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Evolving Catalytic Reaction Sets using Genetic Algorithms

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Outline

1. Pre-genomic Processes
2. Model of a Protocell
3. Computational Protocell Model
4. Artificial Chemistry
5. Evolution of Catalytic Reaction Networks
6. Experimental Results
7. Conclusion

Introduction

Possible steps to natural life	**Self-organizing Protocells** →	**Metabolism** →	**Self-replication**
Corresponding Areas in Artificial Life	**Synthesis of artificial prebiotic chemistries**		**Synthesis of artificial self-replicating systems**

Pre-genomic Processes

What kinds of dynamical processes could lead to the self-organization of protocells (precursors to the first living cells)?

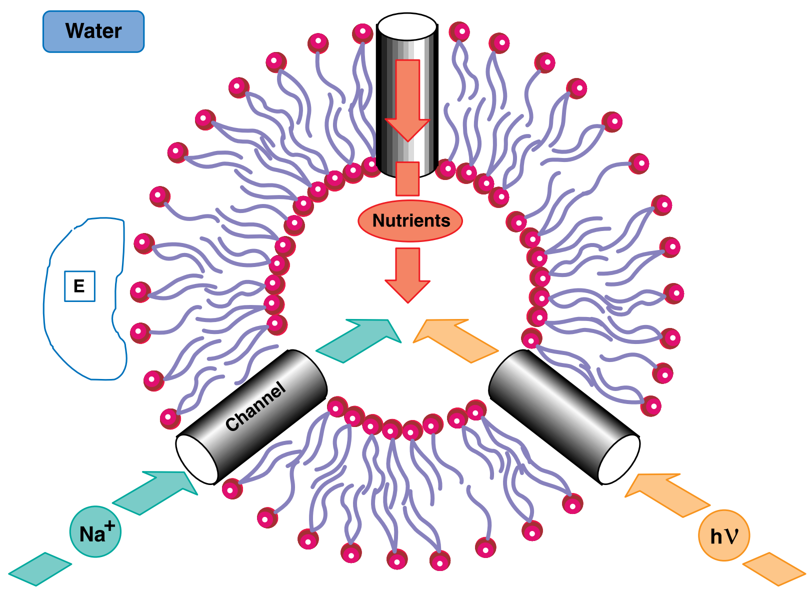
Understanding such processes could potentially be useful for:

- biologists (origins of life hypotheses, astrobiology)
- computer scientists (abstract into useful problem-solving techniques)
- nanotechnologists (molecular self-assembly)

Ongoing interdisciplinary research at NASA Ames Research Center (Astrobiology and Computational Sciences).

Model of a Protocell

Hypothetical protocell: bilayer, amphiphilic membrane

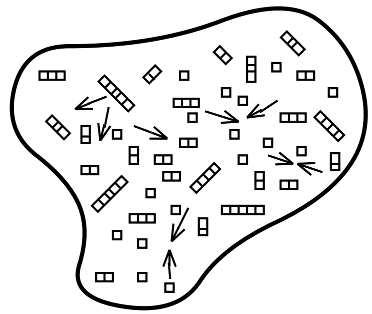


Basic functions (Pohorille, et. al., 1996):

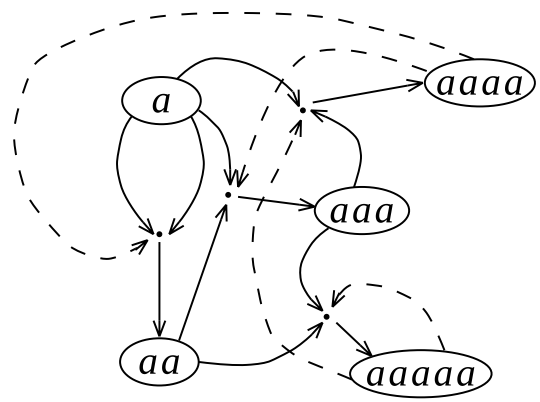
- transport of ions across membranes
- formation of energy source (photoactivated proton gradient) to drive chemical synthesis
- peptide organization for catalytic activity

Simple Computational Protocell Model

Interacting polymers enclosed in a protocell (well-stirred reactor)



Example of a catalytic reaction set: graphical depiction and reaction set. Reverse reactions are not shown explicitly in graph.



$$a + a \overset{aaaa}{\rightleftharpoons} aa \qquad a + aaa \overset{aaaaa}{\rightleftharpoons} aaaa$$

$$a + aa \overset{aaaa}{\rightleftharpoons} aaa \qquad aa + aaa \overset{aaaaa}{\rightleftharpoons} aaaaa$$

Artificial Chemistry

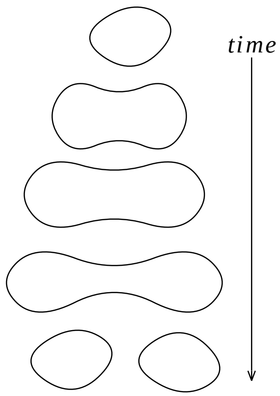
- simplified “polymers”: 1-letter alphabet
- reaction form: $A + B \overset{C}{\rightleftharpoons} P$
- maximum length allowed is 34
- reactions that produce polymers longer than 34-mers are not permitted (illegal)
- polymers are randomly sampled from the reactor (well-stirred condition)
- a chemistry is specified completely by a list 100 reversible reactions and the rules specified above

Problem Description

Objective:

> *Find a set of N reactions that moves a pre-specified initial distribution of polymers to an arbitrary distribution of (longer) polymers.*

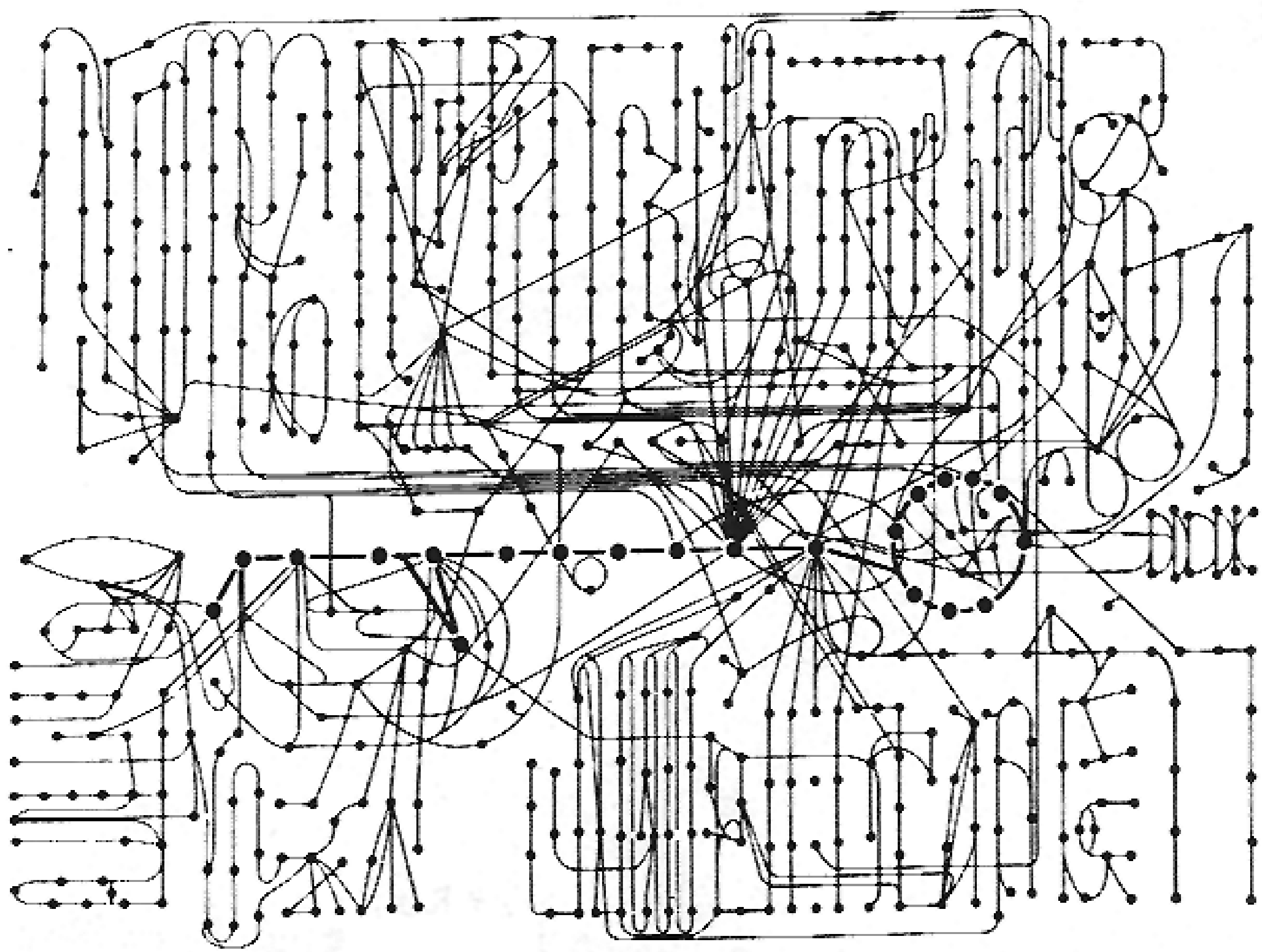
Such "catalytic engines" may have formed in prebiotic protocells and may have been selected as protocells enlarged and divided.



"Programming" such chemistries manually proves difficult.

From past successes in applying GAs to evolving rule-based systems, we used GAs to evolve simple artificial chemistries

“Simplified” view of reaction network for biological cells:

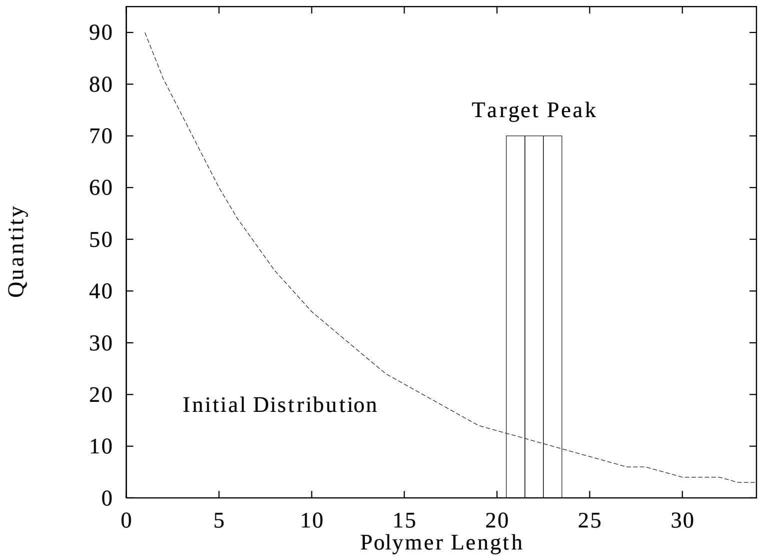


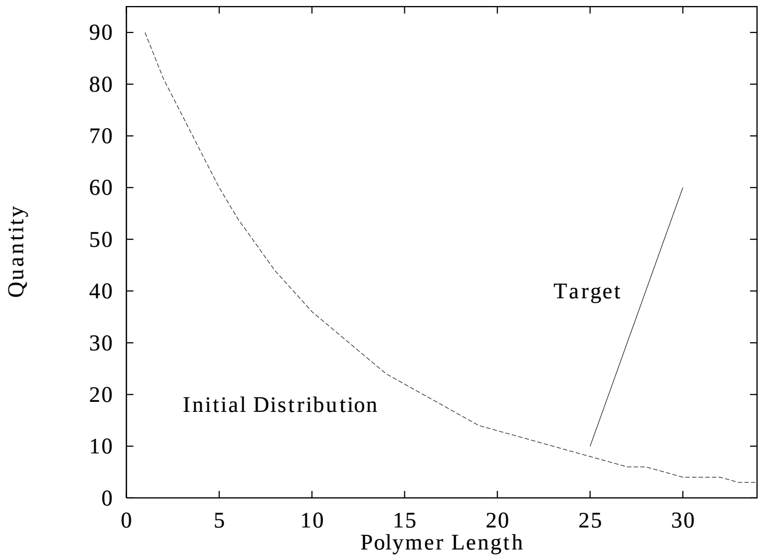
• denotes enzymatic action

from *The Cell*, Alberts, 1983

Two Experiments

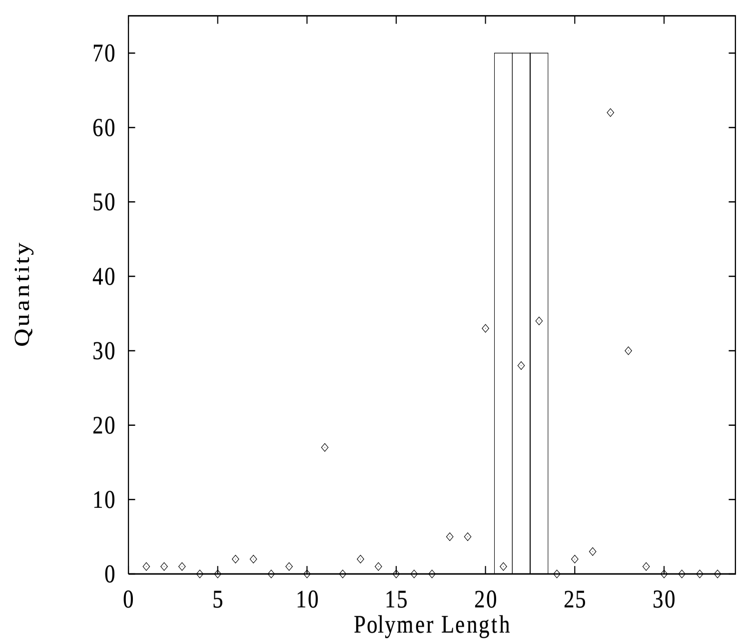
"Peak" and "slope" experiments: both have the same decaying exponential distribution for the initial conditions

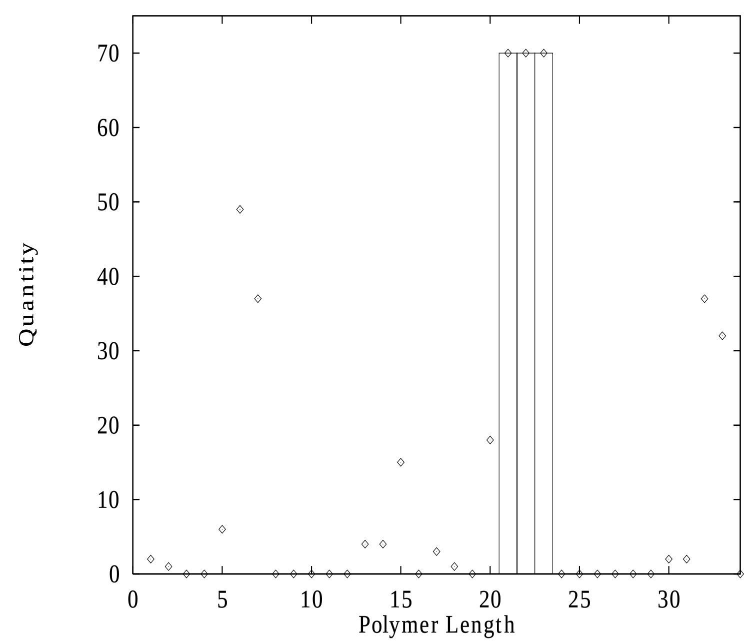




Results

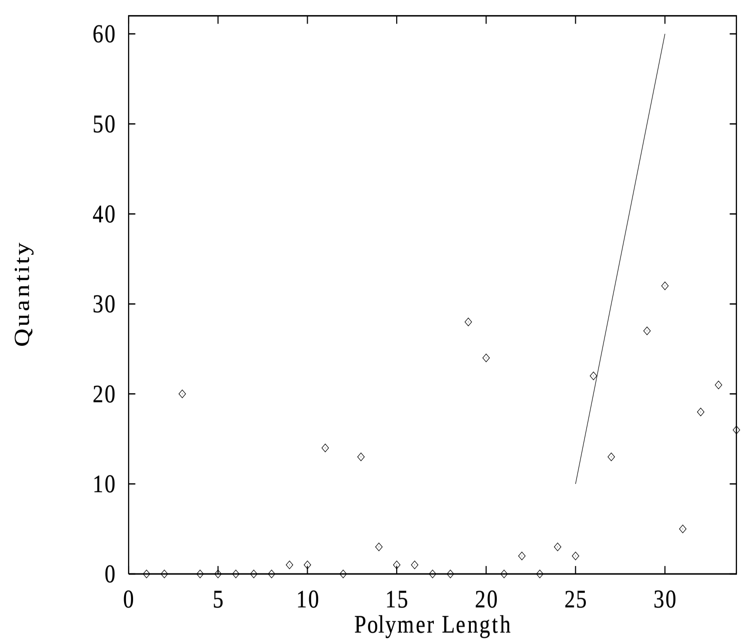
Distributions resulting from best individuals from generations 0 and 166 of the "peak" experiment

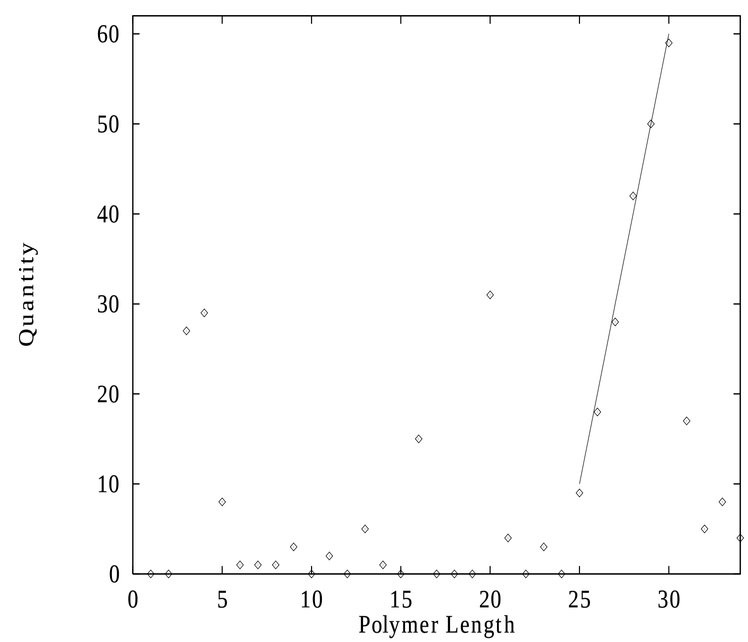




Results

Distributions resulting from best individuals from generations 0 and 118 of the "slope" experiment





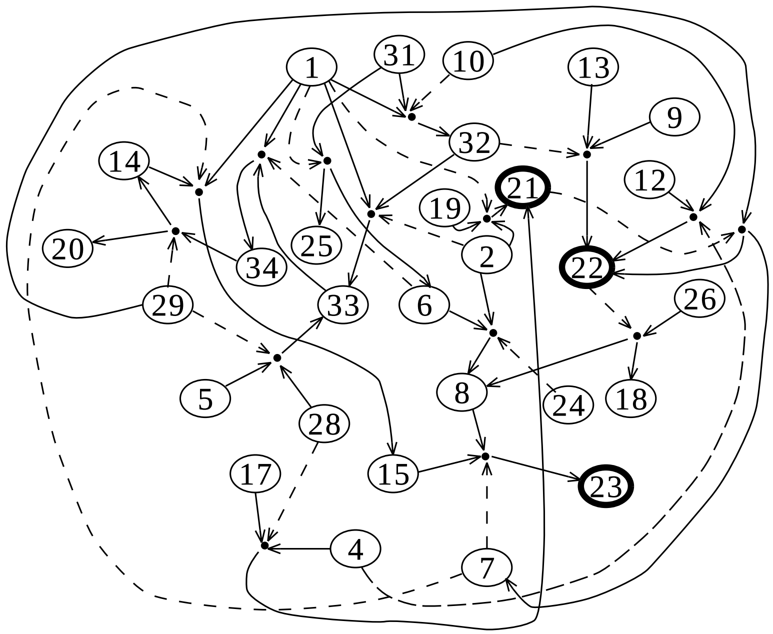
Evolved Reaction Network

Evolved reaction network:

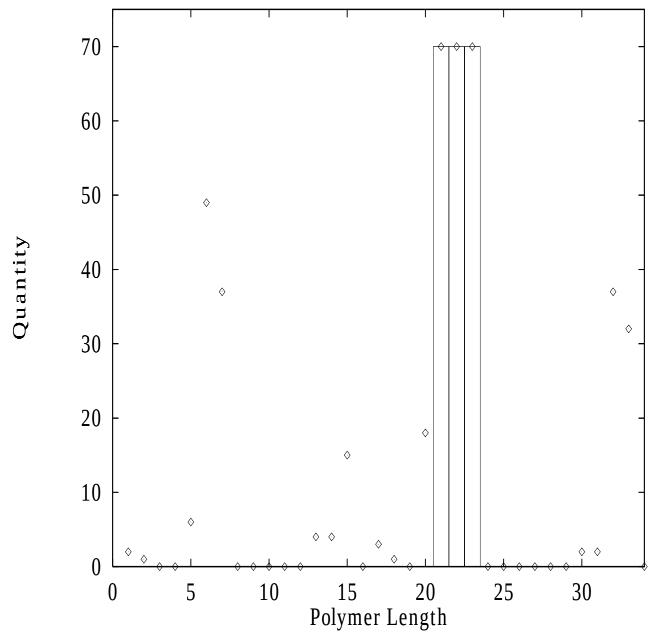
- short cycle formation
- key polymers acting as both reactants and catalysts
- target polymers acting as catalysts

Best found reaction set from 100 GA runs:

partial reaction graph:



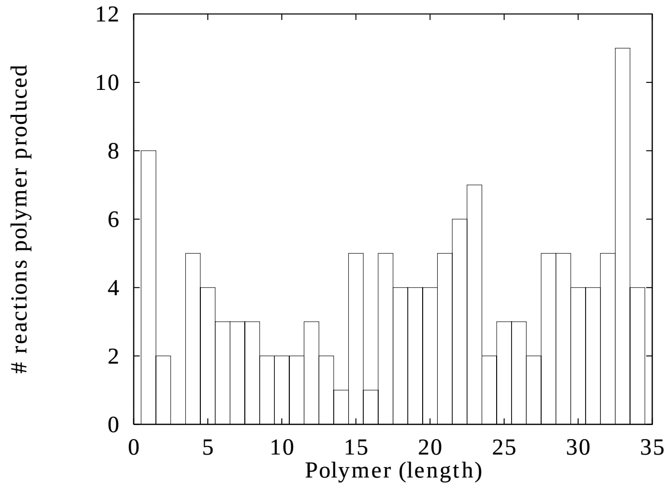
resultant distribution:

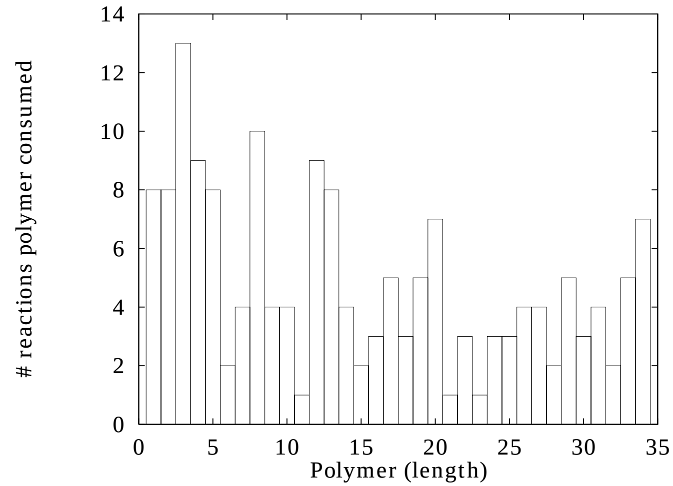


Producer/Consumer Relationship

Polymer production and consumption in the best-found reaction set for the "peak" experiment

Left: net number of times each polymer was a product; Right: net number of times each polymer was consumed





Conclusions

From these early results, we have demonstrated that simple, artificial chemical reaction networks can be synthesized to move a system of polymers into states of increasing complexity.

The reaction sets found are robust in the sense that they produce desirable behavior in equilibrium.

Ongoing efforts:

- restriction to more biochemically plausible reactions
- two and three-letter alphabets and longer polymers
- membrane functionality
- communities of interacting protocells