Self-reproducing entities in an artificial chemistry

Implications of autopoietic and other organisations

PhD Thesis

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I hereby certify that this material, which I now submit for assessment on the programme of study leading to the award of PhD is entirely my own work and has not been taken from the work of others save and to the extent that such work has been cited and acknowledged within the text of my work.

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It turns out that in that terrible year [1937] Andrei Yanuaryevich (one longs to blurt out, "Jaguaryevich") Vyshinsky, availing himself of the most flexible dialectics (of a sort nowadays not permitted either Soviet citizens or electronic calculators, since to them *yes* is *yes* and *no* is *no*), pointed out in a report which became famous in certain circles that it is never possible for mortal men to establish absolute truth, but relative truth only He then proceeded to a further step, which jurists of the last two thousand years had not been willing to take that the truth established by interrogation and trial could not be absolute, but only, so to speak, relative Therefore, when we sign a sentence ordering someone to be shot we can never be *absolutely* certain, but only approximately, in view of certain hypotheses, and in a certain sense, that we are punishing a *guilty* person Thence arose the most practical conclusion that it was useless to seek absolute evidence—for evidence is always relative—or unchallengeable witnesses—for they can say different things at different times The proofs of guilt were *relative*, approximate, and the interrogator could find them, even when there was no evidence and no witness, without leaving his office, "basing his conclusions not only on his own intellect but also on his Party sensitivity, his *moral forces*" (in other words, the superiority of someone who has slept well, has been well fed, and has not been beaten up) "and on his *character*" (i e , his willingness to apply cruelty!)

[ ]

In only one respect did Vyshinsky fail to be consistent and retreat from dialectical logic for some reason, the executioner's *bullet* which he allowed for was not relative but *absolute*

Aleksandr I Solzhenitsyn
The Gulag Archipelago
Part I, Chapter 3 The Interrogation

Abstract

The SCL model system, an artificial chemistry used for the illustration of the concept autopoiesis, is extended to show self-reproducing entities The theory of autopoiesis was developed by the biologists Humberto Maturana and Francisco Varela around 1971 to point out the organisation of living systems One of the aims of this theory is to explain the perceived autonomy of living beings The degree to which the theory succeeds in doing so is investigated Along the way some ambiguities in the theory are pointed out and suggestions for improvements are made The conclusion, however, is that autopoiesis alone is not sufficient for a high degree of autonomy, although it is a step in the right direction Furthermore it is shown that the entities exhibited in the original SCL model system are not autopoietic, whereas in the extended system they are Together with SCL some other real and artificial chemical model systems are investigated with respect to the two concepts autonomy and autopoiesis Furthermore, the utility of autopoiesis as a guiding principle for Artificial Life research is considered The conclusion is that because autopoiesis suffers from too many ambiguities, other concepts in conjunction with some aspects taken from autopoiesis should be preferred In particular, the concept of organisation developed by Fontana and Buss (1994) and the theory of collectively autocatalytic networks advanced by Kauffman (1993) seem to be better starting points when working towards a definition of life or concerning questions of the origin of life Nonetheless, autopoiesis remains useful because some of its variants stress the feature of self-individuation of living beings which the previously mentioned two theories only do to a lesser extent

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1 Introduction

1 1 Artificial Intelligence and Artificial Life research: success or failure?

In a recent article, Rodney Brooks (2001) investigates the achievements of Artificial Intelligence (AI) and Artificial Life (Alife or AL) so far Despite the fact that techniques developed in these fields have found a variety of applications these days, both fields can also be seen as failures because they have not yet lived up to their titles' promises

> At the heart of this disappointment lies the fact that neither AI nor Alife has produced artefacts that could be confused with a living organism for more than an instant AI just does not seem as present or aware as even a simple animal and Alife cannot match the complexities of the simplest forms of life (ibid p 409)

Both in Artificial Intelligence and Artificial Life, strong and weak versions can be distinguished (Pattee 1989, Sober 1992) The strong version claims that it is possible for computers to realise human intelligence or life respectively while the weak version is first of all interested in contributing to the understanding of intelligent and living systems primarily through computer simulations The strong version of Artificial Life is derived from the strong version of Artificial Intelligence, which among philosophers is also know as functionalism (Sober 1992) According to this view, the properties of the mind or living systems are not physical properties themselves and can thus be realised by a multitude of physical systems But since there are no computers which more than a few researchers would feel inclined to call either as intelligent as a human or living, the whole argument about the possibility of realising either strong version is a profoundly philosophical one Critics of strong Artificial Life see functionalism as a variant of idealism and thus incompatible with scientific realism (Pattee 1989)

A noteworthy difference between Artificial Intelligence and Artificial Life is that the former started with the goal to achieve something similar to human intelligence and only has recently begun to include pre-rational intelligence or competence as exhibited for instance by insects (Boden 1996) Artificial Life on the other hand has investigated everything from the origin of life to ecological communities from the beginning In fact, the computational power of today's supercomputers should already be sufficient to simulate a simple life form like

a bacterium in considerable chemical detail (Endy and Brent 2001) However, as the minimal genome project has shown (Hutchison et al 1999), even in the simplest known bacteria about 100 of the 265 to 350 protein-coding genes required for cellular life under laboratory conditions have unknown functions Nonetheless, the simulation of a simple life form seems much closer at hand than demonstrating a computer program that shows human-like intelligence However, this approach won't settle the argument about strong Artificial Life because according to its critics, simulations do not become realisations

> The problem [ ] is that there is a categorical difference between the concept of a realization that is a literal, substantial replacement, and the concept of simulation that is a metaphorical representation of specific structure or behaviour, but that also requires specific differences which allow us to to recognize it as 'standing for' but not realizing the system In these terms, a simulation that becomes more 'lifelike' does not at some degree of perfection become a realization of life (Pattee 1989, p 384)

From the functionalist point of view, detailed simulation is not a useful approach either (Sober 1992, p 377), because one would need to adjust processes from the biochemical medium to the computational medium in order to realise life

> This creates a conceptual problem that requires considerable art to solve ideas and techniques must be learned by studying organic evolution, and then applied to the generation of evolution in a digital medium, without forcing the digital medium into an "un-natural" simulation of the organic world (Ray 1994, sec 4)

Note the choice of words on Ray's side here In his view it requires art to solve the problem, implying that it may not be a purely scientific one In fact, the article that this quotation is taken from is called "An evolutionary approach to synthetic biology Zen and the art of creating life" So far, strong and weak Artificial Life seem to be clearly distinct fields of research

However, simulation of bacteria is actually not what Artificial Life researchers who pursue the weak version typically do Just as strong Artificial Life researchers, they are more interested in ecological interactions and evolution And what probably won't be possible for a long time to come, is the detailed simulation of large communities of ecologically interacting life forms in a complex world and evolutionary phenomena therein Therefore, in order to study ecology or evolution with computer programs, one has to abstract from the processes taking place in biological organisms to make them computationally tractable This

poses a similar problem to the researcher who wants to simulate life as to the one who wants to realise it The danger here is that one abstracts away some of the essential properties of real organisms which are important for the life-like phenomenology they exhibit

1 2 What defines a living system?

Thus, the whole problem touches the definition of living system because no widely accepted one exists (Luisi 1998) Consequently, every choice of abstraction in order to simulate a living system becomes automatically a debatable one The researcher pursuing strong Artificial Life also cannot ignore criticism of the choice of his abstractions, if he is seriously interested in the success of his undertaking and does not want to trivialize the issues at hand This has been pointed out nicely by Pattee (1995b)

> The stronger claims of artificial intelligence and artificial life that a computer can *realize* thought and life are not empirically, or even logically, decidable issues because they hinge entirely on the degree of abstraction one is willing to accept as a realization If we could agree to define life and thought abstractly so as to leave out enough of its material aspects then obviously, by definition, a live, thinking computer is possible (ibid sec 10, original emphasis)

But even if one rejects strong AL and denies that computers could realise life, there is no good reason to deny the possibility of constructing *new physical* life forms, possibly, but not necessarily, from the same components that make up bacteria After all, there is nothing mysterious about biochemical components such as proteins, lipids, carbohydrates or DNA, although they can have quite intricate properties What is complicated is the way in which these components interact so that a well-structured living being is the result Therefore, nobody has yet been able to construct a bacterium from its components, although these are readily available Only the modification of organisms as carried out in the field of genetic engineering is currently feasible and in my view these genetically modified organisms would not qualify as *new* life forms because they are only derivatives of already existing ones It would rather be necessary to construct something living from dead components in order to really have created life anew

Furthermore, it is widely accepted that even the simplest known bacterium cannot have spontaneously arisen from the prebiotic soup and that it must have evolved from more primitive precursors Also, it has been claimed that certain

self-reproducing micelles exhibited in the laboratory are indeed alive (Luisi 1993) These micelles would in fact be new physical life forms, because they don't contain a genetic architecture like all known biological cells do, but only if one accepts a definition of living system that sees the genetic architecture as an accidental property of living systems, or at least as merely a special case of some more general essential property Interestingly, the approach to synthesize life in the laboratory is usually not seen as belonging to the field of Artificial Life, which is mainly concerned with computer models or at best robots As Pattee (1989) puts it " artificial life studies have closer roots in artificial intelligence and computational modelling than in biology itself"

The absence of a widely accepted definition of living system could also be seen as an indicator that there might be something important involved in living systems which is currently outside our scientific understanding (Brooks 2001, p 410) This would not necessarily mean that living systems are subject to some so far unrecognised (or even unrecognisable) physical laws More simply, there could be some kind of mathematical notion or organising principle that is needed in order to understand how living systems really work Such a notion or principle would on the one hand inform researchers interested in simulating life so that they don't abstract essential properties or relations of living systems away On the other hand, it could provide guidance for strong Artificial Life researchers in that it determines how a new life form would have to be organised

One organising principle, called autopoiesis (*Greek* self-production), has been proposed by Maturana and Varela (1973) and is seen as a necessary and sufficient condition that defines a system as living Autopoiesis emphasises the fact that biological organisms produce their own components, whereas for instance man-made machines don't work that way (e g a car) and when their function is production at all (e g a printing press), the product is usually different from any of their components

The need for a theory of biological organisation has also been brought forward by Fontana and Buss (1994, 1996) They see biology's two theories, Darwin's natural selection and Mendel's transmission rules, as insufficient to account for the phenomenology of living systems Because the Modern Synthesis of both theories views the evolutionary process as the displacement of alleles in a gene pool, it assumes the prior existence of organisms and can in particular not explain evolutionary transitions like the one from unicellular to multicellular organisms

Another organising principle is semantic closure (Pattee 1995b) which stresses the matter-symbol complementarity that lies at the heart of the genetic ar-

chitecture of every biological cell The distinction between the two categories matter and symbols is thereby seen as important to avoid ambiguities in the self-referential genetic architecture Unlike autopoiesis, semantic closure is not claimed to be a necessary condition for living systems, although it is a requirement for their autonomy and the open-ended evolution exhibited by populations of them

However, to come back to Artificial Life, other factors could be responsible for the observation that phenomena which are exhibited by computer simulations so far only show a low degree of life-likeness The models of living systems could be below some complexity threshold, or they are sufficiently complex but more computing power is needed (Brooks 2001) Furthermore, when one is interested in modelling the interactions between organisms it becomes necessary to consider not only how the organisms are to be modeled but also how the world in which they are embedded has to be (Taylor 2001)

1 3 What seems to be wrong?

Of course, it is not obvious at the outset, which approach will lead to a significant increase of the life-likeness of computer simulations or even to the realisation of life Furthermore, just to express disappointment with the current state is not enough It is rather necessary to point out in what respects the computer simulations are deficient when compared with the phenomenology of biological life In fact, the failures of Artificial Life can point out the shortcomings of our conceptions of life and thus help to improve them Another approach of criticism is to dispute the abstractions which are made in a given model when one is of the opinion that the phenomenology of real organisms relies on what has been abstracted away

One of the shortcomings of Artificial Life models is seen in the circumstance that they don't address the autonomy of real organisms (Ruiz-Mirazo et al 1999) According to this article, the autonomy of living systems derives from their ability of adaptive self-maintenance brought about by the control they can exert over the transformation of matter Furthermore, this process of self-maintenance must be coupled to a flow of energy through the system (see also Moreno and Ruiz-Mirazo 1999) From this point of view, Artificial Life models must be grounded in the physico-chemical properties of real matter to be of significance to biological problems A similar position has been taken by Pattee (1995a)

> Also, autonomy requires what I call semantic closure [ ] This means

> the organism's measurement, memory, and control constraints must be constructed by the genes of the organism from parts of the artificial physical world (ibid sec 4)

The motivation of Maturana and Varela to develop the theory of autopoiesis comes from their assertion that "Biologists, however, are uncomfortable when they look at the phenomenology of living systems as a whole" (Maturana and Varela 1973, p 74) In particular, this phenomenology encompasses "Autonomy and diversity, the maintenance of identity and the origin of variation in the mode in which this identity is maintained " (ibid p 73) The diversity of living beings is nowadays explained by evolutionary theory, but " autonomy appears so obviously an essential feature of living systems " (ibid p 73) and " autonomy [ ] seems so far to be the most elusive of their properties" (ibid p 73) Furthermore, "Autonomy is the distinctive phenomenology resulting from an autopoietic organization " (Varela et al 1974, section 4) As Fleischaker (1988, sec 3) has put it, "The centrality of autonomy in the original characterization of autopoiesis [ ] was a reaction to the undue emphasis among scientists on genetic determinism and on the supposed passive response to the environment"

Because the question of autonomy is largely neglected in current Artificial Life models, and autopoietic theory claims to explain the autonomy of living systems, this concept with the help of an exploratory computer model is investigated in this thesis to find out if it can improve Artificial Life models

1 4 Organisation of the thesis

The next chapter introduces the theory of autopoiesis along with its central concepts and a description of the original SCL model system, an artificial chemistry designed to illustrate this theory In this chapter several questions concerning the concepts of autopoiesis and the interpretation of SCL are raised while the answers are postponed until the discussion in chapter six Chapter three describes other artificial chemistries and real chemical model systems relevant to the theory of autopoiesis, the questions it raises and related concepts This is followed by a chapter explaining the modifications made to the original SCL system in order to enable the entities therein to self-reproduce Chapter five contains simulation experiments that serve to illustrate this extended model system and investigates some aspects of the phenomenology it displays Although chapters four and five bear comparatively little relevance to the discussion in chapter six, they serve to gain familiarity with some of the finer points which are investigated therein

The central arguments of the discussion, which consider the utility of autopoiesis in characterizing living systems and explaining their autonomy, rather follow the issues introduced in chapters two and three Finally the concluding chapter highlights the central results presented in this thesis in conjunction with a reflection of the process that led to them

2 Autopoiesis and SCL

This chapter starts with a brief characterisation of autopoiesis and a description of the qualitative chemistry implemented by the original SCL system After that, some of the concepts and definitions involved in the theory of autopoiesis are considered together with a preliminary assessment of them and the putative autopoietic entity in SCL

2 1 The Organisation of the Living

The concept of autopoiesis was first extensively elaborated by Maturana and Varela in 1973 As the subtitle "The Organization of the Living" (ibid p 73) indicates, the main intention of their essay is " to disclose the nature of the living organization" (ibid p 75), which the authors hold to be the autopoietic one Although apparently motivated by the operation of biological cells, the concept of autopoietic organisation is rather abstract and doesn't require a specific domain in which the autopoietic unity must be realised This concept can be briefly described as a network of production processes which mutually maintain themselves and a boundary which encloses these processes A possible instance of the first part of this description would be a *collectively* autocatalytic network, discussed in detail by Kauffman (1993) The relation between collective autocatalysis and autopoiesis has been further investigated by McMullin (2000) where he suggests that " autopoiesis can be at least roughly characterised as "collective autocatalysis *plus* spatial individuation"" This characterisation is being used in this thesis, although with the slight clarification that it should be *self*-individuation, as a guiding metaphor when interpreting the theory of autopoiesis as developed by Maturana and Varela, because, as Mingers (1995) has pointed out "The original language of autopoiesis is opaque and convoluted and in a sense closed It is hard to penetrate without much effort " (ibid p ix)

The concept of a collectively autocatalytic network has been developed by Kauffman (1993, part II) for theoretical considerations about the origin of biochemical life It is extremely unlikely that the metabolism of biological cells could have spontaneously arisen, but, as Kauffman argues, it is reasonably likely that some sort of collectively autocatalytic network can spontaneously form itself in a sufficiently diverse mixture of polymers with catalytic properties The crucial point of such a network is, that the production of every member must be catalysed by some member of the network Therefore, this concept relies on the catalytic properties of its members which are envisaged to be polypeptides and/or RNA

sequences Due to the catalytic effects, the whole network can emerge from the background of a (theoretically) infinite number of spontaneous reactions From such collectively autocatalytic networks the metabolism of biological cells has then supposedly developed Because the different metabolisms of biological cells are basically collectively autocatalytic and the paradigmatic example of an autopoietic entity is the biological cell (Maturana and Varela 1973, p 90), the use of this guiding metaphor is warranted All this does not mean that collective autocatalysis plus spatial self-individuation is a necessary condition of autopoiesis but only a sufficient one There might well be autopoietic systems not described by this metaphor but what should be expected of the theory of autopoiesis is that it correctly describes systems characterised by this metaphor

The model described in this thesis is an extension of the SCL (Substrate, Catalyst, Link) computer model developed by McMullin (1997) on the basis of an earlier model developed by Varela et al (1974) that was used to illustrate the concept of autopoiesis SCL has been termed an "artificial chemistry" which means that it is a simulation of a world in which certain elements can be seen as atoms or molecules and certain processes can be seen as reactions between them Some of these processes can be regarded as simplifications of real chemical processes (Varela 1979, sec 3 1 1) but others, especially in the extended version of SCL described here, fail to have any similarity with real chemical processes at all The phenomena which arise in these artificial chemistries can be extensively studied, but this approach has been criticised in (Ruiz-Mirazo et al 1999), mainly because thermodynamic requirements are disregarded in most of them including the one described here However, the approach of the original SCL model system was a minimalistic one (Varela et al 1974, sec 6) and its aim was not to model interactions of molecules in a realistic way Furthermore, because autopoiesis was conceived to be a domain-independent organising principle, it does not matter, at least for demonstration purposes, in which domain it is exhibited

Despite its domain-independent definition, "Autopoiesis in the physical space is necessary and sufficient to characterize a system as a living system " (Maturana and Varela 1973, p 112) Hence, an autopoietic unity in a non-physical domain is not a living system Consequently, autopoietic entities in the SCL system are not living systems, because the particles are interpreted as such by human observers and have no existence independent of the observers Thus they are different from physical particles which, assuming one uses a realist ontology, exist on their own According to Maturana and Varela, "The physical space is defined by components that can be determined by operations that characterize them in

terms of properties such as masses, forces, accelerations, distances, fields, etc" (ibid p 112) Distance is the only of these properties which applies to SCL particles, but even if additional properties were simulated, these particles still wouldn't have an existence of their own

It is important to note that self-reproduction and evolution do not enter into the characterisation of autopoiesis, although the diversity of living beings depends on both processes (Maturana and Varela 1973, p 96) Consequently, self-reproduction is seen as strictly secondary to the establishment of an autopoietic unity and evolution as secondary to self-reproduction This distinguishes autopoiesis from most attempts to define life, which is often done by listing a number of criteria which characterise living beings Such lists usually contain self-reproduction and frequently evolution (Bedau 1996, sec 2)

The rest of this section briefly summarizes what can be observed in SCL so far and what mechanisms are implemented It also preliminarily explains the concept of autopoietic entity with respect to SCL

2 2 The qualitative SCL chemistry

SCL implements a two-dimensional world of lattice positions which "wrap around" at the edges so that the overall topology is toroidal Each position is occupied by one of the four possible particle types which are substrate, catalyst, link and hole Only one particle is allowed per position with the exception that a link can also contain an absorbed substrate particle A substrate can enter a link from any adjacent position leaving a hole where it has been This process is reversed when the absorbed substrate leaves the link to any adjacent position which is occupied by a hole

Links can also spontaneously bond to neighboring links with at most two bonds per link and at most one bond between each adjacent pair Thus, links can form *chains* and when such a chain is closed, it is called a *cluster*, if it consists of less than six links[1], otherwise *membrane*, a link with two bonds is called a *chain link* If a membrane contains one or more catalysts it is referred to as a *cell*[2]

The dynamics in SCL are based on local interactions between neighbouring particles First of all, particles move by swapping their positions with randomly

[1] In the case of a hexagonal lattice, which is used in the extended SCL system, a closed chain of links can only enclose another particle if it consists of more than six links

[2] If there is only one membrane in the world, it is ambiguous what constitutes the interior and what is the environment unless there are catalysts present on only one side of the membrane which then would mark the interior

selected neighbours Thus, there is no notion of momentum or collision Links which have one or two bonds are immobile Consequently, membranes are impermeable to catalysts and links, but permeable to substrates through absorbed substrate particles The bonding process is also influenced by the particles present in the neighbourhood of the two links involved, most notably through a mechanism called chain-based bond inhibition This mechanism inhibits the bond formation between two links if at least one of them has a chain link in its neighborhood Without this mechanism, free links m a cell would tend to bond rendering them immobile

As the name catalyst implies, this particle can catalyse a reaction which is the production of links from substrate particles

$$Catalyst + 2\,Substrate \longrightarrow Catalyst + Link$$

Links also spontaneously disintegrate, if that happens the link in question loses its bonds

Implementation details of the mechanisms described above can be found in (McMullin 1997)

2 3 The autopoietic entity or unity

2 3 1 Necessary concepts

As mentioned above, SCL was developed with the aim of demonstrating a minimal autopoietic unity, which in this framework is the self-production of a cell A more concise definition of unity in general has been given by (Varela et al 1974, section 2) " , a complex system is defined as a unity by the relations between its components which realize the unity as a whole, " Thus, the relations between the components are necessary to define the unity Consequently, the image of a cell in SCL can under this definition not be called an autopoietic unity, but is only a representation of the collection of its components and their spatial relations Maturana and Varela (1973) used the term unity to stress that a unity is brought forward by an act of distinction performed by an observer Distinction and unity are two key concepts in their constructivist epistemology, but whether this kind of epistemology is essential for the theory of autopoiesis won't be investigated here Nevertheless, I continue to use the term unity with two exceptions When referring to the extended SCL system, I use the term autopoietic entity as synonym for cell, because when a cell is present, then by

design of the interactions of particles in SCL the unity is present for the same time period that the cell exists When I otherwise use the term entity, I am talking about unities in the physical domain

Another important concept for the theory of autopoiesis is *organisation* which is used to describe *composite* unities

> [T]he relations that define a system as a unity, and determine the dynamics of interaction and transformations which it may undergo as such a unity, constitute the organization of the system (Maturana and Varela 1973, p 77 and 137)

The organisation of a system specifies its class identity and " if the organization of a system changes, then its identity changes and it becomes a unity of another kind " (Maturana 1980a, p xx) Also, the organisation has to be distinguished from the *structure* of a system which comprises

> [T]he actual relations which hold between the components which integrate a concrete [system] in a given space (Maturana and Varela 1973, p 77 and 138)

The distinction between structure and organisation is made to stress that the same organisation can be realised by systems of different structure

> The organization of a machine (or system) does not specify the properties of the components which realize the machine as a concrete system, it only specifies the relations which these must generate to constitute the machine or system as a unity Therefore, the organization of a machine is independent of the properties of its components which can be any, and a given machine can be realized in many different manners by many different kinds of components In other words, although a given machine can be realized by many different structures, for it to constitute a concrete entity in a given space its actual components must be defined in that space, and have the properties which allow them to generate the relations which define it (Maturana and Varela 1973, p 77)

This is obviously a functionalist position, but it is also made clear that organisation should not be taken to have explanatory value of its own (ibid p 80) Given the importance attributed to the concept of organisation within the autopoietic theory (Fleischaker 1988, sec 2), it is somewhat worrying that the relations which constitute the autopoietic organisation are nowhere specified The only hint provided is the following

> an autopoietic organization constitutes a closed domain of relations specified only with respect to the autopoietic organization that these relations constitute, and, thus, it defines a 'space' in which it can be realized as a concrete system, a space whose dimensions are the relations of production of components that realize it (Maturana and Varela 1973, p 88)

The different kinds of production relations which are taken to be the dimensions of autopoietic space are constitution, specificity and order However, this statement allows two different interpretations One is that there is a circularity in which the organisation and relations mutually constitute each other and the relations are all production relations of any of the three types, but the question then is how this circularity could be resolved or at least be made transparent The alternative interpretation would be that the relations which form a closed domain in autopoietic space have a different type than the production relations that are the dimensions of autopoietic space The open question here is of what type the relations in autopoietic space would be Since not even the type can be derived from the statement above, it cannot provide any insight into the question of which relations actually specify the autopoietic organisation either To make things worse, support for both interpretations can be found as is discussed in section 6 1, but for instance the citation above, that describes the distinction between organisation and structure, contains no hints The components are only required to "generate" the relations which define the organisation, but this would seem compatible with either interpretation of the relations in autopoietic space

Also, because at least all unicellular organisms are supposed to have the autopoietic organisation, they all would have the same identity and the same class It is of course true that they are all living systems, but there are important distinctions between different unicellular organisms, most notably that between prokaryotes and eukaryotes The question then is, whether all unicellular organisms should be seen to have the same organisation and that prokaryotes and eukaryotes just have different structures, or whether they have different organisations, all of which are autopoietic Another way of putting it is to ask whether the autopoietic organisation is unique or whether "autopoietic" is a qualifier which is applicable to a multitude of organisations However, for the purpose of SCL this distinction does not matter, because there is only one type of entity possible at the moment Therefore, the elaboration of this discussion is also postponed until section 6 1

2 3 2 The key to autopoiesis

Basically the same definition of autopoietic unity is given both in (Maturana and Varela 1973, p 78 f) and (Varela 1979, section 2 2 2)

> An autopoietic [machine/system] is organized (defined as a unity) as a network of processes of productions (transformation and destruction) of components that produces the components [which/that] (i) through their interactions and transformations continuously regenerate and realize the network of processes (relations) that produced them, and (ii) constitute it (the machine) as a concrete unity in the space in which they [(the components)/] exist by specifying the topological domain of its realization as such a network [3]

Furthermore, in (Varela et al 1974, sec 9), the authors present a six-point identification key for autopoietic unities which can be summed up in the following way

1 The unity has an identifiable boundary

2 The unity is composed of discrete components

3 The unity is a mechanistic system

4 The boundary of the unity is constituted though preferential neighborhood relations and interactions between its components

5 The boundary components are produced by the unity by interactions of its components, either by transformation of previously produced components, or by transformations and/or coupling of non-component elements that enter the unity through its boundaries

6 All other system components are produced by the unity by interactions of its components as in 5

Contrasting definition and key, two issues become apparent Firstly, no boundary is mentioned in the definition, but there are two points about it in the key This issue is discussed in section 6 1 Secondly, point five and six could be combined into one, but there is, in my view, a questionable exception to point six

[3] There are some minor differences in the exact wording between the two definitions These differences are put in square brackets, what appears before the slash is taken from (Maturana and Varela 1973, p 78 f) whereas what comes after the slash is written in (Varela 1979, section 2 2 2)

which is not mentioned in the list above It is related to the distinction between components of the unity and non-component elements made in point five Both point five and six say that components have to be produced through a process that involves interactions from other components The exception to point six is that non-component elements are allowed as necessary permanent constitutive elements in the production of other components This stands in contradiction to the circularity in the component production which is at the core of the definition of autopoietic unity As long as this exception is kept, the combination of point five and six is not possible Further discussion of this problem follows in section 6 3 1

For the purpose of determining whether real or simulated entities qualify as autopoietic, the identification key is used, because it is more detailed than the definition and appears straightforward to apply Furthermore, the use of collective autocatalysis plus spatial self-individuation as a guiding metaphor is also compatible with the key Spatial self-individuation entails that there is some kind of self-produced boundary and collective autocatalysis means that in the production of components interactions from other components are involved Again, this does not mean that my guiding metaphor is isomorphic to the identification key Collective autocatalysis entails that at the time of the production of a component there must be some kind of interaction from another component which can be interpreted as catalytic effect This seems to be stronger than the requirements of point five and six of the key where it is not explicitly stated that the interaction from another component has to happen at the time of production, the interaction may as well have occurred earlier However, when only non-component elements are involved as substrates of a production step then there should be some interaction from a component necessary to meaningfully call this reaction a production by interactions of components This is just the same as would be required for collective autocatalysis, but when there are components among the substrates then the situation may according to the key be different

2 3 3 The putative autopoietic entity in SCL

In order to further describe the original SCL system and to explain certain design choices of my extensions, I need to mention here, in anticipation of the discussion in section 6 3 1, that in my opinion the original SCL model system does not exhibit any autopoietic entities The operation of a putative autopoietic entity in the original SCL world is as follows The catalyst in the cell produces links which are

trapped inside because of the selective impermeability of the membrane thereby creating a relatively high concentration of free links inside the cell Substrate, however, can enter the cell so that the catalysis reaction continues as long as there is sufficient substrate in the world (and sufficient space in the cell) The substrate particles inside the cell are the non-component elements referred to in point five of the identification key If a chain link in the cell's membrane disintegrates, the membrane is ruptured Since there is a high concentration of free links inside the cell, there is a good chance that one of the free links moves to the rupture site and after formation of new bonds closes the gap All in all, the cell seems to maintain itself for a certain period of time The turn-over of links means that the structure of the putative entity changes whereas its organisation supposedly remains constant

This mode of self-maintenance raises the question whether a cell with a ruptured membrane[4] constitutes an autopoietic entity or not, a complication which was already noted in (McMullin 2000, sec 5), but not resolved In (Varela et al 1974), which describes the very first SCL model system, the authors never explicitly discuss this problem, although it is apparent in the figures 1 and 2 of this article, that gaps in the membrane are temporarily present and that the significant achievement of the autopoietic entity is to repair these gaps Concretely, the caption of figure 2 in this article reads "Ongoing production of links *re-establishes* the unity under changes of form and turnover of components " (emphasis added) This is the first indication that the authors may consider an entity with a ruptured membrane not to be autopoietic, because otherwise this organisation would not be re-established by repair but rather perpetuated through repair

Further support for this point of view comes from the identification key for autopoietic unities itself The relevant points of this key for the question at hand are number one and four Number one requires that the entity must have an identifiable boundary When the membrane is ruptured, the entity is only partially enclosed in an open chain For a human observer it is easy to interpret the gap as a temporary rupture of an envisaged membrane But this alleged membrane only constitutes a boundary for the entity in the mind of the observer For the entity itself, " the components that constitute the boundaries of the unity constitute these boundaries through preferential neighborhood relations *and* interactions between themselves, as determined by their properties in the space of their interactions" (Varela et al 1974, sec 9, emphasis added) In the space of

[4] A cell with a ruptured membrane is a contradiction in itself given my definition of cell, but it should be clear what is meant

interactions of the particles in the SCL world, there are no interactions between the ends of an open chain, which would allow it to constitute a boundary for a possible autopoietic entity In fact, once the membrane of a cell is ruptured, it can't be predicted whether the gap can ever be repaired

Certainly, it is a very conservative point of view to require a constantly intact membrane for an autopoietic entity in SCL, but this is a necessity that follows when one takes point four of the identification key seriously In addition, it spells trouble for the interpretation of the original SCL system, as is further discussed in section 6 3 1 However, this requirement is not problematic for the extended version of SCL due to a change in the mode of self-maintenance and is therefore kept A more detailed description of the phenomena which can be observed in the original SCL world is given in (McMullin and Varela 1997) This article also highlights the importance of the chain-based bond inhibition mechanism which keeps the links inside the cell free and available for repair by preventing them from bonding to each other

All in all, this section has shown that autopoiesis and its concepts are in general not straightforwardly applicable with the possible exception of the identification key In fact, a lot of interpretation is necessary to apply the concepts in a particular situation like for example in SCL This process of interpretation then can lead to varying results which can be seen in the preliminary discussion of the putative autopoietic entity in SCL in this subsection Yet another interpretation of SCL is given in (McMullin 2000) where the author suggests that the entities therein are not autopoietic The reason for this conclusion lies in the circumstance that two adjacent cells in SCL, if they don't disintegrate in the first place, would tend to merge and hence lose their distinct individualities More on this line of reasoning follows in section 6 5

After this preliminary introduction and discussion of autopoiesis and SCL, the next chapter describes several other simulated and real model systems with the purpose of broadening the perspective for the more detailed discussion in chapter six

3 Simulated and real chemistry

Autopoiesis is supposed to be the organisation of the living and the paradigmatic autopoeitic entity is the biological cell Such a cell from a chemical point of view is a vesicle which means that it has a bi-layered membrane that separates an aqueous phase that constitutes its interior from an aqueous environment The chemical properties of the membrane determine its permeability for the molecules and ions that are dissolved in the aqueous solution This selective permeability is very important for the operation of biological cells which is well known A somewhat simpler bounded structure is the micelle where the boundary is a single layer of surfactants that separates phases of different types In a normal micelle, the interior is organic (hydrophobic) and the environment aqueous while in a reverse micelle the interior is aqueous and the environment organic

Because of the separation of interior and environment, both micelles and simple vesicles have a proto-cellular character Furthermore the physico-chemical effects that lead to spontaneous micelle and vesicle formation are at work in biological membranes too Therefore many real and simulated model systems which address micelles and vesicles are under investigation, some of which are described in this chapter

3 1 Self-reproducing micelles in real chemistry

First of all I am describing three experimental setups that allow the demonstration of self-reproducing micelles under laboratory conditions The first two systems (Bachmann et al 1991, systems IIA and IIB) are closely related because the chemical reactions in both are identical and the only difference is that system IIA exhibits normal and system IIB reverse micelles The membranes of the micelles in both systems have octanoate as their primary surfactant but 1-octanol, which is insoluble in water and therefore localized in the organic phase, can occur as co-surfactant In this case, the hydroxyl group of 1-octanol points towards the aqueous phase while the hydrophobic tail remains located inside the membrane The aqueous phase in both cases contains sodium permanganate which in turn is insoluble in the organic phase At the micellar interface the permanganate ion oxidizes the hydroxyl group of 1-octanol and the product of this reaction is octanoate (for the exact reaction equation with all its products see Bachmann et al (1991), fig 1) This production of octanoate molecules leads to the growth of the micelle until it becomes unstable and spontaneously divides The operation of both systems relies crucially on the fact that the two substrates 1-octanol and

permanganate are soluble in different phases only and that the reaction must therefore occur at the micellar interface This also means that the supply of 1-octanol in the micelles or permanganate in the reverse micelles respectively set a limit for the amount of micelles that can be produced

I am describing the third system (Bachmann et al 1991, systems III) in less chemical detail than the previous two because the main difference is that the reaction which leads to the production of surfactant molecules is catalysed by enzymes that are located inside the aqueous phase of the reverse micelles The substrate involved is soluble in the organic phase only so that the reaction, this time a hydrolisation, again takes place at the micellar interface Again, the supply of substrate limits the amount of micelles that are produced All three systems described here are seeded with micelles but another system has been demonstrated (Bachmann, Luisi and Lang 1992) where the first micelles can form in the absence of other compartmental structures

These real model systems set the stage for the artificial chemistries described in the following section In general, artificial chemistries model individual particles and the interactions between them This stands in contrast to, for example, systems of differential equations, which usually model statistical aggregates of particles in continuous space and time Artificial chemistries vary among each other with respect to the spatial resolution and the chemical realism SCL, for instance, contains one particle per lattice position and shows only a low level of chemical realism The choice of spatial resolution and the level of chemical realism depends on the purpose for which each chemistry is constructed I am not giving an exhaustive overview of all artificial chemistries but only describe a few which are selected because they illustrate certain points that are relevant for the discussion

3 2 Concrete artificial chemistries

The artificial chemistries described in this section are explanatory in nature They consider features of real chemistry to different extents and illustrate how the phenomena that can be observed in the model systems arise from those features Like SCL, all artificial chemistries in this section consider two-dimensional worlds, although the way in which they implement space differs between them I refer to these model systems as more concrete artificial chemistries

3 2 1 Self-reproducing proto-cells

This artificial chemistry, described in (Ono and Ikegami 1999), addresses the question how a compartmentalized collectively autocatalytic network can form, self-maintain and self-reproduce, because the acquisition of a cell membrane is widely seen as one of the central steps in the origin of life Without a means of keeping its components from diffusing away, a proto-lifeform would not have been viable This is the same problem addressed by extended SCL, but has been solved in a markedly different way here First of all, many abstract chemicals (particles) are allowed at each lattice position The particles are polarized (similar to an electro-chemical charge) and have an orientation They can move on the lattice, rotate and undergo reactions where they can act as substrates and catalysts Furthermore, all particles have potential energies which because of the charge they carry is not only dependent on the particle type but also on the other particles at the same lattice position The probability of a movement of a particle is then dependent on the difference in potential energy between its old and new position Similarly the likelihood of a transformation depends on the difference in the chemical potential between the substrate and the product but is also modified by catalytic effects Apart from that, all reactions are reversible, but have different base rate constants Consequently, this system offers a higher chemical realism than SCL, but it does not model all properties of real-world thermodynamics For example, there is no notion of the momentum of a particle

There are six different particle types, some of which have similar functions as those in SCL The particle called AA, which plays the role of the catalyst, reproduces itself autocatalytically from a substrate particle (X) and can also catalyse the production of membrane material (M) from X Decay, however, leads eventually to a different particle (Y), which is assumed to have the lowest chemical potential Particle AA is not only the product of the mentioned autocatalytic reaction, but also spontaneously assembles from and disintegrates into singular A particles Finally, there is particle W which plays the role of a solvent and does not participate in any reactions

Starting from a homogeneous initial state, the production processes and repulsion between particles lead to the formation of clusters separated by membrane-like thin films, which are constituted by adjacent lattice positions that predominantly contain M particles If such a membrane is selectively permeable for X and Y but impermeable to AA and A, the X particles are taken in by the cell which leads to growth and eventually division while the Y particles leave the

cell as waste product With the influx of X into the system (and efflux of Y), made possible by the replacement of Y with X at a given rate, ongoing self-reproduction and self-maintenance of the cell-like structures is the result The process of division and the cell shapes that result thereby depend on the strength of repulsion between M particles Different repulsion strengths lead to different membrane flexibilities which is reminiscent of the influence that the composition of a phospholipid membrane has on its fluidity

3 2 2 Micelle formation in continuous space

Another artificial chemistry has been developed by Edwards and Peng (1998), in order to simulate the self-assembly of amphiphilic molecules into micelles The motivation for their model is derived from the generally accepted view that for the emergence of the first biological cells the process of phospholipid self-assembly must have been important However, in their opinion the models used for simulating these processes suffer from unrealistic simplifications to make the problem computationally tractable Thus, in order to better understand self-assembly of lipid aggregates, their system allows the movement of the molecules in a continuous two-dimensional space as a result of intermolecular interactions, which model some of the physical and chemical properties of real phospholipids In particular, the geometric shape of a lipid molecule with its distinction of a hydrophilic head and a hydrophobic tail is modeled as well as the forces that these exert on neighbouring molecules However, because no solvent (water) molecules are represented, the forces are implemented in such a way that they account for this absence An explicit representation of the solvent would certainly be desirable to make the model more realistic but this design choice has probably been made to reduce the computational complexity Also, no chemical reactions are possible in this framework yet Starting from an initial configuration where lipid molecules are scattered randomly on a plane this artificial chemistry then displays the self-assembly process that results in the formation of micelles

3 2 3 LMA micelles

Mayer and Rasmussen (1998) have developed an artificial chemistry that demonstrates the emergence of dynamical hierarchies which in this case is the self-assembly of micelles from polymers and their autocatalytic self-reproduction It is based on the principles of a Lattice Molecular Automaton (LMA) which is a variant of the lattice gas simulation concept (Rasmussen and Smith 1994) In

this model system space is represented by a discrete grid and each position is occupied by either a monomer or vacuum Polymers consist of several monomers that are bonded together and therefore have a specific shape All interactions are directly derived from the laws of physics and are communicated between the lattice positions via propagating information particles Reactions between the molecules (monomers and polymers) are also possible through the formation and breaking of bonds

In the specific case described in (Mayer and Rasmussen 1998) there are three types of monomers One is hydrophobic, the second hydrophilic and the third represents the solvent water The first two types of monomers can be bonded to each other yielding the hydrophobic and amphiphilic polymers that besides water are present in the initial state of this model system From this state the amphiphilic polymers self-assemble into micelles whose surfaces then catalyse the production of new surfactant molecules In general, when the head group of a hydrophobic polymer faces at least two hydrophilic head groups of amphiphilic polymers it is hydrolysed into an amphiphilic polymer and a hydrophobic monomer Because the amphiphilic polymers tend to assemble into micelles the hydrolisation mainly takes place at their surfaces When a new surfactant has been produced it often enlarges the micelle that catalysed its formation until the latter becomes unstable and spontaneously divides This finally is the cause of the ongoing self-reproduction of micelles which lasts until all hydrophobic polymers are used up Thus the surfactants are produced autocatalytically, but it should also be noted that there appears to be no decay of them making the micelles practically immortal In summary, this system illustrates how structures of higher order can emerge from simple molecules and their properties Because of the high level of chemical realism, the way in which and what new structures emerge is a relatively accurate model of what happens in the real world In fact, these LMA micelles resemble those described in section 3 1 quite closely, although the production process for surfactant is rather different

3 3 Abstract artificial chemistries

The more abstract artificial chemistries, as I call them, described in this section are exploratory in nature This means that they don't try to explain how features of real chemistry are involved in certain phenomena but instead abstractly implement selected features and explore issues involving their interactions

3 3 1 AlChemy

In this Algorithmic Chemistry (AlChemy), lambda expressions play the roles of molecules This choice may seem somewhat arcane but lambda calculus is sufficient to represent the two abstractions from real chemistry, transformation and equivalence, that are considered in this model system To make this clear I am briefly describing lambda calculus without being mathematically exact Lambda expressions are sequences over an alphabet of variables and can also contain the two operators abstraction and application The abstraction operator specifies a variable like in the definition of a function Application "cancels out" the abstraction and with the help of syntactical rewrite rules, a lambda expression is reduced to a unique normal form, given that one exists This process of normalization can be seen as computation and the normal form as the result Just as there are infinite loops in computation, a reduction process does not always terminate, and according to Turing's Halting Problem, it is in general not possible to predict if a given lambda expression has a normal form All lambda expressions can be applied to each other, which is taken to be the AlChemy equivalent of chemical transformation Just as in chemistry, where the structures of the substrate molecules determine what the reaction product will be, the syntactical structures of the lambda expressions where one is applied to the other determine what the normal form of the result will be One can thereby think of the reduction process as a chemical process during which subgroups of the substrate molecules are rearranged The second abstraction present in AlChemy, equivalence, results from the fact that different lambda expressions can reduce to the same normal form just like the same product can be the result of chemical reactions involving different substrates Clearly, these two abstractions don't cover several important aspects of real chemistry and Fontana and Buss (1996, sec 2 1 4) are well aware of this In the following subsection a variant of AlChemy is described that addresses some of these shortcomings

As the title of the article (Fontana and Buss 1994) suggests, this abstract chemistry has been conceived in order to embed in it a theory of biological organisation Thus, Fontana and Buss have a similar goal as Maturana and Varela have with autopoiesis, but the former " regard biological organizations as specialized systems of chemical transformation " (Fontana and Buss 1994, sec 2) This differs from the concept of autopoietic organisation because the latter is formulated domain-independently although it is also clear that chemistry is an important domain for the autopoietic organisation because it is in this domain

where the components of biological cells exist

To return to AlChemy itself, unlike in the artificial chemistries described so far there is no underlying space in this system Instead, the simulated lambda-universe can be thought of as something similar to a reactor in which all the expression are assumed to be contained This does not mean though that there are virtual reactor walls which keep the collection of expressions together but instead that there is no space in this lambda-universe and consequently no necessity for special constructs to keep the collection of expressions together The expressions are always present in normal form and reactions are random collisions of two expressions which result in the application of the first expression to the second The normalization process is subject to certain limits which not only ensure that the reduction doesn't get stuck in an infinite loop, but can also be used to forbid certain types of collisions In particular, I am only concerned here with the Level 1 (Fontana and Buss 1994, sec 6 2) operation of AlChemy in which (self-)copying expressions are suppressed Concretely this means that when the normal form of a collision product is the same as one of the colliding expressions the whole collision is assumed to have been "elastic" and is effectively ignored The normal form that results from a successful collision randomly replaces one of the expressions in the reactor With this reaction scheme, expressions which are not continuously reproduced by collisions of existing expressions are eventually removed from the reactor

Under the conditions imposed by Level 1, the emergence of collectively auto-catalytic networks of lambda expressions can be studied In the present context, these networks are described as self-maintaining subsets of organisations The organisation of the network is thereby defined through three properties A grammar that characterises the subspace of all (and possibly infinitely many) expressions which can occur in the organisation, the algebraic structure of interactions (collisions) between expressions and self-maintenance under the conditions imposed by the reactor in which the self-maintaining subset of the organisation resides The organisation thus specifies the class identity through the grammar and the transformations which it may undergo without loss of identity through the algebraic structure under the condition of self-maintenance Therefore, it is an organisation in the sense specified by the autopoietic theory (cf sec 2 3 1)

Likewise, the structure is the self-maintaining subset of an organisation and comprises both the lambda expressions as well as the actual interactions between them Fontana and Buss (1994) don't use the term structure in this sense themselves but instead use it to refer to the sequential composition (inner structure)

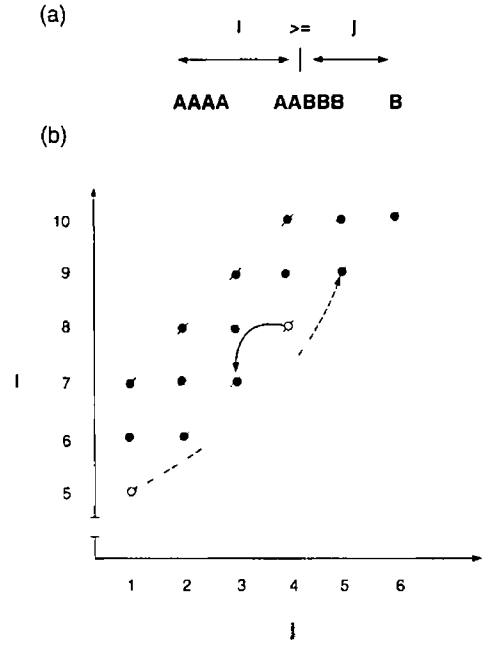

Figure 1 The grammar (a) and algebraic structure (b) of an infinite AlChemy Level 1 organisation as shown in (Fontana and Buss 1994, fig 2) Every point in the plane of subfigure (b) represents a possible component of the self-maintaining subset in the reactor with its inner structure specified by the two coordinates (j,i) according to the grammar in subfigure (a) The two arrows represent the two types of production relations which can occur in this organisation, for details see text

of a lambda expression that determines its functional behaviour upon application Lambda expressions in turn are called objects which correspond to the components in autopoiesis All in all there is a well-defined distinction between structure and organisation in AlChemy Moreover, the organisation can be exactly specified through the grammar and the algebraic structure and remains not in obscurity as the autopoietic organisation does The link between AlChemy and autopoiesis has naturally been recognised by Fontana and Buss (1994, 1996) themselves and is further investigated in section 6 1

An example of an infinite AlChemy organisation is shown in figure 1 It is the lambda calculus independent description of the first example of Level 1 taken from Fontana and Buss (1994, sec 6 2 2) The two types of production relations indicated in figure 1(b) are the following The solid arrow denotes that the application of any expression, that is not at the bottom of a diagonal, to some other expression will result in the production of the lower neighbour on the same diagonal Application of an expression (1,i), which is at the bottom of a diagonal, to another expression (k,l) results in the production of expression (k+1-

1,l+ı-1) which lies upwards on the same diagonal as the latter expression (dashed arrow, this arrow concretely shows the application of (1,5) to itself) This second relationship also entails that the expression (1,1) would produce a copy of any expression it is applied to Under the reaction scheme used for Level 1 such an application would be elastic and hence produce nothing

A set of expressions is said to be self-maintaining, if every expression of this set can be produced by at least one collision between expressions taken from that set Given the two types of production relations present in the given organisation, this is evidently the case Self-maintenance is a necessary condition for the kinetic persistence of an organisation in the lambda reactor, but not a sufficient one because of stochastic events (random removal after collision) in the reactor For instance the organisation shown in figure 1 will under flow conditions over time collapse into one of its suborganisations (see below)

Also the self-maintaimng subset of an organisation does not need to be entirely present in the reactor at given time to ensure its kinetic persistence It may very well be the case that expressions disappear and reappear periodically Consider for example a collection of expressions high up on one of the diagonals in figure 1(b) They will initiate a flow of expressions down the diagonal and at the time the bottom expression is reached the original collection may have very well been replaced Only when the bottom expression is reached can the original expressions be produced again, given they weren't higher than ı steps up the diagonal where ı is the second coordinate of the bottom expression In fact, the lowest ı expressions on every diagonal (except the one which starts at (1,1)) represent finite (sub-)organisations of their own (e g the expressions from (1,5) up to (5,9) in figure 1(b))

The latter organisations also readily illustrate one important concept in Al-Chemy the center of an organisation The center is the smallest self-maintaining subset of an organisation This means that application of all expressions in the center to each other (including themselves) must produce all the expressions of the center For every one of the finite organisations at hand the center is identical with the expressions that make up the organisation itself The main importance of the center derives from the observation that all organisations observed so far possess a single and unique center Moreover, when two organisations are combined the centers combine linearly, but this Level 2 phenomenology of AlChemy (Fontana and Buss 1994, sec 6 4) won't be considered any further here

3 3.2 Combinators

A modified version of AlChemy, described in (di Fenizio 2000), uses combinators instead of lambda expressions Combinatorial logic is a formalism equivalent to lambda calculus with the main difference that combinators are sequences of atoms that don't contain variables The atoms implicitly contain the abstraction operator in that upon application they rearrange following atoms according to certain rules These rules also allow that after an application the expression can split into several subexpressions each of which is independently normalized Compared to AlChemy this situation comes closer to real chemistry where a reaction can have several products Furthermore the number of each of the different atoms in the system remains constant, thus satisfying a conservation law This is achieved by keeping all combinators of length one (atoms) in a pool from which they are taken or can be added When a collision of two randomly chosen combinators occurs then, unlike in AlChemy, the reacting expressions are removed from the reactor During the following normalization process atoms are taken from the pool or are released back to it so that this process can only achieve the normal form if there are always the necessary atoms in the pool If the normal form can be reached, it is released into the reactor, and if not, the whole collision is ignored Also, expressions can with certain probabilities spontaneously disintegrate into the pool or arise from it

Like in AlChemy, self-maintaining subsets of organisations emerge, but with the additional property of acting similar to metabolisms This means that an organisation is capable of using random expressions, which spontaneously arise from the pool of combinator atoms, as material to produce more of its own expressions Furthermore it is not necessary to suppress self-copying expressions because their replicatory advantage is reduced as the reactants in a collision are used up This observation corresponds to a result in AlChemy (Fontana and Buss 1994, sec 6 3) which shows that it is typically sufficient to reduce the probability of copying to 0 75 (i e suppressing only one in four copy-actions) to achieve Level 1 phenomenology

3 4 The status of SCL

There is an important distinction between the more abstract artificial chemistries described in the previous section and the more concrete ones listed before The latter are constructed to exhibit a certain kind of self-organising or self-producing process, which is to a high degree determined by the design of each system The

more abstract chemistries consider the emergence of a multitude of organisations which differ in their grammar and algebraic structure Thereby what kinds of organisations emerge given different reaction rules can be investigated Furthermore it can be studied, if some of these organisations show properties which others don't posses To sum up, the more abstract chemistries allow the emergence of a large variety of organisations and the comparison as well as classification of them

It is also worthwhile to consider whether SCL belongs to the more concrete or the more abstract artificial chemistries On the one hand there are a number of similarities between SCL and the model system described by Ono and Ikegami (1999) which supports the hypotheses that SCL belongs to the more concrete artificial chemistries However, the aim of the latter is to be at least to some extent chemically realistic while in SCL this is a purely circumstantial matter Instead, SCL is an exploratory model system which only seeks to illustrate the concepts involved in the theory of autopoiesis, which brings it closer to the more abstract artificial chemistries that are exploratory as well That AlChemy is explicitly motivated by real chemistry does not change its exploratory nature because its aim is not to explain features of chemistry but instead investigates the emergence of higher level objects like an organisation Because SCL only explores the concept of autopoiesis, the extensions described in the following chapter don't try to be chemically realistic either but are only aimed at opening up the possibility of self-reproduction

4 Self-reproducing entities in SCL-DIV

After the description of other, real and artificial, model systems relevant to the issues considered in this thesis, this chapter returns to the one model system that is specifically designed with autopoiesis in mind, SCL The extended version of SCL, which allows the self-reproduction of the autopoietic entities, is also called SCL-DIV When SCL is used as a designation without one of the qualifiers original or extended, both model systems are referred to

4 1 Requirements

So far, SCL is only concerned with self-maintenance to demonstrate a minimal autopoietic entity As soon as self-reproduction enters the picture, several further requirements become immediately apparent

1 Growth of the membrane is necessary which means that

   (a) firstly bonded links must be allowed to move and

   (b) secondly there has to be a growth mechanism whereby free links can enter and enlarge a membrane

2 Then a fission mechanism is needed so that a membrane can divide into two (or more) daughter membranes

3 To ensure that at least after some divisions there will be more than one daughter membrane containing a catalyst, there must be a means of catalyst replication

As in the original SCL system, all new mechanisms are based on local interactions only However, for three of the new mechanisms (1b, 2 and 3) it is necessary to increase the neighborhood radius from one cell to two cells This is implemented as a particle querying a neighboring particle about the latter particle's neighborhood It is made sure for the mechanisms listed above, that such a query doesn't progress beyond a distance of two cells from where it originated

The following sections outline the new mechanisms and provide implementation notes for each of them insofar as they change or add to the implementation described in (McMullin 1997) Since some of the descriptions use graphical illustrations, figure 2 explains how the different elements of SCL are represented

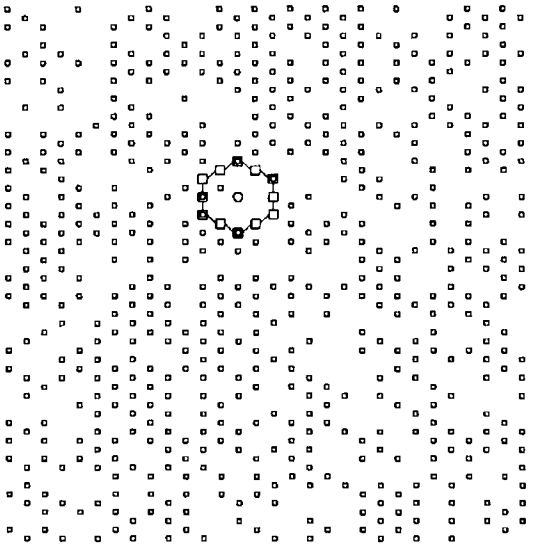

Figure 2 This is a 30 × 30 world containing one cell The large squares are links, the small ones substrates A large square containing a small one shows the presence of an absorbed substrate in this link Bonds between links are represented by lines joining the large squares The circle inside the cell is a catalyst and the membrane consists of twelve links There are currently 591 substrates in total, four of which are absorbed in links If all links and catalysts disintegrated, there would be 619 substrates

4 2 Flexible membranes

A mechanism for requirement 1a can be easily implemented First of all, a chain link can only swap its position with a hole in order to preserve the selective impermeability of the membrane It could also be allowed to swap with substrate particles, but since links are already permeable to those, it would be an unnecessary complication Second, bonds must not be over-stretched by motion which is straightforward to check on a hexagonal lattice This and my personal experience that all mechanisms in SCL can be more easily and unambiguously implemented using a hexagonal lattice as opposed to a rectangular lattice is the reason why the hexagonal lattice is now exclusively used for the extended version of SCL The main advantage of the hexagonal lattice is that all adjacent grid positions are equidistant

It can be argued that membrane flexibility independent of the growth mechanism is not necessary to achieve self-reproduction This is technically true, but membrane flexibility is desirable for at least two reasons First, flexible membranes might lead to configurations that can be exploited for the division process Second, cells should, at least at a later stage, be able to move as wholes

Membrane flexibility represents one step in this direction

Implementation notes Space is still discrete, two-dimensional and has a toroidal topology, but it is now organised as a lattice with a hexagonal neighbourhood

To allow the motion of bonded links a function has been implemented to test if any bonds would be over-stretched in which case the movement won't be allowed This obviously doesn't permit chains of links to move jointly but it is sufficient to make membranes flexible There is a simulation parameter (`acuteBonds`) that controls whether the movement of a bonded link may result in two bonds forming an acute angle (60 degrees) on a link When it is turned off, bonded links can only move if the resulting bond configurations won't include acute angles

4 3 Membrane growth by displacement

A mechanism for membrane growth (1b) is more difficult to devise Since the membrane must stay intact both a free link and a chain link in the membrane have to be moved in synchrony Furthermore, one bond in the membrane has to be broken and two new bonds have to be formed to incorporate the free link into the membrane The overall procedure is illustrated in figure 3 It takes place in one large step so that as far as all further interactions are concerned, the membrane always remains closed Note, that in the actual implementation of displace-growth, two chain links in the membrane are moved Although it would be sufficient to move just one chain link, this would lead to the formation of an acute (60 degree) angle between the two bonds of the link next to the integration site Too many acute angles in the membrane can render it inflexible and eventually rigid which would also stop further growth To prevent this, the chain link next to the link where the acute angle would otherwise form is moved as well

Implementation notes This mechanism can be (de-)activated by setting the boolean simulation parameter `displaceGrowth` accordingly When it is activated, each free link searches its neighbourhood at every time step for an integration site starting from a random position An integration site is a chain link whose bonding partners are chain links and positioned in such a way that they are adjacent to the free link as well If a site is found, the integration process is initiated with a given probability (`displaceGrowthProbability`) and it is randomly determined which

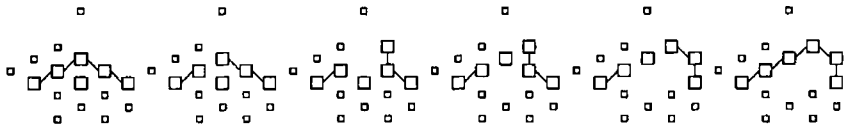

Figure 3 The five steps of the displace-growth mechanism From left to right First, a bond in the chain is removed After that, one single-bonded link moves so that the chain opens itself The free link then moves into the resulting gap Before two new bonds are formed, a second link in the chain is moved to prevent inserting an acute angle into the chain The sequence shown only serves to illustrate the procedure, but as such cannot be observed to take place in the world, because all steps are consecutively executed in one time step so that no other mechanisms can interfere

of the chain links to move besides the one at the integration site If all necessary movements can be carried out without over-stretching any bonds or violating the selective impermeability of the membrane, the process is then completed, otherwise, it will be aborted and the original situation is restored

4 4 Autocatalysis

The next mechanism described here is concerned with the replication of catalysts (requirement 3) In order to achieve this, an autocatalysis reaction is added which effectively turns the catalysts into self-replicators

$$Catalyst + 2\,Link \longrightarrow 2\,Catalyst$$

To prevent an overproduction of catalysts which would reduce the availability of free links for other mechanisms, this reaction is inhibited when more than one catalyst is in the neighborhood of one of the two reacting links Furthermore, if a catalyst has two other catalysts in its neighborhood, it will disintegrate into two links which themselves will disintegrate Spontaneous disintegration of catalysts is not used

Implementation notes Autocatalysis is implemented analogously to the link production mechanism It can be (de-)activated with the boolean simulation parameter `autocatalysis` When it is activated, the rate of production is controlled by the parameter `productionProbability`, which is the same parameter that controls the rate of link production

4 5 Self-maintenance revisited

With the extensions described above (fulfilling requirements 1a, 1b, 3) the membranes in SCL-DIV can now grow and are flexible This poses a problem for the self-maintenance process used in the original SCL system because free links inside the cell are not any more exclusively used to repair potential ruptures in the membrane They can also contribute to membrane growth and are substrates in the autocatalysis reaction Consequently, there are now fewer free links available to repair potential ruptures in an ever growing membrane To make matters worse, if the membrane is ruptured, the gap tends to increase due to the movement of the bonded links (although it is possible that the gap closes itself due to motion) All in all, self-maintenance which relies exclusively on the availability of randomly moving free links to close ruptures has proven unsatisfactory for achieving long-lasting maintenance under these circumstances

One possibility to increase the reliability of the self-maintenance process would be to modify the movement of free links so that they are more likely to stay next to the membrane than some distance away from it in the interior This strategy has been chosen in another modification of SCL, called SCL-GRO (McMullin and Groß 2001) But too few links near the membrane would only marginally increase the reliability and too many links would block the flexibility of the membrane In SCL-GRO, the latter effect leads to a rectangular shape of the growing membrane (cf ibid fig 1) which does not appear to be a configuration that could be easily exploited by some sort of fission mechanism Furthermore, as required by the identification key for autopoiesis (cf sec 2 3 2), the membrane of an autopoietic entity in SCL must always be closed This is not only necessary for conceptual clarity but a membrane can also be easily detected automatically and indicates the probable presence of a cell

For these reasons, spontaneous disintegration of chain links is replaced by a different mechanism which allows the stabilization of chain links without having to explicitly replace them and thus shifts the focus from the repair of ruptures towards the prevention of them This is achieved by a lifetime variable on each link which is decreased at every time step The lifetime units themselves freely diffuse across the lattice and can be collected by free links Every time step, a free link collects all available lifetime units at its position, up to a limit defined for links All mechanisms concerning the lifetime units are implemented so that the total number of them, whether bound in particles or free, is conserved When the lifetime variable of a link becomes zero, the link disintegrates Consequently,

a transfer of lifetime units between links is now sufficient to keep the membrane from rupturing This transfer of lifetime units conforms to the following two rules

1 Free links transfer lifetime units to chain links, if they have a higher lifetime value than the chain link In this case, half of the difference between the lifetime values is transferred

2 Adjacent chain links, which must be bonded to each other, share lifetime units among each other by summing up their lifetime units and distributing them equally among each other

Free links and single bonded links are still subject to spontaneous disintegration like in the original SCL system, only chain links are exempt from this The lifetime units bound by a link are released back to the environment in the event of disintegration

All in all, catalysts are still essential for the maintenance of a cell because without catalysts, all free links will soon have disintegrated This leaves the membrane without a connection to the supply of lifetime units in the environment and it will disintegrate as soon as the lifetime variables of its chain links become zero Furthermore, since membranes of well-maintained cells don't rupture, two (non-growing) cells could exist beside each other for practically indefinite time spans In particular, there is practically no danger of fusion, which would have been a problem in the original SCL system (McMullin 2000)

This lifetime mechanism is also extended to the catalysts, which receive lifetime units from chain links At every time step, a catalyst looks for a random chain link in its neighbourhood and if the chain link contains at least twice the maximal number of lifetime units defined for catalysts a transfer is initiated In this case, as many lifetime units are transferred as needed to increase the lifetime variable of the catalyst to its limit When a new catalyst is produced, its lifetime units are taken from the two links which served as the reactants and any excess beyond the limit for catalysts is released to the environment A catalyst which disintegrates because of the proximity to other catalysts (cf section 4 4) also releases its lifetime units to the environment A schema that summarizes the pathways involved in the transfer of lifetime units is shown in figure 4

As a result, the extension of the lifetime mechanism to catalysts strengthens the complementary relationship between them and the cell membrane Furthermore, if a cell fails to maintain itself, the catalysts often disintegrate before the

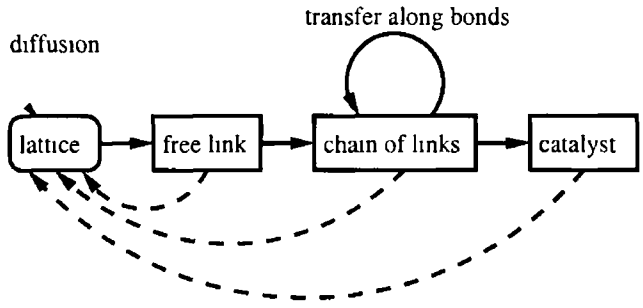

Figure 4 The transfer of lifetime units in SCL-DIV Diffusion of free lifetime units is shown by a dotted arrow while their uptake and transfer among the different particles is shown with solid arrows The dashed arrows represent the loss of lifetime units during every time step

membrane ruptures, because when the chain links themselves contain less than twice the maximal number of lifetime units defined for catalysts, they cease to maintain the catalysts In the original SCL system, a catalyst would usually escape the ruptured cell, leading to the production of links outside the former cell

Implementation notes To activate the new self-maintenance mechanism, both simulation parameters `applyLifespans` and `freeLifetime` have to be set to TRUE Deactivating the former reactivates spontaneous disintegration for chain links as controlled by the parameter `disintegrationProbability` and disables the lifetime count-down as well as the transfer of those units between particles The parameter `freeLifetime` activates the diffusion of free lifetime units on the lattice and makes sure that the total number of lifetime units is conserved

The diffusion of the free lifetime units is scheduled at the beginning of each time step, before the particles perform their step methods (cf McMullin (1997), sec 6 5) All lattice positions are updated simultaneously during the lifetime diffusion step as opposed to the particle diffusion which is achieved by a sequential random walk The diffusion constant is currently fixed in the source code

Both the `Catalyst` and `Link` class have a new instance variable called `lifespan` The value of this variable represents the amount of lifetime units currently held by the particle in question

For links, the collection of lifetime units and distribution to other links is scheduled in the same method which handles the spontaneous disintegration (`doDisintegration`) at every time step The simulation parameter `link2Life-`

Figure 5 Fusion of two clusters creates a membrane The two clusters are aligned so that there is a channel between them where the free links are located

span[5] specifies the maximal number of lifetime units each link can contain The transfer from free to chain links is initiated by the free link, which, starting with a random neighbour, looks for a chain link at every adjacent position and sequentially transfers the appropriate amount of lifetime units, if the conditions are fulfilled (cf rule 1 above) Distribution along bonds is initiated by each chain link and proceeds as described in rule 2 above If the collective amount of lifetime units cannot be equally divided, then the chain link which initiated the process receives the surplus

For catalysts, the search for a random adjacent chain link and a possible transfer of lifetime units is handled by the `step` method itself and proceeds as described above The limit for the number of lifetime units a catalyst can contain is specified by the parameter `catalystLifespan`

4 6 The fission mechanism

There are several ways in which the division of a membrane in SCL-DIV could proceed In biological cells, the cell membrane usually constricts itself creating two daughter cells of either equal or unequal size This constriction is guided by additional molecules inside the cell and would thus be difficult to recreate in the current SCL framework without additional particle types

A fission mechanism, which would rely on the flexibility of the membrane alone to touch itself, would also be prone to failure because a chain link has no way of knowing whether an adjacent chain link, to which it is not bonded, belongs to the same membrane or to a different membrane Therefore such a mechanism would not only lead to cell divisions but probably more often to cell fusions

The fission mechanism implemented instead exploits the fact, that inside a growing cell clusters of chain links tend to form These clusters are the results of free links bonding to each other when they are far enough away from the cell membrane and other clusters so that the chain-based bond inhibition mechanism

[5]It is called `link2Lifespan` because its value is mainly relevant for the lifespan of chain links since free and single-bonded links can still spontaneously disintegrate

doesn't prevent this The clusters usually consist of three or four chain links adjacent to each other which are bonded so that they constitute a closed chain When there is a channel of width one between two such clusters and some further geometric conditions are satisfied, then these two clusters together with two free links which must be in the channel can reorganise their bonds to form a larger single membrane (cf figure 5) If this takes place between a closed chain inside the cell and the outer membrane itself the result will be an incision into the cell If the incision is such that it creates a new channel between itself and the outer membrane then two free links in this channel will trigger the mechanism again so that the membrane will eventually be divided Figure 6 shows a sequence of snapshots from a SCL-DIV run that illustrates the described process Of course, more complicated sequences of fusions and/or incisions can lead to divisions as well

Another possibility for a cell to divide itself using the same mechanism is when both sides of the cell membrane are sufficiently close to each other without any prior incision Then there would be the necessary channel between them in which the presence of two free links could initiate a one-step division (cf figure 7) However, such a configuration is less likely to occur than those described in the previous paragraph Therefore, a cell division usually requires of two or more occurrences of the fission mechanism

Implementation notes Although the boolean simulation parameter which controls this mechanism is called `organizedFission`, because its purpose is to allow cell division, it is a fusion mechanism where two free links and four chain links participate in the integration of the two free links into the chain(s) and the reorganisation of the bonds If switched on, the mechanism is initiated by a free link each time step if there are less than five chain links in its neighbourhood The latter restriction prevents small bulges in the membrane from being split off which would result in an unwanted loss of chain links Then the neighbourhood is searched for an adjacent free link starting from a random position If this other free link has less than five chain links in its neighbourhood as well, both links jointly start from a random position to search for chain links When the first pair of chain links is found, the scan continues to search for a second pair of chain links Both chain links of each pair are at the same neighbour position relative to the free links and the two pairs are at different neighbour positions relative to the free links If all four chain links are distinct and the two sides of the channel are not cross-linked, the reorganisation of the bonds takes place as illustrated in

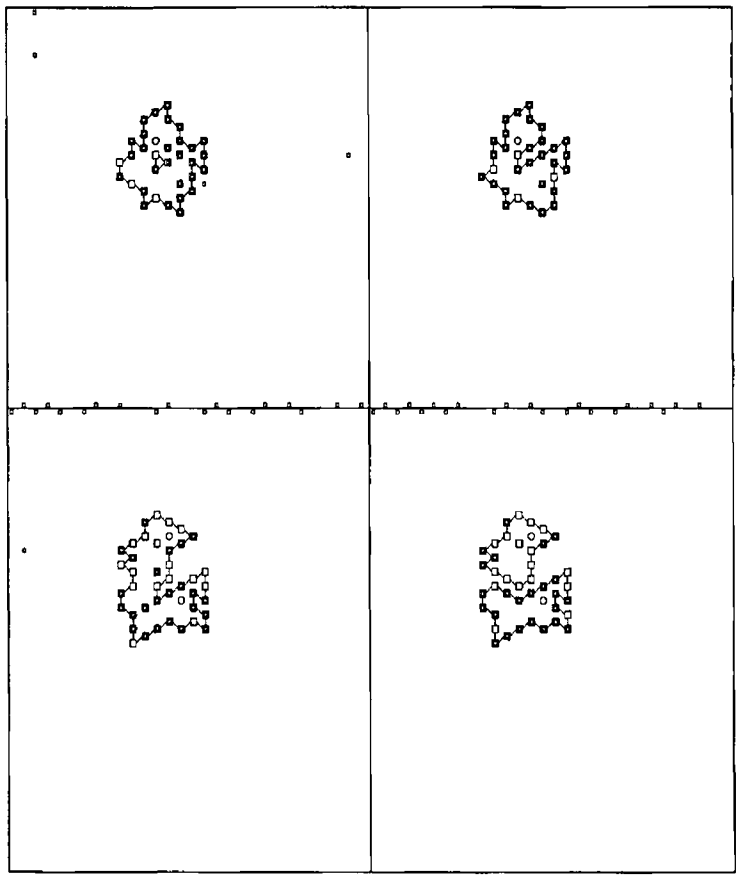

Figure 6 Four snapshots from a run that started with the world shown in figure 2 The upper row shows how an incision into the membrane is formed after it fuses with a cluster This results in the formation of a channel Membrane growth and flexibility then slightly modify this channel but it is basically the site where the cells divide which is shown in the lower row In each row, the left snapshot shows the time step before and the right one the time step after the operation of the fission mechanism

the figures 5 and 7

4 7 Chain motion

Chain motion allows chains of links to move jointly which isn't possible with the mechanism for membrane flexibility alone Although not necessary for self-reproduction, chain motion is desirable for the reason that it can "iron wrinkles out of membranes" What this means is illustrated in figure 8

The reason for this to be desirable is that it prevents the accumulation of acute angles in membranes which can be introduced by the fission mechanism Acute angles which are the result of membrane flexibility can be reversible eliminated,

Figure 7 The division of an hourglass-shaped membrane into two membranes The channel is now made up by two different parts of the same membrane Again, the free links have to be located in this channel

Figure 8 The link which initiates the chain motion is marked with an absorbed substrate Note that at its position there are two adjacent acute angles in the membrane The link moves towards southeast, dragging the link previously southwest of it behind This action eliminates one acute angle from the membrane which wouldn't have been possible with membrane flexibility alone

if no other structures obstruct this, so that they in general don't pose a problem Too many acute angles in a membrane can render it inflexible and also prevent displace-growth Thus, a cell can get stuck in such a "dead end" configuration and achieve immortality Although this has been observed only rarely, there is the conceivable risk that during very long runs one or more such "dead end" cells could accumulate and thereby fix an ever increasing number of links until there are only immortal cells present An example of a world where the one and only cell has achieved immortality is shown in figure 9 In general, since the intention is to demonstrate self-reproducing cells which maintain themselves non-trivially, immortal cells are undesirable

Furthermore, chain motion allows the movement of membranes as wholes by increasing the membrane flexibility However, clusters consisting of three links are still immobile despite chain motion Although extensive use of chain motion would decrease the likelihood of clusters coming into existence through increased chain flexibility and the chain-based bond inhibition mechanism, usually one can expect clusters to be present inside a cell These clusters would through their presence block any far-reaching movements of cells because of the absence of momentum in SCL The same holds for all links, catalysts and substrates inside a cell as well, but their presence is less adverse because these particles constantly change position All in all, the use of chain motion does not make cells as wholes mobile, but only empty membranes Worse still, as noted above, chain motion

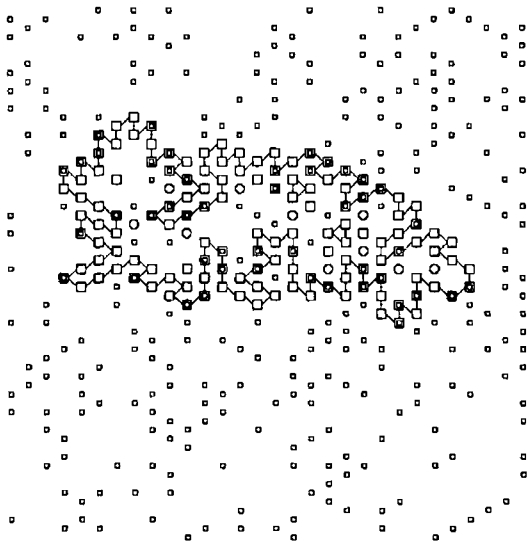

Figure 9 A run which is stuck in a dead end The only cell is practically immortal because of two circumstances Firstly, through membrane flexibility alone no configuration can be reached that would allow displacegrowth to occur Secondly, no new clusters can form in the interior of the cell because of chain-based bond inhibition so that a channel which could be used by the fission mechanism cannot develop The two clusters which are inside the cell were formed earlier before the membrane tightened around them The shown situation remained unchanged for 120,000 time steps before the run was terminated by hand

decreases the likelihood of clusters being formed and can thus hinder cell division (cf section 4 6) Hence, this mechanism must be used with caution

In the light of these restrictions one might wonder whether this mechanism should be used at all, especially so because of its non-local nature Also, kinks in the membrane can be discovered locally by searching for adjacent acute angles and splitting off one of the chain links which make up the kink In figure 8 this would result in splitting off either the chain link marked with an absorbed substrate or the one southwest of it As a matter of fact, a mechanism (`eliminate60probability`) exists in SCL-DIV which achieves just that, but it isn't used in the experiments described in the next section The reason why `chainMotion` is used instead is to highlight the fact that the motion of cells is an important problem that has not yet been satisfactorily solved

Implementation notes Chain motion is implemented independent of the particle motion mechanism and can be initiated by a bonded link only Initiation is controlled by the simulation parameter `chainMotionInitProb` which is used

by bonded links to decide whether to try chain motion each time step If chain motion is initiated, a random neighbour is selected and tested whether it is a hole particle Also, exactly one bond of the initiating link must be over-stretched by its movement, otherwise the process is aborted The over-stretched bond is then used to "drag" the next link Actually, the next link is not immediately dragged but it is recursively tested if the link is dragable, or if it can play the role of the last link in the moving part of the chain When the link is dragable, it is added to a list and the next link is tested A possible last link is either a single bonded link or a link with bonds which form an acute angle If a non-dragable link is encountered, which is the case when it has already moved during the current time step, the whole process is aborted

When a list of links which can move jointly has been found, the geometric mean of the mobility parameters of the participating particles is calculated and used as probability value to decide whether the movement proceeds This follows the procedure for normal particle motion as described in (McMullin 1997, sec 3 2) If motion proceeds, the link which initiated the process is then moved to the lattice position which previously contained the neighbouring hole All the links which have been included in the list during the test phase are then dragged behind and the hole takes up the position which is vacated by the last link that moves Also, all particles which participated in the process become immobile for the rest of the time step

4 8 Other changes in SCL-DIV

The last section of this chapter describes other changes made in SCL-DIV compared to original SCL which are not directly related to the new mechanisms, but still modify some of the original mechanisms in important ways

The mechanism for chain-based bond inhibition is changed, so that it is possible to specify with a simulation parameter (`chainInhibitBondCount`) how many chain links need at least be in the neighbourhood in order to suppress the formation of a bond This allows for a greater flexibility when using this mechanism Catalyst-based bond inhibition can be influenced in the same way with another simulation parameter (`catInhibitBondCount`) Setting either `chainInhibitBondCount` or `catInhibitBondCount` to 6 effectively turns each particular mechanism off Furthermore, the boolean parameter `inhibitOnlyFreeLinks` specifies, whether only free links are affected by the two bond inhibition mechanisms or single-bonded links as well

Substrates, which are inside a link, can now move into other (empty) adjacent links whereas they could only move into adjacent holes in the original SCL system This is achieved by changing the mechanism which implements the emission of substrate particles from links If the adjacent particle, which is randomly chosen during the emission, is a link without an absorbed substrate, then the substrate is transferred to this link The parameter `absorptionProbability` doesn't influence this transfer This extension enables substrates to move through adjacent layers of chain links which is not possible in original SCL

The procedure that implements the bonding of links, is changed significantly The neighbourhood of a link with less than two bonds can now be searched every time step for bonding partners This search is (de-)activated by setting the boolean simulation parameter `scanForBondableNeighbors` accordingly It starts at a random position and continues until a bonding partner is found If no search is conducted, a random adjacent particle is chosen and examined if it can serve as a bonding partner In both cases, when the parameter `acuteBonds` is set to FALSE, a possible neighbour is discounted if bonding to it would result in creating an acute angle between the new and an existing bond Otherwise, the new bond is created and no probabilities are used to control this process so in effect the bond is created with probability one Of course, if no bonding partner is present in the neighbourhood, then no bond can be formed This eager bonding mechanism facilitates cluster formation which is necessary for division

Bond decay, which wasn't present in the model of Varela et al (1974), is removed again so that a bond is only dropped when one of the links which are bonded together disintegrates This is necessary to ensure that the new self-maintenance mechanism can operate as intended

Lastly, in SCL-DIV certain simulation parameters are heritable instead of global as in the original SCL system This means that catalysts can have individual values for those parameters and transmit them to the catalysts and links which they produce Thus cells with different parameter sets can grow and reproduce in the same world

With these new mechanisms and other changes in place, the following chapter describes some aspects of the phenomenology in SCL-DIV and it is illustrated how the mechanisms work together so that self-maintenance and self-reproduction is achieved

5 Phenomena of the SCL-DIV world

This chapter describes what can be observed during runs of the SCL-DIV system The standard parameter set used for the runs is shown in table 1 Any deviation from standard values are mentioned in the relevant sections The mobility factors control the random walks of the particles on the lattice as described in (McMullin 1997) There are other simulation parameters for SCL-DIV as well, but these control currently unused mechanisms and aren't listed here

5 1 Self-maintenance using lifetime units

First of all it is necessary to evaluate the new self-maintenance mechanism before looking at division and the long-term developments Therefore, 200 runs have been conducted starting with the world shown in figure 2 (p 30) The standard parameter set shown in table 1 is used with the exceptions that `autocatalysis` is set to FALSE and `link2Lifespan` reduced to 500 The links in the membrane of the initial cell each contain 500 lifetime units, the catalyst contains 20 and at every lattice position there are 200 free lifetime units All in all, the world contains 186,020 lifetime units The only difference between the runs is that the random number generator is seeded with different values Also, the runs are configured to automatically stop at a limit of 50,000 time steps or when the catalyst disintegrates

Given these numbers, the original cell is at least able to maintain itself for somewhat less than 500 time steps The reason for this is that the transfer of lifetime units from the chain links to the catalyst stops when the chain links in question drop below 40 lifetime units (which is twice the value of `catalystLifespan`) At this point, the catalyst has at best 20 lifetime units left so that it will disintegrate around time step 480 Disintegration prior to this point can happen, when the catalyst doesn't come into contact with the membrane for a sufficiently long time interval Furthermore, the continuous maintenance of the catalyst also draws lifetime units from the membrane so that a minimal lifespan of 480 is an overestimation

The disintegration of the catalyst in these runs is taken as an indicator for the failure of the cell's self-maintenance capability It is a sufficient condition for failure, but not a necessary one because the membrane could have been ruptured prior to that In the case where the membrane was ruptured before the disintegration of the catalyst, the time step during which the rupture occurs is taken to indicate the point of failure

simulation parameter	value	valid range
catalystMobilityFactor	0 1	0 0 - 1 0
linkMobilityFactor	0 1	0 0 - 1 0
substrateMobilityFactor	0 5	0 0 - 1 0
holeMobilityFactor	0 5	0 0 - 1 0
productionProbability	1 0	0 0 - 1 0
disintegrationProbability	0 01	0 0 - 1 0
absorptionProbability	0 5	0 0 - 1 0
emissionProbability	0 5	0 0 - 1 0
chainInhibitBondCount	1	1 - 6
catInhibitBondCount	1	1 - 6
inhibitOnlyFreeLinks	TRUE	TRUE/FALSE
displaceGrowth	TRUE	TRUE/FALSE
displaceGrowthProbability	0 5	0 0 - 1 0
catalystLifespan	20	1 - 2000
link2Lifespan	1000	1 - 5000
scanForBondableNeighbors	TRUE	TRUE/FALSE
autocatalysis	TRUE	TRUE/FALSE
acuteBonds	TRUE	TRUE/FALSE
organizedFission	TRUE	TRUE/FALSE
applyLifespans	TRUE	TRUE/FALSE
freeLifetime	TRUE	TRUE/FALSE
chainMotion	TRUE	TRUE/FALSE
chainMotionInitProb	0 001	0 0 - 1 0

Table 1 Standard values of the simulation parameters The valid range for each parameter is shown in the third column `catalystLifespan` must be smaller than half the `link2Lifespan`

Figure 10 summarizes the lifespans of the cells which were achieved in the 200 different runs Only four of the runs terminated before 500 time steps and in none of them the cell is able to maintain itself until the limit of 50,000 time steps

The statistical parameters, on which figure 10 is based, are shown in table 2 The minimal lifespan for a cell observed in these runs is 453 time steps, which is close to the expectation The second quartile has a range of 3,628 whereas the third quartile has a range of 3,695 This indicates, that the distribution of lifespan values is only slightly skewed close to the median However, the first and fourth quartiles show that further away from the median there is an obvious skew towards the smaller values Thus the probability of failure is higher during the beginning of the run indicating that the start configuration of the cell is not

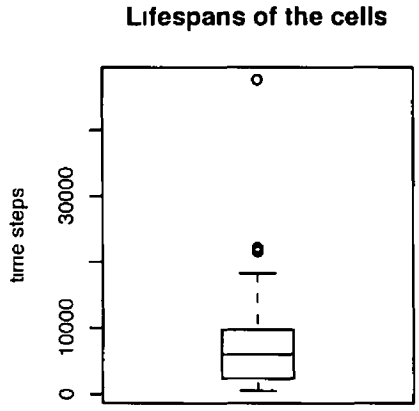

Figure 10 Box-and-whisker plot of the 200 lifespan values obtained by the runs described in the text The box comprises the values contained in the second and third quartile whereas the bar represents the median of the distribution The whiskers extend to the most extreme data point which is no more than 1 5 times the interquartile range from the box The interquartile range is the difference between the highest value in the third quartile and lowest value in the second quartile Outliers beyond the whiskers are represented by circles and if no outlier is present a whisker extends up to the most extreme data point

the most stable one It is also important to note that the lifespans measured are distributed over a large interval which from the minimum to the maximum value spans two orders of magnitude This considerable variation shows that the lifespan is to a great extent influenced by factors that are outside the cell's control One such factor would be the substrate density and another one particle motion that is implemented as a random walk

Further analysis of the runs shows, as can be expected because of the activated fission mechanism, that membrane divisions continually occur But since there is only one catalyst only one of the membranes after a division will be able to persist There are three possible ways, in which the cell will eventually disintegrate First, the membrane can confine the catalyst to an area too small for production of new links to occur Over time, all free links will disappear thereby cutting off the membrane from the supply of free lifetime units Second, a growing cell which doesn't divide can become so large that the catalyst can diffuse around in its interior without touching a chain link so that it will run out of lifetime units and disintegrate The third scenario involves a large cell as well, with the catalyst confined to a small area, but still capable of production (cf upper row of figure

statistic measure	value
minimum	453
1st quartile	2,363
median	5,991
mean	6,804
3rd quartile	9,689
maximum	47,630

Table 2 Summary statistics of the 200 runs The numbers shown indicate the time step at the end of which no membranes are present in the world or the time step during which the catalyst disintegrates, whichever is earlier

13) All the free links produced, will be confined to that area as well and only from that area can lifetime units enter the membrane If the membrane is large, there might not be enough free lifetime units collected in this area to sustain all the links in the membrane Consequently, the membrane will rupture at a position some distance away from the area containing the catalyst In that case, the catalyst still remains confined to this area and produces free links, but these cannot reach the ends of the now open chain Because of spontaneous disintegration, the chain constantly shrinks But until a gap develops, through which the catalyst could escape, there is always the possibility that the chain closes itself or that a new cell is split off from the confinement area through the fission mechanism

To sum up, although the cell is able to maintain itself on average about 15 times the minimum lifespan, it will also eventually disintegrate This demonstrates that, although the new self-maintenance mechanism is more elaborate than the original one, which only relied on the repair of ruptures, it still won't support any sort of trivial immortality It is also important to note, that whereas in the original SCL system due to the process of self-maintenance there is a turn-over of links in the membrane, the turn-over in the extended version involves whole membrane segments This is the case because during division a part of the membrane splits off to form a new one

5 2 Long-term world development

This section describes multiple runs conducted with two different worlds The parameters used for both runs are shown in table 1 which in particular means that compared to the runs described in the previous section the autocatalysis reaction is now activated

statistic measure	value
minimum	167
1st quartile	201 3
median	1354
mean	22,787
3rd quartile	49,917
maximum	90,157

Table 3 Summary statistics of the 52 runs which don't reach the limit of 100,000 time steps The numbers shown indicate the time step during which the last catalyst disintegrated

5 2 1 Small world

This is the same world as used before, shown in figure 2 (p 30) However, the links which constitute the membrane are now initialised with 200 lifetime units each, the other lifetime initialisation values are the same as in the previous section Consequently, there are now 182,420 lifetime units in total in this world 150 runs were conducted with a different seed for the random number generator in each run Runs either terminate when no catalysts are left or when a limit of 100,000 time steps is reached

It turns out that about one third of the runs don't reach the limit of 100,000 time steps because all catalysts have disintegrated before Table 3 shows the statistical parameters for these runs As can be seen, the distribution is now more skewed towards smaller values compared to the one in table 2 One reason for this is that the links making up the membrane are initialised with less lifetime units (200 as opposed to 500) so that the failure rate of the cell early in the run can be expected to be higher Closer analysis of the 52 runs shows that 27 of them fail rather soon with no or only one division occurring Thus the median of the distribution nearly divides these from the other 25 runs which lasted considerably longer as the mean value which is about 16 times higher than the median shows The reason that those 25 runs lasted longer is that autocatalysis is now turned on and the entities can self-reproduce Hence there there can be several cells in the world and a run can still continue when one of them disintegrates Furthermore, the absence of any membranes from the world, although indicating the temporary failure of all autopoietic entities, does not mean that no autopoietic entities can re-emerge again during the remainder of a run Only when all catalysts have disintegrated, no cells can ever arise again

The runs which reached the limit are analysed in the following way For each

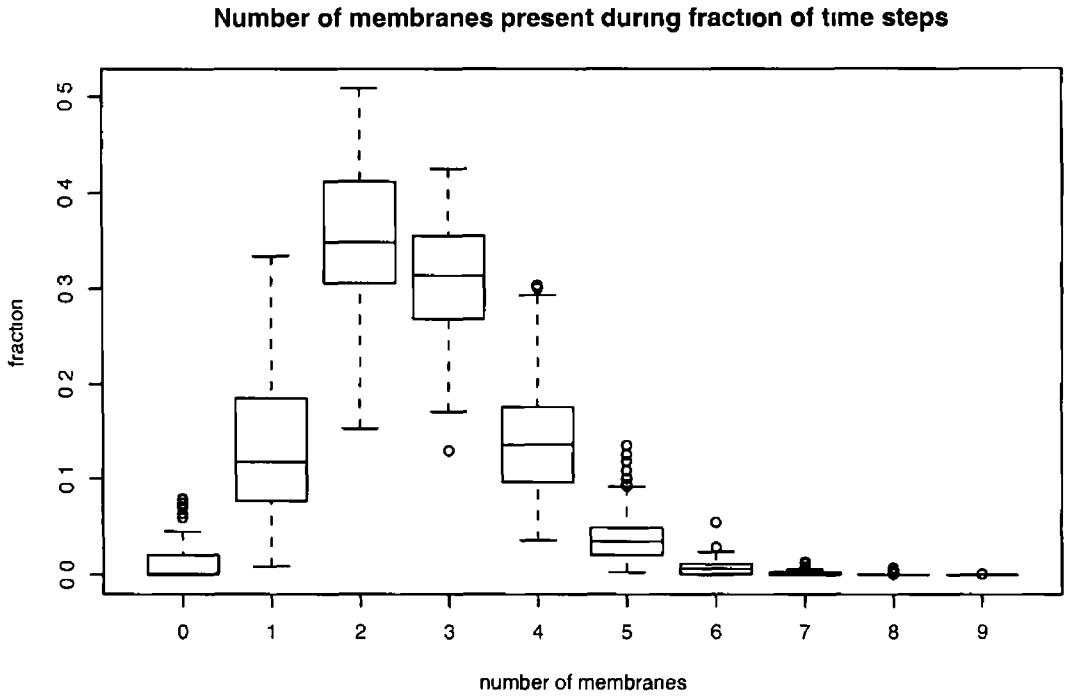

Figure 11 For each number of membranes, the fraction of time steps during which this number of membranes is present is determined separately for each of the 98 runs, ignoring the first 10,000 time steps The fractions from the different runs are represented as a distribution with box-and-whisker plots (set up like in figure 10) for each number of membranes

run it is calculated, how many membranes are present during how many time steps The first 10,000 time steps are not counted to ignore possible peculiarities only characteristic of the initial phase of the run For each value of the number of membranes, the relative frequencies from each run are collected and shown as a box-and-whisker plot in figure 11 It is apparent from this figure that all runs have certain properties in common For instance, during all runs the fraction of time steps when two or three membranes are present is always higher than the fraction of time steps when no or more than five membranes are present Thus it can be said, that for each run there are during the majority of time steps one to five membranes in the world

During 45 of the 98 analysed runs, there is always at least one membrane present However, in the other runs there are periods when no membranes are in the world This, of course, means that there can't be a cell in the world which means that no autopoietic entity can be present during such a period These

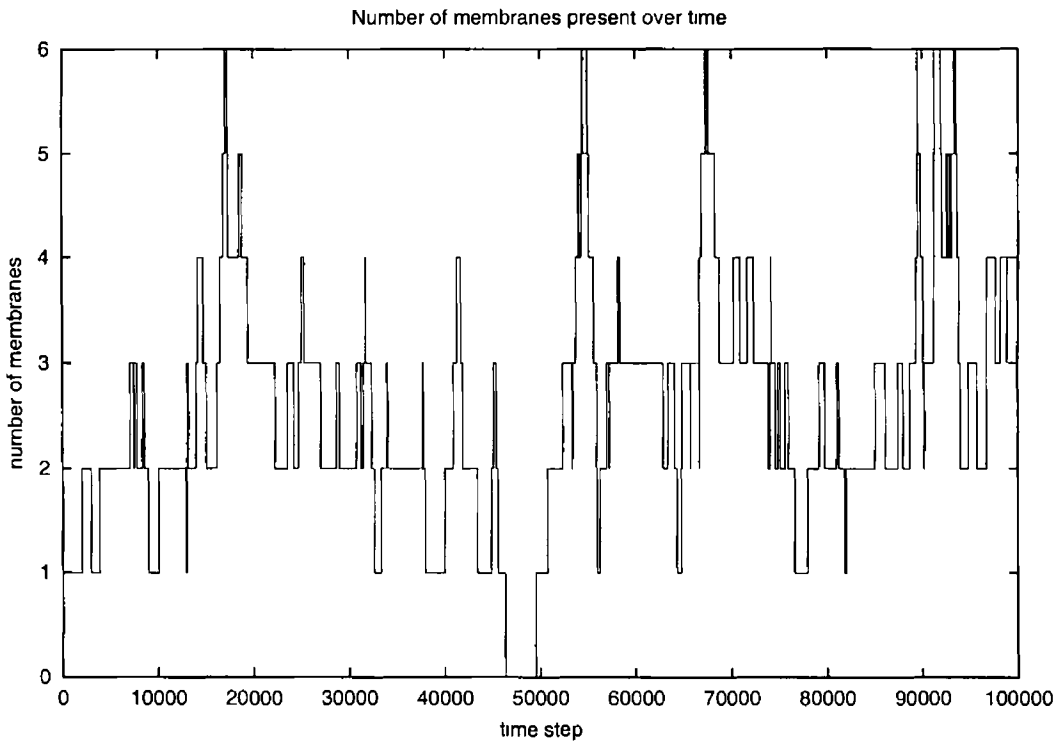

Figure 12 Development of the number of membranes present during one of the runs

periods don't take up more than 8 % of the time steps in any of the analysed runs, so it is apparent that from such a membrane-free period new cells can arise An example of this can be seen in figure 12 Between time step 46,322 and 49,541 there is no membrane present in the world but after this interval of over 3,000 time steps the membrane number increases again, which wouldn't be possible if a cell which then divided had not emerged During a membrane-free period there are typically several catalysts enclosed in one or several open chains of links Since the ends of an open chain are subject to spontaneous disintegration, it will shrink if it doesn't close itself or if a new cell emerges through the fission mechanism For the time interval in question, this is illustrated in figure 13 As can be seen in the upper row, the only cell at this time in the world fails to maintain its membrane because its catalysts are confined to the left part This is the third scenario of cell disintegration described in section 5 1 The three free links at the rupture site shown in the upper right snapshot are in the state of disintegration and therefore cannot form bonds to reestablish the membrane After more than 3,000 time steps, the open chain has considerably shrunk from its ends through both spontaneous disintegration and insufficient lifetime units,

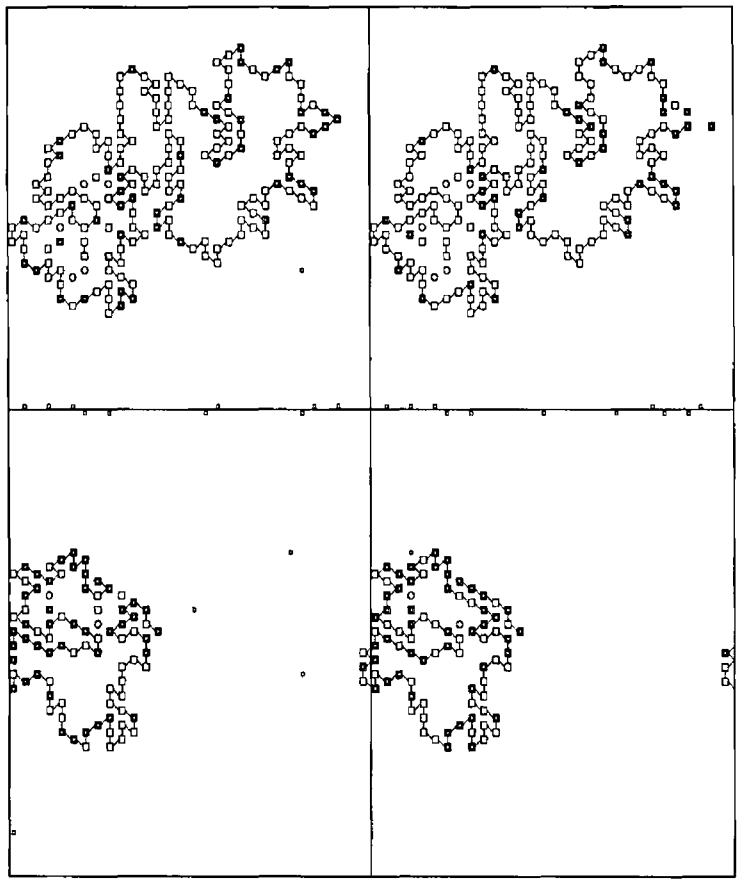

Figure 13 Four snapshots from the run shown in figure 12 The upper row shows the world at time steps 46,322 and 46,323 while the lower row shows time steps 49,540 and 49,541 respectively For details see text

leading to the state shown in the lower left snapshot At this time, the open ends are in a configuration with a channel between them Free links, produced by the catalysts move into this gap and through the fission mechanism the chain closes into a new membrane

A different, hypothetical, explanation for the rise in membrane numbers to six at time step 54,414 (cf figure 12) could be that through the fission mechanism a new membrane is produced without an enclosed catalyst However, it is very unlikely that several empty membranes are produced and maintained by catalysts outside them For this to occur the catalysts would have to be confined between the membranes or otherwise the former would sooner or later diffuse away and disintegrate when cut off from the supply of lifetime units provided by the membranes When the catalysts are confined between the membranes and produce free links then these can get into the channels between the membranes, which can be expected to form because of membrane flexibility Under the operation of the

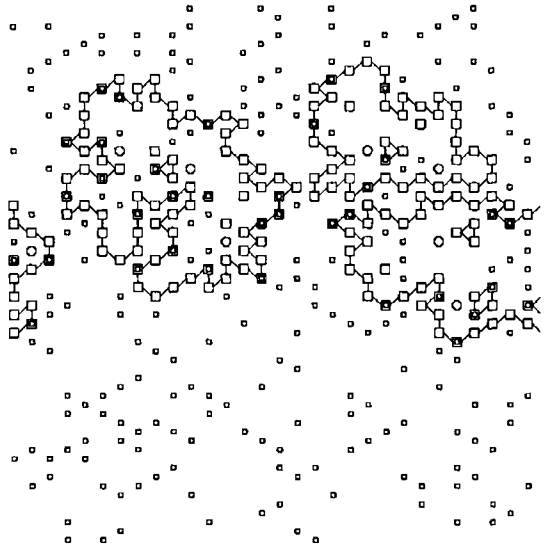

Figure 14 The state of the same world used for figure 12 at the end of time step 100,000

fission mechanism, two membranes then could fuse into one If channels too large for the fission mechanism to operate develop between the empty membranes, for example through chain motion, there is the danger of the catalyst eventually escaping through this channel and soon the membranes would disintegrate All in all, whenever the membrane number falls to zero during a run and later increases again it is reasonable to assume that an autopoietic entity has re-emerged Figure 14 shows the world which is the basis of figure 12 at the end of its run of 100,000 time steps The three cells in the world belong to the lineage established by the cell shown in the lower right snapshot of figure 13

As mentioned earlier, in one third of the runs the population of cells dies out before 100,000 time steps are completed Thus, in a rather small world as used for these runs, it is possible that all autopoietic entities disintegrate one after another, for the reasons given in section 5 1, until none are left During such a period, none of the cells is apparently able to establish a new population of autopoietic entities Obviously, if the world was larger and could support more cells, then it would be more likely that there is always a cell present which is able to process the substrates from disintegrated autopoietic entities, can then divide and establish a new cell population Therefore, the following section investigates such a larger world

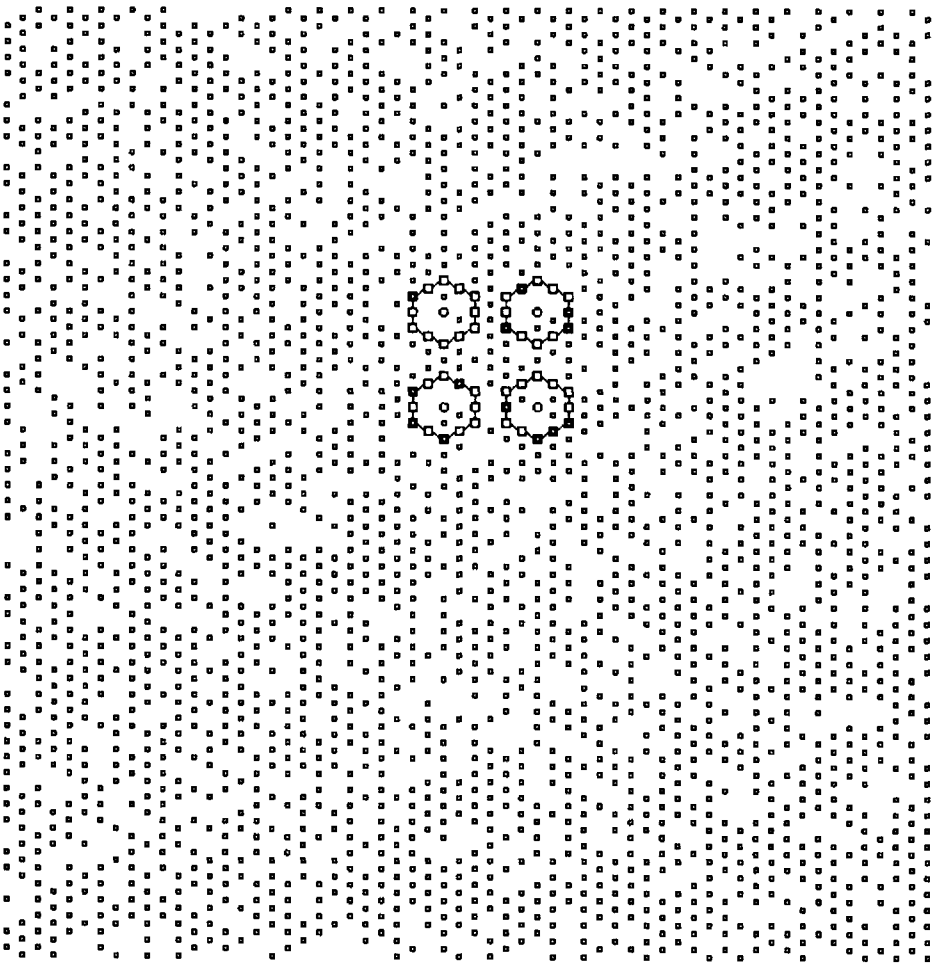

Figure 15 A 60 × 60 world containing four cells The cells have the same size as the one in figure 2 There are currently 2,658 substrates in this world, 13 of which are absorbed in links If all links and catalysts disintegrated, there would be 2770 substrates

5 2 2 Large world

The runs described in this section are conducted in a 60 x 60 world, which is shown in figure 15 It contains four cells which are arranged next to each other in a square The reason why this world is seeded with four cells instead of one as in the previous section is to reduce the likelihood that a run terminates due to early failure as happened in 27 of 150 runs in the small world Each link is initialised with between 997 and 999 lifetime units, each catalyst with 20 and at each lattice position are 100 free lifetime units, in total there are 408,010 lifetime units in this world 50 runs were conducted with this world in the same manner as described in the previous section but the limit is increased to 200,000 time steps One of the runs terminated after 11,019 time steps, the others are combined in the same

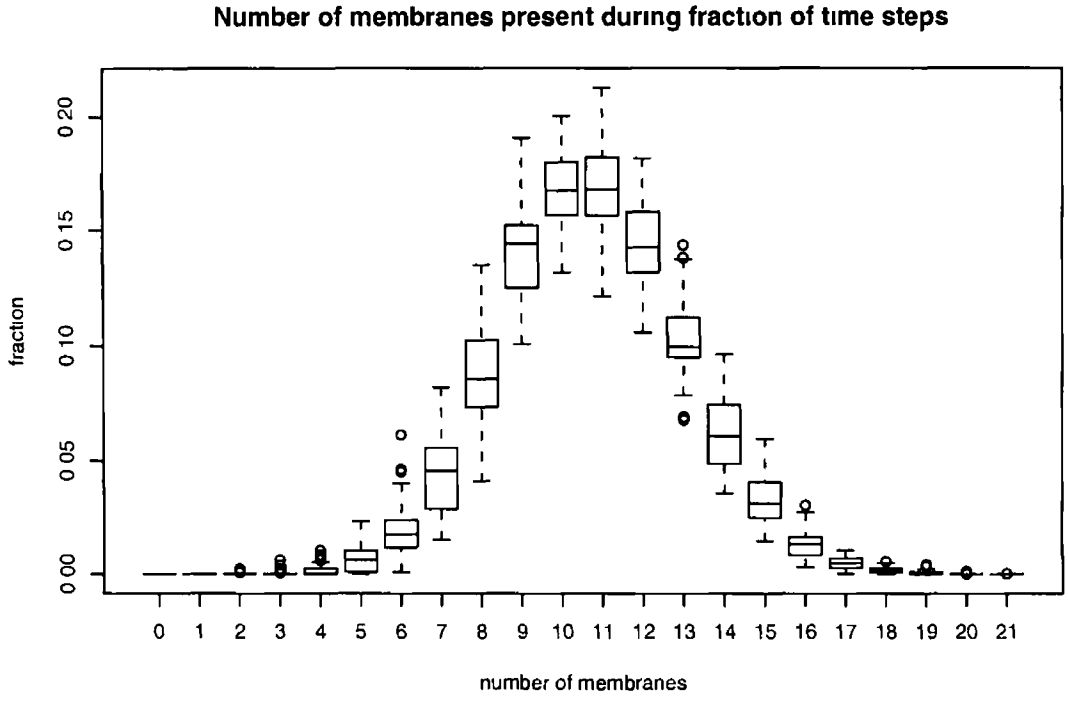

Figure 16: As in figure 11, but each distribution comprises values from 49 runs and the first 20,000 time steps of each run are ignored

way as in the previous section to produce figure 16 This time, the first 20,000 time steps of each run are ignored

First of all, when compared to figure 11, the overall distribution appears now more symmetric and the interquartile ranges have become smaller This can be attributed to the fact that the world is four times larger and supports about four times as many cells Therefore, the range of membrane numbers reaches from two to 21 Also, each run lasted 200,000 time steps which is twice as many as in the previous section These two effects together lead to the result that the fractions for the different runs cluster more closely for each number of membranes Now all runs have in common that during the majority of time steps seven to 15 membranes are present in the world Furthermore, there are significantly more often ten or eleven membranes present than either seven, eight or any from twelve to 15

Also, there aren't any periods in these runs during which there are no membranes present This doesn't mean though, that there is always a cell present, because a few membranes in this large world can be possibly maintained by catalysts outside them But figure 16 makes clear, that there are only very rarely

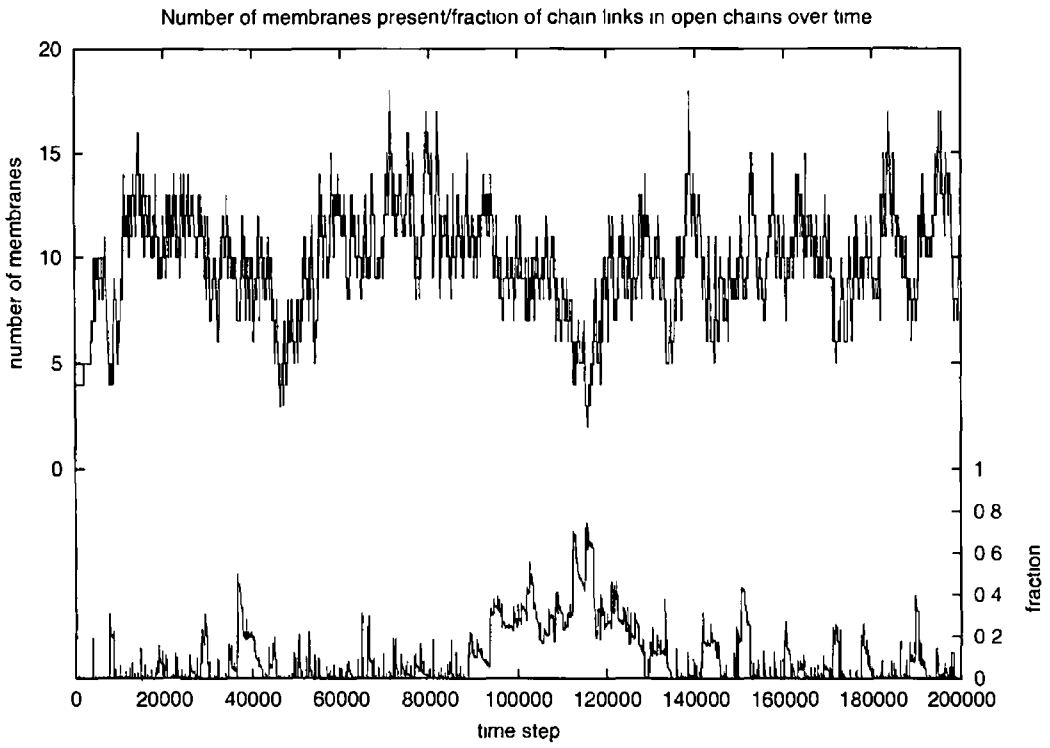

Figure 17 Development of the number of membranes and the fraction of the total number of chain links which are part of an open chain during one of the runs

less than four membranes present and such periods never comprise more than 1 % of the total amount of time steps in any of the runs When four or more membranes are present, then it is reasonably certain that at least one of them is a cell Consequently, as expected, the possibility of the whole population dying out is much reduced and only one of the 50 runs doesn't reach the limit of 200,000 time steps This has to be compared with the 25 of 150 runs in the small world which didn't reach the limit of 100,000 time steps but still were comparatively long-lived Because the large world is seeded with four cells, early failure doesn't occur any more and the rate of later failure relative to the small world is reduced from one in six to one in 50

What happens during periods when relatively few membranes are in the world can be derived from figure 17 The upper graph displays the number of membranes present over time while the lower one shows the corresponding fraction of chain links which are in an open chain As can be seen, from time step 90,000 to 130,000 at least 20 % of the chain links are part of open chains During such a period there would be typically one or several open chains enclosing several catalysts This aggregation then develops into one or several cells under the influence

of the fission mechanism unless it disintegrates when it is not able to contain its catalysts Usually though, such an aggregation is rather short-lived, as can be seen by the multitude of spikes in the lower graph It typically is the result of a growing cell which fails to divide and then breaks open (cf section 5 1) If one of the catalyst escapes, there are also possible effects on the other cells because the catalyst can bounce between the now open chain and an adjacent cell When free links are produced and there is an appropriate channel between the cell and the open chain for the fission mechanism to operate, then as a result the adjacent cell will break open This process can repeat and eventually affect a large part of the world, resulting in a possibly quite long period during which a significant amount of chain links is in open chains A world with these characteristics is shown in figure 18

Comparing the number of membranes with the fraction of chain links in open chains in figure 17 shows that during the longer periods where the fraction of chain links in open chains is high, the number of membranes indeed often drops This can be seen for example around time step 115,000 171,000 and 188,000 On the other hand, around time step 46,000 (cf fig 19), the membrane number drops to three and the fraction of chain links in open chains is low as well The reason for this is that the number of membranes depends on other factors as well For instance, if cells divide successively before growing very large, a lot of membranes can be present whereas if cells grow large without dividing, then rather few membranes are present although most of the chain links are in the membranes Thus, there can be no direct correlation between the two graphs in figure 17 Finally, figure 20 shows a more typical world configuration than those in the previous figures All in all this subsection shows that in a sufficiently large world some autopoietic entities can always be expected to be present Due to ongoing turnover of cells, potentially infinite lineages of them can only be established through ongoing self-reproduction

5 2 3 Population dynamics

The plots in figures 12 and 17 illustrate that there is a complex population dynamic However, the curves show rather erratic fluctuations because there are always some cells disintegrating and other ones reproducing As mentioned, when a cell disintegrates with the catalyst escaping, this has potentially disastrous consequences for the other cells But even without such catastrophes, both division and disintegration are to a significant extent affected by random factors which

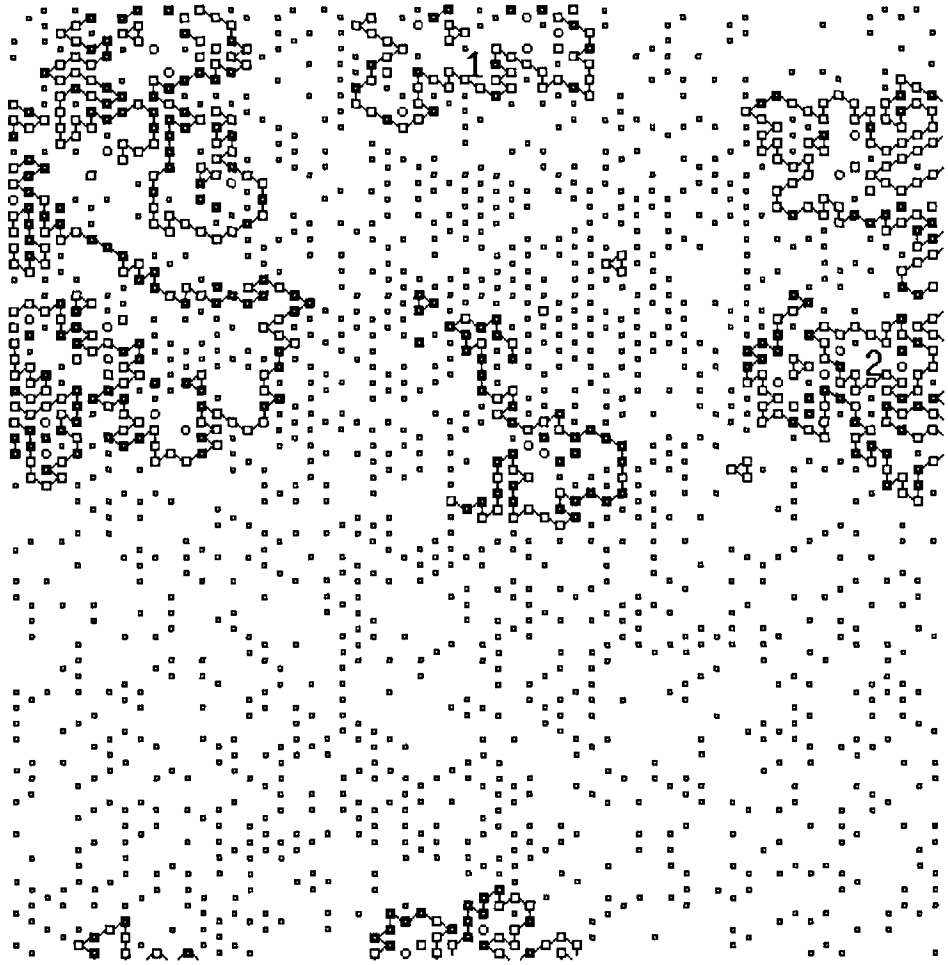

Figure 18 The run displayed in figure 17 at time step 115,475 The only two cells in this world are marked with numbers in their interior Note that cell number two is almost completely surrounded by an open chain that encloses catalysts between it and the cell membrane The open chain in the center is the remnant of a recently disintegrated cell

cannot be controlled by the cells For instance membrane flexibility, which is based on the random walk of links (as far as the bonds allow) influences both division and disintegration of cells For cell division to occur the membrane must form a channel somewhere and awkward membrane configurations can lead to disintegration as discussed in section 5 1 (cf also fig 13) All this leads to significant variability in lifetime and gestation time of the cells

This variability can still be seen when the early stages of the runs in the large world are investigated At the beginning of the run substrate availability, which naturally influences lifetime and gestation time as well, only plays a minor role Nonetheless, even when oscillations in the membrane numbers are removed, then

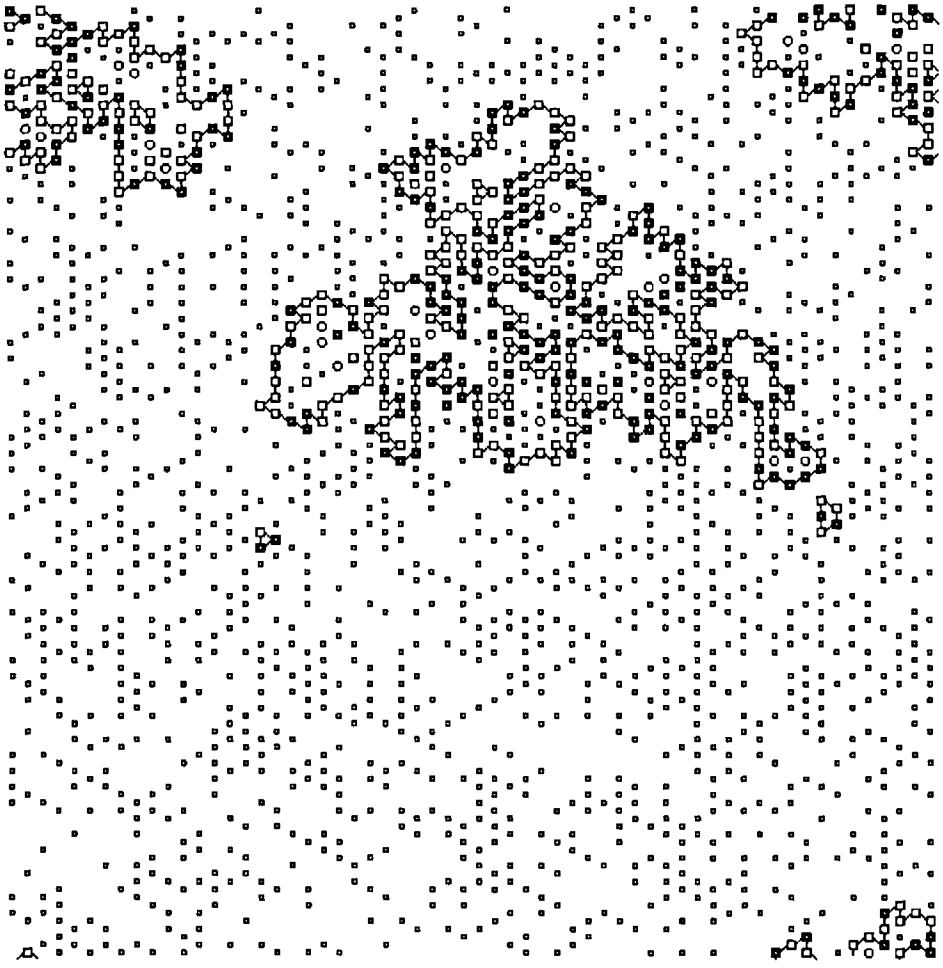

Figure 19 The run displayed in figure 17 at time step 46,290 There are three cells in this world, two of them adjacent to each other in the upper center of the snapshot and the third in the corners All the membranes are rather large and convoluted which is the reason that none of the three cells has divided yet

as shown in figure 21 there are still significant differences between the runs On the other hand it is also apparent from this figure that in several of the runs the membrane number increases in an exponential-like fashion This may seem a little surprising because due to their immobility parent and daughter cell remain adjacent to each other which leads to a colonial growth where cell division is possible in the outermost layer of rings only Because the number of cells in each ring is limited by the diameter of that ring only quadratic growth should be possible However it has to be kept in mind that even in the large world colonies are still so small that they can hardly be said to have separate rings (cf fig 20) Therefore, for the rather small increase from four to eleven membranes, this limiting effect of colonial growth cannot be expected to manifest itself

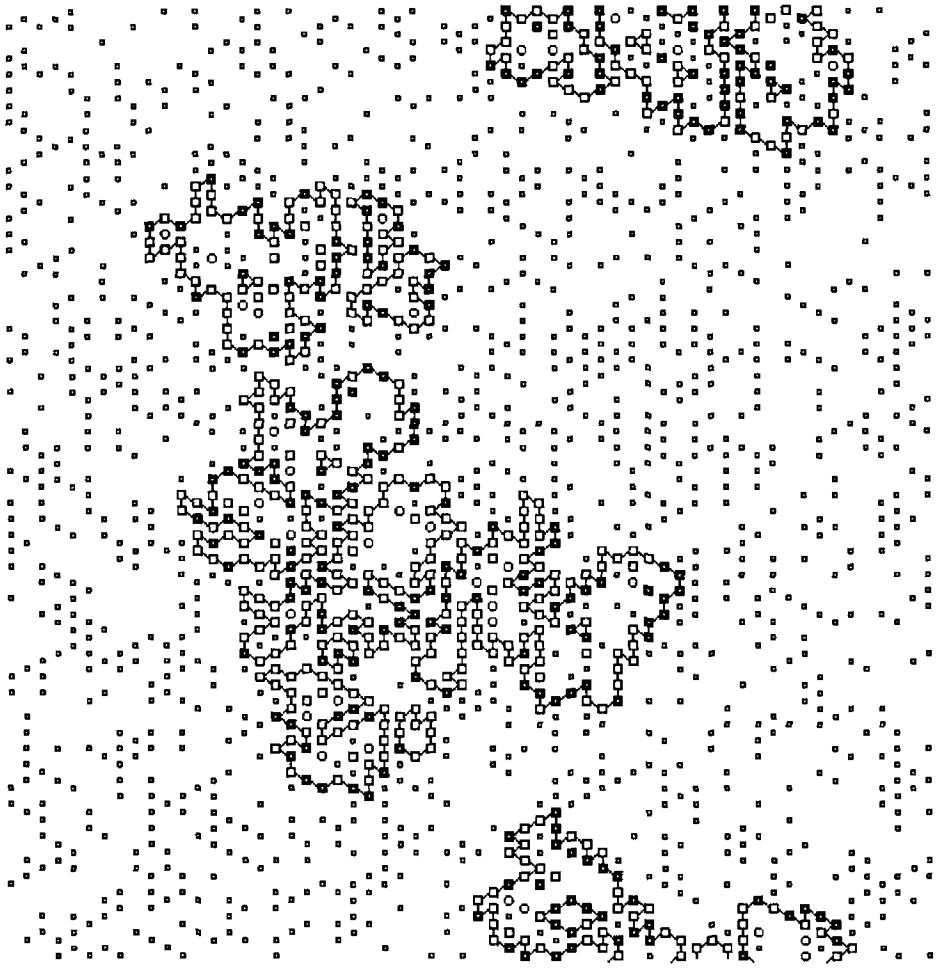

Figure 20 The run displayed in figure 17 at time step 200,000 There are ten cells (13 membranes) in this world, mostly of moderate size Because cells as wholes are immobile, they usually can be found in clusters

5 2 4 Selective displacement and genetic drift

The catalysts in SCL-DIV due to their autocatalytic reproduction are effectively self-replicators Hence they can be used as information carriers for certain simulation parameters that influence the behaviour of catalysts and links Links and catalysts which are produced by a given catalyst then inherit its parameters Thus catalysts can come to act as genomes of the cells This makes it possible to embed cells with different genotypes into the world and investigate whether the resulting phenotypic differences will over time lead to a selective displacement of one of the genotypes

The general possibility of this procedure is demonstrated by an experiment conducted in the large world (cf fig 15) Two of the four cells, the one in the southwest and northeast of the cluster, are initialised with "mutated" cat-

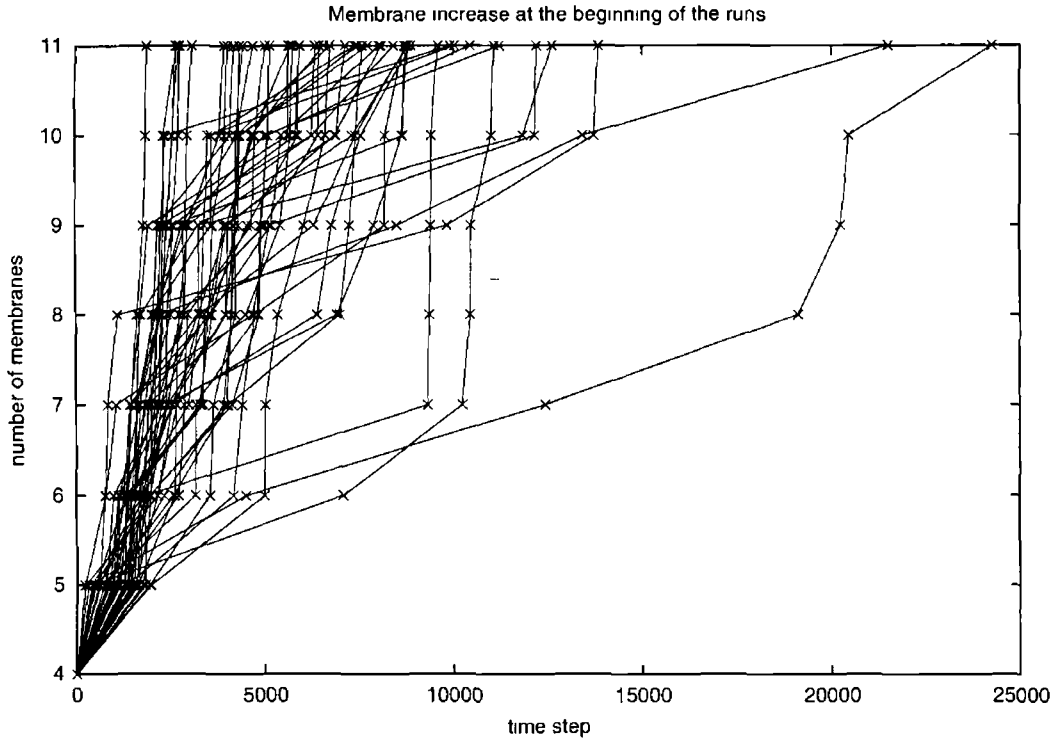

Figure 21 For each of the 49 runs in the large world that reached the limit the time points at which the membrane number successively increases are plotted and connected by lines The last point to in each line is the time point at which for the first time eleven membranes are present in the world Because only the time points at which the membrane number increases are plotted, oscillations in the membrane number are filtered out

alysts that have a reduced `productionProbability` of 0 7 (cf tab 1) In other words, the mutated catalysts have a different allele at the gene locus for `productionProbability` than the normal ones The phenotypic effect of this is that both catalyst and link production are reduced The latter not only entails a slower growth but also a reduced self-maintenance capability because free links are necessary to continuously transfer lifetime units into the membrane The expectation therefore is that, because of the limited resources in the world, the cells with the original parameters will over time outgrow the other ones With constant resources, such a selective displacement would not be possible when the competing populations show quadratic growth (Szathmáry and Maynard Smith 1997, sec 2)

With this setup, 30 runs with differing seeds were conducted in successive intervals of 1,000 time steps After every interval the number of catalysts for

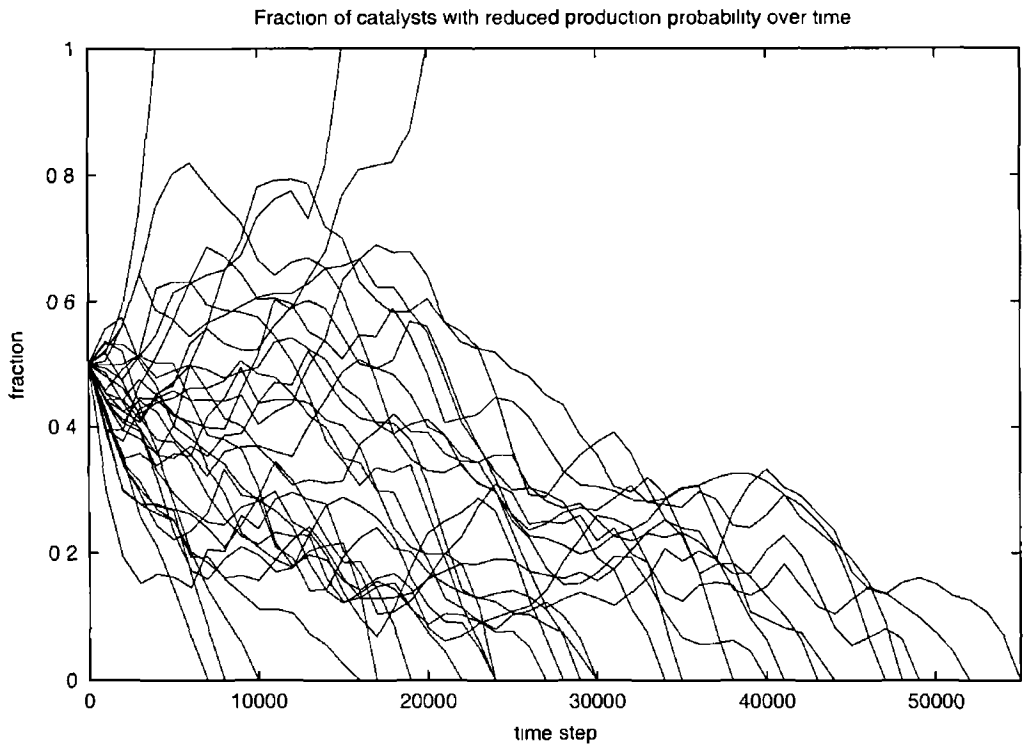

Figure 22 For every run the fraction of catalysts that have a reduced `productionProbability` is calculated after each interval of 1000 time steps Except for the two end points, the floating averages of three adjacent values are plotted and connected by lines

both genotypes is counted and if one of them has dropped to zero the run won't be continued The main result is that only in three of the 30 runs the mutated catalysts displace the original catalysts which consequently "win" the other 27 runs Furthermore it takes no longer than 55,000 time steps in any of the runs until a complete displacement has taken place A more detailed picture of the displacement process can be gained from figures 22 and 23 which show the relative and absolute development of the mutated catalysts First of all it is apparent that the curves show significant fluctuations which can be attributed to genetic drift Nonetheless in the twelve runs that are still undecided after 30,000 time steps the normal catalysts are always in majority which is the result of selection Furthermore, the absolute numbers show that the mutated catalysts multiply and often reach high numbers for prolonged periods of time This indicates that the two mutated seeding cells indeed grow and multiply and not only maintain themselves for a certain time period and then disintegrate

Nonetheless, the results described so far are not completely conclusive because genetic drift in a finite population will sooner or later always lead to the fixation

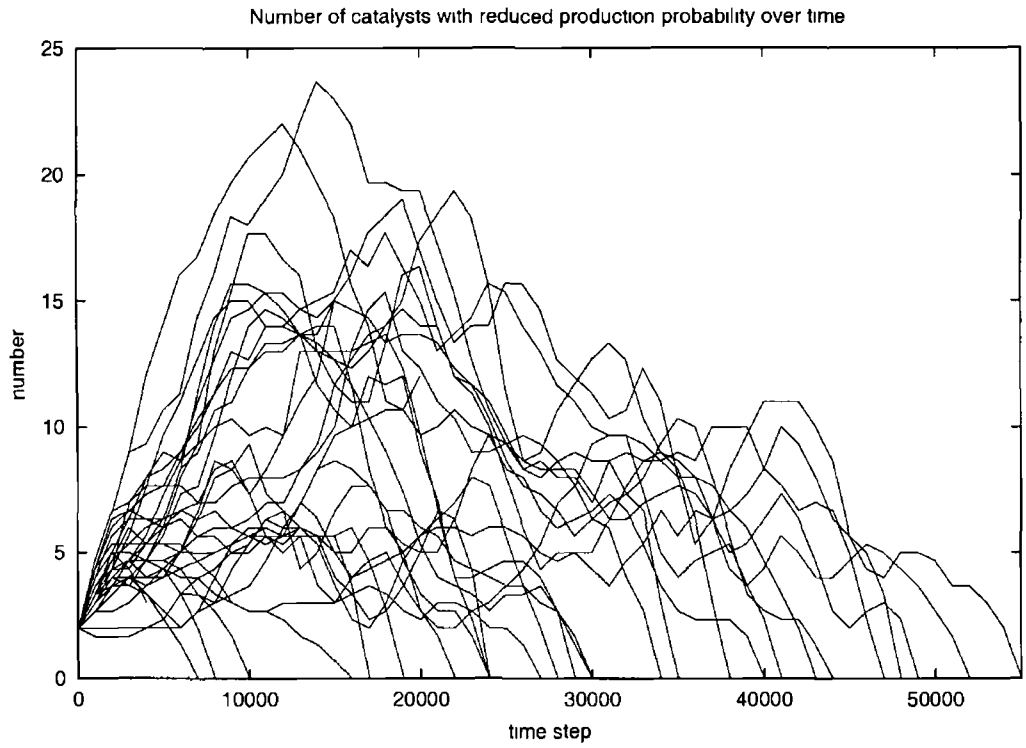

Figure 23 Similar to figure 22, but here the absolute number of catalysts with a reduced `productionProbability` is calculated and averaged every 1000 time steps

of one of the alleles Therefore it is necessary to compare these results with those from an experiment that investigates genetic drift itself This is done with another 30 runs conducted in the same way as above, but the mutated catalysts this time only differ from the original ones with respect to a neutral gene locus The original catalysts carry allele A at this locus while the mutated ones carry allele B Neither allele has any phenotypic effect whatsoever Apart from that, the runs are limited to 150,000 time steps The results of these runs are shown in figure 24 First of all it is apparent that the curves now are more evenly distributed across the range compared to figure 22, which marks the absence of selection Furthermore, until time step 55,000 only eleven runs have been decided, showing that selection leads to a quicker displacement than genetic drift alone After 150,000 time steps a complete displacement has taken place in 26 runs, of which twelve times the mutated allele B succeeds This stands in contrast to the only three runs of the selection experiment "won" by the mutated catalysts Furthermore, those three runs were decided within the first 20,000 time steps, while in the genetic drift case, decisions either way happen during all periods

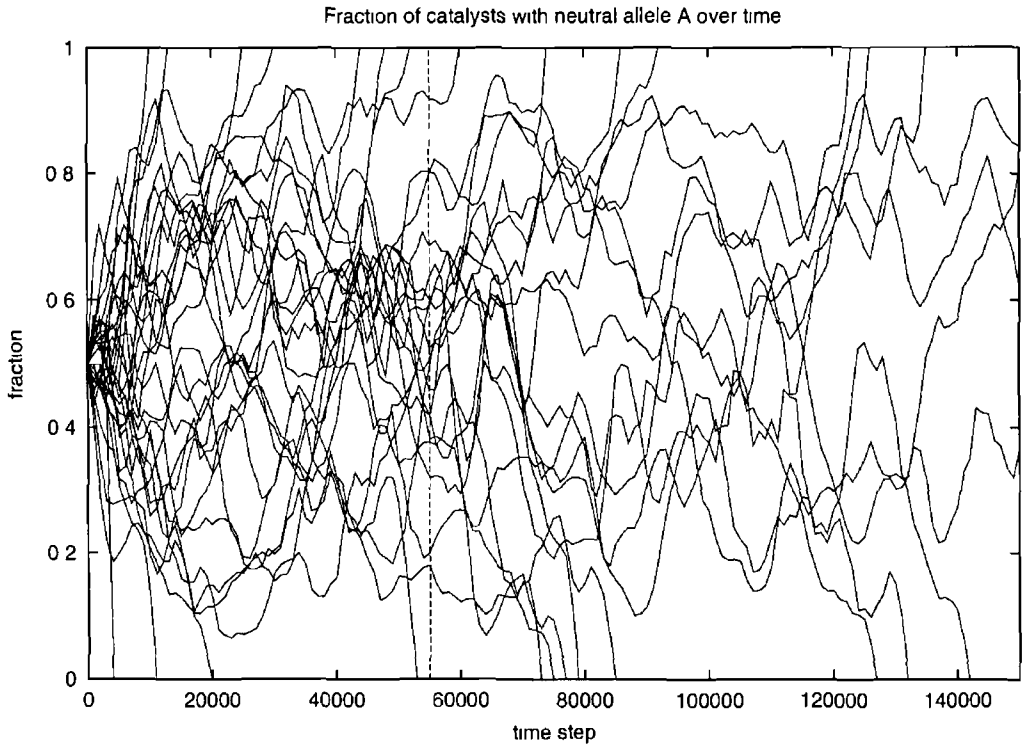

Figure 24 Like figure 22, but here the fraction of one of the two types of catalysts which only differ with respect to a neutral gene locus is calculated and averaged every 1000 time steps The vertical line marks time step 55,000 at which stage all runs in figure 22 had been decided

of the runs This indicates that selection is so strong that a decision towards the cells with a reduced `productionProbability` is only possible if genetic drift in those runs leads to a quick displacement of the original cells Otherwise, reproduction will soon lead to an increase in the number of original cells so that their simultaneous failure becomes unlikely All this shows that even if there was selection present in the genetic drift runs, because some of the seeding cells had some sort of unrecognised heritable (epigenetic) advantage, the force of selection in the runs with the reduced `productionProbability` is significantly stronger

Because this subsection demonstrates selective displacement, an evolutionary process with mutations of the catalysts in SCL-DIV should be possible The situation can then be compared to that of a genetic algorithm, with the difference that in SCL-DIV the fitness function would be implicit while in the former it is explicit But what counts as fit in SCL-DIV is the longevity and fertility of the catalysts which is not necessarily synonymous with the longevity and fertility of cells For instance it would be possible for catalysts to survive in a world more or less evenly filled with clusters and substrate to produce sufficient free links These

would then both provide the clusters with lifetime units to maintain them and indirectly the catalysts and also restore clusters in case of disintegration Although this situation has never occurred as the result of any of the runs conducted so far, it is conceivable that it might occur with a different parameter set

Furthermore, genetic drift is quite significant in the still rather small populations that can be contained in the large world Therefore an even larger world would be advisable to actually conduct an evolutionary run because the fluctuations caused by genetic drift would be smaller in larger populations This of course entails an increased demand for computation time which alone may very well make such an endeavour impracticable with the current implementation of SCL-DIV But since such a run, even if it kept the phenomenology of reproducing cells, would necessarily be a process of limited potential because only existing parameters would be modified and selective displacement has already been demonstrated otherwise, nothing in this direction has been undertaken Therefore the experimental section of this thesis ends here and the next chapter returns to the issues relating to the description of autopoiesis and the original SCL system as well as the other real and simulated model systems

6 Discussion

In this chapter the issues identified in chapter two are investigated further The discussion here is to a large extent based on the issues in chapters two and three which concern the concepts involved in autopoiesis as well as their interpretation and application in the model systems mentioned in this thesis Furthermore the relation between autopoiesis and other concepts of biological organisation is investigated Apart from this, additional considerations concerning the concept of autonomy are presented here as well

6 1 The autopoietic organisation and its boundaries

This section starts with the answer to the question of the uniqueness of the autopoietic organisation raised in section 2 3 1 That the autopoietic organisation is unique can be most easily deduced from Maturana and Varela's (1973) description of evolution

> [H]istory of change in the realization of an *invariant organization* embodied in independent unities sequentially generated through reproductive steps, in which the particular realization of each unity arises as a modification of the preceding one (or ones) which, thus, constitutes both its sequential and historical antecedent (ibid p 136, emphasis added)

Consequently, all living systems only differ in their structure and have the same autopoietic organisation I've already mentioned that this particular organisation is nowhere specified and that it is not even clear what type the relations have that enter its description (cf sec 2 3 1) Having said that, there is a statement in which the autopoietic organisation seems to be indirectly defined

> The autopoietic organization is defined as a unity by a network of productions of components which (i) participate recursively in the same network of productions of components which produced these components and (ii) realize the network of productions as a unity in the space in which the components exist (Varela et al 1974, sec 3)

However, this statement makes some interpretation necessary, because the autopoietic organisation in itself is now taken to be a unity Since otherwise this definition is very similar to the definition of autopoietic system cited on page 14, it is my view that the choice of wording here is misleading, because the organisation is what normally defines a system as a unity (cf sec 2 3 1) and not a

unity in itself I therefore propose that the beginning of this quotation should be changed to this The autopoietic organisation *defines as a unity* a network This change conforms to the usual view taken by Maturana and Varela (1973) that "an autopoietic system is defined as a unity by its autopoietic organization" (ibid p 88, see also p 81) and if it is taken into account, then the statement corresponds closely to the definition of autopoietic system Although this statement doesn't after all help to clarify the autopoietic organisation, it highlights a problem in the definition of autopoietic system which is that even its structure cannot change In the definition on page 14 it is said that the production network is continuously *regenerated* and in the statement above it is the *same* network in which the components recursively participate thereby ruling out any transformations Clearly, in biological cells the network of productions can change over time, for instance when different metabolic pathways are activated Always self-producing the same network would also discount the possibility of evolution In general, since Maturana and Varela (1973) devote a whole chapter of their essay to the diversity of autopoiesis, it is clear that changes of the production relations between the components must be made compatible with autopoiesis

Maybe Maturana and Varela (1973) rather want to convey that the organisation remains unchanged and maybe the network of component production is a synonym for the autopoietic organisation After all, " autopoietic machines are unities whose organization is defined by a *particular* network of processes (relations) of productions of components, the autopoietic network, not by the components themselves or their static relations " (ibid p 79, emphasis added) This entails that the relations which define the autopoietic organisation are in fact production relations Also, " an autopoietic machine is an homeostatic (or rather *relationstatic*) system which has its own organization (defining network of relations) as the fundamental variable which it maintains constant " (ibid p 79, emphasis added) This is the same circularity alluded to in section 2 3 1 which results when the relations that define the autopoietic organisation are the production relations that are the dimensions of autopoietic space However, in the light of the statements cited in this paragraph, this circularity remains obscure because it implies that a system's organisation can enter in the relations between its components Furthermore, " the product of [an autopoietic machine's] operation is [its] own organization " (ibid p 82) Concretely, these statements can be interpreted to say, that interactions between components (e g molecules) have a network of relations as a product This would indeed be a very strange notion of production, and Maturana himself writes in a later article

> The unity of an autopoietic system is the result of the neighbourhood relations and interactions [ ] of its components, and in no way the result of interactions that imply the whole that they produce In other words, nothing takes place in the operation of the autopoietic network with reference to the unity of the network (Maturana 1981, p 23)

Therefore I suggest that the citations taken from Maturana and Varela (1973) in the preceding paragraph should be seen metaphorically So far then, the autopoietic organisation remains obscure amidst a muddle of opaque and convoluted statements It appears to me that the authors have difficulties with their distinction between structure and organisation because all change has been inadvertently ruled out whereas only the organisation is supposed to be invariant This assertion is also corroborated by the fact that in the various definitions of the term "organisation" two variants can be found One variant, to which the definition cited on page 12 belongs only says that some sort of relations must remain constant, while the other variant further requires that these relations must hold between the components of the unity (Maturana 1980a, p xx, Maturana and Varela 1992, p 47) The latter variant implies that the relations which enter the description of the structure and organisation of a unity need not be distinct and an even stronger formulation can be found here

> [T]he relations among components that constitute the organization of a composite unity represent a subset of the relations included in describing its structure (Maturana 1980b, p 48)

Of course the question is now to what other relations, if not to those between the components, the first variant could refer to because it may be just a minor negligence that no reference is made The discussion of a biological cell as an autopoietic system (Maturana and Varela 1973, pp 90-93) contains the answer to this question Here, the authors actually specify what molecules typically embody the three types of production relations (constitution, specificity and order) that are the dimensions of autopoietic space The relations of constitution are established by molecules that determine the the physical neighbourhood of the components, the relations of specificity mainly by nucleic acids and enzymes because of the roles they play in catalysis, and the relations of order by those molecules that control the speed of reactions In this context the autopoietic organisation is taken to be " defined by the *relation of relations* of production " (ibid p 92, emphasis added) and "All the rest - that is, its structure - can vary relations of topology, specificity and order can vary as long as they constitute

a network in autopoietic space" (ibid p 93) These two statements paint a completely different picture of the autopoietic organisation than the ones discussed earlier and it is the current picture that I prefer Firstly, it is now apparent that the relations which constitute the closed domain that defines the autopoietic organisation in autopoietic space have a different type than the production relations which are just the dimensions of that space Secondly and consequently the autopoietic organisation is defined through relations of relations, or, in other words, by *second-order relations* It is clear then that, at least in the case of the autopoietic organisation, the relations that describe it are not a subset of its structure However, it is still not clear which relations concretely define the autopoietic organisation, because it is only required that they define a network in autopoietic space What properties this network must have to be autopoietic is thus still an open question Furthermore, the concept of an autopoietic space with dimensions that are relations seems to be unnecessarily complicated, at least from a mathematical point of view The whole reaction network could just as well be represented by a graph where the nodes are the production relations and the edges show the component interactions that lead to the production of other components The autopoietic organisation would then be a proposition about the connectivity of this graph

The result at this stage is that the autopoietic organisation can't be described using production relations that only belong to the structure of an autopoietic system but that it is instead necessary to talk about second-order relations as the significant relations that define a unity as an autopoietic one These are relations that hold between the relations between the components, and in an autopoietic unity certain second-order relations are kept static because of the operation of the autopoietic unity

An example of such a second-order relation can be found in the list of requirements for collective autocatalysis " it must be the case that every member of the autocatalytic set has at least one of the possible last steps in its formation catalysed by some member of the set " (Kauffman 1993, p 299) This is part of the requirement of catalytic closure and does not say anything specific about any particular production relation that holds between the components Instead, it is a proposition about the collection of the production relations, and this collection can change, as can the components If the principle of catalytic closure is applied in autopoietic space, then the resulting network, assuming it is mathematically represented by a graph, would have to contain one or more circularities For the network of particle transformation in SCL-DIV, this is shown in figure 25

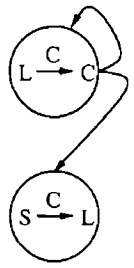

Figure 25 The network of particle transformation in SCL-DIV as a graph The nodes (circles) show the two main production relations where the substrate of the reaction is shown on the left hand side of the arrow and the product on the right hand side Above the arrow is the particle that acts as catalyst of the reaction The edges (arrows which connect nodes) denote catalytic effects The circularity here is due to the autocatalytic production of the catalyst particle and the fact that link particles are the substrate for this reaction is purely circumstantial

Another example that illustrates the relevance of second-order relations are the organisations in AlChemy described by Fontana and Buss (1994), which are characterized by a grammar, algebraic structure and the capability of self-maintenance in the flow reactor Here, the algebraic structure describes *regularities* in the production of lambda expressions (components) upon application (interaction) that ensure closure under collision, which is again *about* production relations But specific production relations themselves don't enter the organisation, although it is necessary to know these relations, which are in fact a subset of the structure, to derive the organisation This can also be seen in figure 1 (p 25) which shows a concrete AlChemy organisation The nodes in this figure are components and not production relations, but it has to be kept in mind that in AlChemy a reaction is generated by the collision of two components alone, without the necessity of some kind of catalyst as in SCL Hence it is sufficient to look at the arrows in this figure to decide whether or not closure is achieved, and this is evidently the case

It is interesting to see how Fontana and Buss (1996) evaluate the relation between their work and autopoiesis

> At minimum, then, our work has converged to a notion similar to that of autopoiesis from an independent angle, quite plausibly, though, we have unwittingly generated a formal interpretation of a heretofore frustratingly elusive notion of considerable importance (ibid sec 3 2)

Indeed, the self-maintaining subsets of organisations in AlChemy are autopoietic and the organisations are, as argued in section 3 3, organisations in the sense of autopoietic theory This means that autopoietic in the context of AlChemy is rather a qualifier applicable to a multitude of organisations than a unique organisation as stipulated by Maturana and Varela (1973) Since their stipulation is founded on an ambiguous concept of autopoietic organisation, it is my opinion that both it and the current definition of autopoiesis should be reconsidered, and that the work of Fontana and Buss (1994, 1996) should be considered as the basis of a revised theory of autopoiesis

The discussion about the relations that describe the autopoietic organisation is also relevant for the consideration of the boundary of an autopoietic unity, an issue already noted in section 2 3 2 In fact, the boundary as some kind of topological barrier, as formulated in the key for autopoietic unities published in (Varela et al 1974), does not exist in this form in (Maturana and Varela 1973) or at least not apparently so On the other hand, the boundaries of the unity are sometimes referred to, but in a rather abstract way "Autopoietic machines are unities because, and only because of their specific autopoietic organization their operations specify their own boundaries in the process of self-production " (ibid p 81) What these boundaries are, is not said, but at least the cell membrane is one of them in the context of biomolecular autopoietic systems (ibid p 91, 109) Whether such a shell-like boundary is a necessity for every autopoietic unity, as it would be according to the identification key, cannot be derived from the statements in (Maturana and Varela 1973) The question then remains, what other kinds of boundaries there are that can delineate an autopoietic unity from its environment Here again it is useful to look at organisations in AlChemy, because they have no shell-like boundary Instead, they endogenously maintain grammatical and functional boundaries which are reflected in their grammar and algebraic structure (Fontana and Buss 1994, sec 8 2 1) Although these boundaries determine whether a given expression is a member of a particular organisation they cannot serve to distinguish different instances of the same organisation Thus these functional boundaries do not allow for self-individuation

Whether Maturana and Varela (1973) in their original essay had functional boundaries in mind that distinguish autopoietic unities from their environment or boundaries that allow for self-individuation remains unclear to me In their view, individuality is seen to stem from the fact that autopoietic unities keep their organisation invariant (ibid p 80) How this can lead to individuality appears particularly obscure to me, because in this context all living systems are

assumed to have the same autopoietic organisation The question is also related to the concept of autopoietic space discussed above, because this opens up the possibility that functional boundaries could be referred to That both types of boundaries are actually considered can be seen in this statement

> Constitutive relations are relations that determine the topology of the autopoietic organization, and hence its physical boundaries (ibid p 91)

Physical boundaries should allow for self-individuation, and the topology of the autopoietic organisation, which I take to be the connectivity between the production relations, specifies a functional boundary in autopoietic space Nonetheless, the mystery only deepens here for me, because it is unclear how a physical boundary (e g a cell membrane) is determined by the connectivity between production relations

In any case, the shell-like boundary as required in the identification key has now widely become accepted as essential for an autopoietic unity (Maturana and Varela 1992, p 46) and thus the whole point has become relatively moot Accordingly, Fontana and Buss (1996) see the situation against this background

> The only claim of Maturana and Varela that is not instantiated in our organizations is their requirement that the system be spatially bounded This is essential for them, for it is the only device by which their "components" may be isolated from the "rest-of-the world" The seeming need for a membrane laid out in space is, in our view, only required because the characterization of autopoietic systems is not built upon a theory of its components (ibid sec 3 2)

How the spatial boundary which is referred to in the quotation has come to manifest itself becomes somewhat clearer in section 6 2 2, and how it is being overemphasised in the field of chemical autopoiesis is criticised in section 6 5 Nonetheless, the spatial boundary is, in my opinion, an important part of autopoiesis that it is necessary to make explicit, because this type of boundary allows self-individuation, which is not possible with the functional boundaries alone The reason that this wasn't done already in (Maturana and Varela 1973) might lie in the domain-independent formulation of the theory of autopoiesis Also, whether the concept of the autopoietic organisation is seen to rely on production relations or second-order relations, it is not clear how to formulate a spatial boundary in terms of such relations alone Only when one considers an autopoietic unity as it

is done in the identification key does it become straightforward to formulate the requirement of a boundary

The last sentence in the quotation above is another criticism of the domain-independent formulation of autopoiesis This formulation only requires that the components which make up autopoietic unities can enter production relations and be transformed in some sort of mechanistic fashion How these mechanics of transformation arise is, unlike in AlChemy where they are determined by the inner structure of the components, left open This leaves the whole theory of autopoiesis underspecified and led to formulations, especially those in connection with the autopoietic space, which are largely unintelligible at least to me Nowadays the domain-independent formulation of autopoiesis appears to play only a role in the undertaking to equate autopoietic with social systems (for criticism of this see Fleischaker 1992 and Mingers 1995, sec 8 2 3) in which spatial boundaries are regarded as dispensable

The necessity of a separation between organisations for further development has also been recognised by Fontana and Buss (1994)

> Note, however, that while [ ] organizations maintain themselves kinetically and constructively, they do not reproduce In no sense can one identify multiple instances of the same [ ] organization in our flow reactor [ ] Reproduction at the new object level requires a means for separating two instances of [an organization] (ibid sec 8 2 1)

Clearly, this self-individuation could be achieved through self-production of a spatial boundary Currently though, there is no notion of space in the lambda-universe of AlChemy and consequently the organisations cannot qualify as autopoietic *entities* because they lack self-individuation

6 2 Autopoiesis and autonomy

Despite the shortcomings of the autopoietic theory discussed in the previous section, the next subsection investigates how the concepts of autopoiesis and autonomy are related according to Maturana and Varela (1973) and Varela et al (1974) Following this, the concept of autonomy developed in Varela (1979) is examined

6 2 1 Autonomy self-maintenance and boundary

Autopoietic entities[6] achieve autonomy, because " they subordinate all changes to the maintenance of their own organization, independently of how profoundly they may otherwise be transformed in the process " (Maturana and Varela 1973, p 80) However, they " do not have inputs or outputs " (ibid p 81) One can view " perturbing independent events as inputs, and the changes of the machine that compensates these perturbations as outputs To do this, however, amounts to treating an autopoietic machine as an allopoietic one " (ibid p 82) The term allopoiesis refers to non-autopoietic systems and connotes that such a system has something else than itself as the product of its operation (ibid p 80) Evidently, the point of view taken by Maturana and Varela here is internalist in the sense presented by Godfrey-Smith (1994, p 318), who sees the whole conception of life as autopoietic in this way The internalist approach regards the processes of a system as controlled by internal constraints and thus resulting from autonomous self-organisation Externalism, in contrast, views the structure of a system as the result of its interactions with the environment

Internalism and externalism don't exclude each other, but rather emphasise different points of view For instance, consider a biological cell that, triggered by a substance in its environment, switches from one metabolic pathway to another The internalist point of view would be that the cell specifies the capability to switch pathways by having some kind of sensor and by having the descriptions for the enzymes of both pathways in its genome In this way, the cell autonomously switches pathways The externalist explanation of this effect would be that the substance in the environment triggered the change of pathways[7] Only both accounts together provide a complete explanation for the observed phenomenon

So far, autopoietic entities are held to be autonomous because their capability of compensating for perturbations (self-maintenance) is only seen from an internalist point of view When taking the externalist approach, one supposedly treats the autopoietic entity as an allopoietic one and the latter are in general regarded to be not autonomous (Maturana and Varela 1973, p 80)

However, the capability of an entity to subordinate changes to the maintenance of its organisation is more a quantitative than a qualitative property

[6] Most citations in this subsection come from a section of (Maturana and Varela 1973) which deals with autopoietic machines I continue to use the term entity because point three of the identification key for autopoietic unities (Varela et al 1974, section 9) requires them to be mechanistic systems

[7] and the capability to do so would be seen as a result of an evolutionary adaptation to the environment

depending on the range of changes it can survive Thus, although self-production lends itself to self-maintenance, any particularly high degree of this capability does not directly follow from the autopoietic organisation alone Concretely, an autopoietic entity with several redundant production pathways can keep its organisation constant under a wider range of perturbations than an entity without redundant production pathways This can for instance be seen in AlChemy organisations where it is possible to half-quantitatively assess the self-repair capability of their structures (self-maintaining subsets in the reactor) Self-repair in AlChemy has to be distinguished from self-maintenance because the latter is a statement about the constructive capabilities of a set of expressions and is only a necessary condition for self-repair (cf sec 3 3 1)

The self-repair capability can now be assessed by investigating the number and size of seeding sets an organisation can maintain in the reactor (Fontana and Buss 1994, sec 6 2 2) A seeding set is basically a subset of the organisation from which the latter can be produced (for an exact definition see ibid sec 5 4), and thus the more seeding sets an organisations contains and the smaller they are, the more robust this organisation will be against perturbations [8] Maybe it is not unreasonable to expect that selective adaptation in a collection of autopoietic entities can lead to an increase in their self-maintenance capability But then this capability cannot be explained in terms of the autopoietic organisation alone

So far it seems that the phenomenon of autonomy remains elusive and that the link to autopoiesis doesn't have much explanatory value Therefore I turn back to the definition of autopoietic organisation and the identification key (cf sec 2 3 2) and investigate the points raised therein as possible sources of autonomy Self-production of the components appears not to be held decisive

> Autocatalytic processes do not constitute autopoietic systems because among other things, they do not determine their topology Their topology is determined by a container that is part of the specification of the system, but which is independent of the operation of autocatalysis [ ] Coupling of independent processes into larger systems is also the rule, these may or may not constitute unities defined by the circumstances of their constitution in a given space, (Maturana and Varela 1973, p 94)

[8] Seeding sets must be capable of producing an organisation under the continuous application of the replacement map After each iteration of the replacement map, the expressions in the set are replaced by those which result from the mutual application of all expressions to each other (including themselves) This is stronger than the random replacement which occurs under flow conditions because unlike in sets, multiple instances of an expression can be present in the reactor Hence not only seeding sets determine the self-repair capability For details see (Fontana and Buss 1994, sec 6 2 2)

A possible illustration of this rather abstract statement would, in my opinion, be the following A collectively autocatalytic network of molecules in a test tube would constitute an entity, because the test tube acts as a boundary However, it is not an autopoietic entity, because the test tube is not produced by the collectively autocatalytic network

The only other reason to call autopoietic entities autonomous is then because they specify their own boundaries (of whatever kind) However, no importance seems to be attributed to the possibility that these boundaries may have important functions (like selective permeability), beyond simply being identifiable Or at least, since Maturana and Varela (1973, chapter II) want to dispense of teleonomic notions, nothing in this direction is explicitly mentioned

Thus, to achieve autonomy by self-producing an *identifiable* boundary alone, appears to be a very restricted notion of this phenomenon Certainly, there must always be some kind of interactions between the boundary and system components of an autopoietic unity Otherwise, the two types of components cannot be said to constitute the unity in one and the same space A similar argument can be made for other elements of the world that are not part of the unity But nowhere do Maturana and Varela (1973) require that the boundary should interact with other elements or components in such a way that autopoiesis is facilitated

Notwithstanding the circumstance that (Maturana and Varela 1973) fails to deliver the promised account of the autonomy of living beings, I assume that self-maintenance of the autopoietic unity and self-production of some kind of boundary are the essential aspects that make it autonomous

6 2 2 Autonomy organisational closure

A rather different take on autonomy in general can be found in (Varela 1979, sec 7 2) First of all, it is stated that a variety of systems are autonomous and hence there are systems which are autonomous but not autopoietic Note, that this was ruled out in (Maturana and Varela 1973) as discussed above The motivation to distinguish between autonomy and autopoiesis comes from the following observation

> the idea of autopoiesis is, by definition, restricted to relations of productions of some kind, and refers to topological boundaries These two conditions are clearly unsatisfactory for other systems exhibiting autonomy (Varela 1979, sec 7 2 3)

Therefore, the following characterisation of autonomous systems is given

> We shall say that autonomous systems are organizationally closed That is, their organization is characterized by processes such that (1) the processes are related as a network, so that they recursively depend on each other in the generation and realization of the processes themselves, and (2) they constitute the system as a unity recognizable in the space (domain) in which the processes exist (Varela 1979, sec 7 2 4)

The closure thesis in (Varela 1979, sec 7 2 5) explicitly states that every autonomous system is organisationally closed However, whether the converse also holds is not made explicit, though in section 7 2 6 Varela says that organisational closure generates a domain of autonomous behaviour Therefore I assume that organisational closure is meant to be a necessary and sufficient condition for autonomy From this it follows that collectively autocatalytic networks can be said to be autonomous and in this specific instance it is the catalytic closure (cf p 67) which fulfills the condition of organisational closure

In general, all autopoietic systems are also autonomous But according to Varela (1979) this autonomy stems from the organisational closure, whereas the self-production of a boundary or the self-maintenance capability in general is not mentioned, although both are arguably a result of organisational closure in an autopoietic unity Again then, the *degree* of a system's self-maintenance capability is independent of organisational closure The self-produced boundary can also be seen as the product of a process participating in organisational closure when the processes are production processes and the boundary is necessary for the organisational closure to hold A self-produced boundary that is not necessary for the organisational closure, and is only a by-product of the processes, is conceivable but would as such be irrelevant to the autonomous (or autopoietic) system in question In summary, the concept of autonomy based on organisational closure is only partly related to the one I derived from autopoiesis in the previous section because it requires no self-produced topological boundary

6 3 SCL, other artificial chemistries and autopoiesis

6 3 1 The original SCL system

Although I have used the term autopoietic entities for cells in the extended SCL system, it needs to be discussed whether these cells really deserve this classification First of all, the question must to be resolved of whether the cells in the

original SCL system qualify as autopoietic entities, because as already indicated in section 2 3, this may not be the case There are two reasons why I hold that it is actually not the case The first is, as already mentioned, that the resulting aggregation after the membrane of a cell ruptures, is not an autopoietic entity It is rather an allopoietic aggregation from which, through the closing of the gap, a *different* cell emerges Thus, the original cell has *not* repaired itself, as would be necessary for the qualification of it as an autopoietic entity, but instead a new one emerges from a previous allopoietic aggregation of components All in all, the cell can neither be said to produce nor to maintain itself As Maturana and Varela put it themselves, " the way the autopoiesis is realized in any given unity may change during its ontogeny, with the sole restriction that this should take place without loss of identity, that is, through *uninterrupted* autopoiesis " (1973, p 98, emphasis added)

The failure of the original SCL cell to exhibit the autopoietic organisation is not merely a side effect of my definition of cell, but stems from the fact that the only possible boundary, in the sense of point four of the identification key (cf p 14), is the closed chain of links with their uninterrupted bonds It is the bonds that are responsible for the interactions between the links in such a way that the latter are constrained to neighbourhood relations in which the bonds are not over-stretched and the membrane is kept closed The argument that an autopoietic entity requires a continuously intact boundary to qualify as such has also been brought forward by Fleischaker (1992)

The second problem with the original SCL system is that the catalyst inside the cell is not produced in any way This poses the question whether the catalyst is to be regarded as a component of the putative autopoietic entity, as has been noted in (McMullin 2000) as well If it does not qualify as a component of the entity, then it would seem to be immediately pointless to talk about self-production or self-maintenance of the entity This possibility is discussed further below, but for now I assume that the catalyst should be regarded as a component In this case, point six of the identification key allows the catalyst as one of " necessary permanent constitutive components in the production of other components " (Varela et al 1974, section 9) This is the exception mentioned in section 2 3, which prevents the combination of points five and six of the identification key It is an exception, if not a contradiction, to the definition of autopoietic unity cited on page 14, which demands that *all* components must be produced through interactions or transformations in which other self-produced components participate, to realise the production network The terms "production", "interaction", "trans-

formation" could be widely interpreted and therefore considered to be vague, but it is obvious that the catalyst in the original SCL system is in no way produced by any kind of process at all and thus cannot qualify as a component without the exception made by point six of the identification key In fact, this exception is not made in (Maturana and Varela 1973), although certain elements, not defined by the autopoietic organisation but necessary for the factual characterisation of components can be taken for granted (ibid p 89) This is different from the exception made in point six of the key, which allows entire components to be taken for granted and not only elements necessary for their factual characterisation Such elements in the metabolism of biological cells would, for example, be the ions, whether dissolved in the cell plasma or bound to molecules, because they cannot be produced by the cell, but are essential for protein folding, signal transduction and other processes These elements can form significant *parts* of components, like in prosthetic groups of enzymes, but can by definition not be components themselves because they cannot be produced by the cell itself

The argument made in the previous paragraph suggests the conclusion that the exception to point six of the identification key was introduced to accommodate the catalyst in the original SCL system To what degree this exception subverts the cited definition of autopoietic organisation is a different question For instance, the mitochondria and plastids of eukaryotes import most of their enzymes from the cytoplasm and produce others themselves Thus, if the exception was allowed, these organelles could be said to be autopoietic, with the possible qualification that they are only partially so [9] But if the one and only component which facilitates the only production process of the "network" is external to it, like in the original SCL cell, then the first requirement of the definition of autopoietic organisation is not only partially but fully violated, because the catalyst as member of the would-be production network is not produced However, it is not entirely correct to say that link production is the only production process because chain elongation would also qualify as one, although as part of a possible autopoietic production network only in so far as an open chain inside an intact cell is concerned But since the open chain as a component is not necessary for the link production process, this doesn't change the situation in any significant way If there was some kind of influence from one of the cell's components that would be necessary during the production step, the situation

[9]However, mitochodria don't synthesize their own membrane lipids which means that they don't have a self-produced boundary and would for this reason not be autopoietic Chloroplasts on the other hand do produce the lipids for their membranes

would be different, but under the current circumstances the cell cannot be called an autopoietic entity

The discussion above has assumed that in original SCL the cell should be considered as the possible autopoietic entity However, when the catalyst is not seen as a component, the situation changes Although the exception in point six of the key seems to imply that the catalyst should have component status, the alternative that the membrane itself is the autopoietic entity must be considered as well Arguably, the diffusion of the substrate through the membrane could be seen as the component interaction that is necessary for the production of links to make them qualify as components too This is possible because the identification key does not require that the interaction from another component has to happen at the time of production Further support for this view comes from the fact that in (Maturana and Varela 1973, p 92) selective permeability has the status of a relation of specificity and can therefore count as a component interaction in a production relation However, if the catalyst is not seen as a component of the entity, then there is no way of distinguishing its interior from the environment and thus it cannot be a unity with respect to the constructivist epistemology in which Maturana and Varela have embedded the theory of autopoiesis But even if one doesn't adopt their philosophy, this whole interpretation where only the membrane is seen as "alive" while the main production process is excluded, would in my opinion be a rather strange view This is why it is proposed in section 2 3 2 that when the substrates of a reaction are non-component elements then there should be some interaction from another component during the production step itself With this modification to the identification key, the rather strange situation here can be ruled out to qualify as autopoiesis

It is therefore my conclusion that the original SCL system does not exhibit any autopoietic entities for two distinct reasons, each of which is alone sufficient to rule out the presence of an autopoietic entity Thus, this model system does not clarify the concept of autopoiesis, but rather obfuscates it The last assertion is exemplified by the interpretation of the results obtained in the APL system, an artificial chemistry similar to SCL but preceding it (Zeleny 1976, 1980) Some of the figures presented in those articles can best be circumscribed using the following quotation

> [The] membrane not only limits the extension of the transformation network that produced its own components but participates in this network If it did not have this spatial arrangement, cell metabolism would disintegrate in a molecular mess that would spread out all over and would

not constitute a discrete unity as a cell (Maturana and Varela 1992, p 46)

The process, which typically leads to the "mess" is embellished by Zeleny (1976) using the following words

> [T]he autopoietic cell keeps renewing itself through a series of oscillations between rupture and closure Its very existence is based on this rhythmical opening and closing We observe that the underlying rules have created a "natural rhythm" of the open system [ ] All living systems, including societies, function through a complex of more or less intricate biorhythms We might preferably talk of *pulsating systems*, since neither permanently closed nor permanently open system are autopoietic, they are nor "alive" (original emphasis)

Needless to say, Zeleny (1976, 1980) does not even notice the problem posed by the permanent catalyst

6 3 2 The SCL-DIV system

After the disappointing conclusion concerning the original SCL system, the immediate question is whether SCL-DIV is any better at exhibiting autopoietic entities Since the mode of self-maintenance is changed, sufficient lifetime units in the membrane are enough to maintain it Links are still turned over because they enter the membrane through the growth mechanism and parts of the membrane split off through the operation of the fission mechanism Despite the turn-over, the membrane remains closed, so that there is always an identifiable boundary that is held together by the bonds between the links Thus, the first problem with the original SCL system is solved

The second problem also does not exist any more, because the autocatalysis reaction now continually produces new catalysts so that they can be viewed as true components of the cell Consequently, the cells in SCL-DIV qualify as autopoietic entities with the added capability of self-reproduction In fact, when the autocatalysis reaction is turned off, as in section 5 1, then the cells lose their status as autopoietic entities because of the second reason explained above But the experiments in section 5 1 were only conducted to assess the new self-maintenance mechanism and the cells exhibited during these runs are not meant to be interpreted as autopoietic entities

There is another noteworthy difference between the original and the extended SCL system concerning the status of the membrane as a whole Displace-growth

in SCL-DIV allows a closed chain to grow, while in the original SCL system only the addition of links to the ends of open chains is possible In fact, displacement-growth can be seen to mimic the self-assembly process of real-world micelles and vesicles This can be interpreted to fulfill a production relation which allows the membrane in the extended SCL system as a whole to qualify as a component of the autopoietic entity The fact that the boundary produces itself strengthens the case of self-production because now not only its components are produced but the whole boundary is as well In such a situation self-reproduction follows almost automatically Only when the entity replaces the exact amount of boundary components that it loses would it be able to maintain itself without reproduction When more boundary components are produced, the result is either explosion or self-reproduction, when too few boundary components are produced, the result is implosion Thus, although self-reproduction is logically secondary to the establishment of the entity itself, it is difficult to see, at least for protocellular biochemical systems, how autopoiesis without self-reproduction should be realised This is also underlined by the experiments with self-reproducing micelles described in section 3 1

6 3 3 Other artificial chemistries

Lastly I examine the artificial chemistries described in chapter three The more abstract ones (Fontana and Buss 1994, di Fenizio 2000) cannot exhibit autopoietic entities, because in both cases the processes are assumed to be taking place in virtual universes without a notion of space so that the emerging organisations cannot have individuality

At first sight, production processes are absent from the system which investigates the self-assembly of micelles in continuous space (Edwards and Peng 1998) However, the insertion of phospholipids into a micelle can be interpreted as a production process where the product is the micelle membrane as a whole But because the phospholipids themselves are not produced by the micelle, they cannot qualify as components Since according to point five of the identification key for autopoiesis (cf p 14) the membrane would have to be constituted by components, these micelles are not autopoietic

In contrast, the proto-cells described in (Ono and Ikegami 1999) clearly are autopoietic entities In this model system, as noted in section 3 2 1, there are particles which have similar functions as the SCL-DIV particles To recapitulate the production network AA catalyses the production of M and also autocat-

alytically produces more AA Thus, the relation between AA and M is the same as that of catalyst and link in SCL-DIV Consequently, AA and M are components of the production network in the sense required by point five and six of the identification key The main difference is that AA and M are produced from the same substrate (X) whereas in SCL-DIV catalysts and links are produced from different ones The M particles constitute the boundaries without explicit bonds like in SCL Instead, preferential neighbourhood relations are the result of the interacting potentials of the particles at different lattice positions, which satisfies point four of the key for autopoietic entities

The LMA micelles exhibited in the model system described in (Mayer and Rasmussen 1998) appear to be autopoietic too, but the situation is more complicated than that because the (amphiphilic) molecules which make up the micelle don't decay Thus, although the micelles produce themselves and also multiply, once a micelle is formed, there is no need for its self-maintenance The production process, which is catalysed by the surface of the micelle, continually makes more surfactant molecules available which then insert themselves, mediated by the different simulated forces, into the micelle This happens until the micelle has become so large that it spontaneously splits into two smaller ones Once the supply of substrates (the hydrophobic polymers) is depleted, the number of micelles remains constant When this has happened, all production processes cease and the notion of autopoiesis seems not applicable any more

However, all this raises the question of whether the self-maintenance of an autopoietic unity is necessary to meet the definitions of autopoiesis (cf p 14 and 64) or if self-reproduction alone is sufficient Another way to put this question is whether autopoiesis requires that the lifetime of the unity is significantly longer than the lifetime of at least some of its components But as argued in section 6 1, the definitions of autopoiesis are problematic because they imply that the same production relations are always maintained Furthermore, the complication that arises with self-reproduction when several unities are the product of the operation of one unity is neither handled by these definitions nor by the identification key (cf p 14) In contrast to the definitions, the key makes no mention of any kind of recurring production processes and self-production of the components is sufficient for autopoiesis Hence with the key alone self-maintenance of components cannot be seen as a necessary condition for autopoiesis When a component disintegrates the whole unity might very well disintegrate and lose its organisation, but as long as the components last, the unity would be autopoietic when those components were self-produced in the first place

Nonetheless, the definitions of autopoiesis refer to recurring production processes which on the face of it implies the necessity of self-maintenance But I would argue that self-reproduction would just as well be a recurring production process which satisfies the definitions The following definition of self-reproduction is given in (Maturana and Varela 1973)

> a unity produces another with a similar[10] organization to its own, through a process that is coupled to the process of its own specifications Only autopoietic systems can self-reproduce (ibid p 137f)

This definition is somewhat problematic because it implies a distinction between the daughter cells where one is the continuation of the parent and the other a side product of the operation of the parent When one considers for instance the division of a bacterium such a distinction certainly doesn't make sense One situation where such a distinction is possible, is between stem cells and their offspring in multi-cellular organisms, but in general it is not a defining feature of self-reproduction But to return to the question at hand, this definition makes clear that self-reproduction qualifies as a production process After all, the components that constitute the offspring directly after division are the ones produced by the parent and not (yet) those that are self-produced This situation has to be taken properly into account and consequently modifies the sense in which self-production has to be understood Hence the recurring production of components for the purpose of self-reproduction would indeed fulfill the requirements set by the definitions of autopoiesis without the self-maintenance of the components as a necessity

Therefore it is my conclusion that the LMA micelles are autopoietic The circumstance that the number of self-reproduction steps is limited due to a limited supply of substrate is of no consequence because this is a situation similar for example to the reproduction of bacteria in a test tube Just because the test tube has a limited supply of nutrients and thus sets bounds to the number of bacteria that can exist wouldn't allow for the conclusion that those bacteria are not alive And just as a population of bacteria in a flow reactor, with constant influx of nutrients and efflux of waste products and bacteria, would exhibit ongoing self-reproduction, the same would result for the LMA micelles if corresponding flow conditions were implemented in this artificial chemistry

[10]This of course implies the possibility of a variety of organisations while in their definition of evolution (cited on page 64) the organisation is assumed to remain invariant

6 4 Artificial chemistries and autonomy

6 4 1 Criteria for autonomy

Since Maturana and Varela (1973) and Varela (1979) already have developed two somewhat different concepts of autonomy, it appears to be a better approach to view autonomy not as an all-or-nothing property but instead to compile a list of criteria with which to judge a system's *degree* of autonomy This approach is taken in (Boden 1995) where the author has put together three aspects that are commonly used by Artificial Life researchers to evaluate the degree of autonomy of a system For as Boden puts it "Autonomy is not an all-or-nothing property It has several dimensions, and many gradations" (1995, p 102) The three aspects are about the way in which a system *controls* its behaviour (Boden 1996, p 10)

1 The extent to which response to the environment is direct (determined only by the present state of the external world) or indirect (mediated by internal mechanisms partly dependent on the system's previous history)

2 The extent to which the controlling mechanisms were self-generated (emergent) rather than externally imposed (implicit in the component properties)

3 The extent to which internal directing mechanisms can be reflected upon, and/or selectively modified

All aspects refer to processes occurring in the system and it can thus be investigated how these relate to the processes exhibited in artificial chemistries However, aspects two and three imply that there exist a variety of processes from which specific ones can be selected by the entities Such a variety can arise through different concatenations of the elementary interactions and/or through a variety of particles when the elementary interactions are dependent on the inner structure of a particle The latter situation is exemplified by the more abstract artificial chemistries (cf sec 3 3) and the former by the more concrete ones (cf sec 3 2)

However, aspect three mainly concerns either evolution, and would then be meaningful for a collection of different systems (entities) only, or the autonomy of the (human) mind Neither are substantially different entities present *together* in any of the artificial chemistries discussed in this thesis nor are they concerned with the (human) mind Thus, aspect three is not relevant for the following discussion The two remaining aspects of autonomy are used together with the three

criteria derived from sections 6 2 1 (self-maintenance, self-produced boundary) and 6 2 2 (organisational closure) in the following section to evaluate the degree of autonomy exhibited by the entities in the different artificial chemistries

6 4 2 Entities in artificial chemistries and their degree of autonomy

Because the cells in the extended SCL system qualify as autopoietic and fulfill the three criteria for autonomy (self-produced boundary through link production, self-maintenance by transfer of lifetime units, organisational closure through collective autocatalysis), they should appear to behave autonomously However, the first aspect from the list above doesn't look very promising when trying to assess the degree of autonomy, because nothing in an SCL-DIV cell is explicitly used as some kind of memory of previous time steps But since cells can take on different shapes, maybe there is some kind of implicit memory For instance, when a cell is embedded in a world with relatively few substrates (because there are many other cells), it usually grows large without dividing The reason for this is that free links are only rarely produced in the cell and chances are low that three such links are available at the same time to bond and form a cluster Instead, the free links continually contribute to a (slow) membrane growth If substrate remains rare, then the cell is likely to break open, with possibly destructive effects on other cells as described in section 5 2 2 When substrate becomes abundant again, the cell may divide more or less quickly depending on the geometric configuration of its membrane Although the shape of the membrane, which can be partly attributed to the availability of substrates in the past, influences the future development of the cell, this is merely an influence and cannot be interpreted as a control process Other kinds of implicit memory don't present themselves, but there might be some I haven't recognised as such

In the other more concrete artificial chemistries, no explicit memory structures are available either and the phenomena observed don't seem to lend themselves for implicit memory structures that, in a meaningful sense, can be said to exert some kind of behavioural control However, for a proper evaluation of a possible implicit memory in the interactions, insufficient data is available, so again there might be something I have overlooked Only in the more abstract artificial chemistries do the types of components (expressions), change over time so that an entity's response to a perturbation depends on the development it has undergone so far Since AlChemy (Fontana and Buss 1994) is described in much more detail than the modified version in (di Fenizio 2000), only the former is discussed here,

although all arguments probably apply to the latter as well because of the close relation between the two

As observed in (Fontana and Buss 1994, sec 6 2 6), once a self-maintaining subset of an organisation has established itself in the reactor, it will move towards the "center" of that organisation and contain it from that point on The center is the smallest self-maintaining subset of an organisation and its continuous presence can be seen as an explicit memory of the organisation because the expressions in the center alone are sufficient to specify the construction of the organisation Since collisions among the expressions of the center regenerate it, its presence ensures its persistence Thus, the center controls its own presence whereas the other expressions can more easily change within the boundary specified by the grammar of the organisation

This leaves only the second aspect as an indicator of autonomy for the more concrete artificial chemistries The controlling mechanisms in SCL-DIV are the ones that are already present in the particle interactions but concatenated in such a way that the cell keeps its organisation However, the same concatenation of interactions can maintain an aggregation of open chains and catalysts confined by loops in the chains or overlapping ends (cf fig 13, p 50) As described in section 5 2, from such an aggregation cells can emerge again and most of the time cells are present This seemingly emergent preference for cells, though, derives from the fact that closed chains are more stable than open ones The reason for this is that the ends of open chains are subject to spontaneous disintegration, whereas in a closed chain no link is Therefore the degree of autonomy exhibited by SCL-DIV cells is somewhat lower than that of the proto-cells described in (Ono and Ikegami 1999) and the LMA micelles described in (Mayer and Rasmussen 1998) because both emerge in a stronger sense of this word The reason for this is that the stability of these emergent structures results from the elementary interactions less directly than in SCL-DIV Furthermore, the production rule for the LMA micelles is emergent because it is a property of its surface, whereas for the proto-cells and SCL-DIV the production rules are already present as particle properties But because the LMA micelles do not (need to) maintain themselves, there is no clear winner between them and the cell-like structures

Given the generality of the artificial chemistry that exhibits the LMA micelles, it appears certainly possible to add a decay process for the surfactants With such a decay process, the production of surfactant molecules would automatically qualify as a self-maintenance process, because without continuous production the micelle would not only be unable to divide, it would also disintegrate Without

the continuous influx of new substrates (and some sort of efflux), all micelles would eventually disintegrate The degree of autonomy for the micelles would then be the highest among the more concrete artificial chemistries The degree of autonomy is lowest for the micelles in (Edwards and Peng 1998) because they neither (need to) maintain themselves nor produce the surfactant they are made of

In summary, among the more concrete artificial chemistries, SCL-DIV only takes the third place with respect to autonomy This leaves AlChemy (Fontana and Buss 1994) as representative of the two more abstract artificial chemistries to be assessed It is my opinion that the self-maintaining subsets of organisations exhibited in AlChemy show a higher degree of autonomy than any of the entities from the more concrete artificial chemistries evaluated so far First of all, AlChemy rates higher under aspect one because of the emergent memory in the form of a center as discussed above With respect to the second aspect, it rates at least as high because the constructive capabilities of the expressions have to be assessed with respect to the organisation in which they occur Once an organisation has emerged, it provides the context for the collisions between expressions These constructive capabilities can be compared to the catalytic capabilities in the more concrete artificial chemistries With the exception of the micelle surface in (Mayer and Rasmussen 1998), none of the catalytic capabilities are emergent

Despite the lack of a self-produced boundary, which prevents their coexistence in the same reactor, these self-maintaining subsets of organisations are organisationally closed sets of expressions The organisation that actually emerges during a run thereby depends only on the initial expressions, the sequence of collisions during a run and the boundary conditions implicit in the normalization process Thus, each organisation has a unique identity and its organisational closure ensures that this identity is maintained The point is that such a unique identity emerges in a world where a wide variety of identities is possible Only then can an organisationally closed system be called truly autonomous because if it did not maintain itself, a change of identity would be the result In the more concrete artificial chemistries, a change of identity is not possible, only the loss of it through disintegration A self-produced boundary would be a natural step to allow different organisations to self-reproduce and coexist Together with heritable variation, an evolutionary process should result, from which organisations with an increased capability of self-maintenance probably would emerge

In conclusion, just to exhibit the autopoietic organisation does not lead to the exhibition of a high degree of autonomy, but organisational closure does indeed

artificial chemistry criterion	SCL-DIV	LMA micelles	proto-cells	micelles in continuous space	AlChemy
organisational closure	+	+	+	-	+
self-maintenance		-		-	
self-produced boundary			+	-	-
emergent production rules	-	+	-	-	+
emergent entity		+ +	++	++	++
explicit memory	-	-	-	-	+

Table 4 Comparison of the different artificial chemistries with respect to the degree in which the entities exhibited by them fulfill the criteria for autonomy The first three criteria are derived from the discussion in section 6 2 Criteria four and five are related to aspect two of the list on page 83 whereas the last criterion is related to the first aspect of the same list

lay the seed for the latter With self-reproduction of autopoietic entities and heritable variation this seed will probably germinate, but whether this is the only way to achieve autonomy is a different question, which is not addressed here Table 4 summarizes the aspects and criteria of autonomy discussed and to what degree they are present in the different artificial chemistries

6 5 Chemical autopoiesis

The approach that Maturana and Varela have taken in developing their theory of autopoiesis has been described by Fleischaker (1988) in the following way

> they start with autopoietic organization as given and locate the living as physical within that organization (ibid p 42)

In sections 6 2 1 and 6 3 1 it became clear that this approach has so far only led to an opaque theory in which even its authors seem unable to find their way around Model systems like SCL, which are motivated by this theory alone, have at best metaphorical value with respect to this theory but are irrelevant to any other field of research The reason for the latter assertion is that the autopoietic theory *in its domain-independent conception* without a theory of its components is severely underspecified Consequently, in what domain one investigates the concept of autopoiesis is entirely arbitrary and model systems like SCL can be criticised on this ground

> If artificial life exists in a computer, the computer milieu must define an artificial physics This must be done explicitly or it will occur by default

> to the program and hardware What is an artificial physics or physics-as-it-might-be? Without principled restrictions this question will not inform philosophy or physics, and will only lead to disputes over nothing more than matters of taste in computational architectures and science fiction (Pattee 1995a, sec 4)

Therefore it seems prudent to also pursue the converse approach and to take real living beings as given and examine if they are autopoietic and elaborate the theory so that at least for biological cells it should be made clear what exactly qualifies as a component and what kinds of processes qualify as production processes A step in this direction has already been taken by Fleischaker (1988) by providing amended criteria of autopoiesis, restricting the concept to the physical domain Only when the usefulness of autopoiesis for the description of living systems can be established, should it be investigated whether this concept can be generalized

Continuing the branch in autopoietic theory initiated by Fleischaker (1988, 1990) leads to the field of chemical autopoiesis (Luisi and Varela 1989[11], Luisi 1993), with the aim to construct minimal living proto-cells in the laboratory guided by autopoiesis as an operational definition of life Clearly, it is necessary to have a definition of life when one attempts to construct new life forms But the choice of autopoiesis, especially when one is looking for intellectual clarity in order to ask consistent experimental questions (Luisi 1993, p 8), is somewhat precarious, given the considerable amount of ambiguity inherent in this particular theory Granted, the micelles described in section 3 1 qualify as self-reproducing autopoietic entities, but the concept of autopoiesis has been reduced to that of a self-bounded entity without taking organisational closure properly into account This can be clearly seen in the following citation, which is part of the discussion of a minimal chemical autopoietic entity

> A *minimal* autopoietic system would require a boundary composed by at least one component, C, it will be characterized by only one entering

[11]The title of this article shows that even Varela isn't faithful to the terminology of his autopoietic theory In the title the micelles are said to be self-replicating, but according to (Maturana and Varela 1973, p 100 f) replication denotes a situation where one unity produces other unities different from itself Since the micelles are autopoietic they should be said to self-reproduce, something that only autopoietic unities are assumed to be capable of (cf p 82 in this thesis) This term is then actually used in the abstract of the article and I use it too when referring to the micellar systems However, the term self-replication has by now firmly established itself in further articles (Bachmann et al 1991, Bachmann, Luisi and Lang 1992, Luisi 1993) This seems to me particularly unfortunate because with replication often the template replication process of nucleic acids is associated, which is clearly different from the reproduction process the micelles undergo

> metabolite, A, and by two unimolecular reactions, a self-generation reaction leading to C (at the expense of A), and a decomposition reaction which transform C into a product P, which then goes out of the boundary. These chemical reactions are determined by the bounded unit, i.e., the transformations of A into C and of C into P take place only inside the boundary, we will assume that such spontaneous reactions are chemically irreversible (i.e., we can neglect the back-reactions). (Luisi 1993, p. 9, original emphasis)

What is missing here is the requirement that the production of C must be facilitated by *interactions* with other components of the entity, as required by point five of the identification key for autopoietic entities, so that organisational closure is achieved. Spatial determination, i.e. confinement of the reactions to the entity's interior is here only necessary, but not sufficient to achieve organisational closure.

Nonetheless, the self-reproducing micelles described in (Bachmann et al. 1991) are indeed autopoietic because the required interactions from other components are present. In all these systems, the production of surfactant takes place at the micellar interface between the organic and aqueous phase and is therefore facilitated by the other surfactant molecules of the entity. How this facilitation works can be seen in (Bachmann et al. 1991, fig. 1). The substrate, from which the surfactant is produced, is aligned in the micellar membrane through interactions with the surfactant molecules in such a way that it can either be hydrolised with the help of a catalyst inside the micelle (system III) or oxidised by permangenate in the aqueous phase (system IIA/B). The fact that in system III the catalyst is not produced by the system does not matter, because, unlike in the original SCL system, interactions with other system components during the production step are given through the process described above. Therefore the catalyst in system III has a status similar to that of an essential co-enzyme in a biological cell. All these systems also comply with my guiding metaphor which involves collective autocatalysis, because the facilitation of hydrolysis/oxidation at the micellar interface can be seen as a catalytic effect (Bachmann et al. 1991, Bachmann, Luisi and Lang 1992). In fact, it is an instance of autocatalysis because the surfactants in the membrane catalyse their own production.

All in all, despite not having captured the aspect of organisational closure correctly in the theoretic foundations, chemical autopoietic entities can be demonstrated in the laboratory. The problems arise when the step from micelles to vesicles is taken. Membranes of vesicles consist of two layers so that there is,

for example, an aqueous phase inside and outside the vesicle and a hydrophobic one inside the membrane between its two layers Thus the production does not necessarily take place in the membrane any more

> The basic idea is to construct lecithin liposomes which host the synthesis of lecithin To accomplish that, the four enzymes which catalyze the so-called salvage synthesis of lecithin are bound to such lecithin liposomes (Luisi 1993, p 17)

In such a vesicle, production would take place in the aqueous phase inside without interaction from other system components during the production step This yields a situation similar to that in the original SCL system and such a vesicle would not be autopoietic, as has been claimed in (Wick and Luisi 1996)

At first sight, it seems obvious that the autopoietic micelles have individuality because of their very nature, and consequently conform to my guiding metaphor But this statement needs some further consideration as far as the aspect of self-individuation is concerned The complication arises because micelles continuously coalesce and divide exchanging their components and contents (Luisi and Varela 1989, p 636) How this complicates the situation can best be seen in the light of a heuristic test for autopoiesis suggested in (McMullin 2000, sec 5), which proceeds as follows Two collectively autocatalytic networks of the same organisation which have been prepared separately are brought into contact with each other If the two reaction networks coexist as two distinct instances, they can be said to be autopoietic Applied to the micelles this test would classify them as not autopoietic However, it has to be kept in mind that the test was suggested to be merely heuristic and not definitive Furthermore, this test would fail to recognise gametes of biological organisms as autopoietic because they fuse with one another as part of their operation One might object here that in sexual reproduction the two gametes have different organisations, male and female However, there are many cases of sexual reproduction without morphologically distinct types of gametes This so-called isogamy does for example occur in many species of single-celled green algae Although even isogametes are usually differentiated physiologically into distinct types, which can be regarded as pseudo-sexes, there are species without such an incompatibility system This is the case of autogamy which together with isogamy is characterised by indistinguishable gametes Therefore, the heuristic test suggested by McMullin (2000) seems only to yield a definite answer when the two reaction networks coexist, while when they fuse the situation has to be regarded as undecidable with this test alone Since the

self-reproducing micelles otherwise fulfill the six points of the key for autopoiesis they should be regarded as autopoietic entities

All this of course has wider implications for the theory of autopoiesis as well While the division of autopoietic unities is at least addressed to some extent in the theory of autopoiesis, although not properly dealt with in detail (cf sec 6 3 3), the possibility of their fusion and the consequences thereof are left unconsidered so far However I won't pursue this thread any further here and instead consider one final aspect concerning autonomy not mentioned yet which concerns the energetic autonomy (Moreno and Ruiz-Mirazo 1999) of living organisms What this exactly means can be understood when a solution of micelles is compared with a solution of bacteria in a test tube The difference between the two *solutions* is that the one with the micelles is thermodynamically stable (Luisi and Varela 1989, p 636) while the one with the bacteria is thermodynamically unstable It is well known that living organisms exist in a state far away from the thermodynamic equilibrium and maintain this state with a complex network of energy flows as well as the temporary storage of chemical energy (e g in the bonds of ATP) Thus the transition of a solution of bacteria towards the thermodynamic equilibrium would entail the disintegration of the components which make up those bacteria and consequently their death This disintegration would proceed by hydrolysis of the components (proteins, polysaccharids, lipids etc) into their constituents (amino acids, sugars, fatty acids, glycerol etc)

This energetic autonomy is not yet present in any of the simulated and real model system discussed in this thesis Whether this type of autonomy is essential for a system to qualify as living, as argued in (Moreno and Ruiz-Mirazo 1999), is a different question Computer simulations clearly can't *realise* this type of autonomy because the electrical energy which is "consumed" when a program is executed does not lead to the production or maintenance of any of the components a computer is made of In the light of this the hypothesis that computer simulations could be alive, as maintained by the computationalist program of strong Artificial Life, would clearly be wrong But since there is no universally accepted definition of life (cf sec 1 2), this question is open to debate However, I feel that a definition of life should make as strong requirements as possible with the currently known life forms Nonetheless the search for and construction (whether material or as computer programs) of "new" life forms should continue, because the results gained thereby are necessary to advance the debate over the definition of life

7 Conclusion

The organisation of this thesis does not entirely reflect the chronological order in which the work on which it is based was carried out At first, the extended SCL model was developed while taking it for granted that the original model already displayed autopoietic entities Of course the problems with the interpretation of the original model, as mainly discussed in section 6 3 1, soon became apparent, but they were not resolved The working hypothesis at this stage was that because the two authors of autopoiesis, Maturana and Varela, (co–)developed this model as an explicit illustration of their theory, it would certainly display autopoietic entities notwithstanding any difficulties with its interpretation But then the extended SCL model led to the insight that with autopoiesis as sole guiding principle it is perfectly possible to construct a completely contrived artificial chemistry that neither offers physical or chemical realism, as present in Mayer and Rasmussen's (1998) artificial chemistry, nor shows the emergence of a (collectively) autocatalytic network from a wide variety of possible reactions, like the more abstract artificial chemistries described in section 3 3 do The reaction network that is exhibited is, in fact, the only possible one Furthermore, the cells in SCL-DIV show a lower degree of autonomy than the entities in most of the other artificial chemistries as discussed in section 6 4 To make things worse, most of these artificial chemistries also exhibit autopoietic entities despite the fact that none of them were directly motivated by autopoiesis This result together with the fact that one of the central motivations of autopoiesis is to explain the autonomy of living beings (cf sec 1 3) led to doubts whether this theory has much explanatory value

At the same time the review of other literature, especially that on collective autocatalysis (Kauffman 1993) and organisation in AlChemy (Fontana and Buss 1994, 1996), led me to the conclusion that both these concepts and that of autopoiesis all represent a similar idea Furthermore, the former two concepts are in my opinion explained more rigorously and clearly, while autopoiesis seems more opaque (Mingers 1995, p ix) and elusive (Fontana and Buss 1996, sec 3 2) This led to the use of collective autocatalysis plus spatial self-individuation, with the latter derived from the identification key for autopoietic unities, as the guiding metaphor for the further theoretical investigation of autopoiesis Although this metaphor most likely contains stronger requirements than those made for autopoiesis, it is argued that systems characterised by this metaphor are autopoietic (cf secs 2 1 and 2 3 2) With the help of this metaphor and the formaliza-

tions of collective autocatalysis and AlChemy, the key concepts of autopoiesis are investigated in section 6 1 and found to be flawed and ambiguous in several places

This does not mean though that these shortcomings cannot be addressed and resolved, but this would raise the question of whether it is really desirable to propose yet another variant of autopoiesis Since the theory of collective autocatalytic networks is available and an interpretation of autopoiesis is possible which renders its concepts almost indistinguishable from those in AlChemy, it seems preferable to continue research into the definition and origin of life with these two theories The usefulness of both theories is evident in section 6 1 where they are applied for the interpretation of the theory of autopoiesis In particular, the concept of organisation in AlChemy seems particularly apt to fill the gap that is left in the theory of autopoiesis due to the fact that the autopoietic organisation is nowhere specified Furthermore, less than clear notions like "autopoietic space" can, at least to some extent, be penetrated

Unlike autopoiesis, both the theory of organisation in AlChemy and that of collective autocatalysis do not exist in a multidude of variants but are instead comparatively concise Indeed, autopoiesis is by now a highly controversial theory which for example can be seen in the forum discussion in the International Journal of General Systems, volume 21 (1992) or by my own criticism of chemical autopoiesis in section 6 5 Worse still, the mentioned forum discussion reveals that some variants of autopoiesis currently in existence are already incommensurable with each other which can easily lead to misunderstandings between the proponents of the different variants generating additional confusion This latter point can readily be seen when one looks at the requirement that autopoietic entities should have some sort of spatial boundary In the field of chemical autopoiesis (cf sec 6 5) this feature is currently regarded as central while when one tries to apply autopoiesis to social systems such spatial boundaries are obviously absent In order not become too much entangled in the different variants of autopoiesis I suggest that in those areas dealing with life-as-we-know-it or simulations thereof instead the concepts of AlChemy and collective autocatalysis should be preferred Both of them are well-defined and although they do not explicitly require spatial self-individuation of their entities, this further demand that is now present in some variants of autopoiesis can readily be integrated If these two concepts prove useful for descriptions of living systems, then it would be interesting to see how they relate to the use of autopoiesis as it is currently explored in other fields of research like law, family therapy or social systems (Mingers 1995)

Notwithstanding my criticism of autopoiesis here, it remains an important although elusive concept This elusiveness derives from its domain-independent formulation that is both the weak and the strong side of this theory That it is the weak side is elaborated in section 6 1 which highlights the resulting ambiguities The strong side of the domain-independent formulation lies in the circumstance that it has the potential to unify areas of research as for example presented in (Mingers 1995) that are currently seen as clearly distinct However, this potential is yet unrealised and instead different variants of autopoiesis have come into existence Furthermore, it is not clear whether this unification is possible at all and the domain-independent formulation of autopoiesis by Maturana and Varela (1973) would allow only a superficial unification since even such a central concept as "autopoietic organisation" is not clearly specified Nonetheless, the idea that such apparently distinct fields like origin of life and social systems could have something essential in common is not only intriguing but would also be revealing if it were the case

To return to the questions of the definition of life and its origin, whether the extended SCL model system would be of any further use when such a research program would follow the path laid out by AlChemy and the theory of collectively autocatalytic networks seems doubtful Although SCL-DIV does exhibit autopoietic entities based on a collectively autocatalytic network, it is a mere illustration Due to the lack of chemical realism, SCL cannot relate to the field of chemical autopoiesis or to weak Artificial Life Despite the fact that the cells in it are not alive, it might be seen as a step towards the realisation of life as defined by autopoiesis, but only if the requirement is dropped that the domain must be the physical one for an autopoietic unity to count as alive But in order to fully integrate SCL into the concepts of AlChemy, the particles would have to be represented with an inner structure with a potential for infinite variations from which their behaviour derives In particular, these representations must admit for some way of meaningful combination in order to allow particle transformation Because the mechanisms in extended SCL are specifically developed and adapted to the one and only reaction network that is present, it is unlikely that they can have a further use when a multitude of reaction networks become possible

The only advancement that SCL-DIV makes beyond the existing artificial chemistries (in the sense defined in section 3 2) is the possibility of selective displacement and hence evolution But as argued in section 5 2 4, such a process would only be of limited potential like in a genetic algorithm Again, the transition to AlChemy-like particles with an inner structure that determines the

behaviour and can be combined with inner structures of other particles would open up a wider range of possible production networks and make an evolutionary process more interesting and also possibly relevant for considerations concerning the early evolution of life The artificial chemistry that currently comes closest to fulfilling the requirements laid out here is that presented in (Mayer and Rasmussen 1998) Although there is currently only one reaction network present in this model system, the potential for a variety of them exists, simply because the interactions are directly derived from physical laws Furthermore, questions regarding the energetic autonomy of proto-lifeforms would automatically addressed by this approach as well The main problem with such a detailed simulation is that the more complex the simulated systems become, the more computation time is needed Apart from that, it would prove difficult to generalise from the results of such simulations which is for example possible with systems like AlChemy (Fontana and Buss 1994, sec 8 3) To repeat a point made in section 1 3, it is not obvious at the outset, which approach will be the most successful one

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Appendix

A SCL-DIV usage guide

This appendix explains how to use the extended SCL model system for the purpose of replicating (as closely as possible) the phenomenology of SCL-DIV that is described in chapters four and five It is neither a technical description of the source code nor a reference guide to all of SCL-DIV's features Also (McMullin 1997) is a useful source of documentation because the extended version of SCL is based on the original version number 0 05 11 which is quite similar to the one documented in that report The ultimate reference of SCL-DIV is naturally the source code It can be downloaded at http //www eeng dcu ie/~alife/src/scl-div/

A 1 Requirements

The extended version of SCL can be compiled and run, theoretically at least, on all platforms that are supported by SWARM version 2 0 or 2 1 (and probably higher as well) SWARM is a multi-platform collection of libraries with the purpose to facilitate and generalize agent-based modeling (see www swarm org) SCL is written in Objective-C which is the original programming language supported by SWARM but since version 2 0 JAVA is supported as well However, the way in which the state of the random number generator is saved in SCL prevents the sharing of world files between different computer architectures The runs conducted in this thesis have been carried out on Intel Pentium computers (Pentium MMX, Pentium II) under the operating system GNU/Linux and it is recommended that a similar setup should be used so that the world files that come with the source code can be loaded into SCL-DIV But also between different x86 compatible architectures and compilers the behaviour of SCL-DIV can vary The reason for this is that lifetime diffusion needs to perform a few floating point operations, which can exhibit slight variations depending on whether the variables are always kept in the CPU registers or are temporarily stored in the memory In general the repeatability of computer simulations, which is one of SWARM's objects, can be quite easily sabotaged by floating point operations The best solution of this problem would probably be to use rational instead of floating point numbers, but the former are not a standard data type in C and would also bring with them a performance penalty It might be a sensible extension to SWARM to provide a rational number data type together with its operations, but whether

exact replication of simulations in the context of agent-based models is really necessary is a different question because in these types of models one is usually interested in some higher-level phenomena which should be robust with respect to small fluctuations

A 2 How to run a simulation

The most convenient way to start a run is to load already existing parameter and world files which come together with the source code [12] This can be done after SCL-DIV has been started or from the command line `scl -p parameterFile -w worldFile` When both files are specified on the command line then always the parameter file is loaded before the world file and this order must be used as well when loading the files in an already running SCL-DIV program [13] After the files have been loaded the simulation can be started or stopped from the standard control panel If you want to use a different seed for the random number generator than the one used in the saved state of the generator call either `reseedRandomNumberGenerator` to get a time-based random seed or `setStateFromSeed` with a specific seed The initial seed either way used to set the state of the random number generator can at any time be retrieved with the message `getInitialSeed` All three messages can be accessed from the `worldManager` window The retrieval of the initial seed is useful when one wants to replicate a run with a saved world as the basis where the random number generator was (randomly) reseeded before the run was started

The following example illustrates this If one wants to replicate the run from which the snapshots in figure 6 are taken, start `scl -p newFission prm -w smallCell200 stt` from a shell Then call `setStateFromSeed` with 2133390192 as argument Now the run itself can be started and at time steps 769 and 1242 the events shown in figure 6 can be observed [14]

The link particles that are shown in the SCL `World` window are coloured in

[12] When a file of either type is loaded often warning messages about unknown instance variables appear on the console These can be ignored

[13] Parameter inheritance in catalysts and links makes it necessary for those particles to carry certain simulation parameters as instance variables When the values of these variables are not specified in the world file the variables will be initialised with values from the `ParameterManager` But the latter values are default values in case a specific parameter has not been loaded beforehand Loading of a parameter file afterwards does not change the values of those parameters that are inherited

[14] Every time the `organizedFission` mechanism (cf sec 4 6) can successfully complete its operation, this is reported at the console, together with the time step during which this has taken place The sequence of these time steps can be effectively regarded as a fingerprint of a run

various ways to convey information about their internal state The standard colour is blue while disintegrating links are bluegrey Links that are part of a membrane are shown in black and when they have too few lifetime units to be able to transfer them to catalysts they are coloured yellow Similarly, catalysts are normally green but bluegrey when they are disintegrating

A 3 The parameter and world files

The parameter file that corresponds to table 1 is called `newFission prm` It is used in all the runs except those without autocatalysis (sec 5 1) where `noAutocat prm` is used together with the world file `noAutocat stt` The world file for all other runs with the small world (fig 2) is `smallCell200 stt` and for the large world (sec 5 2 2) `largeMulti100 stt` The modified large worlds used in section 5 2 4 are `diffProdProb stt` for the selective displacement runs and `geneticDrift stt` for the genetic drift runs