Spontaneous Formation of Proto-cells in an Universal Artificial Chemistry on a Planar Graph

Pietro Speroni di Fenizio[1], Peter Dittrich[1], and Wolfgang Banzhaf[1]

Informatik XI
University of Dortmund
D-44221 Dortmund, Germany
{speroni, dittrich, banzhaf}@LS11.cs.uni-dortmund.de
http://ls11-www.cs.uni-dortmund.de/

Abstract. An artificial chemistry is embedded in a triangular planar graph, that allows the molecules to act only locally along the edges. We observe the formation of effectively separated components in the graph structure. Those components are kept separated by elastic reactions from molecules generated inside the component itself. We interpret those components as self-maintaining proto-cells and the elastic nodes as their proto-membrane. The possibility for these cells to be autopoietic is discussed.

1 Introduction

Presently, much research has been directed towards synthesizing life-like structures in digital media. This goal requires a deeper understanding of the term "alive" and its consequences. Some threads of research have focused on reproduction and have generated programs able to reproduce [6, 11]. Here we follow a different path by focusing on the ability of any living system to self-repair and to keep its identity as an entity separated from its environment [5, 18]. Under those assumption the characteristics of being alive must emerge from the interactions of simpler components. Here we use an artificial chemistry with combinators as molecules. The combinator chemistry is a universal artificial chemistry because it is implicitly defined and it supports universal computation (it can simulate a Turing-machine). In order to permit molecules to generate a "physical" membrane that separates one being from another we embed the artificial chemistry in a graph.

A common feature of artificial chemistries is often the absence of any spatial conditions [4, 5]. Rather, molecules are floating around, randomly colliding with each other. Counter-examples exist, however, either in the form of cellular automata which define a space where to insert the elements [1, 2, 8–10], or by giving a position in a Euclidean space to each element and a range of interaction [13, 20]. Using a cellular automaton (where each cell can hold one molecule) is simple and elegant, but does not permit an unbounded growth of elements in

a particular position. The second alternative is more flexible in this regard, yet the number of interactions that the model has to deal with grows as $n!$ (where n is the local number of elements). This is not efficient and in addition difficult to model, since interactions farer away will often be canceled by the effect of nearer ones.

Here we suggest a different approach in which an artificial chemistry (AC) is embedded in a graph, with each molecule being a vertex of the graph and possible interactions being allowed only along the edges of the graph. We suggest here to use a particular graph, namely, a planar triangular graph. A planar triangular graph can be drawn on a sphere without edge crossing, and with each face being triangular. This particular type of graph can be manipulated by adding and deleting nodes with a minimal local rearrangement of the edges. So we can add nodes near a selected node (like in a 2D model). Yet if we circumscribe a set of connected nodes and insert n new nodes, the number of new relations to be taken into account grows only linearly with n.

Like in many artificial chemistries (and in ours in particular) not all molecules can interact with each other. Special conditions may arise under which different molecules that would have destroyed themselves in a well-stirred reactor can instead coexist [1, 3]. This gives rise to higher organizational levels [7] by allowing the whole graph to split into "effectively" separated components that temporarily act as different reaction vessels. The separation into different components by membrane-like structures has also been identified as an important aspect of "biological" information processing [12] and chemical evolution [17].

In the following, we present the planar triangular graph as a feasible tool to model spatial structures, apply it to an artificial chemistry based on combinators, and then show how separate components arise naturally. These components can be interpreted as proto-cells. For this purpose we also have to defined what a membrane, a cell, and an autopoietic cell are in our system.

2 Basic Definitions and Operators

Let $G =< V, E >$ be a graph. G is planar if (and only if) it can be embedded in a plane without edges crossing each other. Given a planar graph embedded in the plane and a point x, we define the face (of G) to contain x as the set of all the points in the plane which can be reached by x with a Jordan curve and whose points are disjoint from G ([19], p. 64). A face of G is called triangular if there are exactly three vertices which can be reached from a point inside the face, through a Jordan curve. Or equivalently if the equivalent vertex in the dual graph[1] G' has three edges. A planar graph G is triangular if every face is triangular, or equivalently if the dual of every face in G' has exactly three edges.

Given the application-oriented field we are addressing, we will consider in this paper only graphs with at least five nodes. In order to manipulate a graph we need the following operators to add and delete a node: **Add node:** Given

[1] The dual graph of a planar graph G is constructed by inserting a node for every face of G and connecting nodes whose equivalent faces are neighbors.

any planar triangular graph it is always possible to add a node to a face given as a parameter. The new node is added to the list of nodes, and three edges are added connecting the new node the three nodes of the face. This operation destroys the old face given as a parameter and creates three new faces. **Delete node:** Given any triangular planar graph with at least six nodes, and given any node x it is always possible to delete x and the edges that were connected to x. In this way we create a new planar graph G' with all faces triangular except one. Subsequently, it is possible to add edges connecting the nodes of this non-triangular face to restore the triangular planar graph. We start adding edges from the node which has remained with only two edges, since in a triangular planar graph each node possesses at least three connections

We connect the nodes randomly inside the face, taking care never to connect pairs of nodes which are already connected.

2.1 Artificial Chemistry based on Combinators

Any artificial chemistry can be embedded in a graph. In our contribution we use an artificial chemistry based on combinators, described in more detail in [14–16].

Molecules and Reactions: Briefly we say that there is (1) an (infinite) set of potential molecules S and (2) a reaction mechanism which computes the reaction product for two colliding molecules $x, y \in S$. This reaction mechanism can be written as a function $r : S \times S \to S \times S \times \cdots \times S$. So, there may be an arbitrary number of products. We write the function r as an operator[2] $\oplus$. Molecules are built from a substrate of elements called *atoms*. There are seven types of atoms (I, K, W, R, B, C, S), each with a different function. The total number of atoms in the reactor is kept constant during a run. Free atoms (not bounded in molecules) are separately stored and form a global pool.

Dynamics: At every step we pick two neighboring molecules (x, y) and apply the first x to the second $x \oplus y \longrightarrow x(y)$. As described in [14–16], this creates a (multi-)set of new molecules $z_1, \ldots, z_n$. We insert the molecules $z_2, \ldots, z_n$ randomly in the two faces next to the link $x - y$ (Fig. 1). x is replaced with z_1 (the result of the combinator reduction) and y is finally deleted[3]. The process may appear complicated, but has been carefully designed to be coherent for any $n \geq 1$.

3 Results

When observing the behavior of the system, we notice that different molecules tend to cluster in different regions of the graph. At first glance we can immediately notice how the graph helps the system to balance different organizations.

[2] We use the symbol $\oplus$ instead of the symbol + because differently to chemistry the order of the reactants is important to calculate the product(s).

[3] Note that the operation is slightly different from the operation described in [14] where z_1 replaces x and y would be deleted. This change has been enacted to prevent reactions of the type $x \oplus y \longrightarrow x, y$ to switch the molecules. Thus we permit easy diffusion.

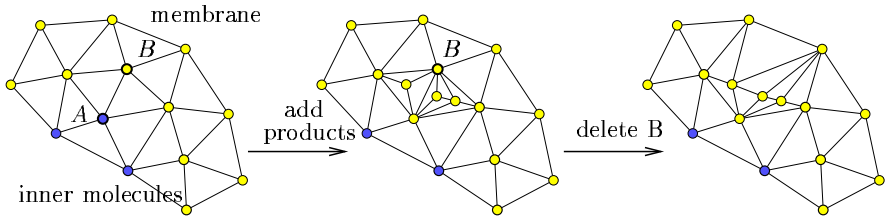


Fig. 1. Illustration of a reaction that creates membrane molecules.

Here, an *organization* is defined as a set of molecules that is closed and self-maintaining. This means that every reaction among molecules of the set produce only molecules of that set, and every molecule of the set is produced by at least one reaction among molecules of the set [5]. So, different organizations can be present at the same time (see Fig. 4, below).

Definition and discovery of the membrane: A first theoretical definition of *membrane molecules* is the set of all molecules who cannot interact with the molecule they are linked with. This definition has a number of flaws: real membrane molecules do interact with their neighbors. Their role is to keep their structure while thus separating inside from outside. We suspect that some molecules in the system do act like membrane molecules of biological cells. The second drawback is more technical. We recall that a reaction is possible if the reduction computation of the expression $x(y)$ halts, and if the number of free atoms (in the global pool) is sufficient to support the computation and the results. For this reason some molecules will be unable to interact, regardless of the number of free atoms, while others are reactive only "sometimes". The first type of links will be called "*absolutely*" elastic; while the second type "*effectively*" elastic. In Fig. 4 the absolutely elastic links are removed before drawing the graph to show the formation of cells. This is imprecise, since the membrane could be much thicker, comprising molecules which in theory could interact, but in practice do not interact because the necessary atoms are missing all the time. In our experiments we have discovered clusters of molecules which were unable to interact and divided the graph into separated regions. Molecules which are absolutely unable to interact with themselves obviously form the raw material for membranes. As soon as such molecules cluster, all inner molecules of these clustered non-reactive molecules will build the membrane. For this reason, here, we define as *membrane molecules* those molecules which are absolutely unable to interact with themselves, regardless of their effective position. Thus, molecules which would build a membrane under the right condition.

Definition of cell: As the membrane molecules appear and start to cluster, the graph looses its homogeneity and starts to divide into different regions. If we delete all absolutely elastic links of a graph G, we will obtain a new graph G'. In this new graph any separated component containing more than one node

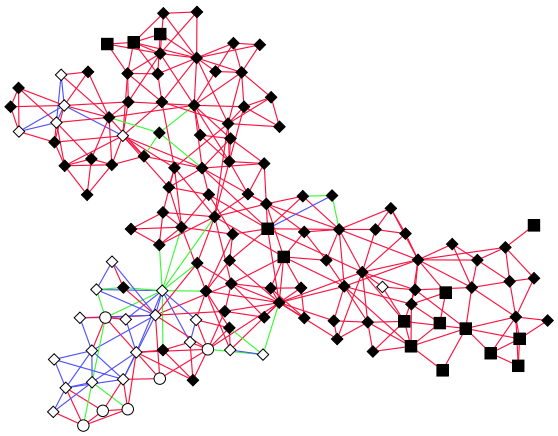


Fig. 2. Example of two cells. Magnification of a sub-graph taken from generation 917. Red edges denote "absolutly" elastic (non-reactive) connections. Membrane molecules: ■(r) and ⧫(y_2). Inner molecules: ◊(b) and ○(g). Note that the lower left cell contains a different inner organization (◊and ○) then the small upper left cell (◊only).

will be regarded as a *cell*. Such a definition is purely geometrical, and in no way infers anything about the nature of the cell, or its possible evolution.

Autopoietic cell: Some cells exhibit stronger properties, so that they can be classified as autopoietic cells (example in Fig. 2). In the following we give a tentative definition of what would be an autopoietic sub-system in an artificial chemistry embedded in a graph. We will call I the set of elements inside a cell, and M the set of elements from its membrane. A cell will be called *autopoietic* if: (1) either I is an organization, and I produces M, or (2) I is an organization and $I \cup M$ produces M or (3) $I \cup M$ is an organization.

We will call such an organization the *cell organization*. Autopoiesis also requires that the cell organization is relatively stable with respect to an influx of random noise, e.g., random molecules. So, we require the system to continuously produces membrane molecules in order to maintain the cell as a separate unit. Under the influx of random molecular noise molecules which cannot interact with the organization will also be generated [16]. Being unable to interact, those molecules will naturally connect to the membrane, and as the membrane grows they will be expelled from the cell. In [16] we explain how metabolic organizations under the influx of random noise sometimes produce long unusable molecules. In our system such molecules would end up being part of the membrane. Under the right conditions (excessive number of atoms which build up membrane molecules), such a membrane could also be overproduced, with the effect of splitting the cell into separate cells. Even if all other requirements are satisfied, not every organization producing membrane molecules would form an autopoietic cell. In our system, if membrane molecules are produced too rapidly,

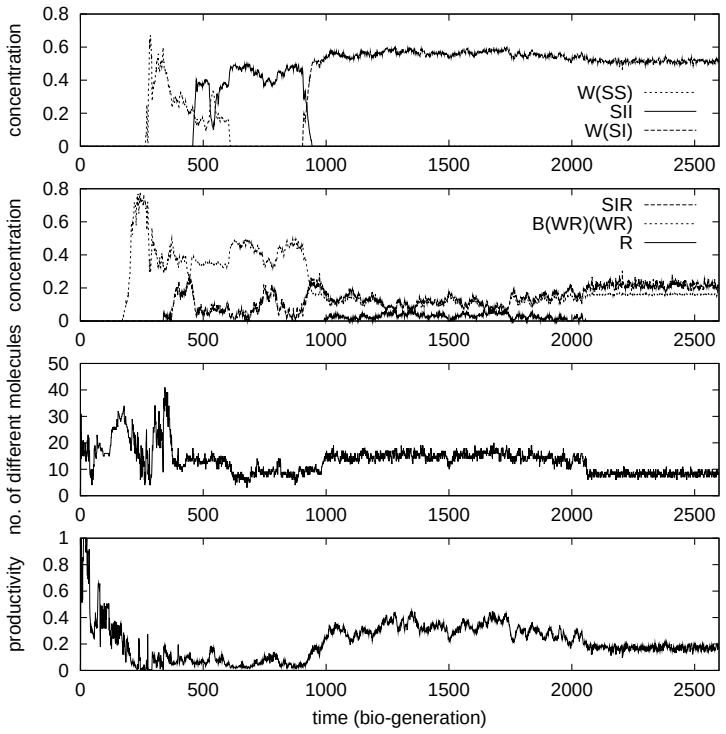


Fig. 3. Time evolution of the concentration of important molecules, number of different molecules (diversity), and productivity (probability that two neighboring molecules can react).

they tend to create big chunks and could not form a smooth membrane, that would otherwise be able to separate the inside from the outside (Fig. 4, middle).

Structure of the process - autopoietic mechanism: We will now discuss in detail a concrete experiment[4] which shows spontaneous formation of autopoietic cells. This will be done by listing its molecules, both the membrane and the inner ones. The main molecules that appeared in this experiment are:

combinator (molecule)	symbol	name	combinator (molecule)	symbol	name
$B(WR)(WR)$	○	g	$W(SS)$	♦	y_1
SIR	◊	b	$S(R(W(SS)))(W(SS))$	●	w
R	□	v_1	SII	■	r
RR	□	v_2	$W(SI)$	♦	y_2

[4] Parameter settings to replicate the experiment: Operation type $x \oplus y \longrightarrow x(y)$. Atoms used: B, C, K, R, I, S, W. Number of atoms: 1000 of each type. The influx of random molecules is exponentially decaying with MinNMolecules = 25, HalfNMolecules = 150. Outflux probability 0.01. Random seed 789. MaxTry = 10000. MaxLength = 100, MaxDepth = 20. Starting number of randomly generated molecules: 150 (initial population size).

The left four being inner molecules; the right four being membrane molecules. Short names are used to ease the following discussion. Two secondary membrane molecules which less frequently appear are:

combinator (molecule)	symbol	name
$S(B(WR)(WR))(B(WR)(WR))$	●	w_2
$S(SIR)(SIR)$	●	w_3

Membrane molecules can never interact with themselves, nor with other membrane molecules. Note that any element of the form $R(x)$ will react with anything else and always creates x by that reaction. Thus $R(x)$ can be seen as an intermediate product. For this reason in our table we will list every molecule $R(R(\dots(x)\dots)$ as x. Some of the inner molecules follow general rules. Let $x, y \in S$ be arbitrary molecules these general rules read: $g \oplus y \longrightarrow 4y$; $R(x) \oplus y \longrightarrow x, y$; $RR(x) \oplus y \longrightarrow R(y), x$.

$b = SIR$ acts differently on any molecule, as can be seen in the following table:

$\oplus$	g	b	v_1	v_2	y_1	w	r	y_2
b	$4g$	$2b$	v_2	v_1, v_2	w	$elastic$	$2r$	$3y_2$

What is missing are the reaction products between membrane molecules and inner molecules:

$\oplus$	g	b	v_1	v_2
y_1	$w_2, 3g$	w_3, b	n.h.	n.h.
w	elastic	elastic	n.h.	n.h.
r	$4g$	$2b$	n.h.	n.h.
y_2	$13g$ elastic de facto	$4b$	v_2	$2v_1, v_2$

Some membrane molecules, interacting with inside molecules create intermediate products w_3 and w_2. Both products cannot interact with themselves, nor with membrane molecules. We list their interaction with inside molecules:

$\oplus$	b	w_3
b	$2b$ elastic	
w_3	$4b$ elastic	

$\oplus$	g	w_2
g	$2g$	$4g$
w_2	$10g$ elastic de facto	elastic

Interactions that do not appear because the corresponding molecules are not present at the same time are marked "n.h." (never happened).

From this tables we can conclude that y_1 cannot be a membrane for b (⧫ and ◊, respectively, in Fig. 4 (a)) since in no way can it be generated by their interaction. b instead can use r (■ in Fig. 4) and y_2 (⧫ in Fig. 4 (b) and (c)) to create cells as it effectively does (Fig. 2)). g (○) can create cells using any of the above membrane molecules. Yet with y_1 and r (■) it generates them smoothly, ending up with an effective membrane (○ and ■). When y_2 appears with g the formation of membrane cannot be as clearly observed as in the other case, since the membrane ends up generating too big clusters. Either this is an

effect of the explosive reaction ($w_2 \oplus g \longrightarrow 10g$), or is an effect of the dynamics. The investigation of the later case is beyond the scope of this paper.

We showed examples from different organizations arising in one run, but where not every membrane molecule was coupled to every organization to generate an effective self-maintaining cell. The other cases seem in all regards autopoietic systems.

Different types of membrane compete: In our experiment we noticed how different types of membrane tend to compete (Fig. 3, upper graph). Since they often use the same type of atoms (S and W) this no surprise. On the other hand, inner molecules can feed upon a bigger variety of atoms, molecules are often divided by the membrane into different cells that do not compete since they feed on different atoms (Fig. 3, second graph from above).

Different runs generate different molecules: Up to now we have spoken about one run only. When more runs are performed, sometimes other cells are generated, based upon different molecules but with similar behavior. Another possible outcome of a run are organizations so different that no membrane is present at all, e.g., where the productivity[5] stabilizes at exactly one.

Since each run generates a totally different experiment, with a completely different behavior, averaging over a number of runs would not give interesting data. For this reason we choose to thoroughly present one run instead. For an analysis of the variability of the possible organization that may appear in different runs see [15].

4 Conclusion

Our results were achieved by permitting any possible molecule to appear in the system (at least in principle). The resulting organizations not only generated a membrane in the "physical" space, but also, through their network of interactions, maintained exactly those molecules which continuously generated the cell.

What we observed is a special case of an autopoietic structure. In a general case the molecules would not be required to remain constant through time. What would remain constant instead is the network of interactions which generate the cell[6]. This is equivalent to saying that a cell can be autopoietic even if it changes its component types, as long as the new components still interact in the same functional way.

In our work the atoms were assumed to have a homogeneous concentration throughout the entire graph. An interesting variation would be to consider them locally in each face. This could give rise to a Darwinian process as cells have to destroy other cell's molecules to free atoms for use in their faces. As we said earlier our results were reached by studying an universal artificial chemistry. Each cell generates its own table of interaction for its molecules. It would be an

[5] Productivity measures the probability that a collision of two molecules is reactive.

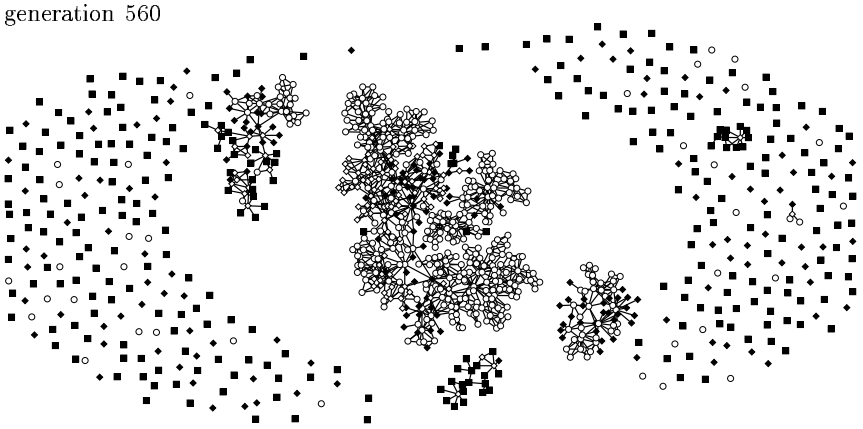
[6] If the molecules remain constant this condition is automatically fulfilled

interesting problem to extract these reaction tables and to use a fast and simple model for studying the evolutionary dynamics of cell assemblies.

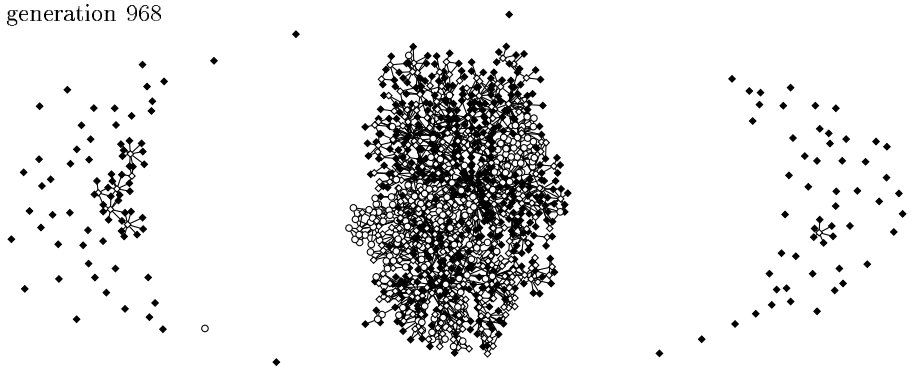
References

1. W. Banzhaf, P. Dittrich, and B. Eller. Selforganization in a system of binary strings with topological interactions. *Physica D*, 125:85–104, 1999.
2. J. Breyer, J. Ackermann, and J. McCaskill Evolving reaction-diffusion ecosystems with self-assembling structure in thin films. *Artificial Life*, 4(1):25–40, 1999.
3. R. Durrett. The importance of being discrete (and spatial). *Theor. Popul. Biol.*, 46:363–394, 1994.
4. J. D. Farmer, S. A. Kauffman, and N. H. Packard Autocatalytic replication of polymers. *Physica D*, 22:50–67, 1986.
5. W. Fontana and L. W. Buss 'The arrival of the fittest': Toward a theory of biological organization. *Bull. Math. Biol.*, 56:1–64, 1994.
6. R. Laing. Some alternative reproductive strategies in artificial molecular machines. *J. Theor. Biol.*, 54:63–84, 1975.
7. B. Mayer and S. Rasmussen. Dynamics and simulation of micellar self-reproduction. *Int. J. Mod. Phys. C*, 11(4):809–826, 2000.
8. B. Mayer and S Rasmussen. The lattice molecular automaton (LMA): A simulation system for constructive molecular dynamics. *Int. J. of Modern Physics C*, 9(1):157–177, 1998.
9. B. McMullin and F. J. Varela Rediscovering computational autopoiesis. In P. Husbands and I. Harvey, editors, *Fourth European Conference on Artificial Life*, pages 38–47, Cambridge, MA, 1997. MIT Press.
10. N. Ono and T. Ikegami. Self-maintenance and self-reproduction in an abstract cell model. *J. Theor. Biol.*, 206(2):243–253, 2000.
11. A. N. Pargellis The spontaneous generation of digital "life". *Physica D*, 91(1-2):86–96, 1996.
12. Gheorghe Paun. Computing with membranes. *J. of Computer and System Sciences*, 61(1):108–143, 2000.
13. M. A. Shackleton and C. S. Winter. A computational architecture based on cellular processing. In M. Holcombe and R. Paton, editors, *Information Processing in Cells and Tissues*, pages 261–272, New York, NY, 1998. Plenum Press.
14. P. Speroni di Fenizio. Building life without cheating. Master's thesis, University of Sussex, Falmer, Brighton, UK, 1999.
15. P. Speroni di Fenizio. A less abstract artficial chemistry. In M. A. Bedau, J. S. McCaskill, N. H. Packard, and S. Rasmussen, editors, *Artificial Life VII*, pages 49–53, Cambridge, MA, 2000. MIT Press.
16. P. Speroni di Fenizio and W. Banzhaf. Metabolic and stable organisations. This volume, 2001.
17. Y. Suzuki and H. Tanaka. Chemical evolution among artificial proto-cells. In M. A. Bedau, J. S. McCaskill, N. H. Packard, and S. Rasmussen, editors, *Artificial Life VII*, pages 54–63, Cambridge, MA, 2000. MIT Press.
18. F. J. Varela, H. R. Maturana, and R. Uribe Autopoiesis: The organization of living systems. *BioSystems*, 5(4):187–196, 1974.
19. R. J. Wilson. *Introduction to Graph Theory*. Oliver and Boyd, Edinburgh, 1972.
20. K.-P. Zauner and M. Conrad. Conformation-driven computing: Simulating the context-conformation-action loop. *Supramolecular Science*, 5(5-6):791–794, 1998.

(a) generation 560



(b) generation 968



(c) generation 1121

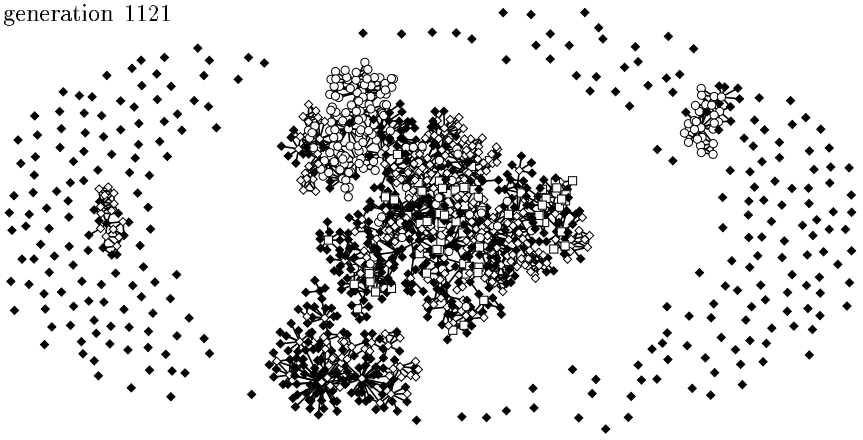


Fig. 4. Two-dimensional embedding of the graph at generation 560, 968, and 1121. Absolutely elastic links are removed before embedding. Note that nearness in the plane does not necessarily infer nearness in the planar graph. The embedding algorithm places nodes without neighbors at the outset of the plane.