Spontaneous Formation of Cells in a Universal Artificial Chemistry on a Planar Graph

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

1 Introduction

Much work has been done in trying to synthesize living structures from a digital background. Doing this would require a deep understanding of the term "alive" and its consequences. Some threads of research have focused on reproduction and generated programs able to reproduce [7, 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 a component separate from its environment [5, 15]. Under those assumption the characteristic of being alive must emerge out of the interaction of simple components. For this reason we use an artificial chemistry with combinators as molecules. This is an universal artificial chemistry because it is implicitly defined and supports universal computation. To permit molecules to generate a "physical" membrane that separates one being from another we embed the artificial chemistry in a graph.

A common theme in artificial chemistries is often the absence of any spatial conditions [4, 6]. Rather, molecules are floating around, randomly colliding with each other. Some important counter-examples exist, however, either using cellular automata to define a space where to insert the elements [1, 2, 8–10], or giving a position in an Euclidean space and a range of interaction to each element [12, 17]. 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, as well as difficult to model, since further interactions 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 through the edges of the graph. We suggest here to use a particular graph, namely, a planar triangular graph. These graphs 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 rearrangements of the edges. This permits to have new nodes added near a selected node (like in a 2D model), yet if we circumscribe a set of connected nodes, and we insert n new nodes in there, 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. Particular conditions may arise under which different molecules that would have destroyed themselves in a well-stirred reactor can instead coexist [1]. This not only gives rise to a higher organizational level, it can also allow the whole graph to split into "effectively" separated components that temporarily act as different reaction vessels.

We present the graph as a possible tool and show how separate components can arise naturally. These components can be interpreted as cells. To do so we will define what a membrane, a cell, and an autopoietic cell are in our system at the beginning of the result section.

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 with no two 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 disjointed from G ([16], 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. We now need some operators which permit us to move from one planar triangular graph to another:

Add node: Given any planar triangular graph it is always possible to add a node. This can be done by choosing the face in which we want to add the node, by adding it to the list of nodes, and by adding three edges from the node to the three vertices of the face. This action destroys the face we are working in, and creates three new faces (Fig. 1 (a)).

[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.

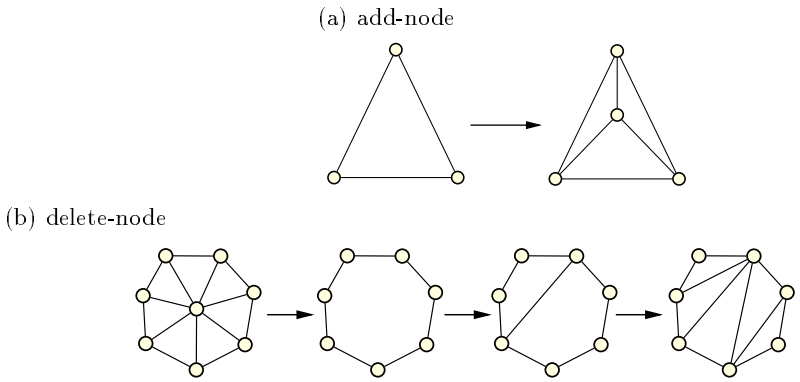

Fig. 1. Illustration of the graph manipulating operators.

Delete node: Given any triangular planar graph with at least 6 nodes, and given any vertex x it always possible to delete x and the edges that were connected to x. By doing this we create a new planar graph G', with all faces triangular except one. It is then possible to add edges between the vertices of this face to generate a new triangular planar graph. Since in a planar triangular graph each node has at least 3 connections we start adding edges from the node which has remained with only two edges. We connect the nodes randomly inside the face, taking care never to connect pairs of nodes which are already connected (Fig. 1 (b)).

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 detail in [13, 14, 3].

[Since the combinator chemistry is described in a separate paper submitted, we would like to point the reviewer to a web site where the paper can be downloaded:
http://www.geocities.com/pietrosperoni/academic/Papers/ecal2001a.ps
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Molecules and Reactions: Briefly we will say that there is (1) a (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 $\oplus$. Molecules are built upon a substrate of elements called atoms. There are seven types of atoms, 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 is described in the Appendix

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 around the link $x - y$ (Fig. 3). x is replaced with z_1 (the result of the computation) and y is finally deleted. The process may appear complicated, but has been carefully designed to be coherent for any $n \geq 1$. Note that the operation is slightly different from the operation described in [13] 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[2]. Thus we permit easy diffusion. Also the artificial chemistry has been changed by adding a new type of atom [14, 3].

3 Results

When observing the behavior of the system it is possible to 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[3], permitting them to be present at the same time (see Fig. 5, 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 holds a number of flaws: real membrane molecules do interact with their neighbors. Their role is that while they interact they keep their structure, 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 in time, and if the number of free atoms 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 figures showing the formation of cells (Fig. 5), the absolutely elastic links are removed before drawing the graph. 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 always missing.

In our experiments we have discovered clusters of molecules which were unable to interact and divided the graph into separate regions. Molecules which are absolutely unable to interact with themselves obviously form the raw material for membranes. As soon as such molecules cluster, all the inner ones will build the membrane. For this reason we often defined as "*membrane molecules*" molecules which are "absolutely" unable to interact with themselves, regardless

[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] Here, an *organization* is defined as a set of molecules which is closed and self-maintaining, that is, 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].

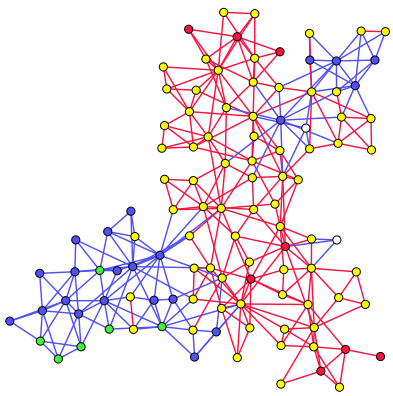

Fig. 2. Example of two cells. Magnification of a sub-graph taken from generation 917. Red edges denote "absolutly" elastic (non-reactive) connections. Membrane molecules: red (r) and yellow (y_2). Inner molecules: blue (b) and green (g). Note that the lower left cell contains a different inner organization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

of their effective position. In such a case what we mean is: molecules who, under the right condition, would build a membrane.

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 consider the graph G, and we delete all its absolutely elastic links we will obtain a new graph G'. In this new graph any separated component made up of more than one node will be regarded as a *cell*. Such a definition is purely geometrical, and in no way infers anything about the nature of the cell, and its possible evolution.

Autopoietic cell: Some cells exhibit stronger properties which made us classify them as autopoietic cells (example in Fig. 2). In the following we make a tentative definition of what would be an autopoietic system for artificial chemistry embedded in a graph. We will call I the set of elements inside a cell, and M the set of elements in 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 organization the *cell organization*. We also require that the cell organization be relatively stable with respect to an influx of random noise (random molecules). Relative to the membrane we require from 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 [3]. Being unable to interact those molecules will naturally connect to the membrane, and as the membrane grow they will be expelled from the cell. In [3] we explain how metabolic orga-

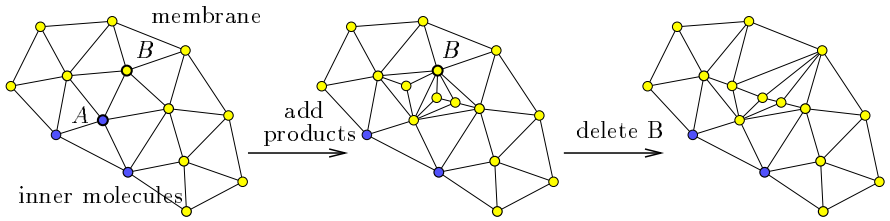

Fig. 3. Illustration of a reaction that creates membrane molecules.

nizations, under the influx of random noise, sometimes produce long unusable molecules. Such molecules would, in our system 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 the membrane molecules are produced too rapidly, they will tend to create big chunks and not a smooth membrane, that would otherwise be able to separate the inside from the outside (Fig. 5, middle).

Structure of the process - autopoietic mechanism:

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

combinator (molecule)	color	name
$B(WR)(WR)$	green	g
SIR	blue	b
R	violet	v_1
RR	violet	v_2
$W(SS)$	yellow	y_1
$S(R(W(SS)))(W(SS))$	white	w
SII	red	r
$W(SI)$	yellow	y_2

The first four being inner molecules; the last four being membrane molecules. Their short name is used to ease the following discussion. Two secondary membrane molecules that less frequently appear are:

[4] Parameter settings for replication of 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. Influx of random molecules 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).

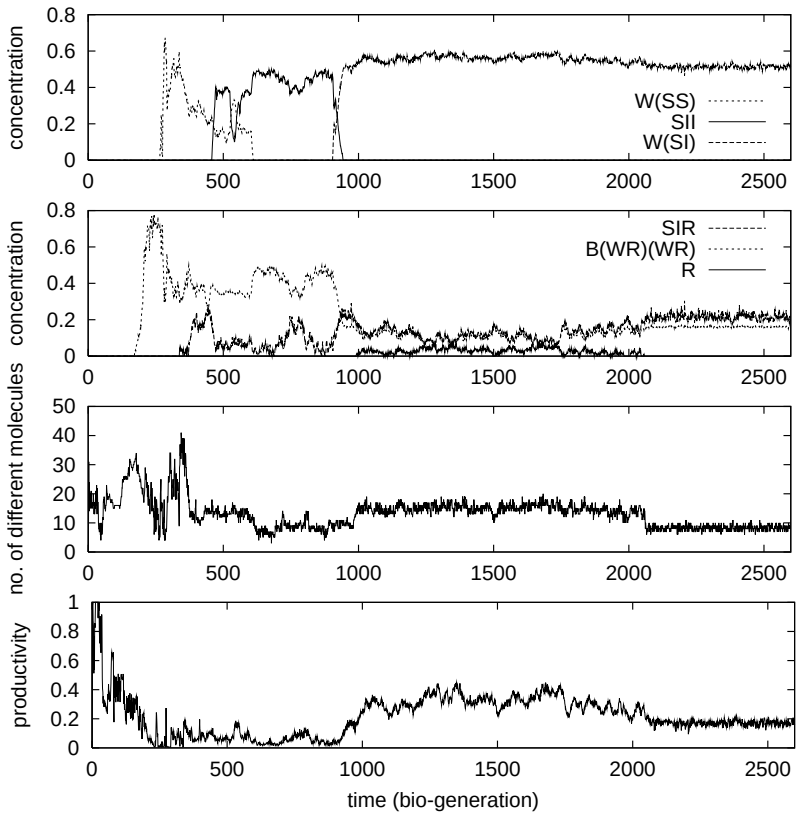

Fig. 4. Time evolution of the concentration of important molecules, number of different molecules (diversity), and productivity (probability that two neighboring molecules can react).

combinator (molecule)	color	name
$S(B(WR)(WR))(B(WR)(WR))$	white	w_2
$S(SIR)(SIR)$	white	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 and creates by that reaction always x. Thus $R(x)$ can be seen as an intermediate product. For this reason in our table we will list every molecule $R(R(...(x)...)$ 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 are 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, acting on the inside created intermediate products w_3, 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 (yellow and blue, respectively, in Fig. 5 (a)) since in no way can it be generated by their interaction. b instead can use r (red in Fig. 5) and y_2 (yellow in Fig. 5 (b) and (c)) to create cells as it effectively does (Fig. 2)). g (green) can create cells using any of the above membrane molecules. Yet with y_1 and r (red) it generates them smoothly, ending up with an effective membrane (green and red). 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 can be coupled with any 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. 4, upper graph). Since they often use the same type of atoms (S and W) this in no surprise. On the other hand inside molecules can feed upon a bigger variety of atoms, also molecules are often divided by the membrane in different cells that do not compete since being fed by different atoms (Fig. 4, second graph from above).

Different runs generate different molecules: Up to now we have spoken only about one run. 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.

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

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 instead to thoroughly present one run. For an analysis of the variability of the possible organization that may appear in different runs see [14].

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 cells molecules to use their atoms 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 interesting problem to extract these reaction tables and use a fast and simple model to study the evolutionary dynamics of cell assemblies.

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

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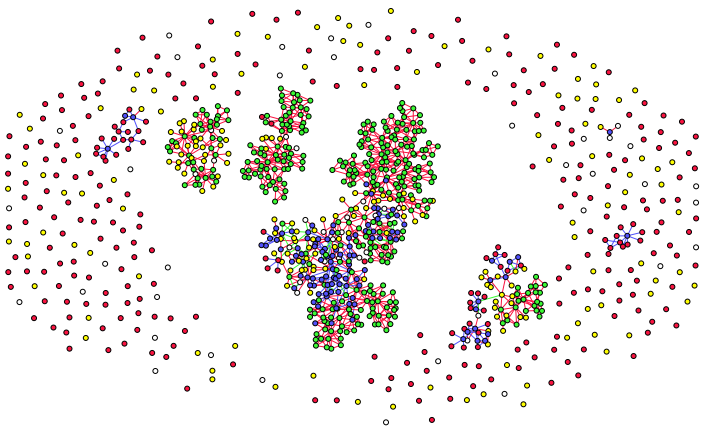
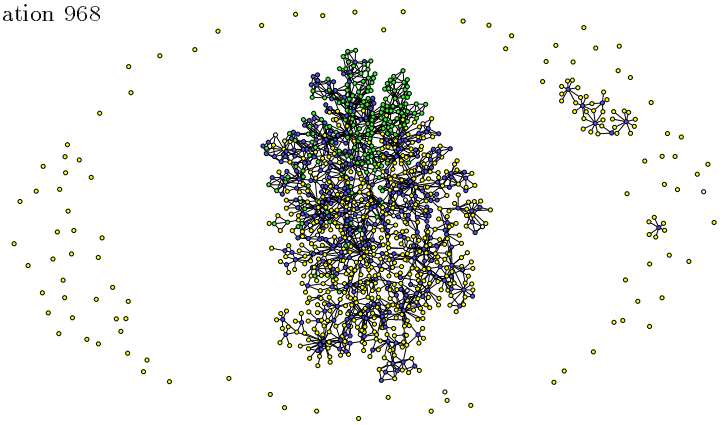
(a) generation 560



(b) generation 968



(c) generation 1121

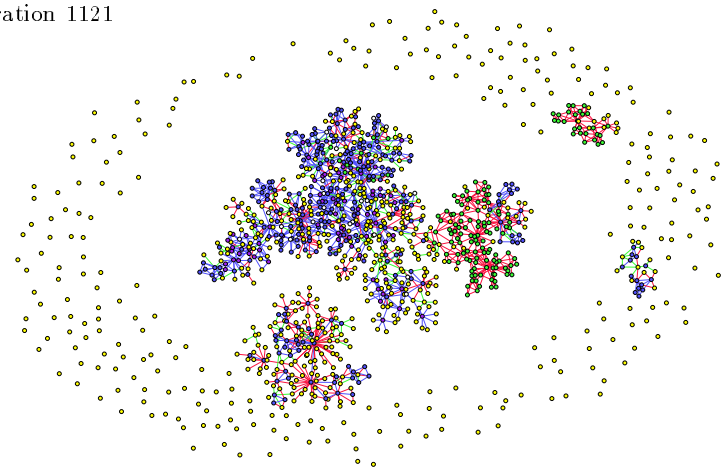


Fig. 5. Two-dimensional embedding of the planar graph at generation 560, 968, and 1121. Noted that nearness in the plane does not necessarily infer nearness in the planar graph. The embedding algorithm places nodes without neighbors at the outset of the plane.