Dynamics of Autocatalytic Reaction Networks IV: Inhomogeneous Replicator Networks

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Abstract

The *inhomogeneous replicator equation* is derived as the continuous time model for parallel first and second order autocatalytic replication of macromolecules in a flow reactor based on mass action kinetics. It is shown that the total concentration of replicating material determines the relative importance of the first order and the second order mechanism. A complete description of the dynamics of the first order model and some special features of the inhomogeneous replicator equation are presented. A minimal prebiotic scenario with the potentiality to develop cooperation is derived from the inhomogeneous replicator equation. In this model cooperation can emerge when the total concentration of replication material exceeds a certain threshold. Below this value, a single species is selected; which one is determined by the rate constants of the first order reaction alone. Above this threshold the second order process becomes important and may lead to cooperative behaviour such as hypercycles.

1. Introduction

Autocatalytic reaction networks which in general involve two classes of catalytic processes – autocatalytic instruction for reproduction and additional material and process specific catalysis – were postulated as models for studies of prebiotic and early biological evolution scenarios (Eigen 1971, Eigen and Schuster 1979). In the last decade it turned out that they serve also as models in very different fields like molecular biology, population genetics, theoretical ecology or dynamical game theory (Schuster and Sigmund 1983). Recent results show that the same type of differential equations is also obtained by non-linear coordinate transformations from models in fluid mechanics and laser theory (Brenig and Goriely 1989). In the present contribution we consider the interaction of the two most simple types of autocatalytic reactions

$$I_k \longrightarrow 2I_k \qquad (I)$$

and

$$I_k + I_j \longrightarrow 2I_k + I_j. \tag{II}$$

The first mechanism (I) considers autocatalytic instruction only. Mechanism (II) two however includes additional catalytic activity of molecules I_j. The first order mechanism implies strong selection. There is only one surviving species (or Quasispecies in the case of erroneous replication) (Eigen, McCaskill and Schuster 1988,1989). The second order mechanism on the other hand allows for very rich dynamics of the corresponding kinetic differential equations. It gives rise to limit cycles or even chaos, it may lead to a single survivor, to a few cooperating species or even to the survival of all species present in the system, depending on rate constants and the initial conditions (Hofbauer and Sigmund 1988, Stadler and Schuster 1990).

There is evidence that RNA is capable not only of replicating according to a first order mechanism but also might serve as a specific catalyst for the replication of other RNA molecules (Doudna and Szostak 1989).

2. The Model

We will consider the reactions (I) and (II) in a flow reactor, i.e. the total concentration of the species I_k is regulated by an unspecific dilution flux $\Phi(t)$. The regualtion may be adjusted such that the total concentration of replicating material in the reaction vessel is held constant. This constraint is known as *constant organization* (Schuster 1986).

Furthermore we approximate the reaction kinetics of (I) and (II) by mass action kinetics (Feinberg 1977). A justification of this ansatz is given in Schuster (1980) and Stadler & Stadler (1991). For mechanism (I) we obtain then the following differential equations

$$\dot{c}_k = c_k(f_k - \Phi_{(I)}) \tag{2.1}$$

The second order autocatalytic model yields

$$\dot{c}_k = c_k\left(\sum_{j=1}^{n} a_{kj}c_j - \Phi_{(II)}\right) \tag{2.2}$$

Constant organization implies $\sum_{k=1}^{n} \dot{c}_k = 0$ and thus

$$\begin{aligned}\Phi_{(I)} &= \frac{1}{c_0}\sum_{i=1}^{n} c_k f_k, \\ \Phi_{(II)} &= \frac{1}{c_0}\sum_{i,j=1}^{n} a_{ij}c_ic_j.\end{aligned} \tag{2.3}$$

Introducing new variables $x_k = c_k/c_0$ we obtain immediately

$$\dot{x}_k = x_k(f_k - \sum_{j=1}^{n} f_j x_j) := \mathcal{L}(x) \tag{2.1$'$}$$

for the first order models (I) and

$$\dot{x}_k = c_0 \cdot x_k\left(\sum_{j=1}^{n} a_{kj}x_j - \sum_{i,j=1}^{n} a_{ij}x_ix_j\right) := c_0\mathcal{R}(x) \tag{2.2$'$}$$

for the second order model (II).

Let us now assume that reactions according to both mechanisms occur simultanously. The "superposition" of the two differential equations (2.1) and (2.2) yields

$$\dot{c}_k = c_k(f_k + \sum_{j=1}^{n} a_{kj} c_j - \Phi). \tag{2.4}$$

In relative coordinates and under the constraint of constant organization equ.(2.4) becomes

$$\dot{x}_k = c_0 \mathcal{R}(x) + \mathcal{L}(x) \tag{2.4'}$$

or equivalently after rescaling the time axis by a factor c_0

$$\dot{x}_k = \mathcal{R}(x) + \frac{1}{c_0}\mathcal{L}(x). \tag{2.4''}$$

We suspect therefore that it will depend on the total concentration c_0 of replicating molecules whether the dynamics are governed by the first order or by the second order mechanism. Equ.(2.4) is a special case of the *replicator equation*

$$\dot{x}_k = x_k \left[\varphi_k(x) - \sum_{j=1}^{n} \varphi_j(x) x_j\right] \tag{2.5}$$

with

$$\varphi_k(x) = f_k + \sum_{j=1}^{n} a_{kj} x_j. \tag{2.6}$$

Now we omit the constraint of constant organization, i.e.

$$c_0 = \sum_{k=1}^{n} c_k$$

is no longer treated as a constant. Instead we assume that $c_0(t)$ is a given function of time or, more generally, that it is given by an additional differential equation

$$\dot{c}_0 = \Theta(x, c_0, t) \tag{2.7}$$

Obviously $\dot{c}_0$ is related with the dilution flux and the internal state of the replicating reaction mixture by

$$\Theta(x, c_0, t) = \sum_{k=1}^{n} c_k \left[f_k + \sum_{j=1} a_{kj} c_j - \Phi\right] \tag{2.8}$$

For the dilution flux Φ we obtain therefore

$$\Phi(x, c_0, t) = \frac{1}{c_0} \cdot \left[\sum_{k=1}^{n} c_k f_k + \sum_{k,j=1}^{n} a_{kj} c_k c_j \right] - \frac{\Theta(c, c_0, t)}{c_0} \tag{2.9}$$

Again we introduce relative coordinates $x_k = c_k/c_0$. For the first derivatives we get

$$\frac{dx_k}{dt} = \frac{d}{dt}\frac{c_k}{c_0} = \frac{\dot{c}_k}{c_0} - \frac{c_k}{c_0} \cdot \frac{\dot{c}_0}{c_0} = \frac{1}{c_0}\left[\dot{c}_k - x_k \cdot \Theta(x, c_0, t)\right] \tag{2.10}$$

Inserting the dilution flux equ.(2.9) into the inhomogeneous model equ.(2.7) and performing the transformation equ.(2.10) again yields equ.(2.4′); the terms containing $\Theta(x, c_0, t)$ cancel.

In order to proof the statements of the following sections we will need a few definitions: The state space, i.e. the set of allowed values of the variables x for all replicator equations is the n-simplex

$$S_n = \left\{ x \in \mathbb{R}^n | x_i \geq 0 \text{ and } \sum_{j=1}^{n} x_j = 1 \right\}. \tag{2.11}$$

All systems of the form of equ.(2.5) leave the surfaces of the simplex invariant. It will be convenient to characterize these surfaces by the coordinates which vanish on them. Let N be the set of the integers 1 through n. We define F_K as the set of all points for which all coordinates x_k with $k \in K$ – and only these – are zero. Formally we may write this as

$$F_K = \{x \in S_n | x_k = 0 \iff k \in K\} \tag{2.12}$$

where the index set K is an arbitrary subset of $\mathcal{N}$. The extension of F_K into the "outer space" where some coordinates are zero will be called

$$\Phi_K = \{x \in \mathbb{R}^n | \sum_{j=1}^{n} x_j = 1 \quad \text{and} \quad x_k = 0 \iff k \in K\}.$$

The closure of F_K and Φ_K will be denoted by $\bar{F}_K$ and $\bar{\Phi}_K$. Equivalently a sub-simplex $\bar{F}_K$ on the boundary of S_n can be characterized by the coordinates which are non-zero in its interior.

3. First Order Replicator Networks

The dynamics of the first order replicator equation

$$\dot{x}_k = x_k(f_k - \sum_{i=1}^{n} x_j f_j) \tag{3.1}$$

are quite simple (Epstein 1979). Equ.(3.1) is the no-mutation limiting case of Eigen's (1971) quasi-species model. In this section we will review its main features as a contrast to the much more involved dynamics of higher order replicator models.

Explicit solutions can be obtained by the non-linear projection (Jones *et al.* 1976)

$$x_k = \frac{y_k}{\sum_{j=1}^{n} y_k} \tag{3.2}$$

from the linear ODE

$$\dot{y}_k = f_k y_k. \tag{3.3}$$

Thus equ.(3.1) is satified by the functions

$$x_k(t) = \frac{x_k(0)e^{f_k t}}{\sum_{j=1}^{n} x_j(0)e^{f_j t}} \tag{3.4}$$

Alternatively equ.(3.1) may be transformed into a topologically equivalent system of linear ordinary differential equations on $\mathbb{R}_+^n$ by means of the transformation (Hofbauer 1981)

$$\mathcal{H} : z_k = x_k/x_p, \qquad k = 1, \ldots, n; \quad k \neq p. \tag{3.5}$$

and a subsequent change in velocity:

$$\dot{z}_k = (f_k - f_n)z_k, \qquad k \neq p \tag{3.6}$$

whenever $x_p \neq 0$. This form simplifies the qualititative analysis of the dynamics even more. Furthermore, Hofbauer's transformation sends the second order replicator equation to a Lotka-Volterra system, thus it is generally applicable to the mutation-free models considered in this contribution.

Lemma 3.1. Any first order replicator network may also be written as second order replicator network with $a_{ij} = f_i - f_j$.

Proof.

$$\dot{x}_k = x_k(f_k \sum_{j=1}^{n} x_j - \sum_{j=1}^{n} f_j x_j \sum_{i=1}^{n} x_i)$$
$$= x_k(\sum_{j=1}^{n} f_k x_j - \sum_{i,j=1}^{n} f_j x_i x_j).$$

Introducing $a'_{kj} := f_k$ for all j we get a second order replicator equation.

It has been shown in a recent paper (Stadler and Schuster 1990) that directed coloured graphs are very useful for classification purposes and for visualizing second order autocatalytic networks:

(i) For each species I_k there is a vertex k.

(ii) Two vertices k and l are joined by an arrow from k to l iff the rate constant a_{lk} is non-zero.

(iii) An arrow from k to l is coloured *black* iff $a_{lk} > 0$ and *white* iff $a_{lk} < 0$.

The following Lemma is then an obvious consequence of Lemma 3.1.

Lemma 3.2. The following two rules assign generalized coloured graphs to first order replicator networks:

(i) A Species I_k corresponds to a vertex k.

(ii) The vertices p and q are connected by a black arrow pointing from p to q iff $f_p < f_q$, and they are connected by a white arrow pointing from p to q iff $f_p > f_q$ holds.

There is a black arrow from p to q iff there is a white arrow from q to p.

Definition. A first order replicator equation is *kinetically degenerated* iff there are at least two parameters f_r and f_s such that $f_r = f_s$.

Theorem 3.1. Let $f_{i_1} = f_{i_2} = \ldots = f_{i_h} =: f$. Then the subsimplex $S_h(\{i_1, i_2, \ldots, i_h\})$ consists entirely of rest points.

Theorem 3.2. Let $\dot{x} = \mathcal{L}(x)$ be a first order replicator equation on S_n. Then the following statements are equivalent.

(i) $\dot{x} = \mathcal{L}(x)$ is nondegenerate.

(ii) Each two vertices are connected by exactly two arrows.

(iii) The rest points of $\dot{x} = \mathcal{L}(x)$ are exactly the corners of the S_n.

(iv) All fixed points of $\dot{x} = \mathcal{L}(x)$ are hyperbolic.

(v) There is no continuum of rest points.

Proof. The fact that kinetic non-degeneracy implies the statements (i) through (iv) has long been known in population genetics (*cf.* Crow and Kimura 1970, Akin

Figure 1: Graphs and phase portraits for the nondegenerate **2, 3, 4** the degenerate cases. of the *2*-, *3*- and *4*-species first order replicator equation. For **2a, 3a** and **4a** two rate constants are equal. In **3b** and **4d** all rate constants are equal and thus the state space consists entirely of rest points. In situation **4b** there are two pairs of equal rate constants and in case **4c** three of them are equal.

1979 or Crow 1986). The converse results are rather easily obtained from the explicit solutions equ.(3.4). A detailed proof can be found in (Stadler 1990).

The following corollary is also well known

Corrolary 1. Let $\dot{x} = \mathcal{L}(x)$ be nondegenerate. Then there is exactly one source and one sink.

Corollary 2. The black arrows of the graph resemble the flow along the edges of S_n.

Theorem 3.4. Let $\dot{x} = \mathcal{L}(x)$ be nondegenerate. Then for any dimension n there is exactly one PP up to homeomorphism and symmetry. All α- and ω-limits are fixed points.

Proof. Without loosing generality we can renumber the coordinates such that

$$f_n > f_{n-1} > f_{n-2} > \ldots > f_2 > f_1. \tag{3.7}$$

Clearly this order is unique. The flow along an egde $< p, q >$ points from p to q iff $p < q$. The unique fixed point of equ.(3.6), the origin, is the image of the corner e_p. It follows from the inequalities (3.7) that the origin is hyperbolic irrespective of the choice of p. Thus there are no α- or ω- limits except the corners of S_n. The flow between them is given by the signs of the differences of the corresponding constants f_k. Therefore there are no bifurcations as long as the ordering (3.7) remains valid – and a change therein can be removed by a symmetry operation.

The dynamics of the second order replicator equation is — in contrast to the simple results reviewed above — overwhelmingly complicated. Only for $n = 2$ (Eigen and Schuster 1979) and $n = 3$ (Bomze 1983, Stadler and Schuster 1990) the classification problem has been solved completely. For models with four or more interacting species the dynamical behaviour can be arbitrarily complicated (Smale 1976). For $n = 4$ for instance, chaos may occur (Gilpin 1978, Arneodo *et al.* 1980, Gardini *et al.* 1989, Schnabl *et al.* 1991). For a recent review on second order replicator equations we refer to the book of Hofbauer and Sigmund (1988).

4. Properties of Inhomogeneous Networks

For the moment we assume constant organization equ.(2.3). This restriction will be dropped in the next section. As for first order replicator networks, we can reduce any inhomogeneous replicator network to a second order replicator equation.

Lemma 1. Any replicator equation of the form $\dot{x} = \frac{1}{c_0}\mathcal{L}(x; f) + \mathcal{R}(x; A)$ can be rewritten as $\dot{x} = \tilde{\mathcal{R}}(x; \tilde{A})$ with

$$\tilde{a}_{ij} = a_{ij} + \frac{1}{c_0}(f_i - f_j). \tag{4.1}$$

Proof. $\sum_{j=1}^{n} a_{kj}x_j - \frac{1}{c_0}f_k = (a_{kj} - \frac{1}{c_0}f_k)x_j =: \sum_{j=1}^{n} a'_{kj}(c_0)x_j$. Furthermore the differential equation does not change if we replace a'_{ij} by $\tilde{a}_{kj} = a'_{kj} - a'_{jj}$.

Let us define

$$\begin{aligned} \omega_p &= a_{pr}a_{rp} + a_{pq}a_{qr} - a_{rq}a_{qr}, \\ \omega_q &= a_{qp}a_{pr} + a_{qr}a_{rp} - a_{pr}a_{rp}, \\ \omega_r &= a_{rp}a_{pq} + a_{rq}a_{qp} - a_{qp}a_{pq}, \\ \omega &= \omega_p + \omega_q + \omega_r. \end{aligned} \tag{4.2}$$

These quantities are related to both coordinates of rest points and to eigenvalues of linearized flows at other rest points; they have proved to be very useful in the analysis of low dimensional second order replicator equations (see Hofbauer and Sigmund 1987, Bomze 1983 and Stadler and Schuster 1991).

Theorem 4.1. (Fixed points on corners, edges and faces of S_n). For an inhomogeneous replicator equation holds:

(i) All corners of S_n are fixed points.

(ii) There is a unique fixed point on an egde $< p, q >$ iff both x_p and x_q are positive, where

$$\begin{aligned} x_p &= \frac{1}{a_{pq} + a_{qp}}[a_{pq} + \frac{1}{c_0}(f_p - f_q)] \quad \text{and} \\ x_q &= \frac{1}{a_{pq} + a_{qp}}[a_{qp} + \frac{1}{c_0}(f_q - f_p)] \end{aligned} \tag{4.3}$$

are the two nonzero coordinates of this rest point.

(iii) The three nonzero coordinates of an equilibrium on a two dimensional face of the simplex are given by

$$
\begin{aligned}
x_p &= \frac{\omega_p}{\omega} + \frac{1}{c_0\omega}\cdot\Big[(a_{rq}+a_{qr})f_p-(a_{pr}+a_{rp}-a_{pq})f_q-(a_{pq}+a_{qr}-a_{pr})f_r\Big]\\
x_q &= \frac{\omega_q}{\omega} + \frac{1}{c_0\omega}\cdot\Big[-(a_{qr}+a_{rp}-a_{qp})f_p+(a_{rp}+a_{pr})f_q-(a_{qp}+a_{pr}-a_{qr})f_r\Big]\\
x_r &= \frac{\omega_r}{\omega} + \frac{1}{c_0\omega}\cdot\Big[-(a_{rq}+a_{qp}-a_{rq})f_p-(a_{rp}+a_{pq}-a_{rq})f_q+(a_{qp}+a_{pq})f_r\Big]
\end{aligned}
\tag{4.4}
$$

(iv) For $c_0 \to \infty$ these formulas reduce to the corresponding expressions for homogeneous second order networks. For sufficiently large values of c_0 fixed points of the inhomogeneous network on F_K exist and are unique if there are unique rest points on F_K for its homogeneous second order part.

Proof. (i) clearly is valid for arbitrary replicator equations (2.5). For $1/c_0 \longrightarrow 0$ the expressions in item (iii) reduce to

$$x_s = \omega_s/\omega \tag{4.5}$$

Equ.(4.5) has been proved in a previous paper (Stadler and Schuster 1991). Thus equ.(4.4) follows from equ.(4.5) by substitution of equ(4.1). An analogous argument holds for equ.(4.3). Item (iv) follows from theorem 4.2 below.

We observe that the coordinates of the rest points on edges and two-dimensional surfaces of S_n are linear functions of $\frac{1}{c_0}$. This result holds for arbitrary rest points of equ.(2.4).

Theorem 4.2. The coordinates of the fixed points of $\dot{x} = \frac{1}{c_0}\mathcal{L}(x;f) + \mathcal{R}(x,A)$ are linear functions of $\frac{1}{c_0}$.

Proof. Let $\eta := \frac{1}{c_0}$ and let $\hat{x}_0$ be a regular fixed point of $\dot{x} = \mathcal{R}(x)$ in F_K. For $k \in \mathcal{N}\setminus K$ we make the ansatz $x_i = x_i^0 + \eta\cdot d_i$. For an interior fixed point we set $K = \emptyset$. Then we find

$$
\begin{aligned}
&\sum_{i=1}^n a_{ki}(x_i^0+\eta d_i) - \eta\sum_{i,j=1}^n a_{ij}(x_i^0 d_j + x_j^0 d_i) - \eta^2\sum_{i,j=1}^n a_{ij}d_i d_j =\\
&-\eta(f_k - \sum_{j=1}^n f_j x_j^0) + \eta^2\sum_{j=1}^n f_j d_j
\end{aligned}
\tag{4.6}
$$

Since η is arbitrary, the contributions of each order of η must vanish separately. For η^0 we get the equation for rest points of the second order replicator field:

$$\sum_{j=1}^n a_{kj}x_j^0 - \sum_{i,j=1}^n a_{ij}x_i^0 x_j^0 = 0. \tag{4.7}$$

which is assumed to hold. Let us now assume that the first order term also vanishes, i.e.

$$\sum_{j=1}^{n} a_{ki}d_i - \sum_{i,j=1}^{n} a_{ij}(x_i^0 d_j + x_j^0 d_i) = -f_k + \sum_{i=1}^{n} f_i x_i^0. \tag{4.8}$$

Now we have to prove, that the second order contributions cancel if (4.7) and (4.8) holds, i.e. that indeed

$$\sum_{i,j=1}^{n} a_{ij}d_i d_j + \sum_{i=1}^{n} f_i d_i = 0. \tag{4.9}$$

To this end we rewrite the first order contribution equ.(4.8) as follows:

$$\sum_{i=1}^{n} a_{ki}d_i + f_k = \sum_{i,j=1}^{n} a_{ij}(x_i^0 d_j + x_j^0 d_i) + \sum_{i=1}^{n} f_i x_i^0. \tag{4.8$'$}$$

Using Lemma 2 below and $L := \mathcal{N} \setminus K$ we can rewrite the second order equation (after substituting the r.h.s of the first order condition for its l.h.s) as

$$\begin{aligned}\sum_{k\in L}\Big[\sum_{i=1}^{n} a_{ki}d_i + f_k\Big]\cdot d_k &= \sum_{k\in L}\Big[\sum_{i,j=1}^{n} a_{ij}(x_i^0 d_j + x_j^0 d_i) + \sum_{i=1}^{n} f_i x_i^0\Big]\cdot d_k = \\ &= \Big[\sum_{i,j=1}^{n} a_{ij}(x_i^0 d_j + x_j^0 d_i) + \sum_{i=1}^{n} f_i x_i^0\Big]\cdot \sum_{k\in L} d_k = \\ &= 0,\end{aligned}$$

since $\sum_{k\in L} d_k = \sum_{k=1}^{n} d_k = 0$. Thus our ansatz in fact solves the equations for the fixed points of the inhomogeneous problem. It follows from continuity that theorem 4.2 remains valid even if there is no unique solution for $d = (d_1, \ldots, d_n)^T$ from the first order equation.

A fixed point in the interior of a boundary face F_K cannot leave this face into the interior of the simplex. It may leave the simplex only along the hyper-plane $\bar{\Phi}_K$ containing F_k as an open subset. Formally we state this as

Lemma 2. Let $x \in F_K$ be a fixed point of $\dot{x} = \mathcal{R}(x)$. Then $d_k = 0$ for any $k \in K$.

We finish this section with a brief discussion of the geometric implications of theorem 4.2 above. Let us denote by $\mathbf{d}(\hat{x}, c_1, c_2)$ the shift of a fixed point, i.e.

$$\mathbf{d}(\hat{x}, c_1, c_2) = \sqrt{\sum_{k=1}^{n} (\hat{x}_k(c_1) - \hat{x}_k(c_2))^2} \tag{4.9}$$

We can write this shift as

$$\mathbf{d}(\hat{x}, c_1, c2) = \mathcal{C}(A, f, K) \cdot (\frac{1}{c_2} - \frac{1}{c_1}) \tag{4.10}$$

where $\mathcal{C}(A, f, K)$ is a constant which depends on the second order coefficients a_{ij}, the first order coefficients f_j and the (sub)simplex in which the fixed point lies. Now let $\hat{x}$ and $\hat{y}$ be two arbitrary fixed points of the second order replicator equation. Then

$$\frac{\mathbf{d}(\hat{x}, c_1, c_2)}{\mathbf{d}(\hat{y}, c_1, c_2)} = K(A, f, K_x, K_y) \tag{4.11}$$

depends on the first and second order coefficients (A, f) and the two faces (K_x, K_y) which contain the rest points, but *not* on the total concentrations c_1 and c_2.

5. The Total Concentration as an Additional Variable

Thus far we have treated c_0 merely as an additional parameter in a second order replicator equation. The work on this contribution however was motivated by the following primordial scenario. Suppose that a "primordial soup" contains macromolecules I_k which can be replicated according to both mechanism (I) and mechanism (II) and that there are non-biological processes very slowly producing raw material for the replicating molecules. Thus the total concentration c_0 of the replicators I_k will be a very slowly increasing function of time:

$$\begin{aligned} \dot{x}_k = \mathcal{L}_k(x) + c_0\mathcal{R}_k(x) \qquad & k = 1, \ldots, n \\ \dot{c}_0 = \Theta(x, c_0, t) \end{aligned} \tag{5.1}$$

This primitive model does not attempt to be realistic, but it is the simplest ansatz that contains the potentiality to "invent" hypercycles and other types of cooperation. Note that the only parameters that enter are the first and second order reaction constants for the replication reactions.

Let us begin with a very simple example. Let $A = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}$ and $f_1 = 2,\ f_2 = 1$. With $x = x_1 = 1 - x_2$ our model reduces to

$$\begin{aligned} \dot{x} &= \mathcal{L}(x) + c_0 \cdot \mathcal{R}(x) = \\ &= x(1-x) + c_0 \cdot x(1-x)(1-2x) = \\ &= x(1-x)(1 + c_0 - 2c_0 \cdot x) \end{aligned} \tag{5.2}$$

For c_0 considered as a parameter the qualitative behaviour of equ.(5.2) is listed in tab.1. It contains two rest points at the ends of the unit interval, one of which is stable for low values of c_0. As c_0 reaches unity, a third equilibrium enters the physically meaningful region via a transcritical bifurcation and "takes over" the stability. In terms of the above scenario this means that for low concentrations of replicating molecules a single species is selected. For larger concentrations however this equilibrium may become unstable and is replaced by a stable state with non-zero concentrations of more than one species.

We assume that variations of c_0 are very slow compared to the selection process in the reaction mixture. Then the system is almost always very close to an ω- limes of the replicator equation (2.4') with $c_0(t)$ considered as a parameter – except perhaps when c_0 is very close to a bifurcation value of the system. We call this

Table 1: Stability of the fixed points for the two species model

	$\hat{x}_1$	$\hat{x}_2$	$\hat{x}_3$
Coordinates	0	1	$\frac{1}{2}(1+\frac{1}{c_0})$
Derivative	$1+c_0$	$-1+c_0$	$\frac{c_0}{2}(1-\frac{1}{c_0^2})$
$c_0<1$	unstable	stable	*unstable*
$c_0>1$	unstable	unstable	stable

Figure 2: Trajectories for the simple two species model **a)** without mutation, equ.(5.2) and **b)** with mutation, equ.(6.6). The abiabatic limit is shown as solid line, numerical solutions are shown as dotted lines for different values of κ: from left to right κ= 0.003,0.03,0.1,0.3,1. Note that the trajectory for κ=0.003 is trapped in x_1=1 without mutation. For $\kappa \geq 0.1$ there is no visible difference between the trajectories with a small mutation rate and without mutation. The mutation rates in **b)** are p=10^{-4} for all off-diagonal entries in both P and $\hat{P}$.

the *adiabatic limit* since the internal state x of the system can be considered as "in equilibrium".

In fig.2a some numerical solutions of the two species model equ.(5.2) are shown. The total concentration is defined by $\Theta(x, c_0, t) = \kappa$ for simplicity. For large values of κ the total concentration becomes very quickly very large and the first order process does not have any significant influence. If κ becomes smaller then 1, the trajectory begins to follow the theoretical line for the adiabatic limit. For very small values of κ the orbit comes so close to the fixed point $x = 1$ that the computer sets $x(t) = 1$ due to round-off errors. It does not "feel" then that this equilibrium becomes unstable for $c_0 \geq 1$.

It is easy to predict the long-time behaviour of small inhomogeneous networks in the adiabatic limit. One has to know only the ω-limit of equ.(2.4) belonging to the initial value $(x_1(0), \ldots, x_n(0))$ for the parameter value $c_0(0)$ and to trace its path as c_0 varies. As c_0 varies from 0 to approximately infinity, this path begins at the unique stable state of the first order replicator equation and ends up in one of the ω- limits of the second order model. In between it is often, but not

Figure 3: Changes in the dynamical behaviour of inhogeneous three species models as c_0 increases in the adiabatic limit. All six models have the same second order matrix A (equ(5.2)) but different permutations of the first order rate constants f_i.In the first, second and sixth example first a two-membered hypercycle if formed which incorporates a third species when c_0 reaches a second threshold. In the other three cases evolution avoids cooperative behaviour although the differential equations would allow for it. Sinks, sources and saddles are denoted by $\bullet$,$\circ$ and $\oplus$ resp. Centers (which are surrounded by a continuum of periodic orbits are shown as $\odot$ and a single periodic trajectory.

always, uniquely defined and therefore it is predetermined which ω-limit of the second order replicator equation will be reached.

Such an analysis has been performed for six 3-species systems (fig.3) with common second order rate constants and different first order constants:

$$A = \begin{pmatrix} 0 & 6 & -4 \\ -3 & 0 & 5 \\ -1 & 3 & 0 \end{pmatrix}, \quad f_a = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \tag{5.3}$$

and the other 5 permutations of $1, 2, 3$ as entries in the first order parameter vectors f_b through f_f. If $c_0(0)$ is small enough (as in this example), the whole information on the initial value is extincted, for the trajectories rapidly approach the unique stable corner of the first order system. Depending on which corner of the simplex this is, the system can reach different attractors as c_0 becomes large.

The history of a hypercycle is fairly simple in this scenario. For very low concentrations there is a single selfreplicating species. As its concentration increases it becomes unstable against a second species. The second order coupling of these two species may allow them to coexist – a hypercycle with 2 species is formed (fig.2a). This process of incorporation of a mutant with suitable reaction constants into the hypercycle A when c_0 exceeds a certain threshold may be repeated (fig.3).

Although a rigorous treatment of the adiabatic limit for arbitrary functions $\Theta(c_0, t, \kappa)$ seems to be very complicated since it has been shown that even a very slowly varying central parameter may drastically change the bifurcation properties of the system, we can treat the cases in which c_0 converges towards a limit $\bar{c}$ for $t \to \infty$.

Theorem 5.1 Let $c_0(t)$ be such that either

$$\|c_0(t) - \bar{c}\| < K/t^\alpha \quad \text{or} \quad \|\frac{1}{c_0(t)} - \frac{1}{\bar{c}}\| < K/t^\alpha$$

for some constant $\bar{c}$ and $\alpha > 1$ and $t > \tau_0$ Let furhermore

$$\dot{x} = \mathcal{L}(x) + c(t)\mathcal{R}(x) = \hat{F}(x) + (c_0(t) - \bar{c})\mathcal{R}(x)$$

or (for the second case)

$$\dot{x} = \frac{1}{c_0(t)}\mathcal{L}(x) + \mathcal{R}(x) = \hat{F}(x) + (\frac{1}{c_0(t)} - \frac{1}{\bar{c}})\mathcal{L}(x)$$

By $y(t)$ we denote the solutions of the homogeneous system $\dot{y} = \hat{F}(y)$. Furthermore we require that $\hat{F}$ is structurally stable. Then for almost all initial conditions there is a τ_0 such that $\omega(x(0))$ (under the full dynamics) and $\omega(y(\tau_0))$ under the homogeneous dynamics $\dot{y} = \hat{F}(y)$ are equal.

bf Proof.

$$\|x(t) - \int_\alpha^t \hat{F}(x(\tau))d\tau\| \leq \|\mathcal{R}\| \int_\alpha^t (c_0(\tau) - \bar{c})d\tau \leq K\|\frac{1}{1-\alpha} \cdot T^{1-\alpha} \to 0$$

as $T \to 0$. Thus for τ_0 sufficiently large the solutions of the perturbed system approximate the solutions of $\dot{y} = \hat{F}(y)$ with initial condition $y(\tau_0) = x(\tau_0)$ arbitrarily close. Provided there is a neighborhood of $y(\tau_0)$ such that all solutions in this neighborhood converge to the same ω-limit this implies $\omega(x(\tau_0)) = \omega(y(\tau_0))$. In a structurally stable vector fields $\hat{F}$ this is the case for almost all initial conditions. The second case follows immediately from the first one.

This in fact gives a a rigorous result for the simple case of exponentially growing total concentration:

Corollary. If $\mathcal{R}$ is structurally stable, then for almost all initial condition x_0 the system (2.4") converges towards an ω-limit of $\dot{y} = \mathcal{R}(y)$. In case of 2- or 3-species models this holds for almost all second order replicator fields.

6. Including Mutation

We have assumed thus far that the replication process is accurate. In nature, however, infinitely accurate processes do no occur. Miscopying – mutation – is an unavoidable by-product. We assume that mutations occur only as erroneous copying. This means the reaction

$$I_k \longrightarrow I_l + I_k$$

occurs with a probability $\hat{p}_{lk}$ and

$$I_k + I_j \longrightarrow I_l + I_k + I_j$$

occurs with a probability p_{lk} and reaction rate constants f_k and a_{kj}, resp. The matrices P and $\hat{P}$ containing the above mutation probabilites must fulfil

$$\sum_{l=1}^{n} p_{lk} = \sum_{l=1}^{n} \hat{p}_{lk} = 1. \tag{6.1}$$

The differential equation for this more realistic model reads

$$\dot{c}_k = \sum_{i,j=1}^{n} p_{ki} a_{ij} c_i c_j + \sum_{j=1}^{n} \hat{p}_{kj} f_j c_j - c_k \Phi. \tag{6.2}$$

With $c_0 = \sum_{j=1}^{n} c_j$ we find

$$\Phi = \frac{1}{c_0} \cdot \left\{ \sum_{i,j,k=1}^{n} p_{ki} a_{ij} c_i c_j + \sum_{k,j=1}^{n} \hat{p}_{kj} f_j c_j \right\} - \frac{\dot{c}_0}{c_0} \tag{6.3}$$

Since P and $\hat{P}$ are stochastic matrices this expression simplifies to

$$\Phi = \frac{1}{c_0} \cdot \left\{ \sum_{i,j=1}^{n} a_{ij} c_i c_j + \sum_{j=1}^{n} f_j c_f \right\} - \frac{\dot{c}_0}{c_0}. \tag{6.4}$$

As usual we introduce relative coordinates $x_k = \frac{c_k}{c_0}$. Then we find

$$\dot{x}_k = c_0 \cdot \sum_{i,j=1}^{n} a_{ij} x_i x_j (p_{ki} - x_k) + \sum_{j=1}^{n} f_j x_j (\hat{p}_{kj} - x_k). \tag{6.5}$$

Using that P and $\hat{P}$ are stochastic matrices we may split the above equation into an inhomogeneous replicator field and a mutation field:

$$\begin{aligned}\dot{x}_k = c_0 \cdot x_k[\sum_{j=1}^{n} a_{kj}x_j - \sum_{i,j=1}^{n} a_{ij}x_ix_j] + x_k[f_k - \sum_{i=1}^{n} f_ix_i]+ \\ + \sum_{i,j=1}^{n} \Big\{[a_{ij}p_{ki}c_0 + \hat{p}_{ki}f_i]x_ix_j - [a_{kj}p_{ik}c_0 + \hat{p}_{ik}f_k]x_jx_k\Big\}\end{aligned} \tag{6.6}$$

The pure first order model

$$\dot{x}_k = x_k[f_k - \sum_{i=1}^{n} f_ix_i] + \sum_{i=1}^{n}[\hat{p}_{ki}f_i]x_i - \hat{p}_{ik}f_k]x_k]$$

is the well-known *Quasispecies* model (Eigen 1971). It can be solved explicitly by perturbation methods (Thompson and McBride 1974). For a recent review of this model see Eigen *et al.* (1989).

The second line of equ.(6.6) fulfils the requirements for a meaningful mutation model if $\hat{P}$ is irreducible and $f_k > 0$ for all k (Stadler and Schuster 1991). Then we have a unique, globally stable rest point in the interior of the simplex. In general it is not possible to reduce the inhomogeneous selection mutation problem stated here to a homogeneous problem. Let us introduce the following abbreviation:

$$Q^j_{ki} = p_{ki}a_{ij}c_0 + \hat{p}_{ki}f_j. \tag{6.7}$$

The mutation field reads then

$$\mathcal{M}^I_k(x; c_0) = \sum_{j=1}^{n} x_j \sum_{i=1}^{n}[Q^j_{ki}x_i - Q^j_{ik}x_k]. \tag{6.8}$$

With the averages

$$\bar{Q}_{ki} = \sum_{j=1}^{n} Q^j_{ki}x_j$$

equ.(6.8) takes the same form as the most simple mutation models

$$\mathcal{M}_k(x) = \sum_{i=1}^{m}[\bar{Q}_{ki}x_i - \bar{Q}_{ik}x_k]. \tag{6.9}$$

Since the replication part may be expressed in terms of homogeneous linear functions in any case, with $a'_{ij} = a_{ij}c_0 + f_j$, one can do so with the entire equation iff one can extract these factors a'_{ij} in the definition of Q^j_{ki}. This is possible iff $P = \hat{P}$, i.e. iff the mutation probabilities are the same for catalytic and the noncatalytic replication mechanism.

Numerical investigations (fig.2b) show that for small mutation rates the inhomogenous evolution equations with and without mutation show one major difference. In the presence of mutation the trajectories are not trapped by fixed points on the boundary of the simplex, but follow for slowly changing c_0 very closely the adiabatic limit curves calculated from the selection-only model equ.(2.4). This behaviour is readily understood in term of a perturbation theory for selection mutation models (Stadler and Schuster 1991): Mutation breaks the transcritical bifurcations of the pure replicator equations into a pair of saddle-node bifurcations. Thus a stable equilibrium disappears at certain threshold of c_0 and the trajectory is "freed". For a slightly different value of c_0 however another stable equilibrium is created in the second saddle node bifurcation, and it is located very near to the previous one. Thus it will usually "catch" the trajectory again. Thus trapping in unstable equilibria is prevented and the system follows the adiabatic limit very closely.

Note that this property does not depend on the particular form of the mutation model, but only on some rather weak conditions required for meaningful mutation models (Stadler and Schuster 1991).

7. Conclusions

The prebiotic scenario presented in this contribution is a minimal model to study the origin of cooperation. It is shown that cooperation can, but need not, emerge simple by increasing the total concentration of selfreplicating molecules. For low concentrations the dynamics are governed by first order autocatalytic reactions which lead to strict selection. Apart from nongeneric cases only one single species survives. This first order regime "erases" the initial conditions completely. When the concentration of selfreplicating material exceeds a certain threshold, however, this strong selective pressure may be overcome by features characteristic for second order autocatalysis. Cross-catalysis of two species may lead to coexistence. Since a second order replicator equation allows in general for more than one ω-limit, the long time behavior of the inhomogeneous model with slowly growing total concentration depends on both the first order and the second order rate constants, but not on the initial conditions.

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TABLES

Table 1: Stability of the fixed points for the two species model

	$\hat{x}_1$	$\hat{x}_2$	$\hat{x}_3$
Coordinates	0	1	$\frac{1}{2}(1+\frac{1}{c_0})$
Derivative	$1+c_0$	$-1+c_0$	$\frac{c_0}{2}(1-\frac{1}{c_0^2})$
$c_0 < 1$	unstable	stable	*unstable*
$c_0 > 1$	unstable	unstable	stable

Figure Captions

Figure 1. Graphs and phase portraits for the nondegenerate **2, 3, 4** the degenerate cases. of the *2*-, *3*- and *4*-species first order replicator equation. For **2a, 3a** and **4a** two rate constants are equal. In **3b** and **4d** all rate constants are equal and thus the state space consists entirely of rest points. In situation **4b** there are two pairs of equal rate constants and in case **4c** three of them are equal.

Figure 2. Trajectories for the simple two species model **a)** without mutation, equ.(5.2) and **b)** with mutation, equ.(6.6). The abiabatic limit is shown as solid line, numerical solutions are shown as dotted lines for different values of κ: from left to right $\kappa = 0.003, 0.03, 0.1, 0.3, 1$. Note that the trajectory for $\kappa = 0.003$ is trapped in $x_1 = 1$ without mutation. For $\kappa \geq 0.1$ there is no visible difference between the trajectories with a small mutation rate and without mutation. The mutation rates in **b)** are $p = 10^{-4}$ for all off-diagonal entries in both P and $\hat{P}$.

Figure 3. Changes in the dynamical behaviour of inhogeneous three species models as c_0 increases in the adiabatic limit. All six models have the same second order matrix A (equ(5.2)) but different permutations of the first order rate constants f_i.In the first, second and sixth example first a two-membered hypercycle if formed which incorporates a third species when c_0 reaches a second threshold. In the other three cases evolution avoids cooperative behaviour although the differential equations would allow for it. Sinks, sources and saddles are denoted by $\bullet$,$\circ$ and $\oplus$ resp. Centers (which are surrounded by a continuum of periodic orbits are shown as $\odot$ and a single periodic trajectory.