\lambda_{+,-} = \frac{1}{2}\left(-\frac{(k_1+k_2)\tau_1\tau_2}{k_1\tau_2+k2_t a u_1} \pm \sqrt{\frac{(k_1+k_2)^2\tau_1^2\tau_2^2}{(k_1\tau_2+k_2\tau_1)^2} - \frac{4k_1k_2\tau_1\tau_2}{k_1\tau_2+k_2\tau_1}}\right). \tag{86}$$

5.1.3 Mutualistic Model for three species

For the mutualistic model we get very large and not-at-all easy to handle formulas for the characteristic polynomial. Since it was impossible to factor this polynomial into nicer looking terms, the Routh-Hurwitz conditions had to be applied in order to get information about the stability of the eigenvalues.

For the characteristic polynomial is of fourth order, we get

$$\mathcal{P}_4 = a_4\lambda^4 + a_3\lambda^3 + a_2\lambda^2 + a_1\lambda + a_0$$

where the coefficients are:

$$\begin{aligned}
a_4 &= 1 \\
a_3 &= \frac{1}{\Gamma} 2\left(k_1k_2 + k_1k_3 + k_2k_3\right)\tau_1\tau_2\tau_3 \\
a_2 &= \frac{1}{\Gamma}\Big(\tau_1\tau_2\tau_3\left(k_1k_2 + k_1k_3 + k_2k_3\right)^2 \\
&+ k_1k_2^2k_3^2\tau_1\tau_2 + k_1^2k_2^2k_3\tau_1\tau_3 + k_1^2k_2^2k_3\tau_2\tau_3 \\
a_1 &= \frac{1}{\Gamma}k_1k_2k_3(k_1k_2 + k_1k_3 + k_2k_3)\tau_1^2\tau_2^2\tau_3^2 \\
a_0 &= \frac{1}{\Gamma}k_1^2k_2^2k_3^2\tau_1^2\tau_2^2\tau_3^2 \\
\Gamma &= (k_2k_3\tau_1\tau_2 + k_1k_2\tau_1\tau_3 + k_1k_3\tau_2\tau_3)^2
\end{aligned} \tag{87}$$

So we get the following conditions for eigenvalues with negative real part

$$\begin{aligned}
3\left(k_1k_2^2k_3^2\tau_1\tau_2 + k_1^2k_2^2k_3\tau_1\tau_3 + k_1^2k_2k_3^2\tau_2\tau_3\right) \quad < \\
2\tau_1\tau_2\tau_3\left(k_1^2k_2^2 + k_1^2k_3^2 + k_2^2k_3^2 + k_1^2k_2k_3 + k_1k_2^2k_3 + k_1k_2k_3^2\right)
\end{aligned} \tag{88}$$

Since this condition is not very illustrative and but for numerical application, is not very useful, it is convenient to consider two special cases, where either k_i or τ_i are equal.

- **Case 1:** $k_1 = k_2 = k_3 = k$
  The equation (88) reduces to the much simpler condition

$$k = \frac{6\tau_1\tau_2\tau_3}{\tau_1\tau_2 + \tau_1\tau_3 + \tau_2\tau_3}. \tag{89}$$

- **Case 2:** $\tau_1 = \tau_2 = \tau_3 = \tau$
  Here equation (88) gives

$$\tau = \frac{3k_1k_2k_3}{2\left(k_1k_2 + k_1k_3 + k_2k_3\right)}. \tag{90}$$

Here the critical values are calculated, where primary Hopf-Bifurcations occur. For equal reaction constants, we get (104).

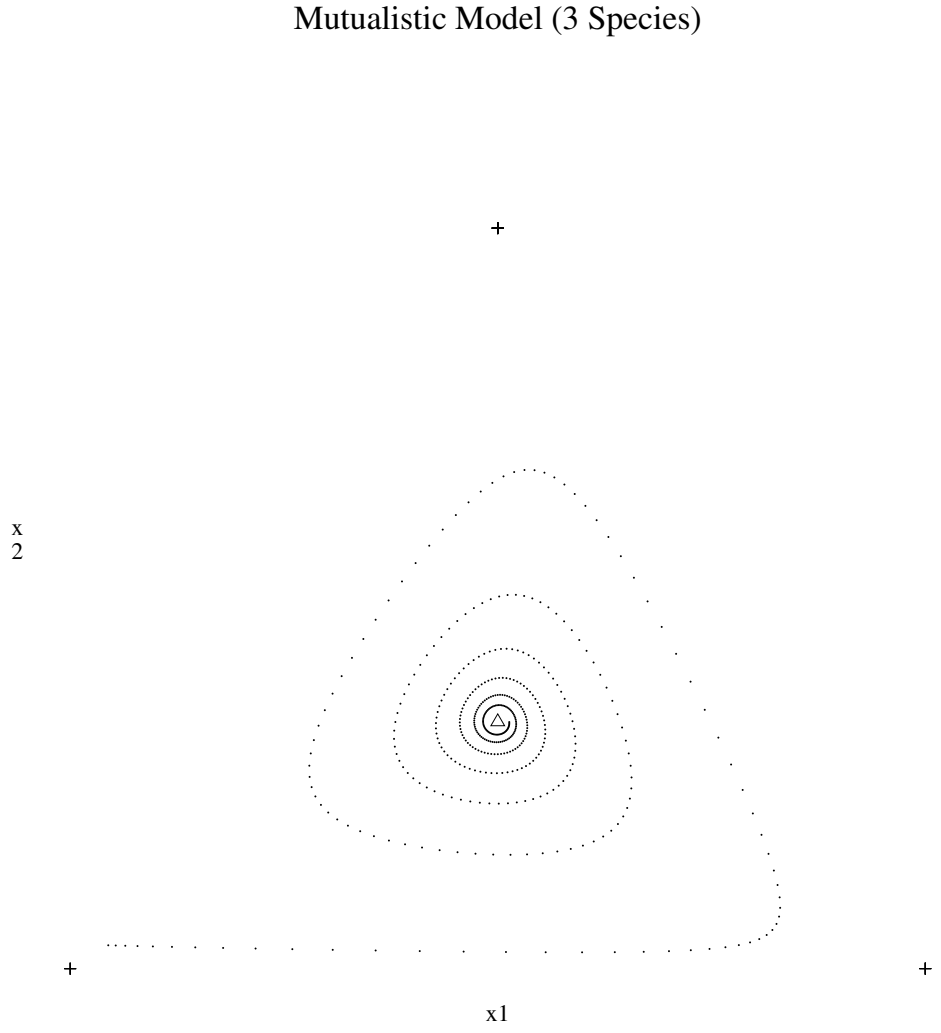

Figure 7: Example for phase portrait of mutualistic model under constant organization. A fixed point is shown; x-part

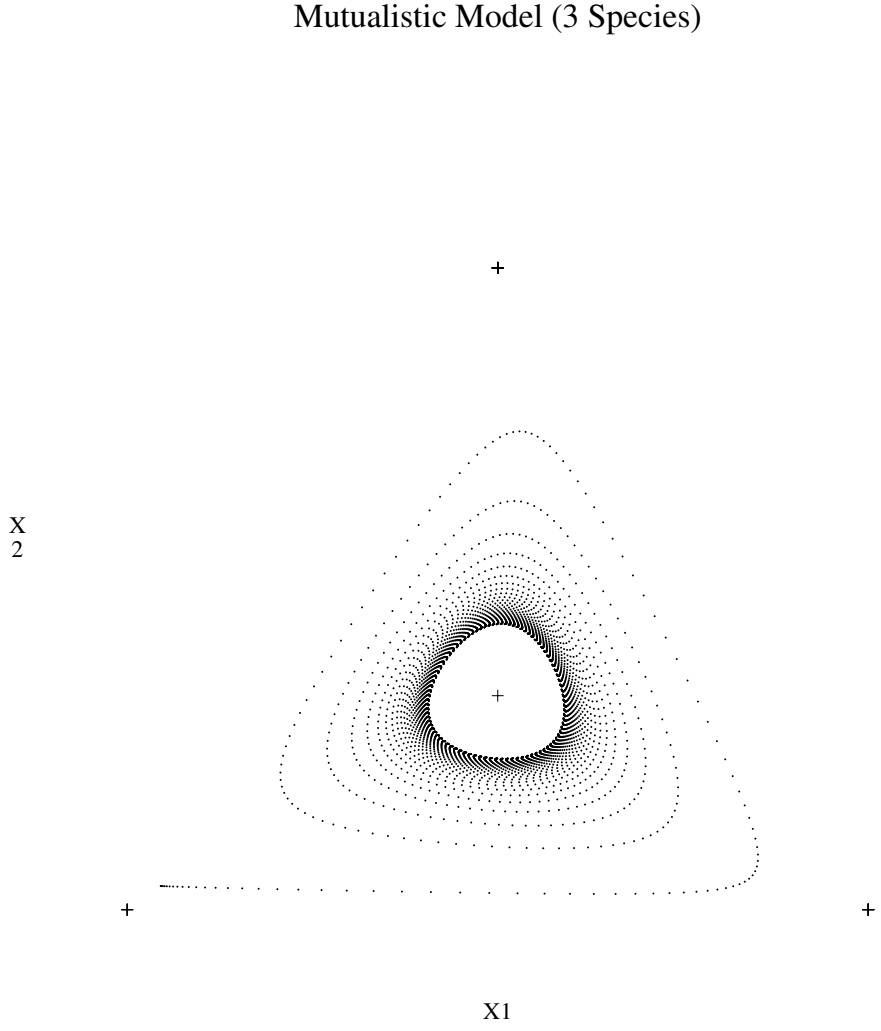

Figure 8: Example for phase portrait of mutualistic model under constant organization. A limit cycle is shown; x-part

5.2 Mutualistic Model in the CSTR

$$\begin{aligned} A + X_i + T_{i-1} &\xrightarrow{k_i} 2X_i + T_{i-1} \\ B + X_i &\xrightarrow{\tau_i} X_i + T_i \\ X_i &\xrightarrow{r} \star \\ T_i &\xrightarrow{r} \star \\ A &\xrightarrow{r} \star \\ B &\xrightarrow{r} \star \end{aligned} \tag{91}$$

The kinetic equations read:

$$\begin{aligned} \dot{a} &= -a\sum_{j=1}^{n} k_j x_j t_{j-1} + r(a_0 - a) \\ \dot{b} &= -b\sum_{j=1}^{n} \tau_j x_j + r(b_0 - b) \\ \dot{x}_i &= x_i(k_i a t_{i-1} - r) \\ \dot{t}_i &= \tau_i b x_i - t_i r \end{aligned} \tag{92}$$

For t $\longrightarrow \infty$ the total concentrations become

$$a + \sum_{i=1}^{n} x_1 \longrightarrow a_0 \qquad \text{and} \qquad b + \sum_{i=1}^{n} t_i \longrightarrow b_0 \tag{93}$$

such that

$$\bar{a} = a_0 - \sum_{i=1}^{n} x_i \qquad \text{and} \qquad \bar{b} = b_0 - \sum_{i=1}^{n} t_i \tag{94}$$

There are two inner fixed points with

$$\bar{t}_i = \frac{r}{k_{i+1}\bar{a}} \tag{95}$$

$$\bar{x}_i = \frac{r^2}{k_{i+1}\tau_1 \bar{a}\bar{b}} \tag{96}$$

Let

$$\lambda = \sum_{i=1}^{n} \frac{1}{k_i} \quad \text{and} \quad \kappa = \sum_{i=1}^{n} \frac{1}{k_{i+1}\tau_i} \tag{97}$$

Since the chances from the competitive model are completely packed into λ and κ, we are glad to leave equation (48) until equation (54) untouched and use them also for the mutualistic type of replication.

5.2.1 Stability Analysis

For the sake of simplicity in the following part only the symbols of the variables a , b , x , t instead of the equilibrium concentrations $\bar{a}$, $\bar{b}$,$\bar{x}$ and $\bar{t}$ are used. Since the simplices exist only at the equilibrium points, there can arise no error from that.

$$\lambda_A = \begin{cases} -nkxt & : \quad j = 0 \\ 0 & : \quad j \neq 0 \end{cases} \qquad \lambda_B = \begin{cases} kx(1-nx) & : \quad j = 0 \\ kx(1-nx)e^{\left(\frac{-2\pi ij}{n}\right)} & : \quad j \neq 0 \end{cases}$$

$$\lambda_C = \tau(1-nt) \qquad \lambda_D = \begin{cases} -x\tau - r & : \quad j = 0 \\ -x\tau & : \quad j \neq 0 \end{cases}$$

- **j=0 :**

$$\Lambda_{0,\pm} = \frac{-nkxt - r \pm \sqrt{(nkxt)^2 + 4\frac{x}{t}r\tau b}}{2} \tag{98}$$

- **j $\neq$ 0 :**

$$\Lambda_{j,\pm} = \frac{-r \pm \sqrt{r^2 + 4\frac{x}{t}re^{\left(\frac{-2\pi ij}{n}\right)}}}{2} \tag{99}$$

If we use condition (81) to calculate the real part of the eigenvalues we get

$$\Re(\Lambda) = \frac{1}{2} - r + \sqrt{\frac{1}{2}\left(r^2 + \frac{4xr\tau b}{t}\cos(\varphi) + r\sqrt{\Phi}\right)} \tag{100}$$

$$\Phi = r^2 + \frac{8xr\tau b}{t}\cos(\varphi) + \left(\frac{x\tau b}{t}\right)^2$$

$$\varphi = \frac{-2\pi j}{n} = \frac{2\pi\,(n-1)\,j}{n} \tag{101}$$

As can be easily seen equation (100) can be simplified to

$$\left(r^2 - \frac{4xr\tau b}{t}\cos(\varphi)\right)^2 = r^2\left(r^2 + \frac{8xr\tau b}{t}\cos(\varphi) + \frac{16x^2\tau^2 b^2}{t^2}\right), \tag{102}$$

which gives after some more simplifications

$$-r\cos(\varphi) = \frac{\tau b}{t}\sin^2(\varphi). \tag{103}$$

So finally the condition for vanishing real part of the eigenvalues (99) is

$$\left(\frac{r}{\tau}\right)_{crit} = \frac{\bar{b}}{\bar{t}} \cdot \frac{\sin^2\left(\frac{2\pi(n-1)j}{n}\right)}{\cos\left(\frac{2\pi(n-1)j}{n}\right)}. \tag{104}$$

5.3 Mutualistic Model with Regeneration

The chemical schema looks like

$$\begin{aligned} B + X_i &\xrightarrow{\tau_i} X_i + T_i \\ A + X_i + T_{i-1} &\xrightarrow{k_i} 2X_i + T_{i-1} \\ X_i &\xrightarrow{g_i} A \\ T_i &\xrightarrow{\gamma_i} B \end{aligned} \tag{105}$$

The kinetic equations are

$$\begin{aligned} \dot{x}_i &= x_i\left(k_i a t_{i-1} - g_i\right) \\ \dot{t}_i &= \tau_i b x_i - \gamma_i t_i \\ \dot{a} &= \sum_{i=1}^{n} x_i\left(g_i - k_i a t_{i-1}\right) \\ \dot{b} &= \sum_{i=1}^{n}\left(\gamma_i t_i - b x_i \tau_i\right) \end{aligned} \tag{106}$$

This model is again restricted to the simplices (63). If we have

$$\lambda = \sum_{j=1}^{n} \frac{\gamma_j g_{j+1}}{\tau_j k_{j+1}} \quad \text{and} \quad \kappa = \sum_{j=1}^{n} \frac{g_j}{k_j}, \tag{107}$$

then the inner equilibria of (106) are the same as (69) and (70) with

$$\bar{x}_i = \frac{\gamma_i \bar{t}_i}{\tau_i \bar{b}} = \frac{\gamma_i g_{i+1}}{k_{i+1}\tau_i \bar{a}\bar{b}} \tag{108}$$

$$\bar{t}_i = \frac{g_{i+1}}{k_{i+1}\bar{a}}. \tag{109}$$

5.3.1 Stability Analysis

Once again, only the eigenvalues with equal reaction constants at the inner fixed points are calculated.

- **j=0:**

$$\Lambda_{j=0_\pm} = \frac{-nkxt - \gamma \pm \sqrt{\left((\gamma - nkxt)^2 + 4\frac{xg}{t}\tau(1-nt)\right)}}{2} \tag{110}$$

- **j ≠ 0:**

$$\Lambda_{j\neq 0_{pm}} = \frac{-\gamma \pm \sqrt{\gamma^2 + \frac{xg}{t}\tau(1-nt)e^{\frac{2\pi i(n-1)j}{n}}}}{2} \tag{111}$$

So we get for the real part of (111)

$$\Re(\Lambda) = \frac{1}{2}\left(-\gamma + \sqrt{\frac{1}{2}\left(\gamma^2 + \frac{xg\tau(1-nt)}{t}\cos(\varphi) + \sqrt{\Phi}\right)}\right) \tag{112}$$

$$\Phi = \gamma^4 + \frac{2\gamma^2 xg\tau(1-nt)}{t}\cos(\varphi) + \left(\frac{xg\tau(1-nt)}{t}\right)^2$$

$$\varphi = \frac{2\pi(n-1)j}{n} \tag{113}$$

Some transformations give finally the condition for vanishing real part:

$$\left(\frac{\gamma}{g\tau}\right)_{crit.} = -\frac{\bar{x}\bar{b}}{4\bar{t}} \cdot \frac{\sin^2\left(\frac{2\pi(n-1)j}{n}\right)}{\cos\left(\frac{2\pi(n-1)j}{n}\right)}. \tag{114}$$

6 Mutation

Since the famous work of Darwin [10] we know that selection alone is not sufficient for the development of new species, but there also has to be mutation. So we have the "Quasi-species"[12], [13], where selection works on. As we have seen, the Replicator-related models are quite complicated to deal with, and mutation does not make it easier ...

The general model for a network with replication is:

$$\begin{array}{rcl} (B) + X_k & \stackrel{Q^{\sim}_{km}\tau_k}{\longrightarrow} & X_k + T_k + T_m \\ (A) + X_k + T_l & \stackrel{Q^{x}_{km}a_{kl}}{\longrightarrow} & X_k + X_m + T_l \\ X_k & \stackrel{\Phi^x}{\longrightarrow} & \star \\ T_k & \stackrel{\Phi^{\sim}}{\longrightarrow} & \star \end{array} \tag{115}$$

Once more there are n replicating species with genes X_k and gene-products T_k, where $k = 1,\ldots n$. A and B denote the low-molecular substrates. This time replication is erroneous and we introduce a mutation matrix $\mathbf{Q}$ whose elements Q_{kl} represent the fraction of replications with X_l as a template and X_k as copy. Since replication has to be necessarily either correct or erroneous, $\mathbf{Q}$ is a column-stochastic matrix [72] :

$$\sum_{k=1}^{n} Q_{kl} = 1 \qquad \forall k = 1, 2, \ldots, n. \tag{116}$$

Again the kinetic equations can be derived:

$$\begin{aligned} \dot{x}_k &= \sum_{j=1}^{n} Q^{x}_{kj} x_j \sum_{i=1}^{n} a_{ji} t_i - x_k \Phi^x \\ \dot{t}_k &= \sum_{j=1}^{n} Q^{\sim}_{kj} \tau_j x_j - t_k \Phi^{\sim} \end{aligned} \tag{117}$$

where the fluxes Φ^x and $\Phi^{\sim}$ are the same as (5).

Using condition (116) is is possible to part (117) into the replication-parts $\mathcal{R}$ and $\mathcal{T}$ and mutation part $\mathcal{M}$, such that

$$\begin{aligned} \dot{x}_k &= \mathcal{R} + \mathcal{M}^x \\ \dot{t}_k &= \mathcal{T} + \mathcal{M}^{\sim}, \end{aligned} \tag{118}$$

which gives finally

$$\begin{aligned} \dot{x}_k &= x_k\left((\mathbf{A}t)_k - \Phi^x\right) + \sum_{j\neq k}\left[Q^x_{kj}x_j(\mathbf{A}t)_j - Q^x_{jk}x_k(\mathbf{A}t)_k\right] \qquad (119)\\ \dot{t}_k &= \tau_k x_k - t_k\Phi^{\sim} + \sum_{j\neq k}\left[Q^{\sim}_{kj}\tau_j x_j - Q^{\sim}_{jk}\tau_k x_k\right] \end{aligned}$$

The mutation matrices $\mathbf{Q}^x$ and $\mathbf{Q}^{\sim}$ have the form

$$\mathbf{Q}^i = \begin{pmatrix} 1-n\epsilon^i & \epsilon^i & \dots & \epsilon^i \\ \epsilon^i & 1-n\epsilon^i & \dots & \epsilon^i \\ \vdots & \vdots & \ddots & \vdots \\ \epsilon^i & \epsilon^i & \dots & 1-n\epsilon^i \end{pmatrix} \qquad (120)$$

so that (119) finally becomes

$$\begin{aligned} \dot{x}_k &= x_k\left((\mathbf{A}t)_k - \Phi^x\right) + \epsilon^x \cdot \sum_{j\neq k}\left[x_j(\mathbf{A}t)_j - x_k(\mathbf{A}t)_k\right] \qquad (121)\\ \dot{t}_k &= \tau_k x_k - t_k\Phi^{\sim} + \epsilon^{\sim} \cdot \sum_{j\neq k}\left[\tau_j x_j - \tau_k x_k\right] \end{aligned}$$

Mutation can be controlled by two parameters ϵ^x and $\epsilon^{\sim}$. In the case of vanishing mutation ($\epsilon^i \to 0$) we simply get the replication terms $\mathcal{R}$ and $\mathcal{T}$. So there are three possible cases:

1. Errors due to translation: These do not create new genes and thus will never create new species. The only effect is a change of the components of the selection matrix.

2. Errors due to replication: New species can be created and thus this sort of mutation is the interesting one.

3. Errors due to both sorts of reaction.

Definition 6.1 $\mathbf{x} = (x_1, \dots, x_n, t_1, \dots, t_n)$ *denotes the concentrations of the species* X_k *and* T_k*, where* $k = 1, \dots, n$.

Definition 6.2 *The set* $\mathcal{S}_\mathbf{n} = \mathcal{S}^x_n \oplus \mathcal{S}^{\sim}_n$*, according to the conditions* $\sum_{j=1}^n x_j = 1$ *and* $\sum_{j=1}^n t_j = 1$*, is partitioned into interior (int* $\mathcal{S}_\mathbf{n}$*) and boundary (bd* $\mathcal{S}_\mathbf{n}$*) of sub-simplices on which one or more species* $\mathbf{x_i}$ *are non-existing.*

Boundary sets are invariant since:

$$x_k = 0 \Rightarrow \dot{x}_k = 0 \Rightarrow \ddot{x}_k = 0 \ldots$$

holds for equation (3). So the following notations are used:

Definition 6.3 *$\bar{F}_K$ is the sub-simplex on with all species X_k, $k \in K$ are missing. The index K comprises all possible combinations of vanishing concentrations,*

$$K \in J \quad with \quad J = \mathcal{P}(\mathcal{N}) \setminus \{\emptyset, \mathcal{N}\},$$

where $\mathcal{P}(\mathcal{N})$ is the power set of $\mathcal{N} = \{1, 2, \ldots, n\}$. Thus $\bar{F}_K = \mathcal{S}_m(\mathcal{N} \setminus K)$ with $m = \#(\mathcal{N} \setminus K) = n - \#K$. The interior of the (sub)simplex $\mathcal{S}_m$ is denoted by F_K.

Theorem 6.1 (Rest point-Migration-Theorem (RPM) [72]) *Let $\bar{\mathbf{x}}= (x_1, \ldots, x_n, t_1, \ldots, t_n)$, $\epsilon = (\epsilon^x, \epsilon^\sim)$ and $\bar{\mathbf{x}}_\mathbf{0}$ be a rest point of equation (117) which lies on bd $\mathcal{S}_n$, say $\bar{\mathbf{x}}_\mathbf{0} \in F_K$, and let $\mathcal{M} = (\mathcal{M}^x, \mathcal{M}^\sim)$ be a mutation field, with corresponding mutation parameters ϵ^x and $\epsilon^\sim$, for which $\mathcal{M}_k(\bar{\mathbf{x}}_\mathbf{0}, \epsilon) > 0$ holds for all $k \in K$. Then the following statements are true for sufficiently small values of the perturbation parameter $\epsilon > 0$:*

1. *If the rest point $\bar{\mathbf{x}}_\mathbf{0}$ is regular then*

$$\bar{\mathbf{x}}(\epsilon) \in \ int\ \mathcal{S}_n \Leftrightarrow \ the\ transversal\ eigenspace\ E_T(\bar{\mathbf{x}}_\mathbf{0})\ is\ stable.$$

2. *If the transversal eigenspace $E_T(\bar{\mathbf{x}}_\mathbf{0})$ has at least one positive eigenvalue, $\lambda_l > 0$, then all fixed points $\bar{\mathbf{x}}_\mathbf{j}$ derived from $\bar{\mathbf{x}}_\mathbf{0}$ lie outside the simplex $\mathcal{S}_n$.*

Proof: equivalent to the proof of the rest point migration theorem, given in Stadler and Schuster [72].

Models with general selection matrices are not particularly suitable for analytical treatment, thus it is necessary to restrain the problem to circulant selection matrices $\mathbf{A}$. Therefore, once more the competitive- and mutualistic model are investigated.

Theorem 6.2 *For equal reaction constants, ($k_i = k$, and $\tau_i = \tau$), the inner rest point is: $\mathcal{P}_{int} = (\ldots, \frac{1}{n}, \ldots)$.*

Proof: This can be checked very easily. ■

6.1 Competitive model with Mutation

Here (121) has the much simpler form

$$\begin{aligned} \dot{x}_k &= x_k \left(k_k t_k - \sum_{l=1}^{n} x_l k_l t_l \right) + \epsilon^x \left(-(n-1) k_k x_k t_k + \sum_{j \neq k} k_j x_j t_j \right) \\ \dot{t}_k &= \tau_k x_k - t_k \sum_{l=1}^{n} \tau_l x_l + \epsilon^{\sim} \left(-(n-1) + \tau_k x_k \sum_{j \neq k} (\tau_j x_j \right) \end{aligned} \tag{122}$$

All transversal eigenvalues are negative, so the rest points of all sub-simplices will have to move into the interior, according to the RPM. Since there is no chance to obtain analytical results for the full system, once more only the case with equal reaction constants was investigated, so $k_i = k$ and $\tau_i = \tau$. The block structure of the Jacobian keeps circulant, because the mutation matrix was assumed to be circulant.

So we get the following eigenvalues for the Jacobian at the inner rest point $\mathcal{P}_{int}$:

- **j=0:**

$$\Lambda_{0_+} = -\frac{k}{n} \quad \text{and} \quad \Lambda_{0_-} = -\tau \tag{123}$$

  These are again the external eigenvalues, which do not influence the behavior of the dynamical system.

- **j $\neq$ 0 :**

$$\Lambda_{j\pm} = \frac{-k\epsilon^x - \tau \pm \sqrt{(\tau - k\epsilon^x)^2 + 4\frac{k\tau}{n}(1 - n\epsilon^x)(1 - n\epsilon^{\sim})}}{2} \tag{124}$$

Note that in the limit of vanishing mutation we get the same eigenvalues as in the unperturbed case.

Thus it is possible to calculate the critical values for ϵ^x and $\epsilon^\sim$, where the inner fixed point becomes a sink.

$$\epsilon^x_{crit} = \frac{n\epsilon^\sim - 1}{n(n\epsilon^\sim - 2)} \tag{125}$$

or

$$\epsilon^\sim_{crit} = \frac{2n\epsilon^x - 1}{n(n\epsilon^x - 1)} \tag{126}$$

If we consider the case where either ϵ^x or $\epsilon^\sim$ are zero, very simple conditions for the critical values can be derived.

$$\hat{\epsilon}^x_{crit} = \frac{1}{2n} \qquad \text{or} \qquad \hat{\epsilon}^\sim_{crit} = \frac{1}{n} \tag{127}$$

- **Case1:** $\epsilon^\sim = 0$
  The typical behavior in this case is that the originally one-dimensional rest points remain sinks for values less than ϵ^x_{crit}. Then all rest points collapse and only one sink remains.

- **Case2:** $\epsilon^x = 0$
  Here the subcritical case is the same as above, but the rest points will not vanish.

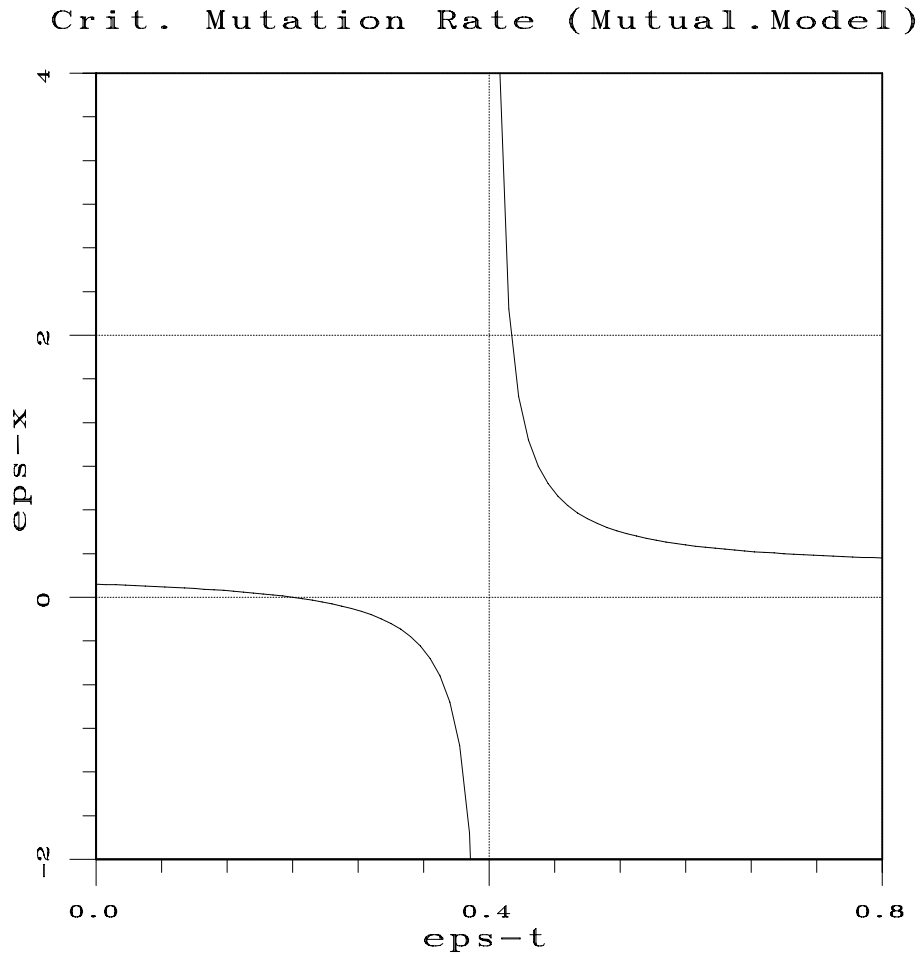

Figure 9: Plot of ϵ^x against $\epsilon^{\sim}$ for $n = 5$;

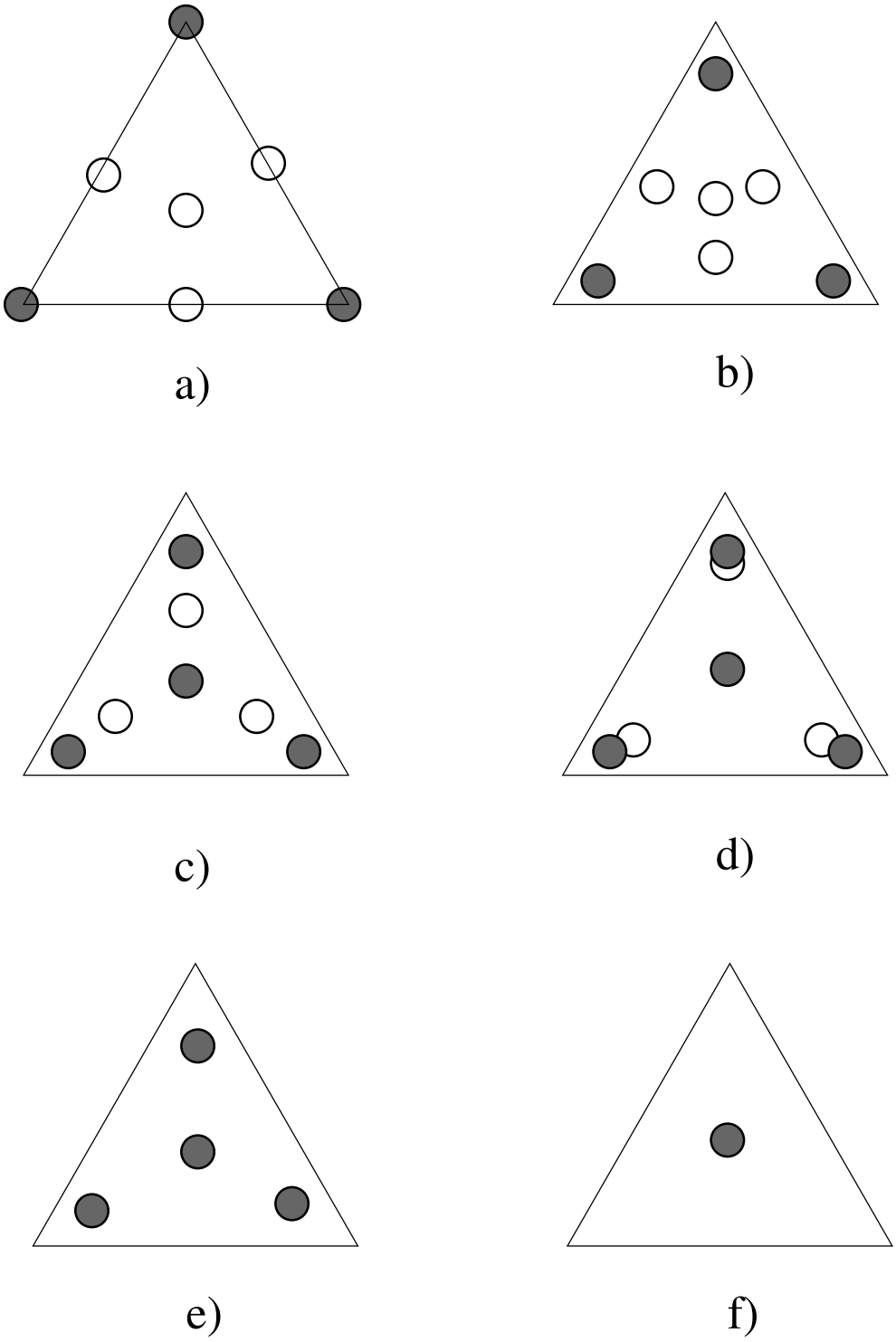

Figure 10: The development of the fixed points of the competitive model for various values of ϵ^x, where $\epsilon^{\sim} = 0$ for $n = 3$: a) no mutation; b) subcritical values for ϵ^x; c)–f) transcritical value for ϵ^x; $\bullet$:Sink; $\circ$: Saddle

6.2 Mutualistic model with Mutation

Equation (121) reads this time:

$$\begin{aligned}\dot{x}_k &= x_k\left(k_k t_{k-1} - \sum_{l=1}^{n} x_l k_l t_{l-1}\right) + \epsilon^x\left(-(n-1)k_k x_k t_{k-1} + \sum_{j\neq k} k_j x_j t_{j-1}\right)\\ \dot{t}_k &= \tau_k x_k - t_k \sum_{l=1}^{n} \tau_l x_l + \epsilon^{\sim}\left(-(n-1) + \tau_k x_k \sum_{j\neq k}(\tau_j x_j\right)\end{aligned} \tag{128}$$

The mutualistic model has the same external eigenvalues but for $j \neq 0$ we get

$$\Lambda_{j\pm} = \frac{-k\epsilon^x - \tau \pm \sqrt{(\tau - k\epsilon^x)^2 + 4\frac{k\tau}{n}(1-n\epsilon^x)(1-n\epsilon^{\sim})e^{-2\pi\imath j/n}}}{2} \tag{129}$$

The critical values for the mutation coefficients have been calculated explicitly, but they are of third order and the results are much too complicated to be stated here.

So just a very special case is treated with $n = 3$. Then we have

$$\begin{aligned}\hat{\epsilon}^x_{crit} &= -\frac{1}{9} - \frac{\tau}{6\,k} + \\ &+ \frac{\alpha^{\frac{1}{3}}}{18\,k} + \frac{4\,k^2 - 168\,k\,\tau - 99\,\tau^2}{18\,\alpha^{\frac{1}{3}}\,k}\end{aligned} \tag{130}$$

where

$$\alpha = (-8k^3 + 990k^2\tau + 108k\tau^2 + 459\tau^3 + 23^{5/2}(\tau(k+3\tau)^2\sqrt{\beta}))$$

and

$$\beta = -8k^3 + 711k^2\tau + 486k\tau^2 + 135\tau^3$$

It's interesting that the mutation parameter ϵ^x has no influence on the phase-portraits, if the condition for the existence of a limit cycle (83) is not fulfilled. So, if there is a stable equilibrium, it will remain.

When there is a limit cycle, small values of ϵ^x will not change the phase portraits until the critical mutation rate is reached. Above that value the inner rest point is stable again.

In this example the Hopf-bifurcation occurs at $k = 2\,\tau$, and we can see that $\epsilon^x(2) = 0$.

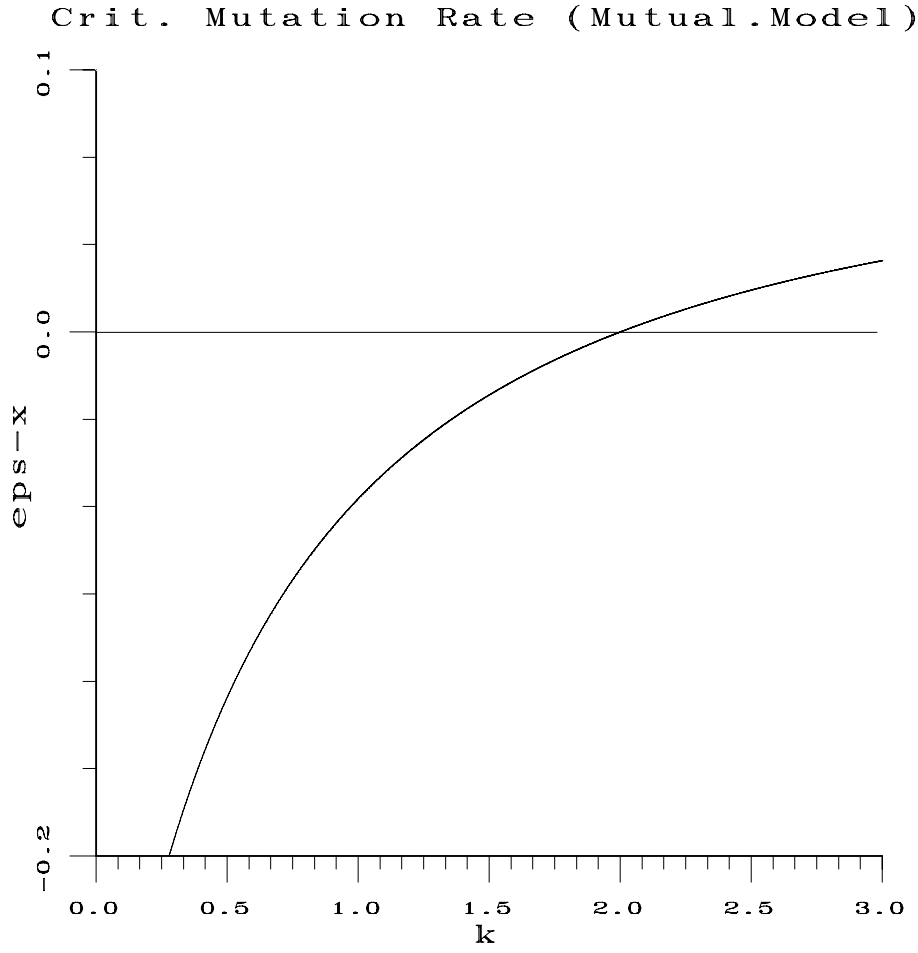

Figure 11: The critical mutation-rate ϵ^x for $\tau = 1$. The critical value is defined only for transcritical values of k. (The Critical value for the existence of limit cycles was $k = 2\tau$.)

7 A Strange Attractor

The four species Replicator system shows chaotic dynamics for certain parameter values [56]. According to [33] Hofbauer this auto-catalytic network with four species is – apart from a transformation of the time scale – equivalent to a three-species Lotka-Volterra equation. Possible existence of very complex dynamical behavior in Lotka-Volterra models was predicted by Smale [64]. Two distinct chaotic attractors were found in Lotka-Volterra equations for three species: Vance [79] discovered a "quasi-cyclic" trajectory in a one predator two prey model, which was uncovered by Gilpin [28] to be a strange attractor, and Arneodo, Coullet and Tresser [76] found a one parameter family of strange attractors (ACT-attractor).

Both the ACT family and the Vance-Gilpin attractor (VG) correspond to non-robust phase-portraits because of zero or almost zero (see e.g. A_{24} or A_{43} in A_V) off-diagonal elements in the reaction matrices A below.

The VG model has a replication matrix

$$A_{VG} = \begin{pmatrix} 0 & 0.063 & 0 & 0.437 \\ 0.537 & 0 & -0.036 & -0.001 \\ -0.535 & 0.38 & 0 & 0.655 \\ 0.536 & -0.032 & -0.004 & 0 \end{pmatrix}$$

and the ACT attractors are found at

$$A_{ACT} = \begin{pmatrix} 0 & 0.5 & -0.1 & 0.1 \\ 1.1 & 0 & -0.6 & 0 \\ -0.5 & 1 & 0 & 0 \\ 1.7+\mu & -1-\mu & -0.2 & 0 \end{pmatrix}$$

Note that the parameter μ which corresponds to $\mu - 1.5$ in the papers of Arneodo *et al.* [1, 2].

The connective model, that was constructed by Schnabl at. al. [51] was used.

$$A(\mu, \nu) =$$

$$\begin{pmatrix} 0 & 0.5-0.437\nu & -0.1+0.1\nu & 0.1+0.337\nu \\ 1.1-0.563\nu & 0 & -0.6+0.564\nu & -0.001\nu \\ -0.5-0.035\nu & 1-0.62\nu & 0 & 0.655\nu \\ 1.7+\mu-1.164\nu & -1-\mu+0.968\nu & -0.2+0.196\nu & 0 \end{pmatrix}$$

All three matrices of replication constants fulfill $\sum_{j=1}^{4} A_{ij} = 0.5$

With the method of [80] the following Ljapunow exponents were calculated.

The dependences of the parameter μ and τ are shown. Because this problem is 2 n dimensional in this case, the calculation of Ljapunow exponents was very time-consuming. So it was impossible to perform very detailed studies of the chaotic attractor.

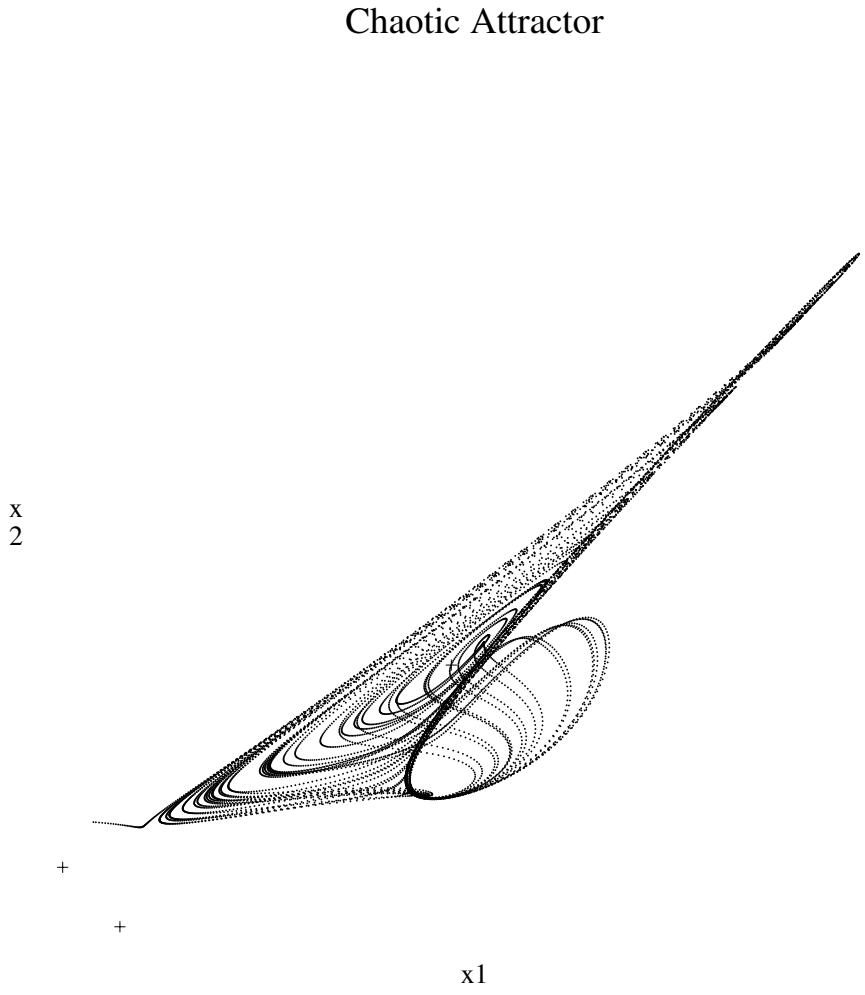

Figure 12: Example for phase portrait of chaotic model under constant organization; x-part μ = -0.1; $\nu = 0$; $\tau = 2$;

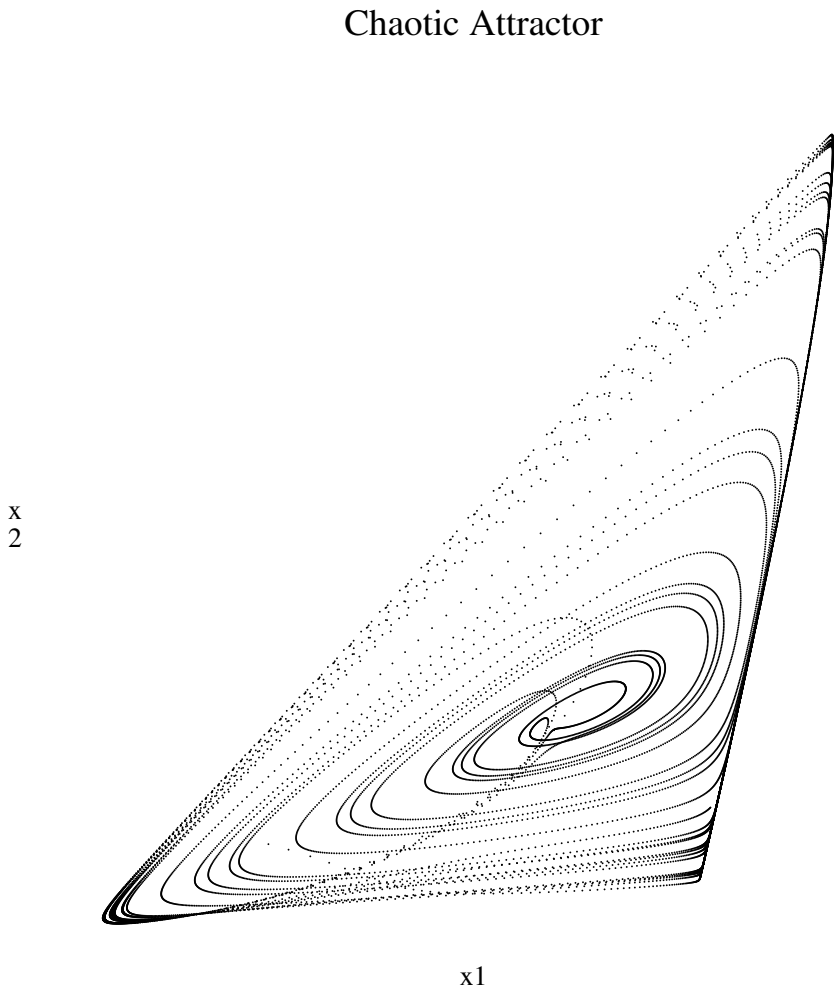

Figure 13: Example for phase portrait of chaotic model under constant organization; x-part $\mu = 0$; $\nu = 1$; $\tau = 2$;

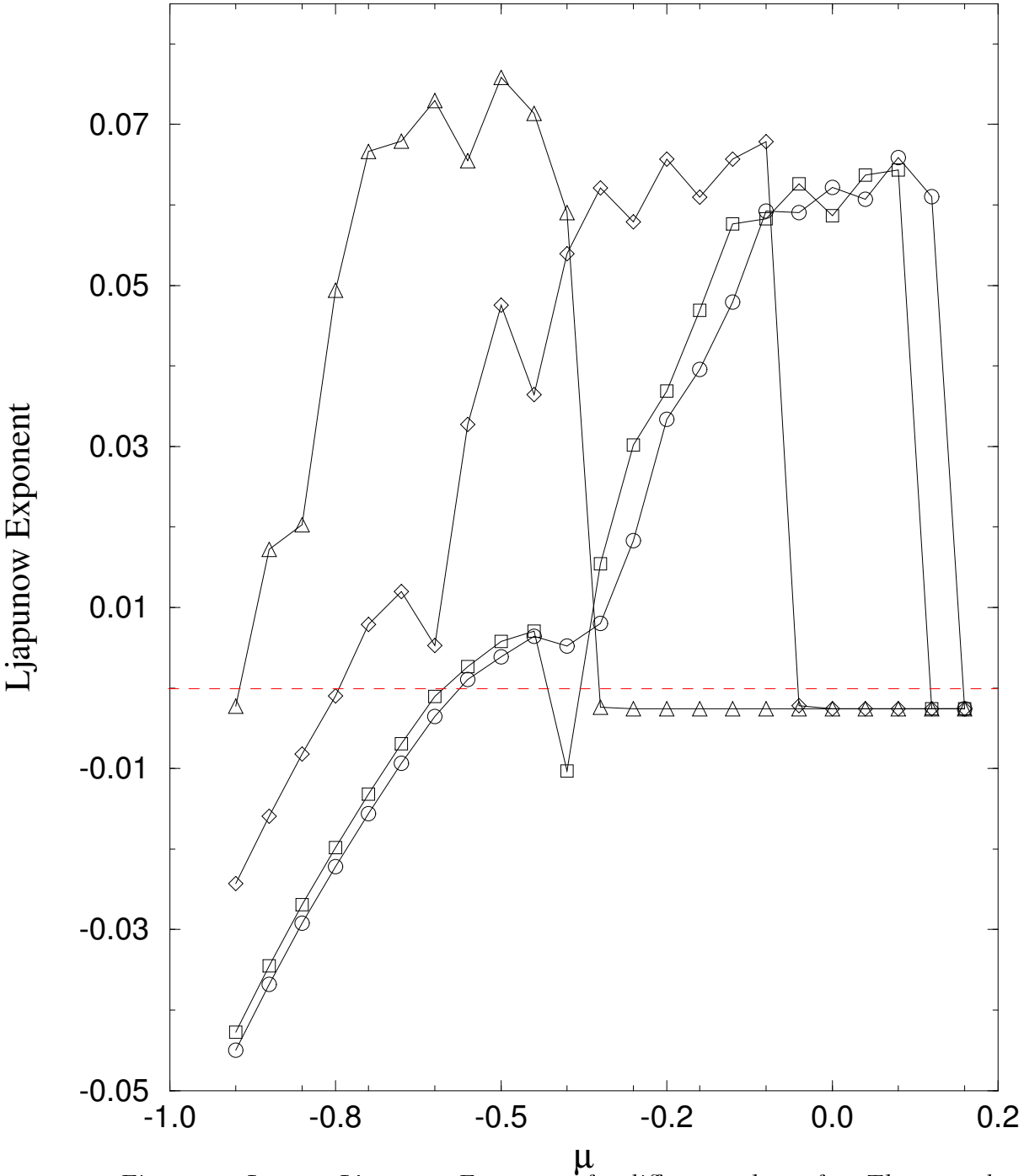

Figure 14: Largest Ljapunow Exponents for different values of μ. The second parameter ν was set to zero. The symbols denote to $\circ : \tau = 10$; $\square : \tau = 5$; $\diamond : \tau = 1$; $\triangle : \tau = 0.5$

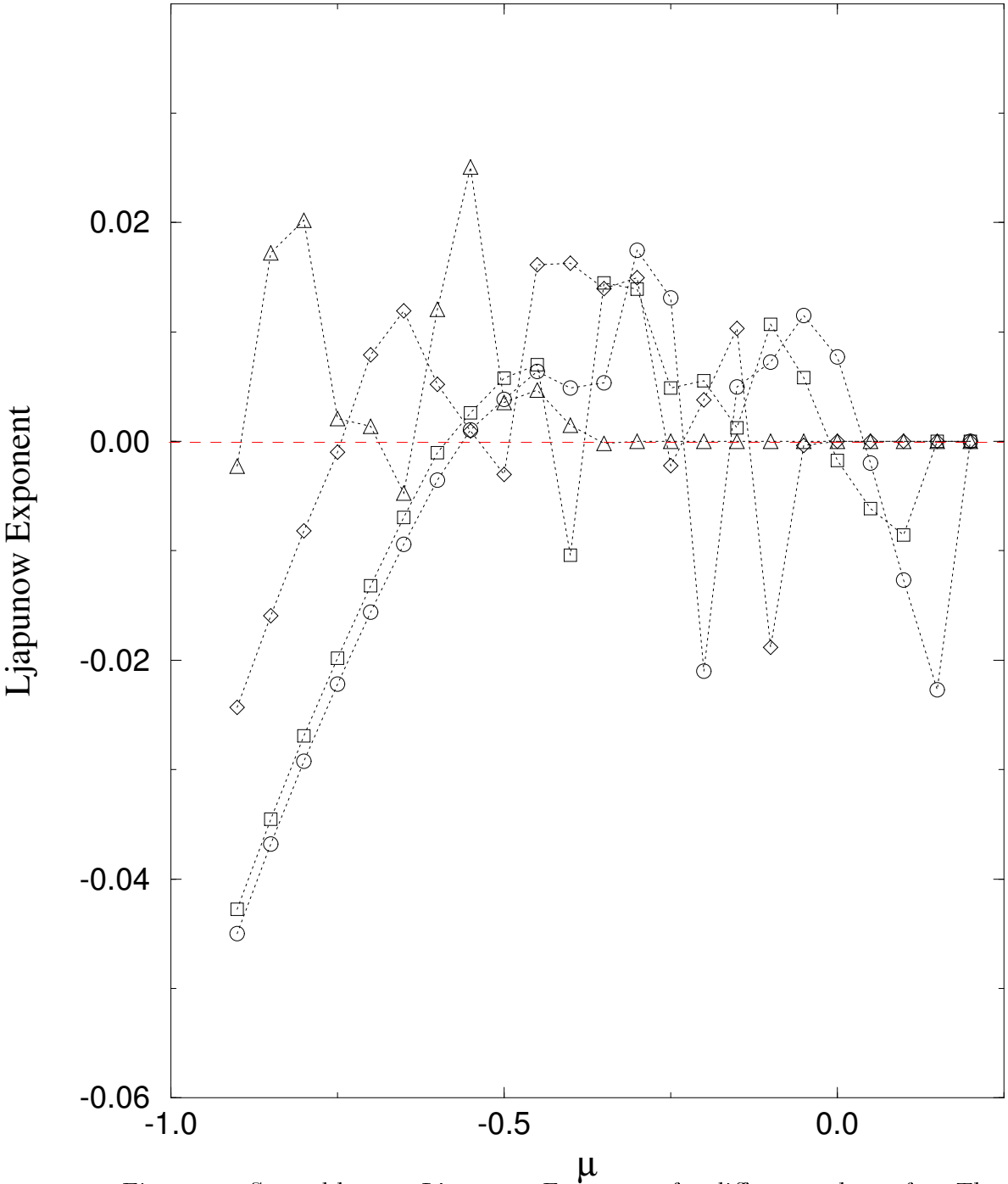

Figure 15: Second largest Ljapunow Exponents for different values of μ. The second parameter ν was set to zero. The symbols denote to $\circ$: $\tau = 10$; $\square$: $\tau = 5$; $\diamond$: $\tau = 1$; $\triangle$: $\tau = 0.5$

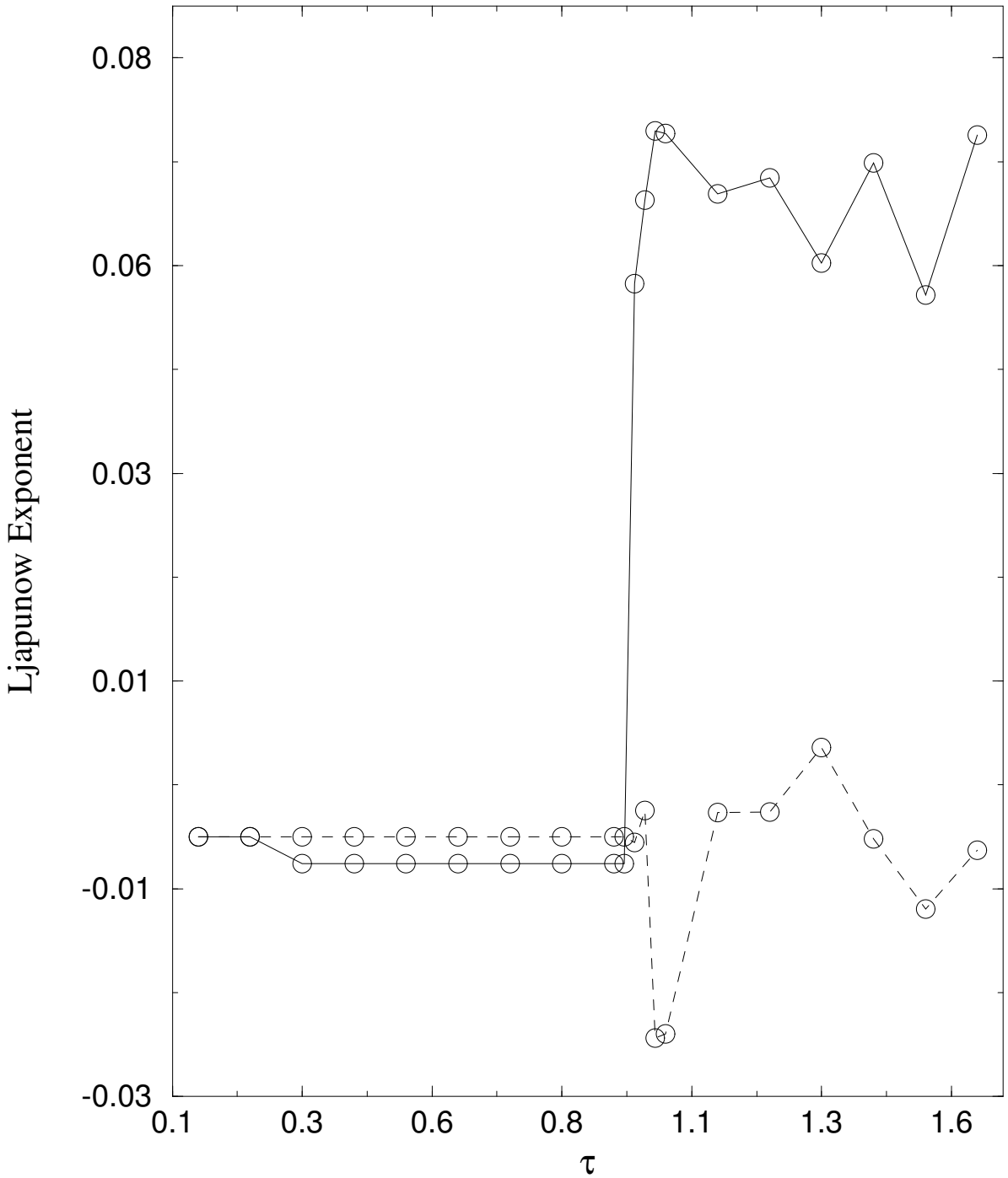

Figure 16: Dependence of the chaotic attractor for $\mu = 0.01$ and $\nu = 0$ of the parameter τ.Only the two largest exponents are shown.

8 Diffusion

The system of differential equations we are concerned with is the spatial discretization of the partial differential equation system. The discretization of the spatial domain in the context of reaction diffusion equations is central to a seminar paper by Turing [77], The instability at the homogeneous state due to diffusion hence is often called *Turing-instability.*

A Turing -instability which is also called *pitchfork bifurcation* occurs when one real eigenvalue goes through zero, while all other eigenvalues have negative real part. There, the lowest coefficient of the characteristic polynomial vanishes, hence A - D becomes singular. For a D slightly beyond the bifurcation value, the homogeneous solution becomes instable, and a stationary inhomogeneous solution can become stable.

The reactions take place under the assumption of regeneration, because under constant organization the species A and B are in great excess and diffusion processes are impossible by default. Also the CSTR is not suitable for diffusion, because of the constant stirring, that is not compatible with diffusion. For a different model see [45].

For the diffusion part only the competitive and the mutualistic system were choosen. The one dimensional space consists of 100 cells and no-flux boundaries were choosen.

8.1 Competitive Model with Diffusion

$$\begin{aligned} B + X_i &\xrightarrow{\tau_i} X_i + T_i \\ A + X_i + T_i &\xrightarrow{k_i} 2X_i + T_i \\ X_i &\xrightarrow{g_i} A \\ T_i &\xrightarrow{\gamma_i} B \end{aligned} \tag{131}$$

The kinetic equations become partial differential equations.

$$\begin{aligned} \dot{x}_i &= x_i\left(k_i a t_i - g_i\right) + D_{x_i}\nabla^2 x_i \\ \dot{t}_i &= \tau_i b x_i - \gamma_i t_i + D_{t_i}\nabla^2 t_i \\ \dot{a} &= \sum_{i=1}^{n} x_i\left(g_i - k_i a t_i\right) + D_a \nabla^2 a \end{aligned} \tag{132}$$

$$\dot{b} = \sum_{i=1}^{n} (\gamma_i t_i - b x_i \tau_i) + D_b \nabla^2 b$$

Here we restrict ourselves to the simplest possible case, where diffusion is only one-dimensional, and the diffusion coefficients of all species are the same : $D_{x_i} = D_x$ and $D_{t_i} = D_t$. Then only the case with equal reaction constants was considered: $k_i = k$; $\tau_i = \tau$; $g_i = g$ and $\gamma_i = \gamma$. Finally ξ is the spatial coordinate. So the simplified equations (132) read:

$$\begin{aligned} \dot{x}_i &= x_i (k a t_i - g) + D_x \frac{\partial^2 x_i}{\partial \xi^2} \\ \dot{t}_i &= \tau b x_i - \gamma t_i + D_t \frac{\partial^2 t_i}{\partial \xi^2} \\ \dot{a} &= \sum_{i=1}^{n} x_i (g - k a t_i) + D_a \frac{\partial^2 a}{\partial \xi^2} \\ \dot{b} &= \sum_{i=1}^{n} (\gamma t_i - b x_i \tau) + D_b \frac{\partial^2 b}{\partial \xi^2} \end{aligned} \tag{133}$$

All numerical work was done with the `STAR`-program package from Ch. Streissler [73].

The competitive model shows two different behaviors: for sufficiently large diffusion coefficients only a spatial homogeneous solution exists, while for small coefficients each cell decides, which one-dimensional equilibrium is reached.

Coefficient	figure (17)	figure (18)
k_i	0.90	0.90
τ_i	0.87	0.87
g_i	0.20	0.20
γ_i	0.20	0.20
D_x	1.0e-6	1.0e-6
D_t	1.0e-6	1.0e-6
D_a	1.0e-1	1.0e-6
D_b	1.0e-1	1.0e-6

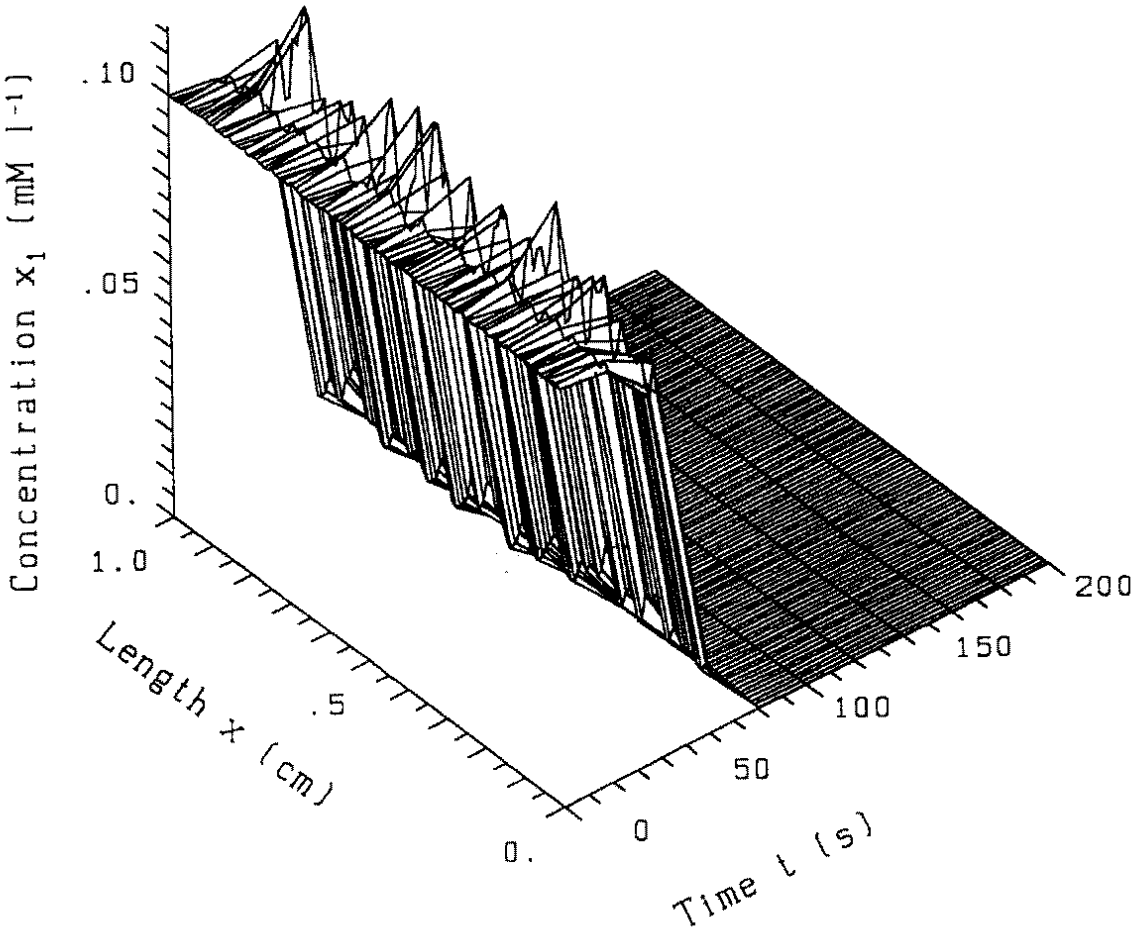

Figure 17: Competitive model: a)

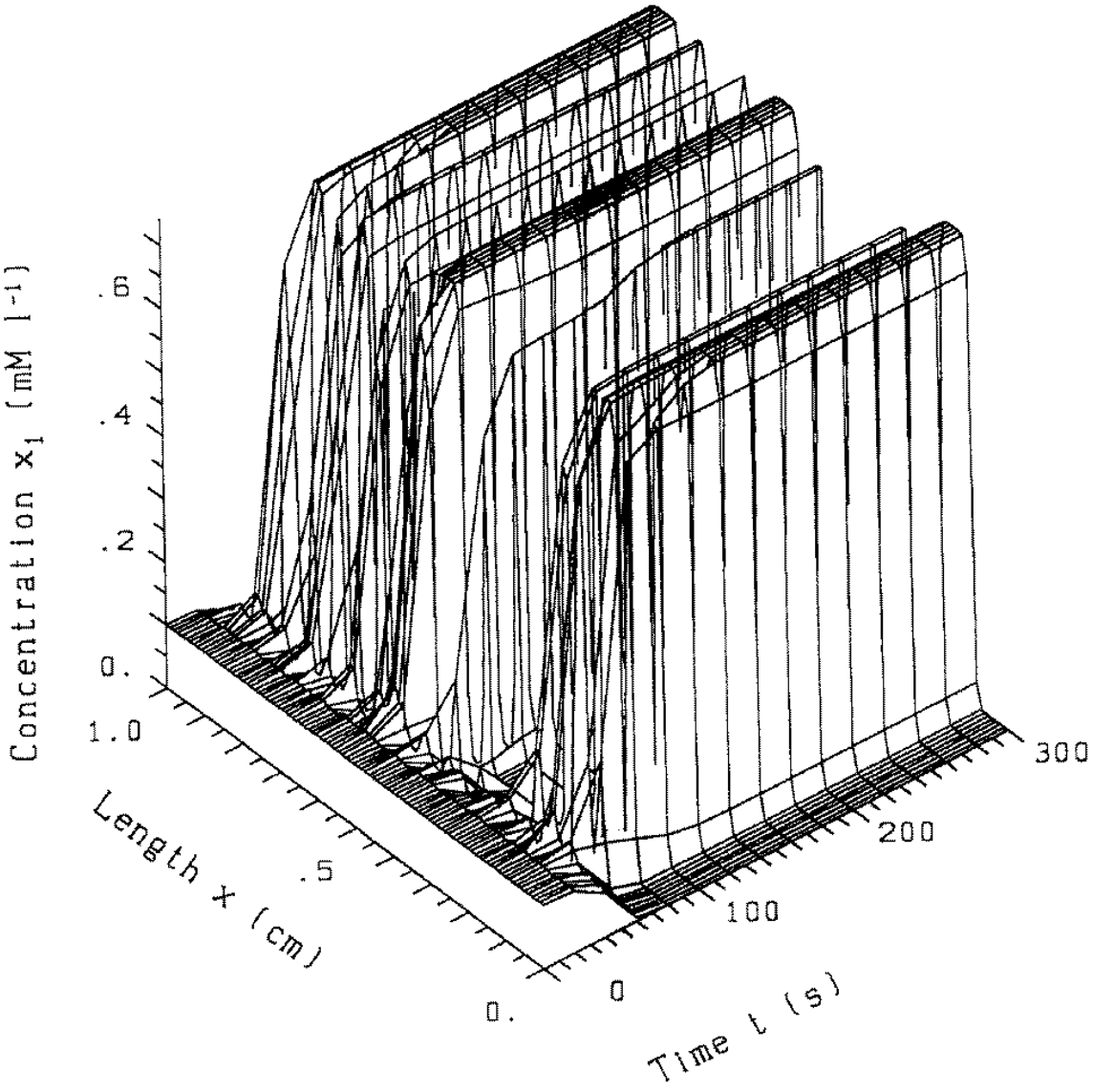

Figure 18: Competitive model: b)

8.2 Mutualistic Model with Diffusion

Here we have

$$\begin{aligned}
\dot{x}_i &= x_i\left(kat_{i-1} - g\right) + D_x\frac{\partial^2 x_i}{\partial\xi^2} \\
\dot{t}_i &= \tau b x_i - \gamma t_i + D_t\frac{\partial^2 t_i}{\partial\xi^2} \\
\dot{a} &= \sum_{i=1}^{n} x_i\left(g - kat_{i-1}\right) + D_a\frac{\partial^2 a}{\partial\xi^2} \\
\dot{b} &= \sum_{i=1}^{n}\left(\gamma t_i - b x_i\tau\right) + D_b\frac{\partial^2 b}{\partial\xi^2}
\end{aligned} \tag{134}$$

The eigenvalues for $j \neq 0$ do not depend on the diffusion coefficients, but for $j = 0$ a critical value for the occurrence of a pitchfork bifurcation could be derived:

$$\begin{aligned}
D_{x,crit} &= \frac{-g + akt}{\kappa} + \frac{kt\left(g - akt\right)x}{D_a\kappa^2 + k\kappa nt} + \\
&+ \frac{abk\tau^2x^2\left(-\left(D_a\kappa n\right) - kn^2t + ktx\right)}{\kappa\left(D_a\kappa + knt\right)\left(D_b\gamma\kappa + D_tD_b\kappa^2 - \gamma\tau x + \gamma n\tau x + D_t\kappa n\tau x\right)} + \\
&+ \frac{abk\tau x\left(D_a\kappa n + kn^2t - ktx\right)\left(D_b\kappa + n\tau x\right)}{\kappa\left(D_a\kappa + knt\right)\left(D_b\gamma\kappa + D_tD_b\kappa^2 - \gamma\tau x + \gamma n\tau x + D_t\kappa n\tau x\right)}
\end{aligned} \tag{135}$$

The numerical results show that the diffusion coefficients alone can introduce a very interesting behavior: We start with at limit cycle and very low diffusion coefficients. A periodic, but spatially homogeneous pattern is formed fig.(19). When increasing the diffusion-rate of the monomers a and b a bit, very interesting spatially non-homogeneous pattern were formed; fig. (20). By increasing D_a and D_b we finally can detect a non-periodic spatially inhomogeneous pattern as shown in fig. (23).

Coefficient	figure (19)	figure (20)	figure (21)	figure (22)	figure (23)
k_i	0.90				
τ_i	0.75				
g_i	0.10				
γ_i	0.12				
D_x	1.0e-5				
D_t	1.0e-5				
D_a	5.0e-6	5.0e-5	5.0e-4	5.0e-3	5.0e-2
D_b	5.0e-6	5.0e-5	5.0e-4	5.0e-3	5.0e-2
Behavior:					
Space	○	●	●	●	●
Time	■	■	■	■	□

○ ... homogeneous

● ... inhomogeneous

■ ... periodic

□ ... constant

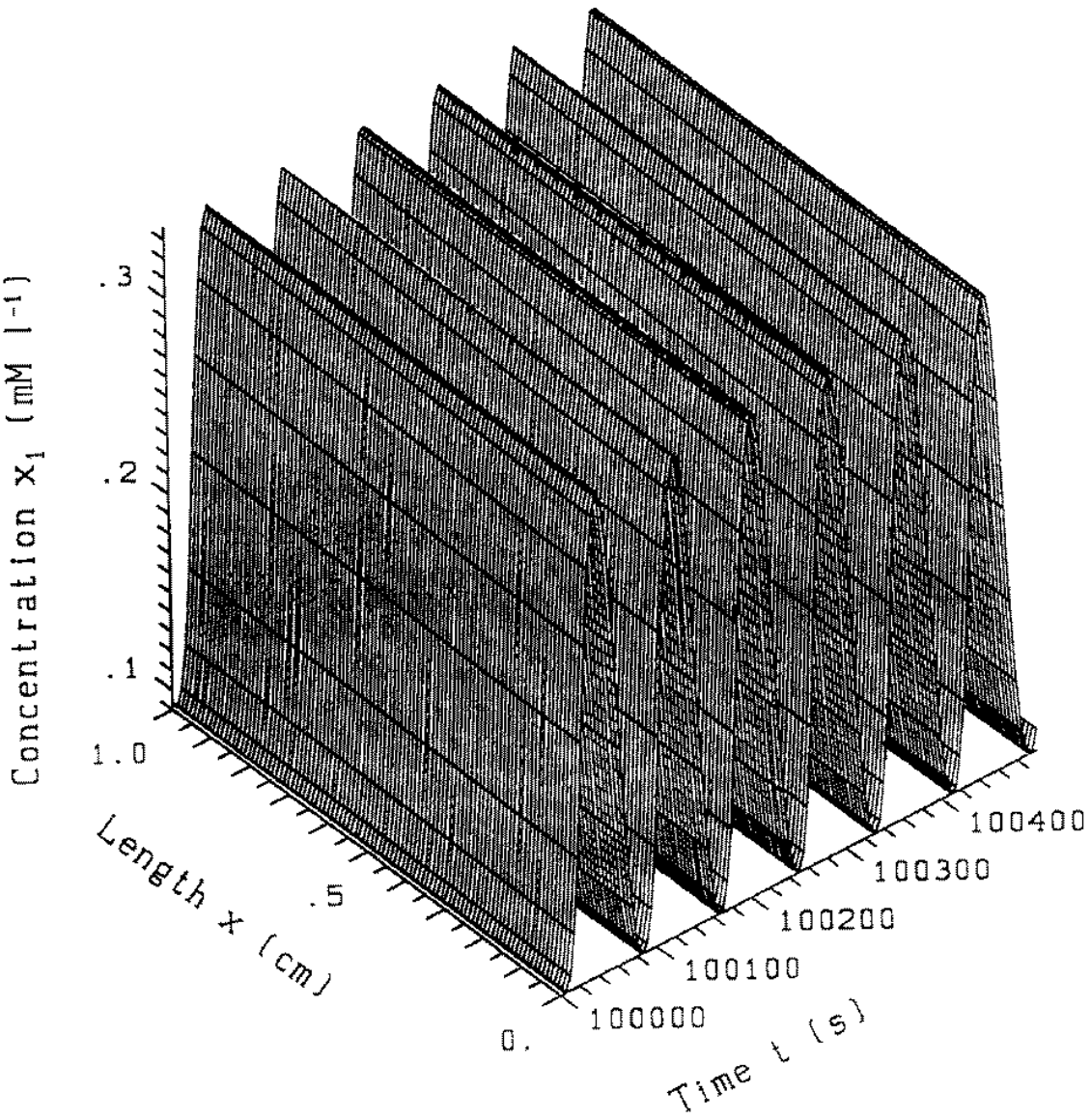

Figure 19: Mutualistic model: a)

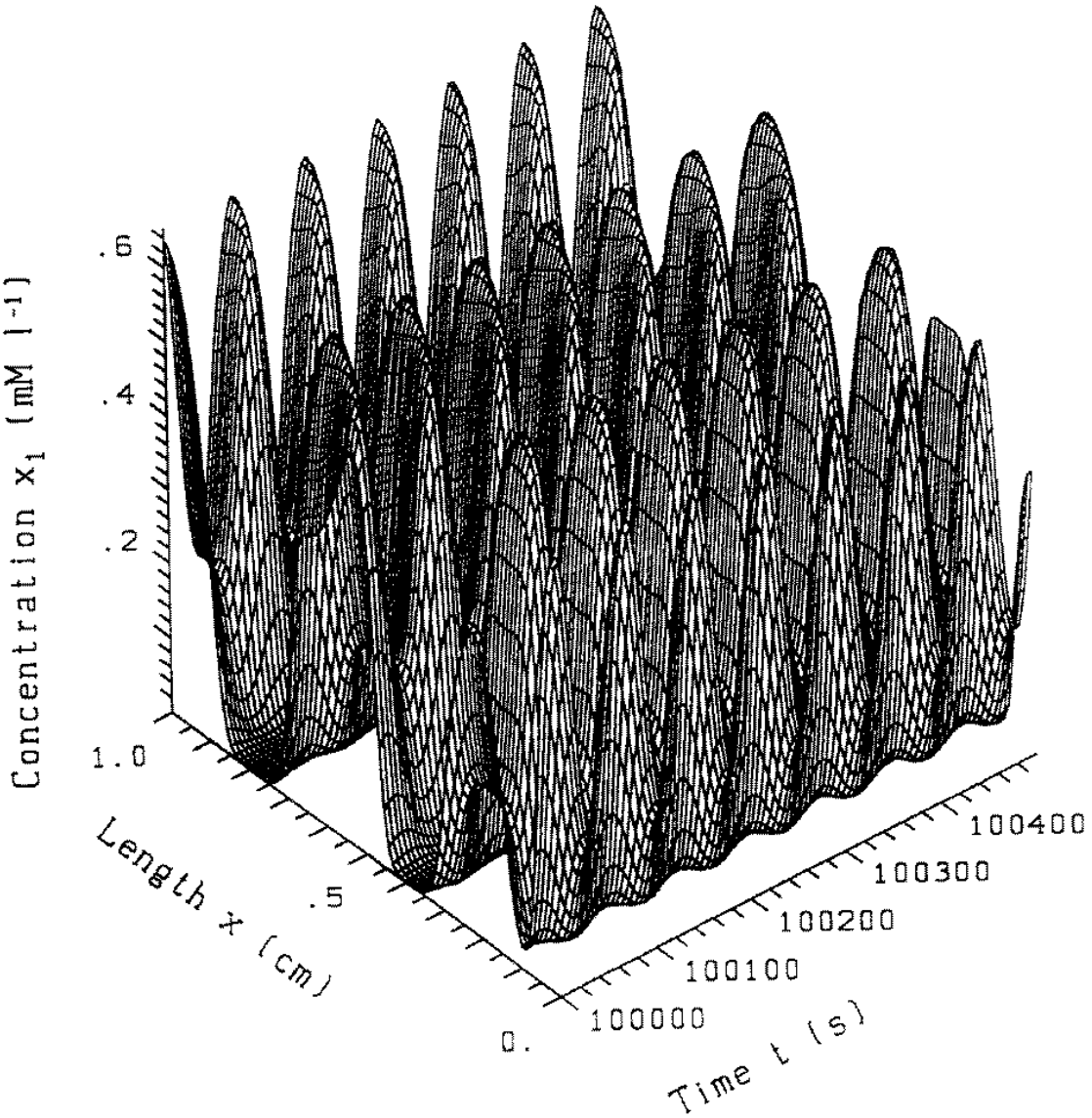

Figure 20: Mutualistic model: b)

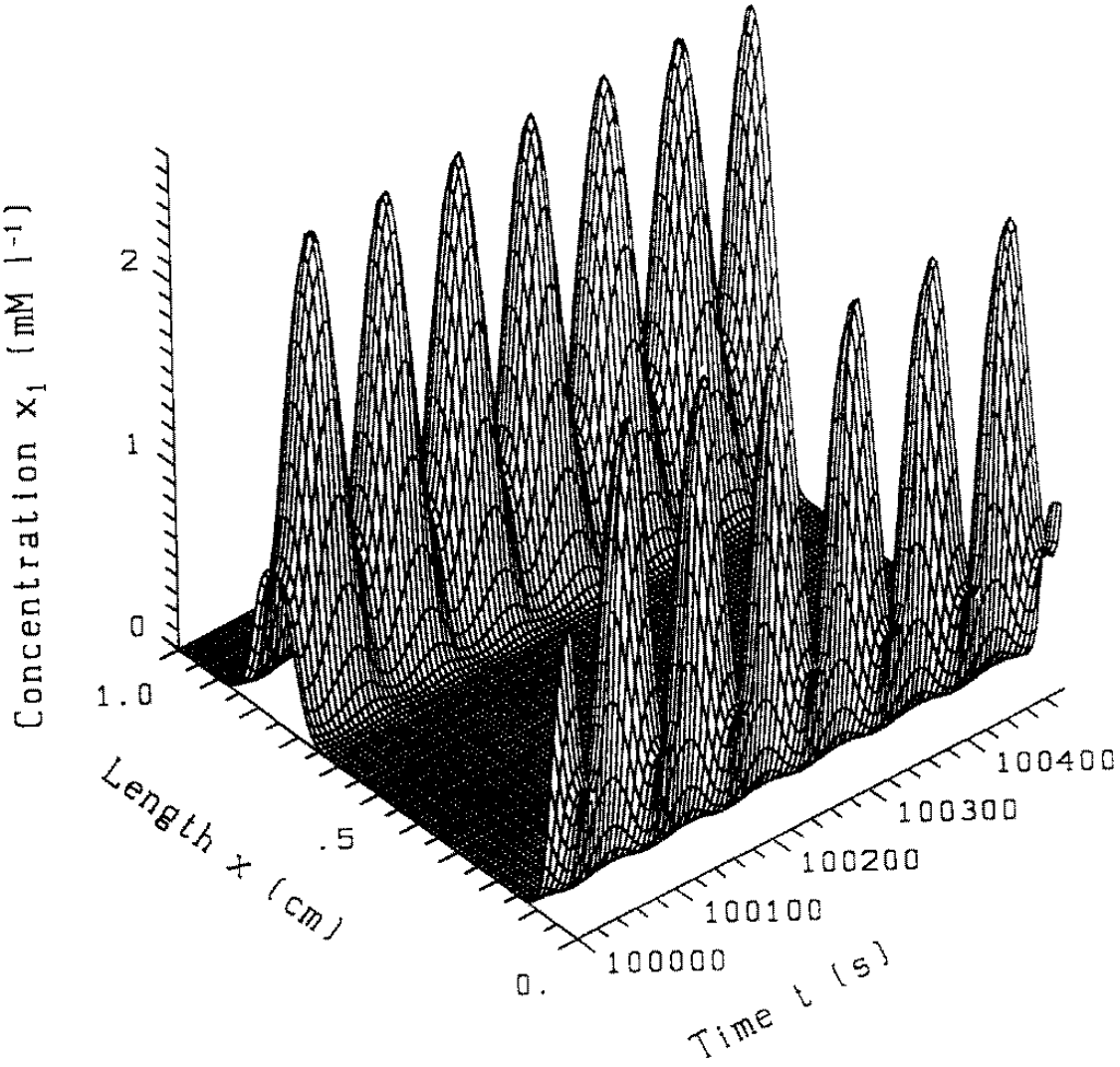

Figure 21: Mutualistic model: c)

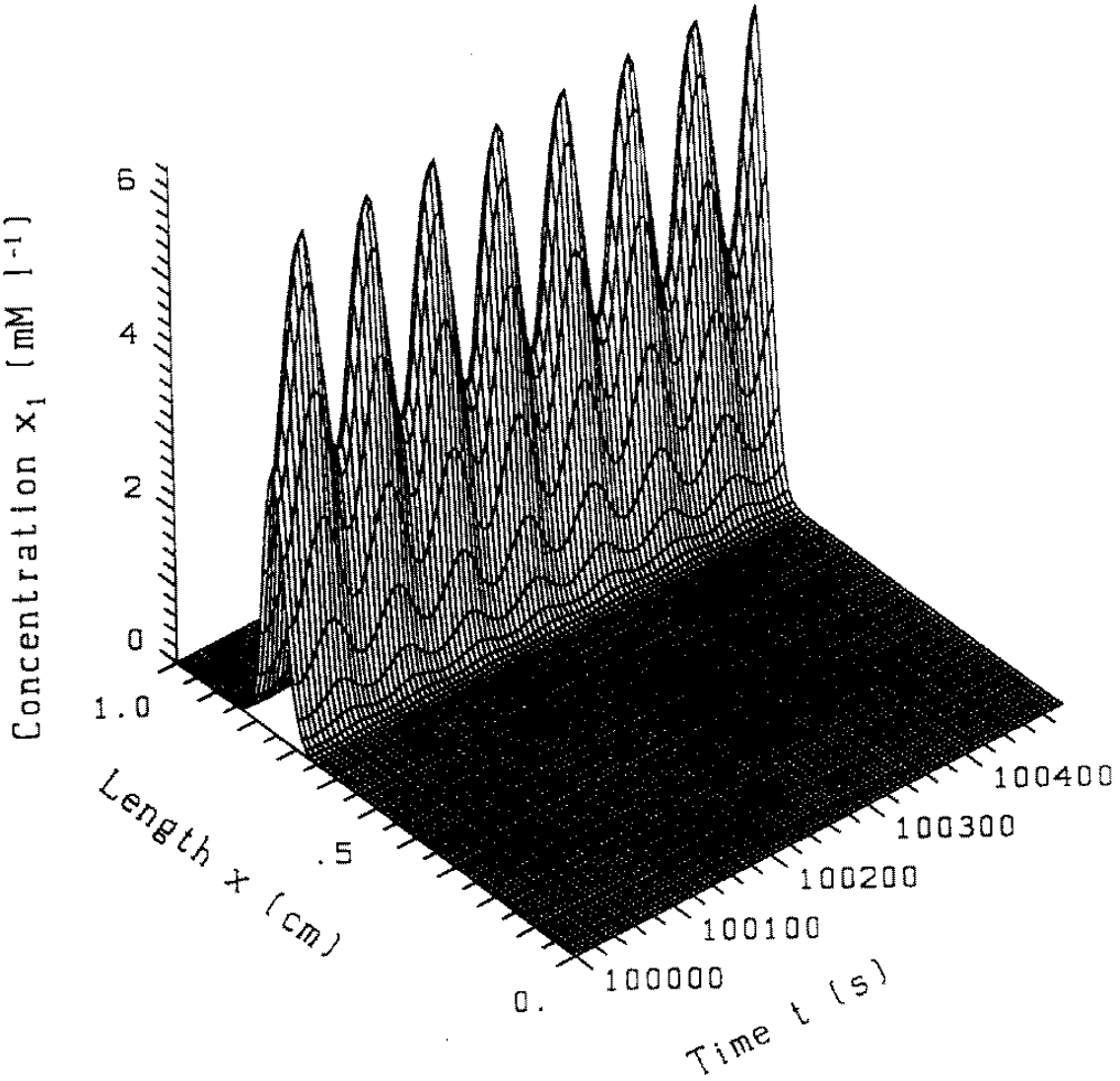

Figure 22: Mutualistic model: d)

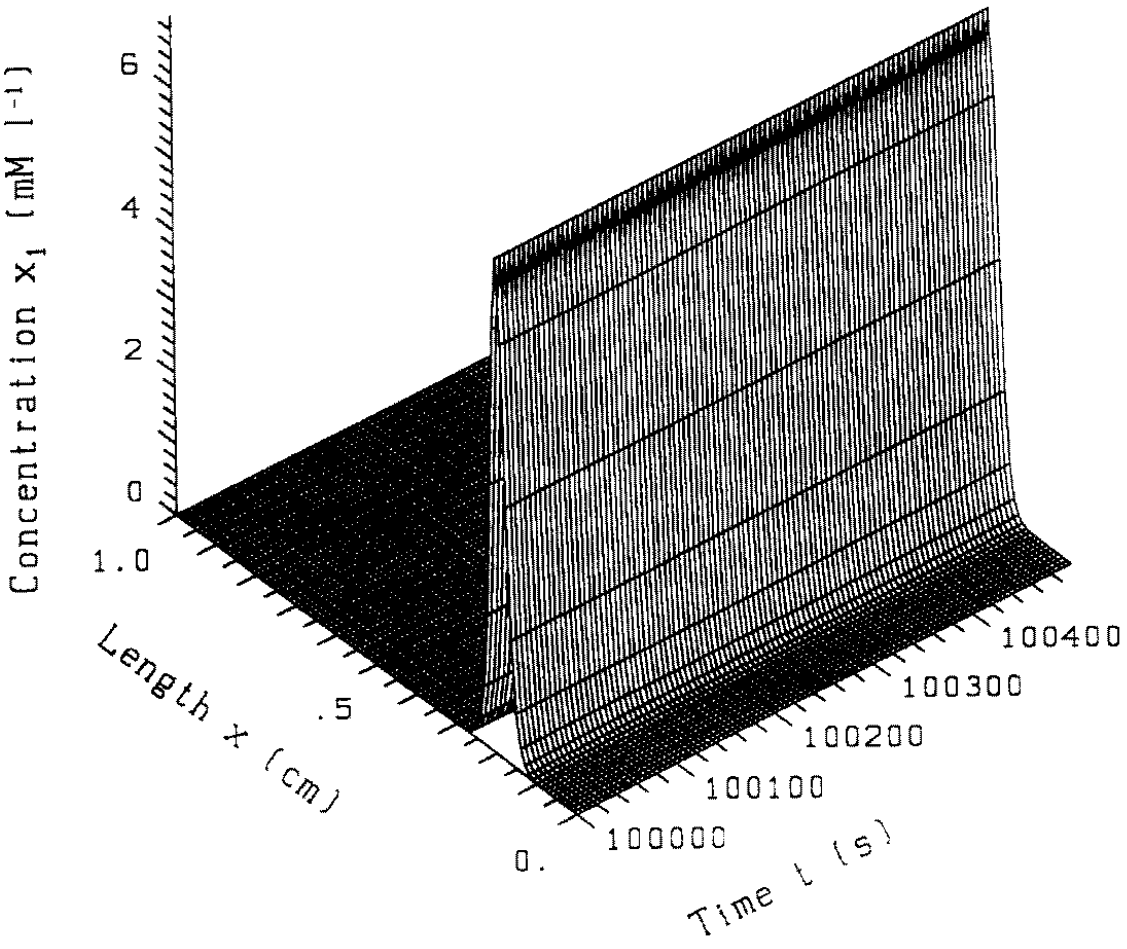

Figure 23: Mutualistic model: e)

9 Conclusions and Outlook

In this work replicator-related catalytic networks have been studied under the assumption of a separate translation step. Particularly some simpler cases with circulant selection matrices have been investigated under various boundary conditions, namely

- a competitive model and
- a mutualistic model.

The long time behavior of these models has been studied under the following boundary conditions:

1. evolution reactor,
2. continuously stirred tank reactor, and
3. regeneration.

These models give rise to different mathematical expressions, because the evolution reactor always provides the substrate in great excess, whereas the other two models deal with limited substrate concentration. Thus monomer-concentrations have to be considered explicitly in the kinetic differential equations.

Some effort has been spent to solve the general case of the competitive model under constant organization. Although no inductive proof can be given, numerical results seem to confirm the considered formula.

The competitive model displays the same type of behavior for all three models of boundary conditions: only one species survives. So only the corners of the simplex, where all but one species vanish, are stable equilibria. Depending on the values of the rate constants, basins of attraction with different size decide which species has the best chance to survive. Nevertheless, the dynamical behavior of the system is completely determined by the initial values.

In the mutualistic model, the rate constants decide whether there is a stable interior equilibrium, or a stable limit cycle. In all three cases, conditions for the existence of Hopf-bifurcations were derived.

Mutation for both replication and translation has been considered. The erroneous translation only produces new proteins, but cannot create non-existing genes and therefore influences only the rate constants of the selection matrix and, in general, has no great influence on the replicating species.

Erroneous replication is capable of regenerating extinct species and creating new ones, because new arising genes induce the production of their translation products and thus influence the overall behavior of the system.

Critical values for the mutation parameters at bifurcation points have been derived in both cases.

A chaotic attractor of the system with translation exists in almost the same region of parameter space as in the pure replicator-equation. For increasing values of the translation constants, the detailed dynamical behavior of the attractor becomes similar to the replication-case.

The influence of diffusion has been investigated as well. By means of numerical integration a very interesting type of bifurcation was found for the mutualistic system, which depends only on the diffusion coefficients of the substrates. Starting with a limit cycle and very low diffusion coefficients of the substrates, spatially homogeneous, but temporally periodic solutions are obtained. By increasing the diffusion coefficients, the solutions become unstable in space and forms patches. A further increase in the diffusion coefficients finally creates a stationary, spatially inhomogeneous solution.

Perspectives:

Some more analytical results seem to be possible. More intensive numerical and some analytical work should be done concerning the effects of diffusion. The interaction of mutation and diffusion is an interesting topic to work on and also the influence of diffusion upon the strange attractor might be investigated. By means of singular perturbation theory, the connection to the replicator-model might be derived. Some other models of translation may be investigated.

References

[1] A. Arneodo, P. Coullet, J. Peyraud, and C. Tresser. Strange attractors in volterra equations for species competition. *J. math .Biol.*, 14:153–157, 1982.

[2] A. Arneodo, P. Coullet, and C. Tresser. Occurance of strange attractors in three- dimensional volterra equations. *Phys. Lett.*, 79A:259–263, 1980.

[3] G. Bennetin, L. Galgani, A. Giorgilli, and J.-M. Strelcyn. Lyapunow characteristic exponents for smooth dynamical systems and for hamiltonian systems ; a method for computing all of them. *Meccania*, 15:9–21, 1980.

[4] A. Berman and R. J. Plemmons. *Nonnegative Matrices in the Mathematical Sciences.* Academic Press, New york, London, San Francisco, 1979.

[5] G. Bouligand. Ensembles impropres et nombre dimensionell. *Bull. Sciences Math.*, II-52:320–334 & 361–374, 1928.

[6] S. A. Campbell and P. Holmes. Heteroclinic cycles and modulated travelling waves in a system with D_4 symmetry. *Physica D*, pages 52–78, 1992.

[7] T. Cech. RNA as an enzyme. *Scientific American*, 11:76–84, November 1986.

[8] T. R. Cech. Conserved sequences and structures of group I introns : building an active site for RNA catalysis - a review. *Gene*, 73:259–271, 1988.

[9] L. S. Dai. On the existence, uniqueness, and global asymptotic stability of the periodic solution of the modified michaelis menten mechanism. *J. Diff. Equ.*, 31:392–417, 1979.

[10] C. Darwin. *The Origin of Species.* reprinted in Penguin Classics, 1859.

[11] U. Dressler and J. D. Farmer. Generalized lyapunow exponents corresponding to higher derivatives. *Physica D*, 59:365–377, 1992.

[12] M. Eigen. Selforganization of matter and the evolution of biological macromolecules. *Die Naturwissenschaften*, 10:465–523, 1971.

[13] M. Eigen, J. McCaskill, and P. Schuster. Molecular Quasi-Species. *Journal of Physical Chemistry*, 92:6881–6891, 1988.

[14] M. Eigen, J. McCaskill, and P. Schuster. The molecular Quasispecies. volume 75, pages 149 – 263. J. Wiley & Sons, 1989.

[15] M. Eigen and P. Schuster. The hypercycle A: A principle of natural self-organization : Emergence of the hypercycle. *Naturwissenschaften*, 64:541–565, 1977.

[16] M. Eigen and P. Schuster. The Hpercycle B: The abstract hypercycle. *Naturwissenschaften*, 65:7–41, 1978.

[17] M. Eigen and P. Schuster. The hypercycle C: The realistic hypercycle. *Naturwissenschaften*, 65:341–369, 1978.

[18] M. Eigen and P. Schuster. Stages of emerging life – five principles of early organization. *J. Mol. Evol.*, 19:47–61, 1982.

[19] M. Eigen, P. Schuster, K. Sigmund, and R. Wolff. Elementary step dynamics of catalytic hypercycles. *BioSystems*, 13(1-22), 1980.

[20] J. D. Farmer, E. Ott, and J. Yorke. The dimension of chaotic attractors. *Physica*, 7D, 1983.

[21] P. C. Fife. *Mathematical Aspects of Reacting and Diffusing Systems.* Number 28. Springer, Berlin,Heidelberg,New York, 1979.

[22] W. Fontana, T. Griesmacher, W. Schnabl, P. Stadler, and P. Schuster. Statistics of landscapes based on free energies, replication and degredation rate constants of RNA secondary structures. *Monatshefte der Chemie*, 122:795–819, 1991.

[23] W. Fontana, W. Schnabl, and P. Schuster. Physical aspects of evolutionary optimization and adaption. *Physical Review A*, 40(6):3301–3321, Sep. 1989.

[24] W. Fontana and P. Schuster. A computer model of evolutionary optimization. *Biophysical Chemistry*, 26:123–147, 1987.

[25] D. Gallez and A. Babloyantz. Lyapunow exponents for nonuniform attractors. *Physics Letters*, 161:247–254, 1991.

[26] F. R. Gantmacher. *Applications of the Thoery of Matrices.* Interscience Publishers, New York, 1959.

[27] R. gencay and W. D. Dechert. An algorithm for n lyapunow exponents of an n-dimensional unknown dynamical system. *Physica D*, 59:142–157, 1992.

[28] M. E. Gilpin. Spiral chaos in a predator pray system. *Amer. Nat.*, 133:306–308, 1978.

[29] P. Glansdorff and I. Prigogine. *Thermodynamic Theory of Structure, Stability and Fluctuations.* John Wiley, New York, 1971.

[30] J. Guggenheimer and P. Holmes. *Nonlinear Oscillations, Dynamical Systems ond bifurkations of Vector Fields.* Springer, New York,Berlin,Tokyo, 1983.

[31] R. Hecht. PhD thesis, Universität Wien, 1994.

[32] M. W. Hirsch and S. Smale. *Differential Equations, Dynamical Systems and Linear Algebra.* Academic Press, 1974.

[33] J. Hofbauer. On the occurance of limit cycles in the lotka- volterra equation. *Nonlinear Analysis*, 5:1003–1007, 1981.

[34] J. Hofbauer, P. Schuster, K.Sigmund, and R. wolff. Dynamical systems under constant organisation II: Homogeneous growth functions of degree p=2. *Siam. J. Appl. Math.*, 38(2):282–304, 1980.

[35] J. Hofbauer and K. Sigmund. *The Theory of Evolution and Dynamical Systems.* Cambridge University Press, New York, Port Chester, Melbourne, Sidney, 1988.

[36] K. Kishimoto, M. Mimura, and K. Yoshida. Stable spatio-temporal oscillations of diffusive lotka-volterra system with three or more species. *J. Math. Biol.*, 18:213–221, 1983.

[37] A. N. Kolmogorov and V. M. Tihomirov. Epsilon- entropy and epsilon-capacity of sets in funktional spaces. *Amer. Math. Soc. Translations*, 17:277–364, 1959.

[38] E. N. Lorenz. Lyapunow numbers and the local structure of attractors. *Physica 17D*, pages 279–294, 1985.

[39] T. R. Malthus. *An Essay on the Principal of Population.1798.* Penguin Books, 1970.

[40] B. B. Mandelbrot. *The Fractal Geometry of Nature.* Freeman & Co., New York, 1983.

[41] J. D. Murray. *Mathematical Biology.* Springer, 1989.

[42] G. Nicolis and F. Baras. Nonequilibrium dynamics in chemical systems. *Physica D*, pages 345–348, 1985.

[43] G. Nicolis and I. Prigogine. *Self-organisation in non-equilibrium systems.* John Wiley, New York, 1977.

[44] A. I. Oparin. *The Origin of Life on the Earth.* Oliver & Boyd, Edinbourgh, 1957.

[45] J. J. Perraud, A. De Wit, E. Dulos, P. De Kepler, G. dewel, and P. Borckmans. One - dimensional "Spirals": Novel asynchronous chemical wave sources. *Physical Review Letters*, 71(8):1272–1275, 1993.

[46] P. E. Phillipson and P. Schuster. Analytical solution of coupled nonlinear rate equations.II. kinetics of positive catalytic feedback loops. *J. chem Phys.*, 79(8):3807–3817, 1983.

[47] L. Pontrjagin and L. Schnirelman. Sur une propriet'e metique de la dimension. *Annals of Math.*, 33:156–162, 1932.

[48] I. Prigogine and R. Lefever. Symmetry breaking instabilities in dissipative systems ii. *J. Chem. Phys.*, 48:1665–1700, 1968.

[49] F. Schlögel. Chemical Reaction Models for Non-Equilibrium Phase Transitions. *Z. Physik*, 253:147 – 161, 1972.

[50] F. Schlögl. On thermodynamics near a steady state. *Z. Physik*, 248(446-458), 1971.

[51] W. Schnabl, P. F. Stadler, C. Forst, and P. Schuster. Full characterization of a strange attractor: Chaotic dynamics in low dimensional replicator systems. *Physica D*, 48:65 – 90, 1991.

[52] P. Schuster. Coevolution of proteins and nucleic acids.

[53] P. Schuster. Dynamics of molecular evolution. *Physica D*, 22:100 – 119, 1986.

[54] P. Schuster. Mechanisms of molecular evolution. In S. W. Fox, editor, *Selforganization*, pages 57 – 91. 1986.

[55] P. Schuster. Evolution von Molekülen und einfachen viren. Ein Beitrag zur Festveranstaltung: Theoretische Grundlagen und Probleme der Biologie, Jena, März 1987.

[56] P. Schuster. Structure and dynamics of replication - mutation systems. *Physica Scripta*, 35:402–416, 1987.

[57] P. Schuster. Dynamics of autocatalytical reaction networks. In A. Perelson and S. Kauffman, editors, *Molecular Evolution on Rugged Landscapes*, volume IX, pages 281–306. SFI studies in the sciences of complexity, 1991.

[58] P. Schuster, S. A. Kauffman, P. F. Stadler, and R. Hecht. A two species model for coevolution. *in prep.*, 1993.

[59] P. Schuster and K. Sigmund. Replicator dynamics. *J. theor. Biol.*, 100:533–538, 1983.

[60] P. Schuster and K. Sigmund. Dynamics of evolutionary optimization. *Berichte der Bunsen-Gesellschaft für physikalische Chemie*, 89:668–682, 1985.

[61] P. Schuster, K. Sigmund, and R. Wolff. Dynamical systems under constant organisation I.topologigal analysis of a family of non-linear differential equations - a model for catalytic hypercycles. *Bull. Math. Biophys.*, 40:743–769, 1978.

[62] P. Schuster, K. Sigmund, and R. Wolff. Dynamical systems under constant organisation III.cooperative ond competitive behaviour of hypercycles. *J. Diff. Equ.*, 32:357–368, 1979.

[63] P. Schuster, K. Sigmund, and R. Wolff. Mass action kinetics of selfreplication in flow reactors. *J. Math. Anal. App.*, 78(1):88–112, 1980.

[64] S. Smale. On the differential equations of species competition. *J. math. Biol.*, 3:5–7, 1976.

[65] R. V. Sole and J. Valls. Characterisation of spatiotemporal chaos from macrospopic measures. *Physics Letters*, 161:241–246, 1991.

[66] R. V. Sole and J. Valls. Spiral waves, chaos and multiple attractors in lattice models of interacting populations. *Phys. Lett. A*, 166:123–128, 1992.

[67] P. Stadler. *Selection, Mutation and Catalysis.* PhD thesis, Universität Wien, 1990.

[68] P. F. Stadler. Complementary replication. *Mathematical Biosciences*, 107:83–109, 1991.

[69] P. F. Stadler. Dynamics of autocatalytic reaction networks IV: Inhomogenous replicator neworks. *BioSystems*, 26:1–19, 1991.

[70] P. F. Stadler and J. C. Nuno. On a class of selection mutation equations. The influence of mutation on autocatalytic reaction networks. *Bull. Math. Biol.*, subm., 1992.

[71] P. F. Stadler and P. Schuster. Dynamics of small autocatalytic reaction networks. I: Bifurcations, permanence and exclusion. *Bull. Math. Biol.*, 52, no.4:485–508, 1990.

[72] P. F. Stadler and P. Schuster. Mutation in autocatalytic networks - an analysis based on perturbation theory. *J. Math. Biol.*, 30:597–631, 1992.

[73] C. Streissler. *Autocatalytic Networks under Diffusion.* PhD thesis, Universität Wien, 1992.

[74] G. C. W. Swabin. Chaos in a periadically forced predator-prey ecosystem model. *Math. Biosciences*, 113:91–113, 1993.

[75] J. Swetina and P. Schuster. A model for polynucleotide replication. *Biophys.Chem.*, 16:329–345, 1982.

[76] C. Tressner. Homoclinic orbits for flows in r^3. *J. Phys. France*, 45:837, 1984.

[77] A. M. Turing. The chemical basis of morphogenesis. *Bul. Math. Biol.*, 52(1/2):153–197, 1990.

[78] H. C. Urey. The plants, their origin and development. New Haven, 1952.

[79] R. R. Vance. Predation and resource partitioning in one predator - two pray model communities. *Amer. Nat.*, 112:987–813, 1978.

[80] A. Wolf, J. B. Swift, H. L. Swine, and J. A. Vastano. Determining Lyapunow exponents from a time series. *Physica D*, pages 285–317, 1985.