

SELF-ORGANIZATION AND EVOLUTION IN A SIMULATED CROSS CATALYZED NETWORK

A. HUNDING and ROBIN ENGELHARDT

*Department of Chemistry, H. C. Ørsted Institute C116, University of Copenhagen,
Universitetsparken 5, DK 2100, Copenhagen Ø, Denmark
(e-mail: kel3ah@unidhp.uni-c.dk; kel3re@unidhp.uni-c.dk)*

(Received 12 November, 1998)

Abstract. Motivated by an alternative to the concept of a prebiotic soup in the form of interacting crystal growth close to hot vents, we investigate a model system in which the growth rate of a particular entity is modified (enhanced or reduced) by other entities present, thus forming a web of cross catalysis. Initially random interactions are imposed, but the entities compete for a common source, and some entities may thus vanish in the competition. New entities, or mutations (error copies), with randomly selected interactions to the web are then introduced, and the concentrations of the entities are followed as solutions to stiff ordinary differential equations. Entities with positive growth may create new related entities with slightly randomly modified interactions to the web. Extinctions, wild-type survival and replacement, and self-organization to sustain periodic external variations, are studied. It is shown that even systems with mostly cross-inhibition and no initial autocatalysis may eventually create highly stable self-organized systems. We find that an already established cross catalyzed system often wins over a selfreplicating invader (or mutant).

Keywords: genetic takeover, hydrothermal, mineral origin of life, quasispecies

1. Introduction

The idea by Cairns-Smith that life originated from self-organizing crystallization processes is explored here. This theory (Cairns-Smith, 1982) has recently become more attractive with the discovery that a possible common ancestor of life as we know it seems to be closely related to hyperthermophiles, and that large communities of such cells are abundant today in deep subterranean bacterial ecosystems, notably in hydrothermal systems. (See Walter, 1996). Such a cradle for the origin of life on Earth or other planets is believed to be much less sensitive to outside catastrophes like meteorite impact than a possible surface related prebiotic soup.

Self-replicating entities based on nucleic acids are experimentally difficult to realize, and such an RNA world may have emerged from a more primitive setting. Alternatively, reliable self-replication is abundant in crystallization processes and such processes may be kinetically much faster in a hot setting than in the originally proposed context of vital muds. Moreover it is widely felt that focusing on processes needed for the system to work bypasses the problem that many related and



equally probable processes presumably would act as inhibitors of the few necessary ones.

In the present study, we do not rely on an information system dependent on precise copying of particular crystal defects. Also we explicitly study the effect of having an overwhelming negative influence on the growth of a particular species due to inhibitory interactions from other species. Autocatalysis is thus not an intrinsic property from the outset, but may be an emergent property.

2. Evolution with Mutual Interactions, Invaders and Mutants

The kinetics for a large system of interdependent crystal entities is dependent on many details, which cannot at present be captured by tractable model systems. The feature of most interest here is that the rate of growth of a particular crystal entity is not necessarily autocatalytic i.e. proportional to the amount present, but may depend on the surface area, degree of saturation, or local diffusion properties of the medium (Sultan *et al.*, 1990).

We have restricted ourselves to a much simplified set of kinetic equations, which to leading order may nevertheless incorporate essential elements of a system characterized by interdependent growth or decay.

The basic rate equation for the amount per volume unit of a specific crystal entity y_i is thus taken here to be dependent on interactions from the other entities and a common source m , for which the entities compete. In its simplest form (to be extended below), such a system may evolve due to the equations

$$\frac{dy_i}{dt} = m \sum_{j=1}^N A_{ij} B_{ij} y_j - k_i y_i \quad (1)$$

We take the amount of m present equal to a basis value v minus the total amount used up in the y -entities, and thus

$$\frac{dy_i}{dt} = \left(v - \sum_{j=1}^N y_j \right) \sum_{j=1}^N A_{ij} B_{ij} y_j - k_i y_i \quad (2)$$

$$\frac{dm}{dt} = - \sum_{j=1}^N \frac{dy_j}{dt} \quad (3)$$

The elements A_{ij} contain the interaction strength of entity y_j upon the rate of y_i , and this may be taken to be a positive or a negative number. The B_{ij} elements are either 0 or 1 that is, the nonzero B elements act as connectivity elements. The k_i elements are, for the time being, simple first order rate constants for degradation of y_i .

We initialize the system as follows. v and system size N are kept constant in a simulation. Also the number of nonzero B elements per row is kept constant to K . If we choose K much less than system size N , the rate of any entity y_i only depends on interactions from relatively few other entities, but we will also discuss systems with K approaching N . For the i 'th rate, we thus choose K randomly selected j 's, for which $B_{ij} = 1$. For the same j 's, we select randomly chosen values for A_{ij} from, say, a uniform distribution between $-L_1$ and $+L_2$. Indeed, we use the interval $-\sigma$ to $2.0 - \sigma$ – or with parameter σ about 1.90, to be varied below. Finally the particular k_i is generated as a random real number between 0 and 1. The system is now defined and integrated with initial values of the y_i 's much less than v , usually $1.0 \times 10^{-6} \ll v = 15.0$.

Numerical aspects of the integration will be described in a section below, suffice is here to say that we use a stiff ODE solver. The behaviour of the solution as function of time is now basically as follows. Originally, most (if not all) rates may be negative, and the corresponding entities thus decay and may eventually die out. If a few nondecaying entities are present, their growths increase the term Σy_j , but this in turn diminish the value of $m = v - \Sigma y$. Thus the growth of a few species may aggravate the decay of other species. When a particular decaying y_i vanishes (or rather, goes below a critical low concentration such as 10^{-2} times its initial value), it is replaced by a new entity (an invader), and its connectivity to all species are redefined by random elements as described for initialization above. Also the value of k_i is replaced.

The initial phase is thus characterized by many extinctions and perhaps growth of a few entities. For successful entities, we introduce related entities ('mutants' or slightly deviating copies) as follows. We monitor any positive partial rate ($m \Sigma A B y$), and if its accumulated magnitude over one or several time steps exceeds a predefined threshold, we decide that an error copy has appeared. To keep system size N constant, we find the smallest y_j and replace it with the error copy. The interactions of the mutant is defined to be closely related to those of its originator. Say y_k mutates and the mutant is introduced as entity y_j . We thus copy B 's for entity k into species j , and replace one 0 with 1 (or vice versa) in the mutant.

Extensions to this basic model will be discussed in later sections.

3. Dynamical Properties of the Simple Model

The simple model may suffice to familiarize the reader with some of the properties, we want to examine in the extended model to be introduced in later sections.

Most studies were carried out with entity number N around 100, although values as high as 512 were attained. In all studies the source term v equals 15.0, and all entities were started with the value $y_i = 1.0 \times 10^{-6}$ that is much smaller than their possible maximum $y_i \approx v = 15.0$. The time evolution of all entities were followed, but for practical reasons, only eleven entities are shown in the following

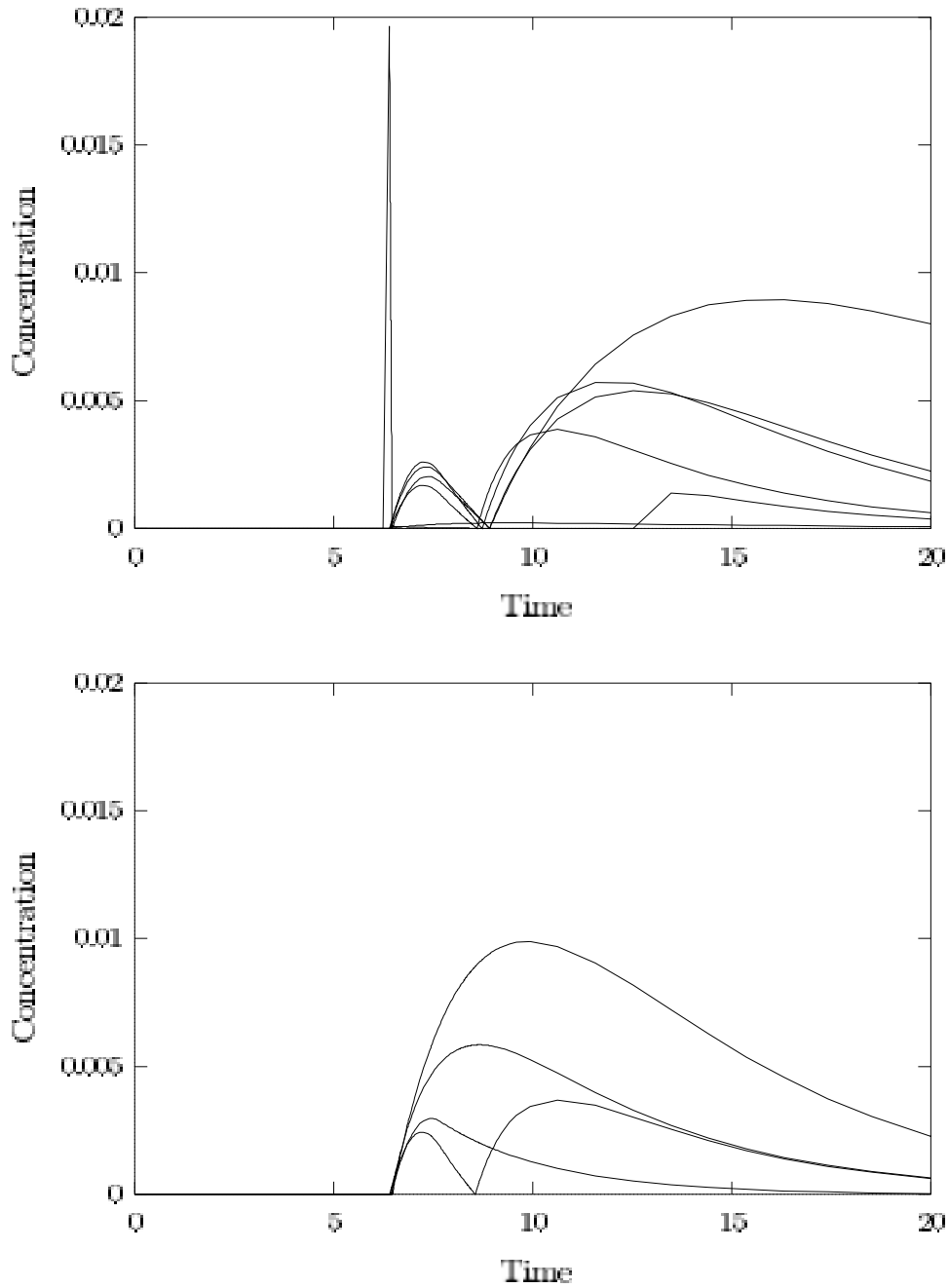


Figure 1. Concentration of entities versus time. Only 11 entities out of $N = 95$ are displayed for convenience. Medium connectivity $K = 12$, of which approx. 3.5% are positive elements in the connection matrix A . Source $v = 15.0$. For a long initiation time, $T < 6.0$, all entities stay small, after which a certain entity grows fast, only to be outcompeted soon after by others. At about $T = 8.5$ some of the entities shown go extinct, and are replaced by invaders or mutants (error copies) of the more successful entities.

figures. The differential equations were integrated with variable step lengths, to ensure that the local solution of each entity was computed to relative accuracy 1.0×10^{-5} . In Figure 1 a typical solution is depicted, where the onset of sustained growth of some entities are shown. Here, $N = 95$ and the number K of nonzero elements per row in matrix A is taken as 12 that is a particular entity y_i has its rate defined by 12 randomly selected entities. The interaction elements in the A matrix were taken as uniform random numbers between -1.93 and $+0.07$ that is 7 out of every 200 computed elements, or 3.5%, are positive. Thus in each row of A the probability for encountering a single positive element is moderate and the special case of autocatalysis, i.e. a positive diagonal element, is even less. The initial phase of the time evolution of the system is thus characterized by many entities with negative rate, and these entities vanish on a time scale smaller than that shown in Figure 1.

Indeed, about half the depicted subpopulation diminishes fast and dies out in the short time span $T < 0.02$. They are replaced by invaders with randomly chosen parameters as described above, about half of which also vanish over a somewhat longer time span $0.02 < T < 0.12$. However a few of the invaders manage to stay approximately stationary, albeit with very low concentration, for a much longer time span.

During this initial phase none of the entities may have a nonzero (let alone a positive) diagonal A element, and thus none of the entities have autocatalysis. It is found, however, that such communities may have cross catalysis through the off-diagonal elements, and thus some entities with mutual sustained growth.

Indeed in the present run, no autocatalysis is present at the onset of rapid growth about $T \approx 6$, but some entities increase orders of magnitude on a time scale of about 0.3, which is indicative of how steep the growth may be in the following figures. The rise and fall of entities seen in Figure 2 occur in a system, in which autocatalysis still not has occurred. Only about $T = 7000$ is a single such entity present, but it is unlikely to be among the highest concentrations, since mutations of this entity then would have proliferated, and many autocatalytic entities subsequently recorded. Instead we find that this entity is absent for $7500 < T < 18\,500$. A new autocatalytic entity appears for $T = 19\,000$ only to die out again. Only after $T = 22\,500$ one or two autocatalytic entities are consistently present.

Invaders are common initially, but when the entity community is characterized by enough members with high concentrations, the value of the source term $m = v - \sum y_i$ is very small, and thus a newborn invader may have kinetics dominated by its first order rate $-k_i y_i$, in other words, it rapidly goes extinct again. Only if the invader happens to have the right connections to high concentration entities, it may start to grow. Unsuccessful invaders are replaced with mutants selected from the most abundant entities. Thus the predominant innovation in the system comes from mutants. When a mutant is introduced, the entity with lowest current concentration is removed, and the entity to mutate is selected among the remaining entities with probabilities proportional to their current concentrations.

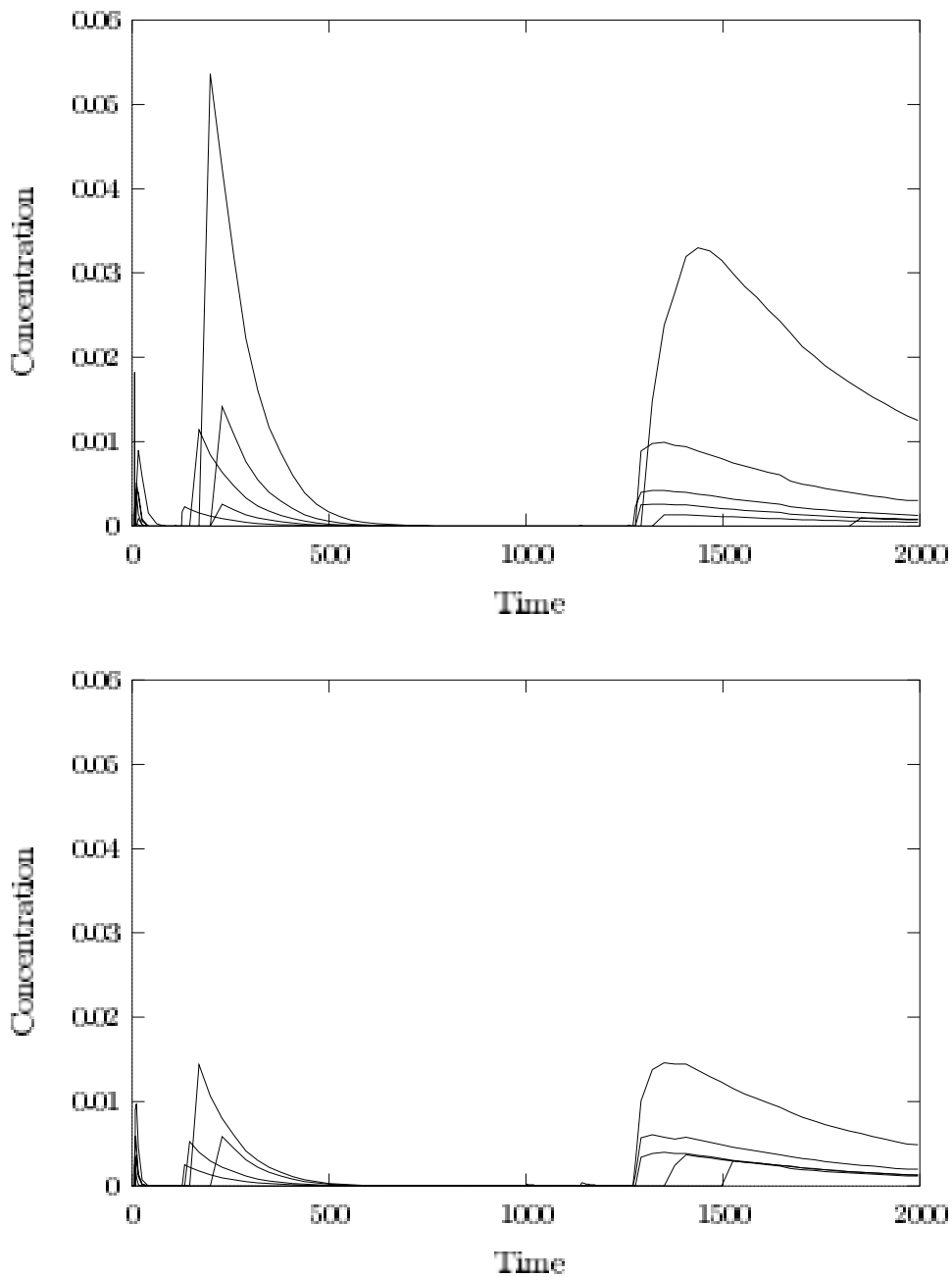


Figure 2. Concentration of entities versus time. Again, only 11 entities out of $N = 95$ are displayed for convenience. Parameters as in Figure 1, but two orders of magnitude longer time. The entities which grew up in Figure 1, have gone extinct at about $T = 100$. A series of mutants enters between $T = 150$ and 250 , only to go almost extinct by $T = 600$. A new set of mutants enters after $T = 1250$. The more successful entities create mutants (error copies), which may stay in the population until the entity with the lowest current concentration is replaced by the introduction of yet another mutant. Entities with a common root have kinetical parameters, which on average yields a wild type entity, around which they cluster.

To keep track of the origin of a mutant, we introduce a Hamming sequence and distance as follows. At birth of an entity (invader or mutant) it is assigned a binary code with 775 bits, its Hamming sequence. When a mutant is created from a preexisting entity, the new Hamming sequence is changed one (randomly selected) bit from the original sequence. In due time, this entity may mutate to create an entity with Hamming distance 2 from the original, etc. The average Hamming sequence of the community is said to be the wild type. Often an entity with this sequence is indeed present, but this need not be so. The distribution of Hamming distances from the current wild type may be recorded over time. If all entities present originated from the same entity, or its mutants, the distribution has a peak close to Hamming distance zero (the wild type).

Such a cluster of related entities is known as a quasispecies (see Novak, 1992). However, if two unrelated species have coexisted for a substantial time, they may both have many mutants, and these quasispecies show up as two strong peaks, both of which are quite distant from the mean sequence in the community, the wild type. This no longer represents a single strong survivor in the community. A recording over time of Hamming distances from the current wild type is shown in Figure 4. One quasispecies may replace another quasispecies during the evolution.

As already stated, none of the quasispecies in Figure 3 are characterized by entities with autocatalysis, the large majority of the entities present do not have positive diagonal A -elements. Also quasispecies often exist over a substantial longer period of time than the life time of the individual entities.

Generally it is found that quasispecies build around entities with autocatalysis may outcompete other quasispecies, which do not exhibit such direct catalysis. However the reverse is also true. Thus we find that it is unnecessary to wait for the occurrence of an entity with autocatalysis in order to have self-sustained growth and surviving quasispecies. We will revert to this in more detail in sections below.

4. Crystals as Candidates for Cross Catalysed Network

With the above results in mind, we may discuss whether communities based on crystals could display some of the phenomena found in the simple model above. Many general properties found in growing crystal communities are already mentioned in substantial detail in (Cairns-Smith, 1982). Small changes in the crystallization environment may yield quite some changes in porosity, flow rates, ion exchange properties, and so on. One type of crystal may be helpful to nucleate another types growth. Great variety of micromorphologies may arise from local changes in permeability, pH etc. Crystals displaying outgrowth in long threads may yield particular three dimensional structures and defects depending on conditions set by other entities in the surrounding, and the break up rate of such threads and the transport of such seeds in the system may be a common primitive proliferation mechanism.

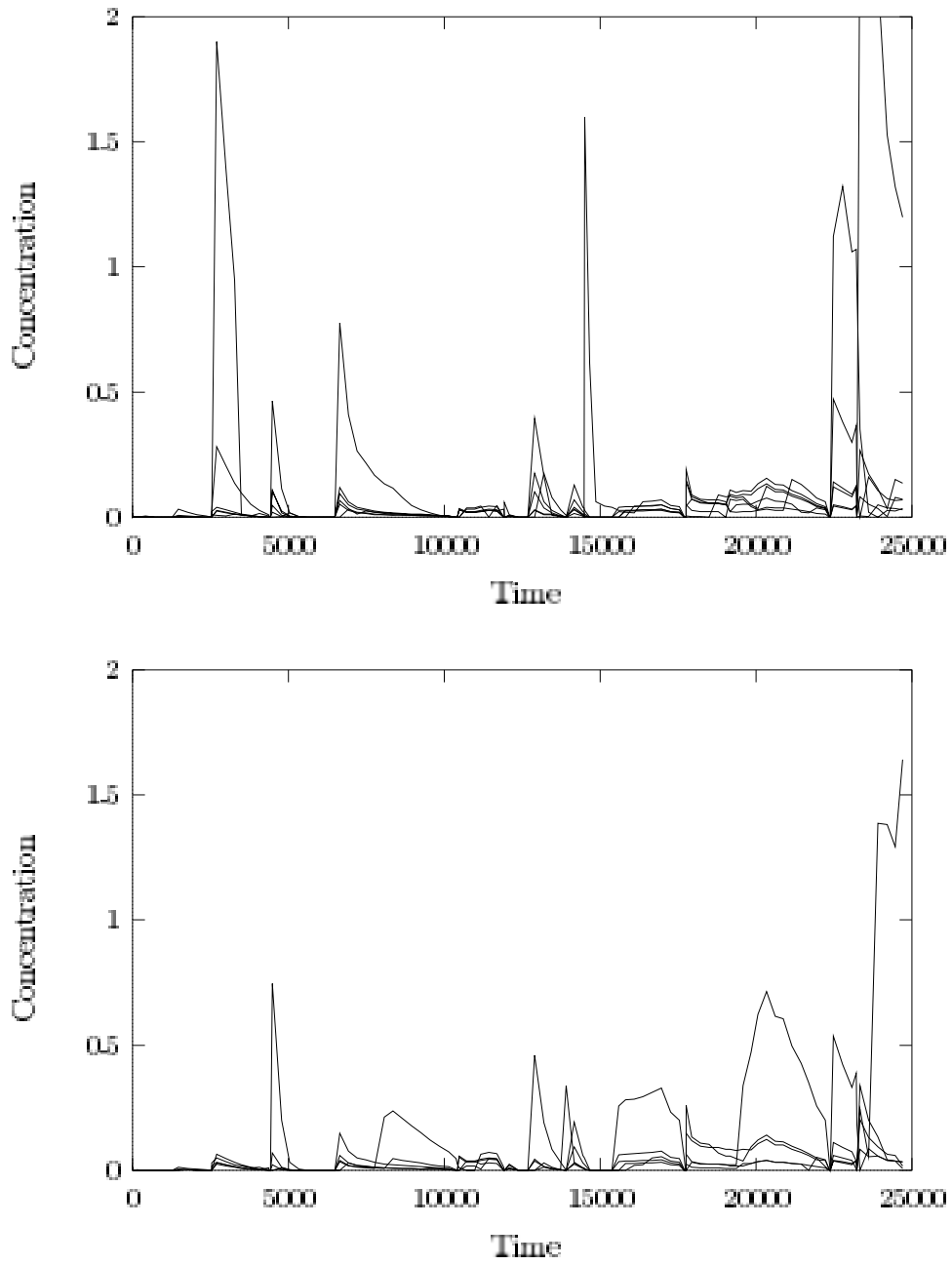


Figure 3. Concentration of entities versus time. Parameters as in Figure 1, but time now extends to $T = 25\,000$. The system does not come to a rest.

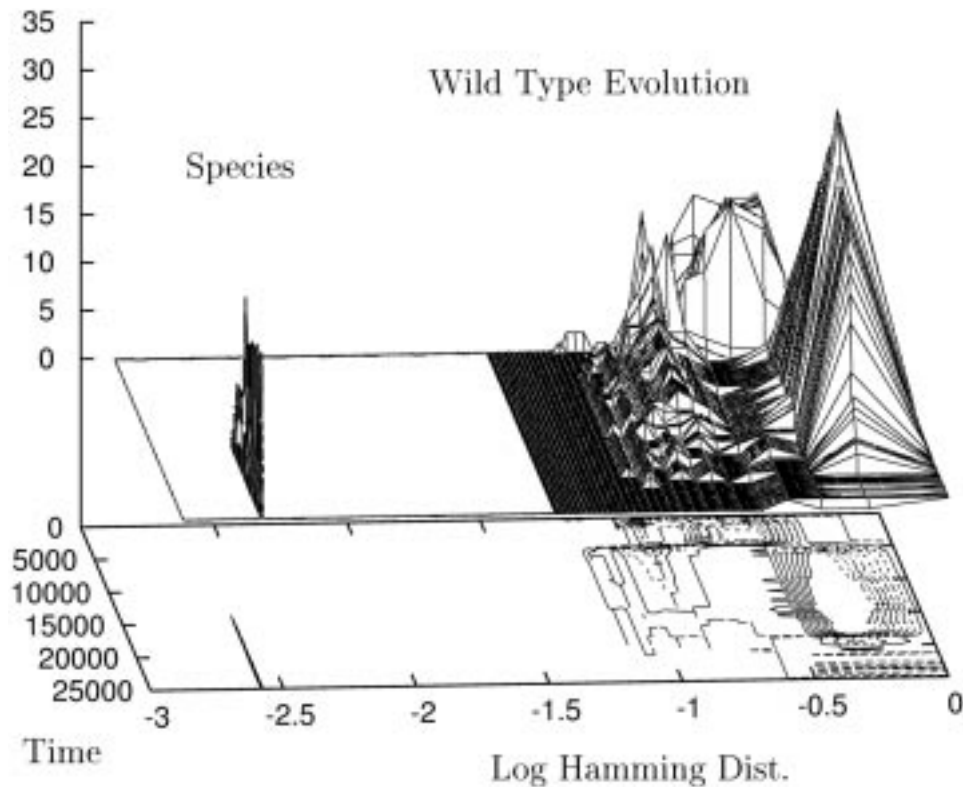


Figure 4. Quasispecies competition during evolution. The wild type has properties as the average entity. Hamming distance for an entity is defined as number of mutations from the wildtype. Abscissa is logarithm of (Hamming distance plus one). Initially, entities are scattered with random hamming distance to the mean, but soon a few entities outgrow the rest, and mutations of these entities dominate. Up to about $T = 5000$, the wild type is determined by two quasispecies, each with a (log) distance of about 0.6. After $T = 5000$ one of these grows at the others expense, and thus the dominant quasispecies appears closer to the wildtype, while the other appears (relatively) to have moved to (log) distance of 0.9. These two quasispecies coexist for a long time. At about $T = 14\ 000$, a successful invader, with distance 380 (log distance approx. 2.6), starts to create yet another quasispecies. At $T = 25\ 000$, the two former quasispecies are much reduced, one has disappeared, but the other has still a few, high concentration, entities present, which still define the wild type of the entire population.

The point is that crystal growth may generate three dimensional structures, which may be modified in a reliable way by activators and inhibitors as described above. This feature is not present in just any net of entities, say, based on reactions of small inorganic molecules. In this respect the modifiable micro structure of crystals is related to the three dimensional structure of small RNA's or proteins. This property of crystals is well established and widely explored for making efficient catalysts in industry. It is thus not just the overall chemical composition of such catalysts, which is important, but to a large extent, the conditions prevailing,

when the catalyst is made. This defines the impurities, active catalytic sites, micro structure etc., which make the difference between just an inorganic compound and an efficient catalyst with the same overall chemical composition.

In general the resulting rate for a particular entity is thus not necessarily linked to exponential, autocatalytic growth, which is one reason we have chosen to build our model without such explicit terms. Also the interactions may or may not be nonlinear, but we have chosen not to build in highly nonlinear off-on rates from the outset, as this might be seen as bypassing the problem of how such well-tuned control arose in the first place. Our model simply supposes that the growth or dissolution of some entities in the community has impact on the possibility for growth of other entities, and we have chosen a very simple first-order model for such interactions. It seems more interesting to study the possible onset of self-organization in a net based (initially at least) on such very simple interactions, rather than nets with build-in elaborate off-on control systems from the outset.

As previously stated, we do not incorporate entities with autocatalysis from the outset, and our finding that sustained mutual growth and long time survival of quasispecies build on such non autocatalytic interactions is likely to be a feature, which may thus arise in real systems as well. Notably this is found also for systems, in which the mutual interactions are predominantly inhibitory.

Also we find coexistence over substantial time periods of quasispecies, and the phenomenon of take-over presupposed in (Cairns-Smith, 1982). It is thus conceivable that a predominant dynamical structure in the system is replaced over time with another dynamical structure, which arises within the system with a minor role initially.

5. Extended Model. Cyclic Environmental Conditions

Self-organization in crystal communities was originally suggested for a clay environment, but such a vital mud scenario has been replaced by an environment related to deep underground hot vents. Speculations on the origin of an initial energy source to keep the system far from equilibrium and make the eventual necessary organic polymerization processes feasible have pointed to the possibility of harvesting energy from cyclical heating/cooling processes. Indeed it has been proposed that the first organisms were such heat engines (Muller, 1995).

The dynamical properties of the entities in our simple model may thus be extended to a situation, in which the environment, and thus the parameters in the system, undergo cyclic variations. One may wonder whether the established self-organization in the system may survive such changes, and if so study possible adaptations to the cyclic environmental conditions. Also we will present the obtained results in the form of averages over many (100) runs, rather than details connected to a single run as above.

Generally all parameters in the system may change up or down according to very different rules. We have chosen a very simplified form for the implementation of a time variation, which would create a significant constraint on the rate of each entity. We only redefine the k_i 's to be slowly cyclically varying with time. Thus

$$k_i(t) = k_i^0 \left(\frac{\cos(\omega t) + 1}{2} \right) \quad (4)$$

with period of this cycle taken to be very long (say, 5000) (See Figure 8).

This choice makes the explicit first order rate constants vary between k_i^0 and zero at the bottom of the cycle. After the initial phase, where m has dropped from its initial value to almost zero, this imposes substantial stress on entities, which may have done well during a phase with small k 's, but which then face an enlarged degradation rate during the peak of the cycle.

We will discuss the results in terms of the three parameters N , the system size; K , the connectivity; and σ , the shift parameter, which monitors the relative amount of negative versus positive random elements in the A -matrix. Recall that K usually is taken substantially less than N , typical values being $(N, K) = (64, 12)$ which is a medium to highly connected system, or $(N, K) = (256, 3)$ which is a system with low connectivity. Elements of A are generated, as stated earlier, as a uniform distribution between $-\sigma$ and $2.0 - \sigma$. Thus $\sigma = 1.0$ means elements between -1 and $+1$, $\sigma = 1.90$ means elements between -1.90 and $+0.10$ that is only $0.10/2.0$ or 5% are positive. We will use σ values mostly between 1.80 and 1.95. The simulations were carried out then for fixed values of N , K , σ , but different seeds to the random number generator, and the results for 100 such runs were averaged.

First we discuss *extinctions*. The number of extinctions per unit time (the extinction rate) is high initially as discussed earlier, but when a growth system has stabilized the extinction rate comes down. A mutation, or a successful invader, may lead to further extinctions. As we would expect from the introduced cyclic variation of the outgoing rates k_i , Equation (4), this cyclic variation tends to destabilize the system, and an increased extinction rate is observed when the k_i 's peak. See Figure 5 or Figure 8.

The magnitude of this cyclic extinction rate is dependent upon the connectivity and σ as well. In medium to highly connected systems $(N, K) = (64, 12)$, a dramatic (about 20 fold) increase in extinction rate magnitude is observed, when the average number of positive A elements is reduced from 20% ($\sigma = 1.60$) to 2.5% ($\sigma = 1.95$). Thus in such highly connected systems, a small relative amount of positive connection elements has a profound effect on the extinction rate encountered (see Figure 5). Each time an extinction occurs, an invader is introduced, but if this invader at birth has a negative rate, and thus goes extinct shortly, it is replaced by a mutation instead. The number of successful invaders is remarkably small, even in systems displaying a high rate of extinctions. For the high-extinction system in lower part of Figure 5, rate of successful invaders never exceeds 0.02 and mostly stay around 0.005.

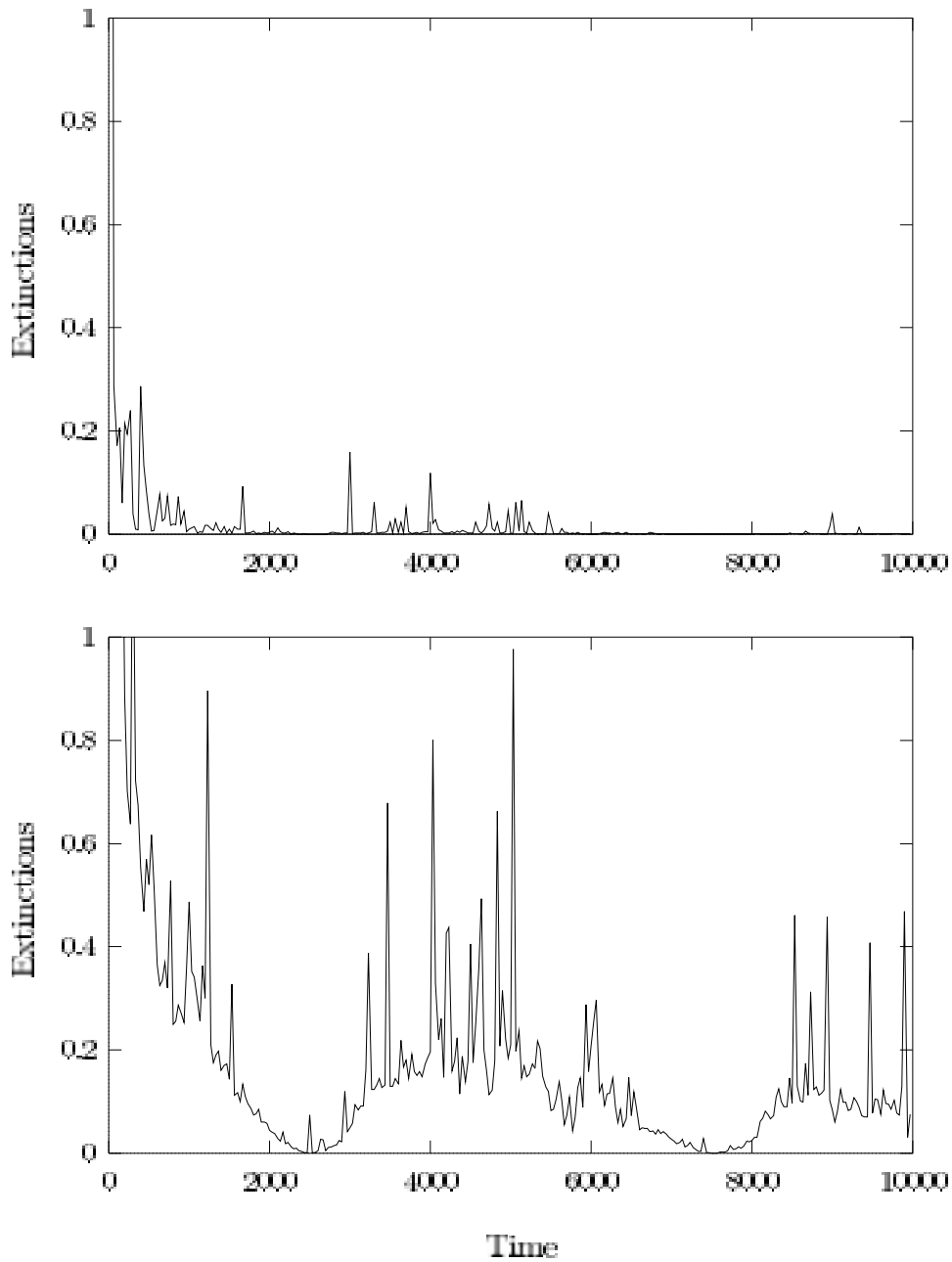


Figure 5. Extinctions versus time. For medium to highly connected systems, $(N, K) = (64, 12)$, with relatively many (20%) positive elements in the connection matrix A , the extinction rate is only moderate, and it cycles in time with the cyclic alteration of the outgoing rates k_i^0 . These extinctions tend to diminish with the number of cycles (upper figure). With number of positive elements diminished to 5%, a substantial increase in extinction rate through the cycles is observed (lower curve). See also Figure 8.

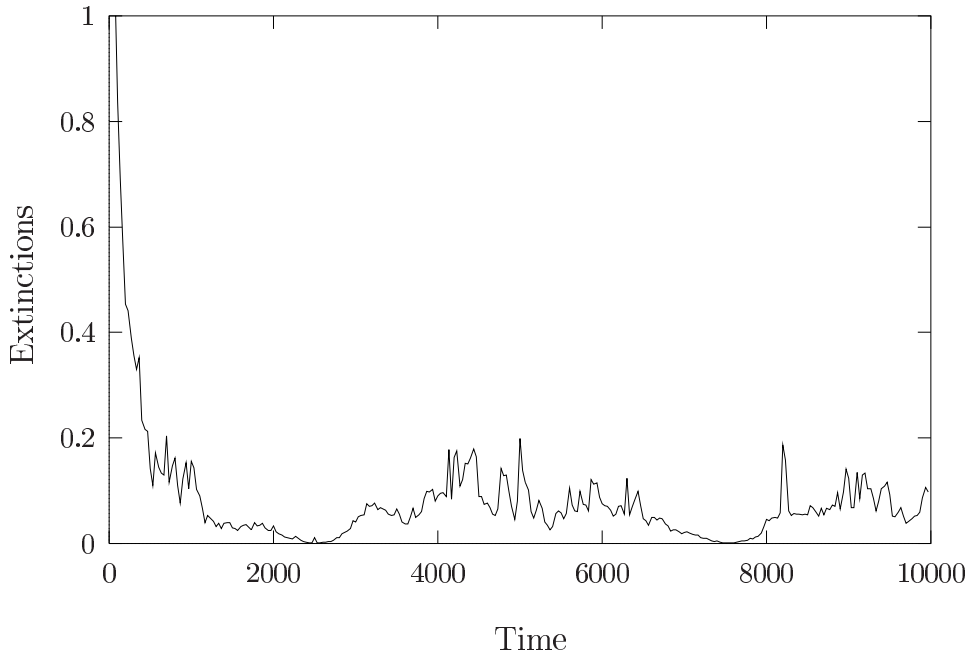


Figure 6. Extinctions versus time. With lower connectivity, here $(N, K) = (128, 3)$, and 5% positive elements (i.e. $\sigma = 1.90$), the extinction rate decreases again, compare Figure 5.

However in systems with low connectivity, $(N, K) = (128, 3)$ a much smaller extinction rate is encountered, and it stays low even for $\sigma = 1.95$ (see Figure 6).

Indeed in such systems of low connectivity, the extinction rate is so low that the total number of extinctions during a particular run is less than the system size N . Thus the source of renewal in the system is predominantly entering through mutations.

Next we have followed the *diagonal terms* during the simulations. For a particular run, we record at fixed time intervals, if the system has any positive elements in the diagonal. For all 100 runs with fixed parameters (N, K, σ) , the fraction of runs, which has no positive diagonal elements at time t is recorded. This fraction is $nD(0)$. We monitor the number of positive elements in the diagonal as well, but slightly differently. If at time t the system has one or more (d) positive diagonal elements, the relative number d/N is recorded, and after completion of all runs, the mean such fraction at time t is depicted as $nD(p)$.

For medium to highly connected systems, $(N, K) = (64, 12)$, we observe an increase with time of $nD(p)$, thus reflecting an increased abundance of autocatalytic members. This abundance tends to grow faster when extinctions start to grow during the cyclic variations of the k_i 's, with subsequent relative stasis when extinctions come down again. In such highly connected systems, the relative number of positive diagonal elements present ($nD(p)$) grows from 0 to about 0.3 for σ values between 1.6 and 1.8, only to show slower growth for $\sigma = 1.95$, presumably

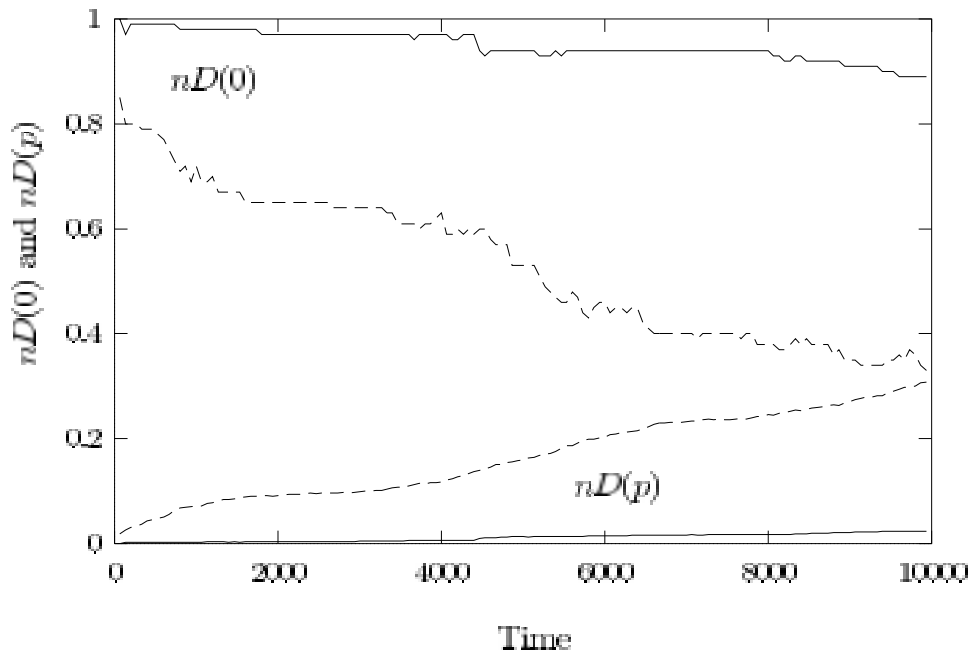


Figure 7. Diagonal terms in the connectivity matrix A . The fraction of runs at time t , for which no positive diagonal A -element is present, is depicted as $nD(0)$. It decreases with time. If at time t , a system has d positive diagonal elements, the fraction d/N (i.e. relative to system size) is recorded. Depicted is the mean of this fraction $nD(p)$ over 100 runs. Usually $nD(p)$ increases with time, but for low connectivity and/or low number of positive randomly generated A -elements, $nD(p)$ stays low and the system is dominated by entities, which have no positive diagonal elements and the system is thus not autocatalytic. Dashed curves: Medium to high connectivity, $(N, K) = (64, 12)$ and $\sigma = 1.90$ that is 5% positive random A -elements. Solid curves: Low connectivity and lower number of positive elements, $(N, K) = (128, 6)$ and $\sigma = 1.95$.

due to the smaller probability of creating positive elements now, but despite the vastly increased extinction (mutation) rate, as discussed above. On the other hand, the fraction of runs, which at time t has no positive diagonal elements ($nD(0)$), in general decreases over time, but the final value increases a lot, from about 0.2 to 0.8, when σ varies from 1.6 to 1.95.

For systems with lower connectivity, $(N, K) = (64, 3)$ or $(N, K) = (128, 6)$, both with $\sigma = 1.8$, $nD(p)$ curves are somewhat lower, but $nD(0)$ curves are about twice as high. For even lower connectivity, $(N, K) = (128, 3)$, $(N, K) = (256, 6)$ or eventually $(N, K) = (256, 3)$ $nD(p)$ only goes up to about 0.1 (128, 3) or eventually, much lower values as 0.04 (256, 3). Correspondingly $nD(0)$ decreases, eventually to about 0.7 (see Figure 7). If σ additionally is increased, from 1.80 to 1.95, $nD(p)$ as expected is very low, going from 0.1 to less than 0.01 (128, 3), with corresponding high sustained values of $nD(0)$, about 0.98 throughout the simulation.

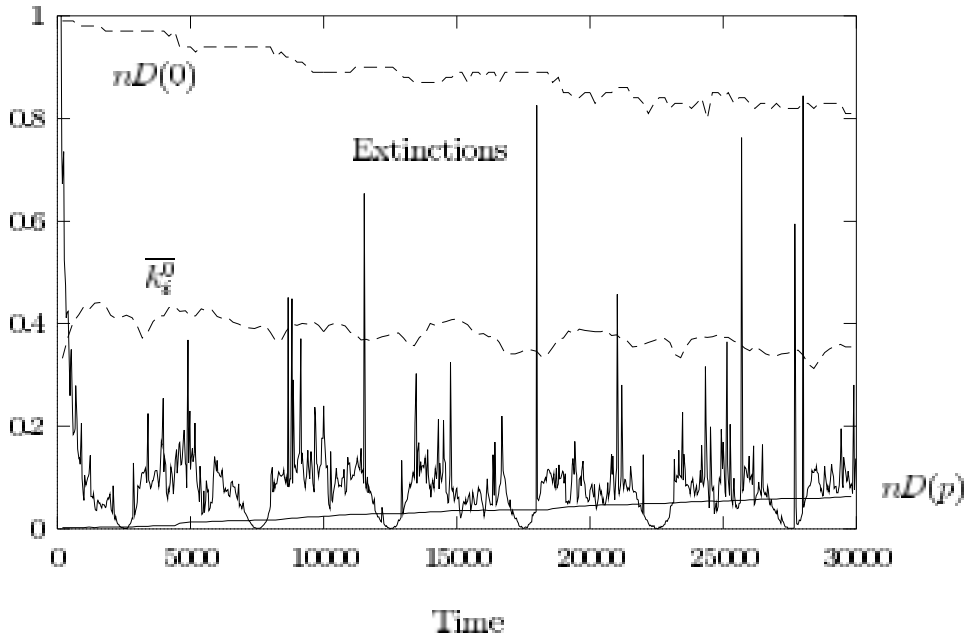


Figure 8. Cyclic variation of extinction rate for very long times. The extinctions do not die out significantly in this system of low connectivity $(N, K) = (128, 6)$, $\sigma = 1.95$. Also shown are $nD(0)$ (top), $nD(p)$ (bottom) and the mean outgoing rate k_i^0 .

In conclusion, lower connectivity (smaller K relative to N) and a decreasing percentage (less than 5%) of positive connection elements (σ approaching 2.00) display runs in which entities with autocatalysis (positive diagonal elements) play a minor role. Increasingly, in such runs, the entire system consists of entities, for which no such autocatalytic entities are present at all. Nevertheless these systems have a low extinction rate, as observed above, and successful invaders are rare. Thus these systems are not prone to be overtaken by invaders, or mutants, with autocatalytic terms, but self-sustained even with predominant negative elements in the connection matrix A .

6. Numerical Method

Before we enter the discussion, we provide some information for the reader interested in the details of our numerical method.

The numerical integration of the differential equations was performed with a stiff solver of Rosenbrock type, with variable step size control. Indeed, integration step length h may vary from about $h = 10^{-5}$ during periods with high extinction rate, to about $h \simeq 1$ during periods of quasistationarity. For sampling purposes (recording of $nD(0)$ and $nD(p)$, say) we restricted h to at most 1.

The Newton iterations in each time step, necessary with implicit stiff integration schemes, involve the solution of N linear equations $Mx = b$ with matrix M nonsymmetric. The condition number was evaluated and a reduction in step size h made if necessary.

We made a crude estimate of the time for which the next extinction would occur (based on linear extrapolation of current rates and concentrations). We restricted h to a fraction of this limit. This feature to a large degree prevents the ODE solver to compute negative concentrations.

Also, our choice (after a small initiation period) to discard invaders with negative initial growth has a substantial effect on computation speed. When such invaders were followed in preliminary versions of the code, these invaders would go extinct shortly, only to be replaced largely by new shortlived invaders, thus restricting h .

7. Discussion

Previous studies of the dynamical properties of nets of entities with cross coupled interactions belong largely to two classes, cellular automaton models and small systems of differential equations. In (Kauffman and Johnsen, 1991), a key paper exploring a cellular automaton approach, a coupled system of genes restricted to off-on states is studied. Many papers on related models have appeared (see Bastolla and Parisi, 1998).

The confinement to off or on states of the entities present make such models comparatively easy to program, and fairly large communities of entities may be studied. However, with our model, we would like to study systems more closely related to actual chemistry. In such systems, it is not the system with lowest fitness (defined as the lowest rate) which is most prone to vanish. Rather it is an entity with low current concentration and low (negative) rate. Thus a restriction to off-on states may introduce peculiarities, which may not be found in systems, where the individual entities past history is taken into account. An entity may during the past have grown to a level, where it by far is dominant in the community, yet its current rate may be close to zero (quasistationarity). It is not obvious that invaders with comparatively very small concentrations, but current higher rates, may outcompete the dominant entity.

Networks of interacting entities described by differential equations in the context of the dynamics of small sets of self-replicating polymers have been much studied (Stadler *et al.*, 1993, 1995; Phillipson and Schuster, 1994; Happel and Stadler, 1998) on the basis of the so-called second order replicator equation, which is equivalent to the Lotka-Volterra equation (Hofbauer and Sigmund, 1998)

$$\frac{dy_i}{dt} = y_i \left(k_i + \sum a_{ij} y_j \right) \quad (5)$$

Our simple growth equation, however, is not of the special Lotka-Volterra type, but the rhs is a more general bilinear form. The size N of interacting entities studied here is substantially higher than those reported above.

The present work shows that cross coupled kinetic systems without explicit autocatalysis and with predominant inhibitory interactions may selforganize nonetheless, and have stable quasispecies over time intervals much longer than lifetimes of individual entities. Interactions are not from the outset of a strongly nonlinear off-on nature, rather simple linear interactions are invoked, but due to competition for a common source, nonlinear dynamics is encountered. Thus the emergent organization is not based on the property of a selfreplicating molecule (like RNA) or other intrinsically autocatalytic such entity.

Medium or highly connected systems have a high probability of creating entities with positive diagonal elements, and such autocatalytic nets are close to the systems already investigated in other works. We have thus concentrated on systems with relatively low connectivity $K \ll N$, and a low density of positive interaction elements. In our system, growth starts in a system with no positive diagonal elements as a rule. Although autocatalytic invaders may appear, mostly they are not successful, once a cross catalyzed system has grown up. Thus such a system is not prone to be overtaken by the appearance of an autocatalytic entity. Indeed, such invaders are mostly unsuccessful (they have negative growth from birth), and in our algorithm they are replaced by mutants. We thus find that an already established cross catalyzed system wins over a selfreplicating invader (or mutant).

We have not investigated extinction patterns for power law relationships, nor have we plotted lifetime distributions. One of us (R. E.) has recently published such data for a related model

$$\frac{dy_i}{dt} = \frac{1}{K_i} \sum_{j=1}^N A_{ij} B_{ij} y_j (\kappa - y_j) \quad (6)$$

with variable connectivity K for each species, and upper bound due to $m = v - \sum y_j$ replaced by a carrying capacity κ , i.e. a system with logistic growth (Engelhardt, 1998). One finds a power law distribution for extinction patterns with exponent $\beta \simeq 1$, and lifetime distributions of power law shape, but with exponent dependent on system size N . We have omitted such power law studies here, since data following such laws may be found even for systems without selforganizing underlying mechanisms (Newmann, 1997).

Our aim has rather been to investigate the selforganizing potential of a cross coupled system, in which as little as possible has been predefined. Thus we have very simple interactions (linear couplings), predominantly inhibitory, and competition among entities is introduced simply by feeding all entities from a common source, which may be almost depleted by the entities' growth.

The essential system feature is not just the imposed interactions of the entities. Rather it is the capability of an entity to mutate (or error copy) to an entity, which

has *related* interactions to the other entities. This property has been found for small strands of RNA, and small variations in the primary sequence yields (model) secondary structures related to the original (Schuster, 1993; Grüner *et al.*, 1996).

Thus the *shape* of RNA entities may be modified gradually by such mutations. We have presupposed that crystal entities may influence each others growth in a similar graded way due to changes in the crystallization medium, thereby creating related entities with different impurities, microstructure and interactions. Such systems may display robust selforganization, as shown here. On the other hand, such graded interactions is *not* a feature of just any set of small chemical compounds. Although such entities also initially show connections in their growth properties, generally such small molecules are unable to produce related species with only small changes in their molecular constitution and interactions. Thus our model equations do not describe such a small molecule system, but may capture some features of an interconnected crystal community.

In our model, we would not see self-organization, if the initial $v\Sigma AB\gamma$ term is much smaller than the outgoing $k_i y_i$ term. Growth is made possible through a value of $v > k_i$. This is to say that the initial conditions are such that net crystallization (rather than dissolution) is presupposed, but then the (mostly inhibitory) interactions among entities define, which (if any) entities are actually growing. Cross catalysis with mostly negative connections is possible, as the inhibitor of an inhibitor is in effect an activator.

We may comment on an aspect of crystal communities versus a community of small RNA (or protein) strings. For the latter macromolecules, it has been shown that each of the most common structures may be realized with a huge number of primary sequences. Thus the total system may ‘diffuse’ around in primary sequence space, but remain neutral with respect to its essential property, its structure class. (A model for evolution on a fitness landscape with a tunable degree of neutrality was recently published by one of us (see Newman and Engelhardt, 1998). However, only a few mutations are required to create a member of another structure class, and thus the majority of common structures, i.e. ‘shape space’, may be covered from any given sequence with only very few mutations. This aspect is one of the key features of the immune system (Smith *et al.*, 1997). It is not obvious that a pure crystal community has the same property, and thus the ‘shape space’ it may cover is presumably much more restricted. With the build in of molecular connections based on phosphate chains and sugar kinks, as suggested by Cairns-Smith, a much more flexible crystal community may emerge. The initial pure crystal community may however have properties captured already by our simple model.

Acknowledgement

This work was supported by The Danish Research Councils, Grant No. 9313362.

References

- Bastolla, U. and Parisi, G.: 1998, *Physica D* **115**, 219.
- Cains-Smith, A. G.: 1982, *Genetic Takeover and the Mineral Origins of Life*, Cambridge University Press, Cambridge.
- Engelhardt, R.: 1998, *Emergent Percolating Nets in Evolution*, HCØ Tryk, Copenhagen.
- Grüner, W., Giegerich, R., Strothmann, D., Reidys, C., Weber, J., Hofacker, I. L. and Schuster, P.: 1996, *Monatshefte Chemie* **127**, 355 and 375.
- Happel, R. and Stadler, P. F.: 1998, *J. Theoret. Biol.* **195**, 329.
- Hofbauer, J. and Sigmund, K.: 1998, *Evolutionary Games and Population Dynamics*, Cambridge University Press, Cambridge.
- Kauffman, S. A. and Johnsen, S.: 1991, *J. Theor. Biol.* **149**, 467.
- Muller, A. W. J.: 1995, *Prog. Biophys. Molec. Biol.* **63**, 193.
- Newman, M. E. J.: 1997, *J. Theor. Biol.* **189**, 235.
- Newman, M. E. J. and Engelhardt, R.: 1998, *Proc. R. Soc. Lond.* **B 265**, 1333.
- Nowak, M. A.: 1992, *Trends Ecol. Evol.* **7**, 118.
- Phillipson, P. E. and Schuster, P.: 1994, *J. Math. Biol.* **32**, 545.
- Schuster, P.: 1993, *Origins of Life* **23**, 373.
- Smith, D. J., Forrest, S., Hightower, R. R. and Perelson, A.: 1997, *J. Theoret. Biol.* **189**, 141.
- Stadler, P. F., Fontana, W. and Miller, J. H.: 1993, *Physica D* **63**, 378.
- Stadler, P. F., Schnabl, W., Forst, C. and Schuster, P.: 1995, *Bull. Math. Biol.* **57**, 21.
- Sultan, R., Ortoleva, P., Depasquale, F. and Tartaglia, P.: 1990, *Earth-Sci. Rev.* **29**, 163.
- Walter, M. R.: 1996, *Evolution of Hydrothermal Ecosystems on Earth (and Mars?)*, Ciba Foundation Symposium 202, Wiley, New York.