MOLNETS: AN ARTIFICIAL CHEMISTRY BASED ON NEURAL NETWORKS

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ABSTRACT

The fundamental problem in the evolution of matter is to understand how structure-function relationships are formed and increase in complexity from the molecular level all the way to a genetic system. We have created a system where structure-function relationships arise naturally and without the need of ad hoc function assignments to given structures. The idea was inspired by neural networks, where the structure of the net embodies specific computational properties. In this system networks interact with other network to create connections between the inputs of one net and the outputs of another. The newly created net then recomputes its own synaptic weights, based on anti-hebbian rules. As a result some connections may be cut, and multiple nets can emerge as products of a 'reaction'. The idea is to study emergent reaction behaviors, based on simple rules that constitute a pseudophysics of the system. These simple rules are parameterized to produce behaviors that emulate chemical reactions. We find that these simple rules show a gradual increase in the size and complexity of molecules. We have been building a virtual artificial chemistry laboratory for discovering interesting reactions and for testing further ideas on the evolution of primitive molecules. Some of these ideas include the potential effect of membranes and selective diffusion according to molecular size.

INTRODUCTION

The fundamental problem in the evolution of matter is to understand how structure-function relationships are formed and increase in complexity from the molecular level all the way to a genetic system.

In this context, the genetic system is a point of arrival rather than the starting point for evolution. From this point on the rules of the 'game' are reasonably clear and evolution can be understood. Our question instead is what 'game' is being played at the very early stages of the evolution of matter? How are rules created and how are they 'fixed' in the system?

In order to approach these questions without the insurmountable computational obstacle of simulating a real prebiotic milieu, we have created a system where structure-function relationships arise naturally and without the need of ad hoc function assignments to given structures. The idea was inspired by neural networks, where the structure of the net embodies specific computational properties. One changes either the topology of the net or the synaptic weights, and the computational properties change.

This basic idea is modified by having networks interact with other network to create connections between the inputs of one net and the outputs of another. The newly created net then re-computes its own synaptic weights, based on anti-hebbian rules. As a result some connections may be cut, and multiple nets can emerge as products of a 'reaction'.

The idea is to study emergent reaction behaviors, based on simple rules that constitute a pseudophysics of the system.

BACKGROUND

This approach to the study of self-organization is based on the well established notion of an artificial chemistry, but we believe that use of neural network structures for our system is still largely unexplored. The abstract definition of an artificial chemistry typically involves a set of molecules, the rules of molecular interactions, and an algorithm to describe how the rules are applied to form a "reactor soup" (Dittrich *et al.*, 2001). Objects and rules specify a population dynamics, i.e. how object will appear, change in time, combine with other objects, etc. Some examples of objects are numbers (Ehrenfest and Ehrenfest 1907), bits strings (Dittrich and Banzhaf, 1998, Segovia and Colombano 2001), lambda-expressions (Fontana, 1992, Fontana and Buss, 1996) and other abstract structures. Rules may be based on string matching, arithmetic, matrix multiplication, lambda calculus, cellular automata etc. while the system dynamic can be determined by ordinary differential equations, difference equations, detailed collision simulation, self-organization topologies and others.

It must be noted that the motivations of artificial chemistry can be varied as well, ranging from biological models of origins of life phenomena (Colombano 1977, Eigen and Schuster 1977, Stassinopoulos *et al.* 1998) to biological adaptation and chemical information processing (Segovia and Colombano *op. cit.*, Zauner and Conrad 2002, Ziegler et al.) to logics (Morris 1989).

The challenge in all biological models is to produce phenomena that have enough analogies with their real biological counterparts to be able to shed light on their nature. This is not the same as attempting to build explicit simulations of these phenomena. The problem with explicit simulations is that they are often computationally intractable. For example, as stated in the introduction, even

modeling the folding of a single protein is still a major computational challenge. Detailed modeling of a large number of protein interactions will remain beyond the capabilities of computational technology for the foreseeable future. One can also make the argument that even when detailed simulation is possible a real understanding can only be achieved by providing suitable abstractions.

THE MOLNET SYSTEM

In an artificial chemistry context Molnets provide an abstraction for structure function relationships where function arises naturally from the system's pseudophysics, while retaining fast computational properties. The rules and structures are especially designed to bring out analogies with the protein world.

Here are some fundamental rules for Molecular Networks (Molnets):

1) Molnet nodes correspond to "atoms". They have a charge positive(+) or negative(-) and they are connected by "bonds".
2) Bonds have a direction and weight. From the point of view of each atom they can be input or output bonds. The value of the bond weights is between 0 and 1.
3) Atoms have type INPUT, OUTPUT, or HIDDEN, depending on the relative numbers of input and output bonds.
4) Molecular reactions consist in the forming of temporary bonds between the input and output atoms of each molecule. Bond strengths are then re-computed according to weight changing rules (see below) and new molecular structures are produced as a result of the reaction.
5) Weight changing rules are anti-hebbian, i.e. activation with opposite charges result in increased bond strength.

RESULTS

These simple rules are parameterized to produce behaviors that emulate chemical reactions. In particular we are interested in the emulation of the production of proteins in a pre-biotic "soup". In these case each node corresponds to an amino-acid, rather than a single atom, and a molnet corresponds to a protein.

We find that these simple rules show a gradual increase in the size of molecules up to an average value that depends on the initial population size (figure 1).

Some typical reactions are shown in figures 2 and 3. Figure 2 shows a reaction of the form A + B -> C. This is the type of reaction responsible for size growth in the initial soup. Figure 3 shows a reaction of type A + B -> C + D.

We have been building a virtual artificial chemistry laboratory for discovering interesting reactions and for testing further ideas on the evolution of primitive molecules.

Some of these ideas include the potential effect of membranes and selective diffusion according to molecular size. Figure 4 shows a typical reaction chamber,where the rectangles represent closed membranes which allow the passage of small molecules while blocking the passage of larger ones. The circles represent the reaction range for a molecule that is selected for reaction with its neighboring molecules. One molecule is selected at random for reaction at each time step.

FUTURE DIRECTIONS

The system shows interesting behavior even at this very simple level of rules, but it is clear that a much richer chemistry is needed in order to make observations that might be meaningful in the context of a prebiotic chemistry. The first obvious requirement is to incorporate energy in an explicit manner. At present vicinity is sufficient to trigger a reaction and no energy considerations are made. An explicit representation of energy will open the possibility to observe some form of metabolism within our reactor. Metabolism and some form of self-catalysis are necessary conditions for the continuing evolution of Molnet systems.

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REFERENCES

Colombano, S.P. "Towards a Theory of the Origin of the Genetic Code: the Complementary Roles of Chemical and Logical Constraints". PhD Dissertation, State University of N.Y. at Buffalo. 1977.

Dittrich, P. and Banzhaf W. “Self Evolution in a constructive binary string system”. Artificial Life, 4(2), 203-220. 1998.

Dittrich, P., and Ziegler, J., and Banzhaf W. Artificial Chemistries-A Review. Artificial Life, **7**(3):225-275. 2001.

Ehrenfest, P. and Ehrenfest, T. “Ueber zwei bekannte Einwaende gegen Bolzmannsche H-Theorem” Physikalische Zeitschrift, 8(9), 1907.

Eigen, M and Schuster, P. “The hypercycle: a principle of natural self-organization, part a.” Naturwissenschaften, 64(11) 541-565. 1977.

Fontana W. “Algorithmic chemistry”. In Langton, C.G., Taylor, C., Farmer, J.D., and Rasmussen, S. editors. Artificial Life II, pp:159-210. Redwood City, CA., Addison-Wesley. 1992.

Fontana, W. and Buss, L.W. “The barrier of objects: From dynamical systems to bounded organization”. In Casti, J. and Karlqvist, A. editors, “Boundaries and Barriers’, pp 56-116. Addison-Wesley, 1996.

Morris, H.C. “Typogenetics: A logic for artificial life” In Langton, C.G., editor, Artificial Life, pp 341-368. Addison-Wesley, 1989.

Segovia-Juarez, J. and Colombano, S. Mutation buffering capabilities of the hypernetwork model. Third NASA/DoD Workshop on Evolvable Hardware. 12-14 July 2001. Long Beach, CA., USA, pp 7-13, 2001.

Stassinopoulos, D., Colombano, S. P., Lohn, J. D., Haith,G. L., Scargle, J. and Liang, S. ``Spatial autocatalytic dynamics: an approach to modelling prebiotic evolution,'' Proceedings of the International Conference of Complex Systems , Nashua. Oct. 1998.

Zauner, K-P. and Conrad, M. “Conformation driven computing: Simulating the context-conformation-action loop” Supramolecular Science, 5(5-6), 791-794. 1998.

Ziegler, J., Dittrich, P., and Banzhaf, W. “Towards a metabolic robot controller”. In Holcombe, M. and Paton, R., editors, Information Processing in Cells and Tissues. pp 305-318, New York, Plenum Press, 1998.

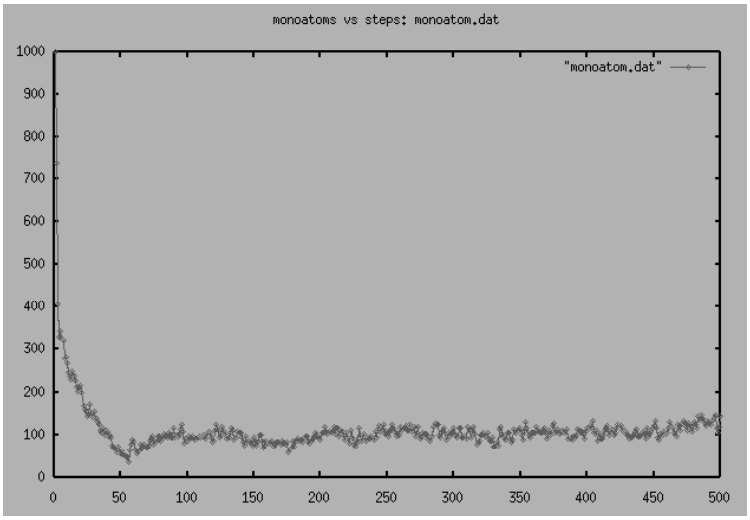
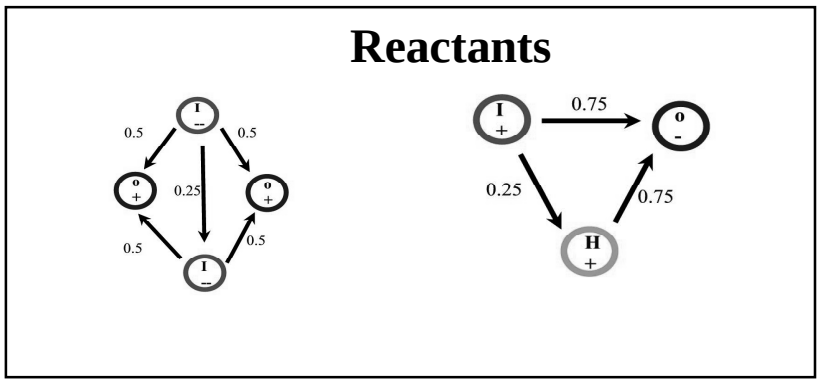
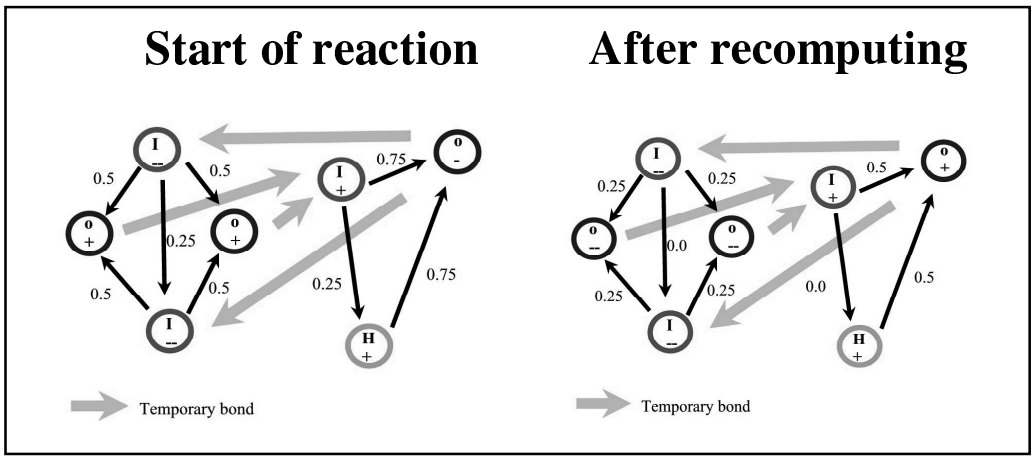


Figure 1. A vat starting with a 1000 single-atom molecules settles down to about 100 molecules of average size 10.





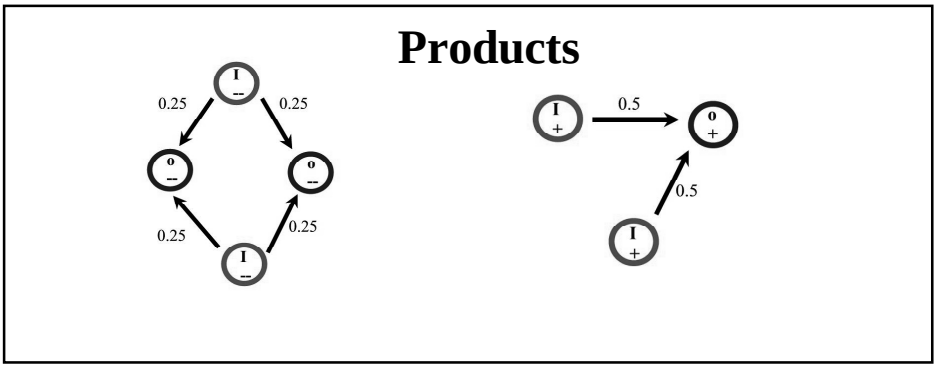
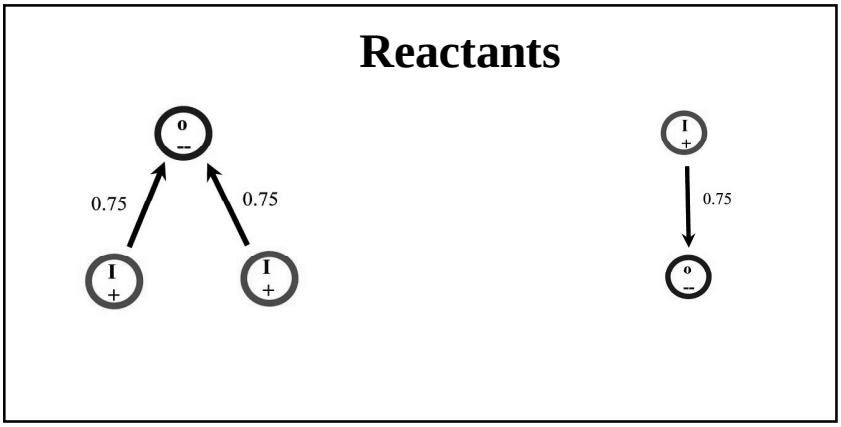
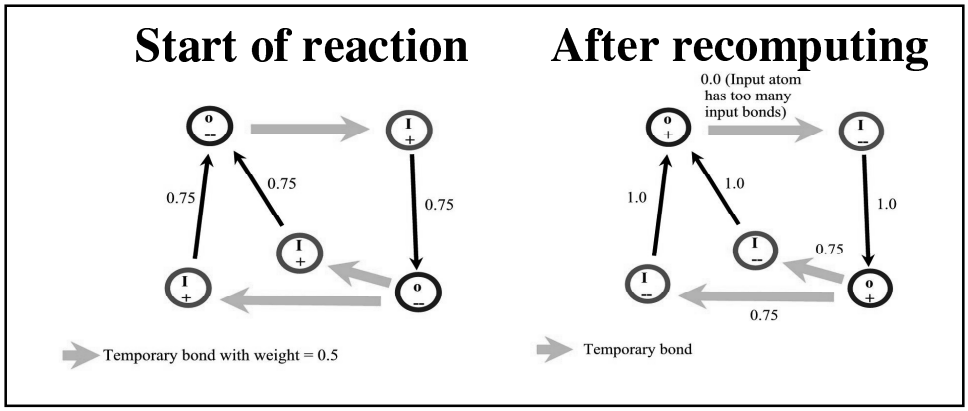


Figure 2. Top: intial molecules. Midde: reaction and temporary bonds before and after recomputing. Bottom: reaction products.





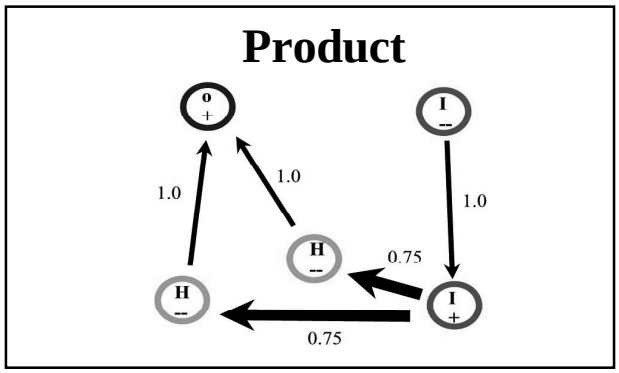


Figure 3. Top: Initial reactants. Middle: reactions and temporary bonds before and after recomputing. Bottom: final reaction product.

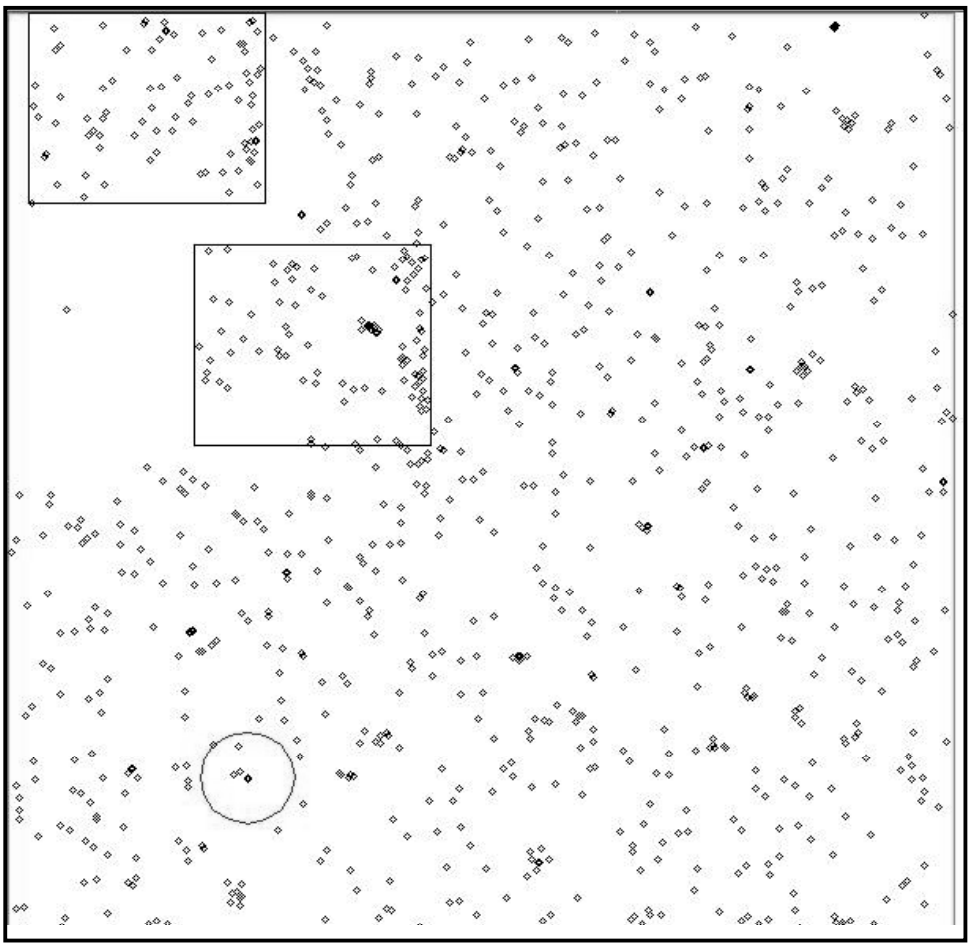


Figure 4. A typical reaction vat showing randomly distributed molecules. The rectangles are “membranes”. The circle in the lower left side is the reaction range of the molecule at the center.