SimSoup: Molecules Designed for Switchable Autocatalytic Memory

Abstract

A Chemical Memory System

- This work shows a memory system based on reaction processes in an artificial chemistry
- The system consists of multiple chemical memory units co-existing in the same physical environment
- Each unit can be switched between three states corresponding to different autocatalytic reaction processes
- Switching occurs when an external stimulus triggers the autocatalytic reaction process for a new state; an associated inhibiting process stops activity for the old state
- The system has memory. This is evident from the persistence of the new state following a stimulus

Molecular Structures for Memory Processes

- Artificial molecular structures *designed* to support the autocatalytic and inhibiting processes are shown
- The SimSoup artificial chemistry simulator is used to confirm the memory system behaviour

Origin of Life and Biological/Chemical IT Uses

- The work provides a 'proof of concept' for *metabolism based inheritance* in Origin of Life scenarios not reliant on 'smart' template molecules such as DNA and RNA
- With the advent of engineering at the molecular level, it may be possible to transfer the concepts from an *in silico* environment to a 'real' chemical environment

Introduction

Background and Motivation

Inheritance at the Origin of Life

- Contemporary organisms and viruses use DNA or RNA template molecules for inheritance
- These molecules are too complex to be plausible in the pre-biotic world
- Some Origin of Life theories envisage metabolism based inheritance in which protocells or lipid enclosed droplets without template molecules reproduced by growth and division
- Variations in metabolism would have led to differences in fitness that would drive evolution
- Successful variations in metabolism would have to be 're-membered' and inherited
- The SimSoup project is investigating possible mechanisms for this

Biological and Chemical Computing

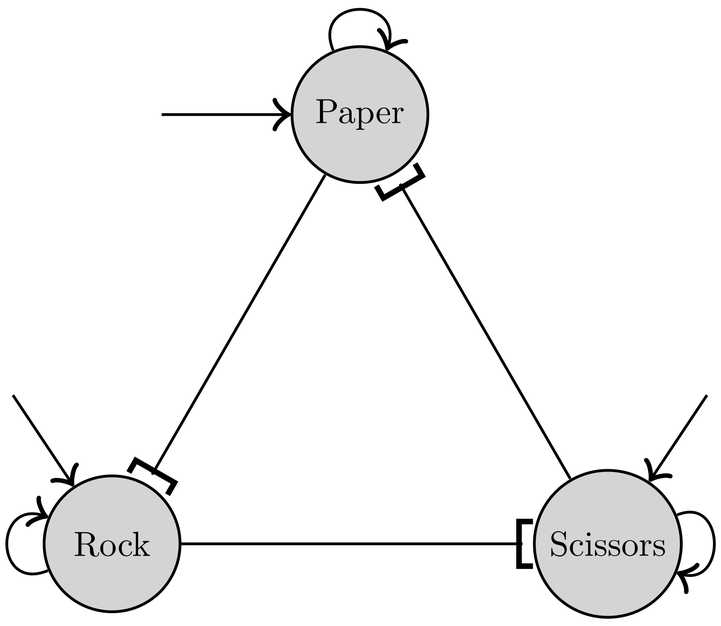
- A key challenge for the newer field of biological and chemical computing is the development of memory systems using components that can be readily constructed
- Such systems may be used for various purposes, including an inheritance mechanism for artificial evolution
- The simple memory mechanisms being investigated here is relevant to this

SimSoup Artificial Chemistry Model

- *Molecules* are two dimensional rigid structures built from *Atoms* bonded together such that they occupy fixed positions on a square 'board'
- Each square contains at most one Atom
- Each Atom Type has a defined maximum number of bonds
- Bond angles are always either 90° or 180°, and bond lengths are all equal
- Bonding is broadly consistent with valence theory
- Molecules join or split to form Molecules of different types
- Splitting occurs by breaking the weakest set of bonds that hold the Molecule into a single unit
- A split (eg $D \rightarrow E + F$) is called a *Fission Interaction*
- A join (eg $A + B \rightarrow C$), is a *Construction Interaction*
- Bond strengths are usually fixed according to the Atom Types, but some are *Perturbable*; they can be weakened or strengthened by other nearby Atoms
- Constructions and Fissions occur in a well-mixed *Reactor*

Memory Unit Outline

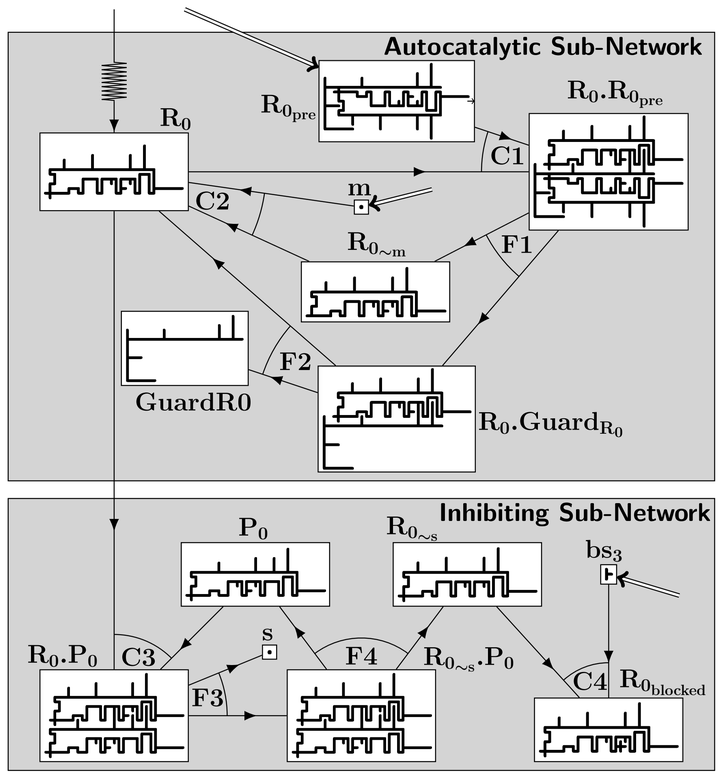
Concept: Rock-Paper-Scissors



- A memory unit has three possible active states; 'Rock', 'Paper' and 'Scissors'
- 'Loopback' arrows indicate autocatalytic feedback
- Straight arrows indicate external activating stimuli
- Lines terminated with '[' signify that activity for one state inhibits another
- Switching occurs when an external stimulus activates a new state, which simultaneously inhibits ('kills') the old state

Overview Of Memory Unit Design

Chemical Network and Molecular Structure 'Thumbnails' for Rock State of Memory Unit 0



- The figure shows both the structure of the (artificial) chemical network, and a 'thumbnail' structure diagram for each Molecule Type involved in maintaining and inhibiting the zeroth memory unit's 'Rock' state, Rock_0
- Labelled arcs between lines joining Molecule Types identify Constructions and Fissions
- Zig-zag arrow indicates an external activating stimulus
- Double arrows indicate a constant supply
- Overall Reactions:

$$\text{Autocatalytic: } R_{0_{pre}} + m \xrightarrow{R_0} R_0 + \text{Guard}_{R_0}$$

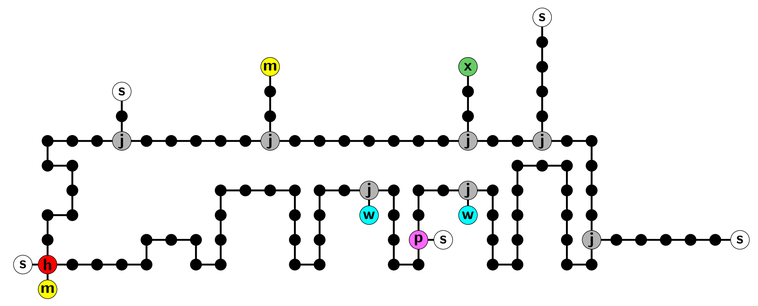
$$\text{Inhibiting: } R_0 + bs_3 \xrightarrow{P_0} R_{0_{blocked}} + s$$

Operation Of The Memory Unit

- A supply of $R_{0_{pre}}$, m and bs_3 is provided as 'food'
- The Autocatalytic Sub-Network is activated by a short stimulus of R_0 Molecules
- An excess of R_0 is produced, and so the Autocatalytic Sub-Network activity is self maintaining
- A later stimulus of P_0 activates the Paper_0 state
- This combines with R_0 to produce $R_0.P_0$ in the Inhibiting Sub-Network
- Subsequent Interactions F3, F4 and C4 disable R_0 by converting it to $R_{0_{blocked}}$. This inhibits the Rock_0 Autocatalytic Sub-Network, enabling Paper_0 to take over

Memory Unit Molecules

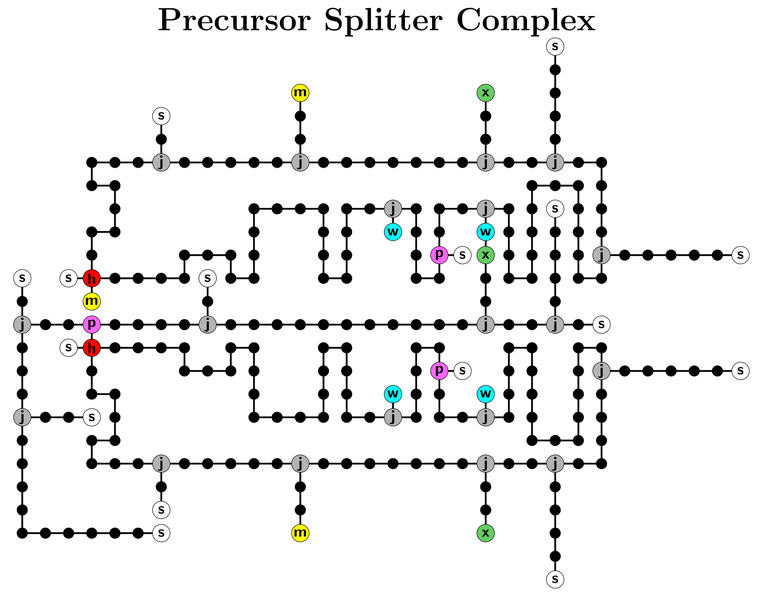
R_0: Core Molecule Type for the Rock_0 State[a]



- The three central recesses are key to the operation of the 'Rock-Paper-Scissors' mechanism

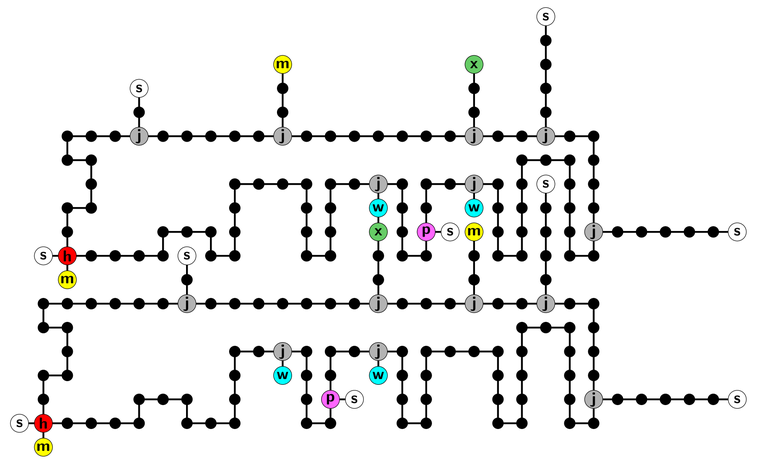
[a] Different Atom Types are shown with different colours. Eg 'Assemblite' is **black**, Hookite is **red**

Precursor Splitter Complex



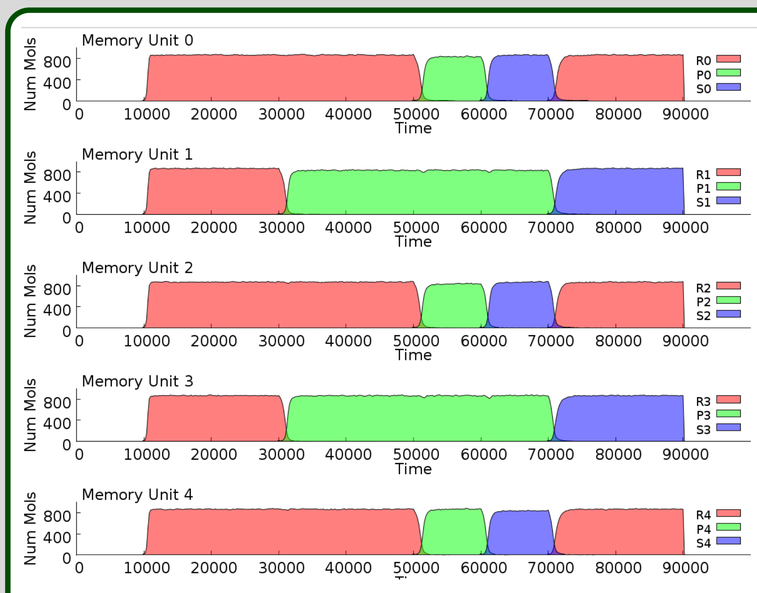
- The figure shows $R_0.R_{0_{pre}}$, the *Precursor Splitter Complex* for the Rock_0 Autocatalytic Sub-Network
- Top part is R_0. Lower part is $R_{0_{pre}}$, the *Precursor* for R_0
- The Precursor splits at the perturbed p–h bond

Core-Core Complex



- The figure shows *Core-Core Complex* $R_0.P_0$, the result of Construction C3. After F3, F4 and C4, R_0 is blocked
- This is the basis of the Inhibiting Sub-Network

Results



- A system of five co-existing memory units is switched between different states. For example, stimuli for P1 and P3 at time 30000 switch the system to state R0P1R2P3R4[a]

[a] These are 'stop press' results, based on improved versions of the Molecules shown above

Conclusions and Prospects

- An (artificial) chemical system can be switched between alternative states
- It has memory; it 'remembers' a new state
- The author would like to hear from anyone interested in translating this to 'real' chemistry