Molecules Designed For Network Memory And Evolution

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Presentation Objectives

Objectives For This Presentation

- Introduce SimSoup artificial chemistry model and simulator
- Show a ‘proof of concept’ design for a chemical memory bank implemented using a metabolic network
- Show initial SimSoup results for the design
- Ask: Can a metabolic memory bank be built using real molecules?

SimSoup Model

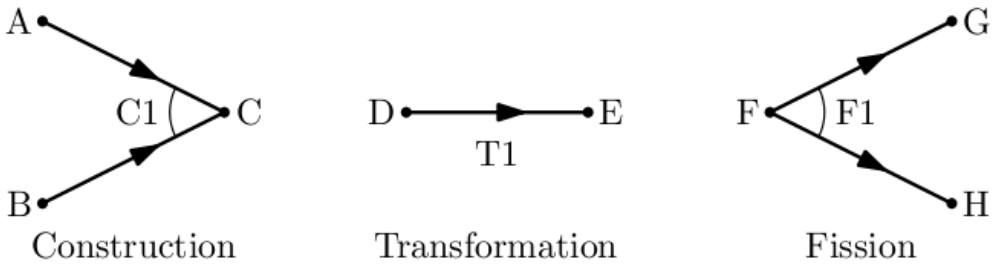
The SimSoup Project and Simulation Model

- The SimSoup project was initiated to investigate non-genetic mechanisms for evolution relevant to the Origin Of Life
- SimSoup is also the name of the artificial chemistry simulator that has been developed[a]

[a] The open source code is available at http://www.simsoup.info/SimSoup_Download_Page.html

SimSoup Model
Network Elements

Three Forms Of Interaction In SimSoup



$A + B \rightarrow C$ $D \rightarrow E$ $F \rightarrow G + H$

- Three forms of Interaction are possible in SimSoup[a]
  - Construction[b]: Two Molecules join
  - Transformation[c]: A Molecule re-arranges
  - Fission: A Molecule splits
- Interactions combine to form complex reactions

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[a] Constructions and Fissions in real chemistry can have more products.

[b] Termolecular reactions are rare.

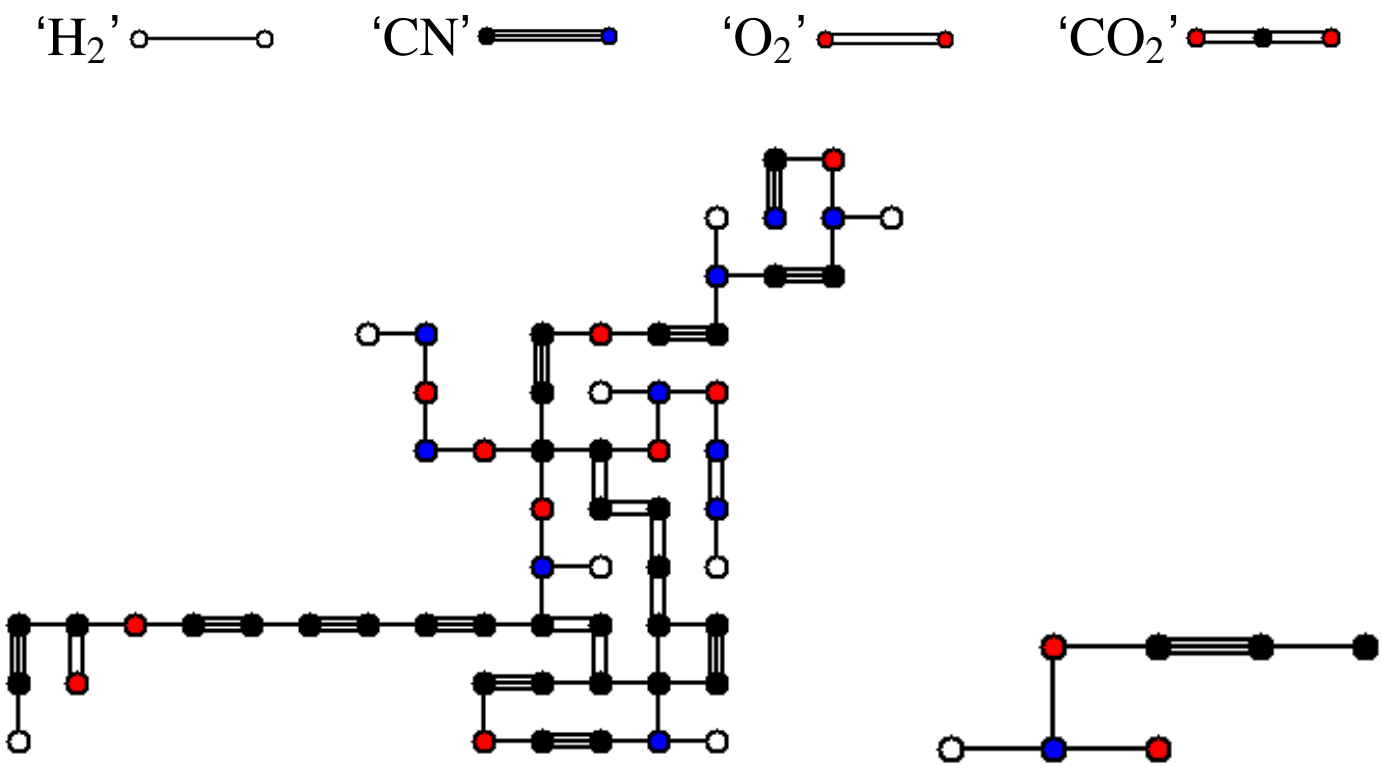
[c] Not implemented in latest version of SimSoup with molecular structure.

Molecular Structure In SimSoup

- Molecules are rigid two dimensional structures
  - Atoms are placed in a ‘board’ layout
  - All bond lengths are equal
  - All bond angles are 90° or 180°
  - Each board location can have at most one Atom
  - Each Bond has a Bond Order and a Bond Enthalpy (*bond strength*)
  - Bonds must satisfy valence bonding rules
  - Bonds can be perturbed (strengthened / weakened) by nearby atomic configurations

SimSoup Model
Molecular Structure

Some Molecules Constructed By SimSoup



SimSoup Model
Joining And Splitting

Joining And Splitting Molecule Types

- Molecules Split and Join according to rules analogous to real chemistry
- Joining: According to valence rules. Maximize total bond enthalpy. Atoms cannot overlap[a]
- Splitting: Break bonds with least total enthalpy

[a] In the current version of SimSoup, a Mass limitation is in place to limit computation.

The SimSoup Network Is Effectively Unlimited

- Molecule Types and associated Interaction Types are 'discovered' in an open-ended way
- The SimSoup chemical network is effectively unlimited

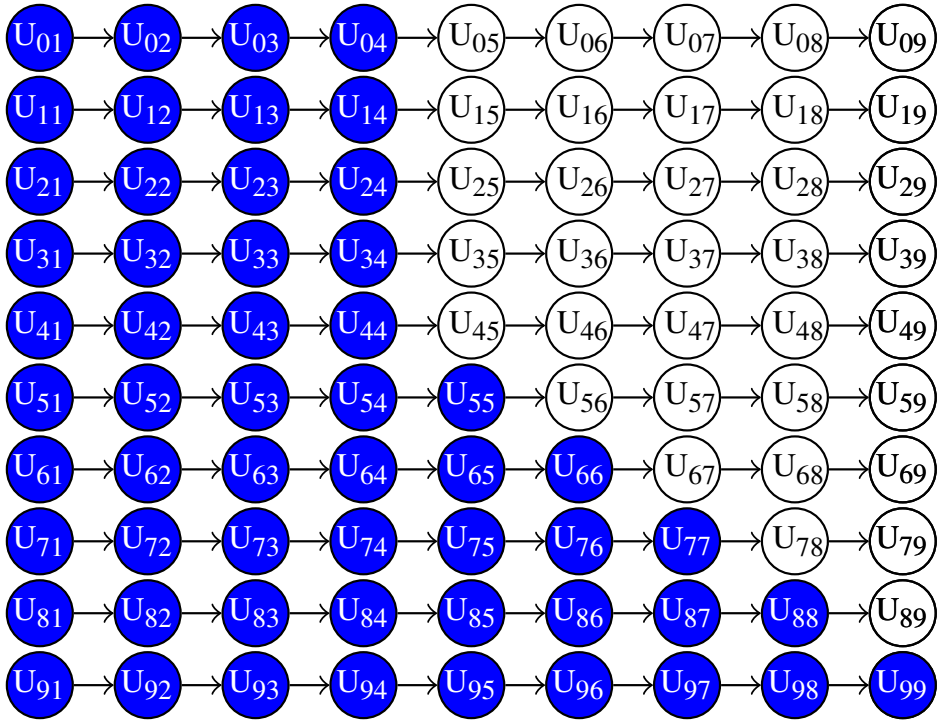
Memory Bank Design

Memory Bank Requirements

- All Molecules and Interactions must exist in the same environment - perhaps in a droplet
- The memory bank must have many alternative states
- The states of the metabolic network must be self maintaining
- Molecules and Interactions supporting different states must not interfere with one-another (no ‘side-reactions’)

Memory Bank Design
Overall Network

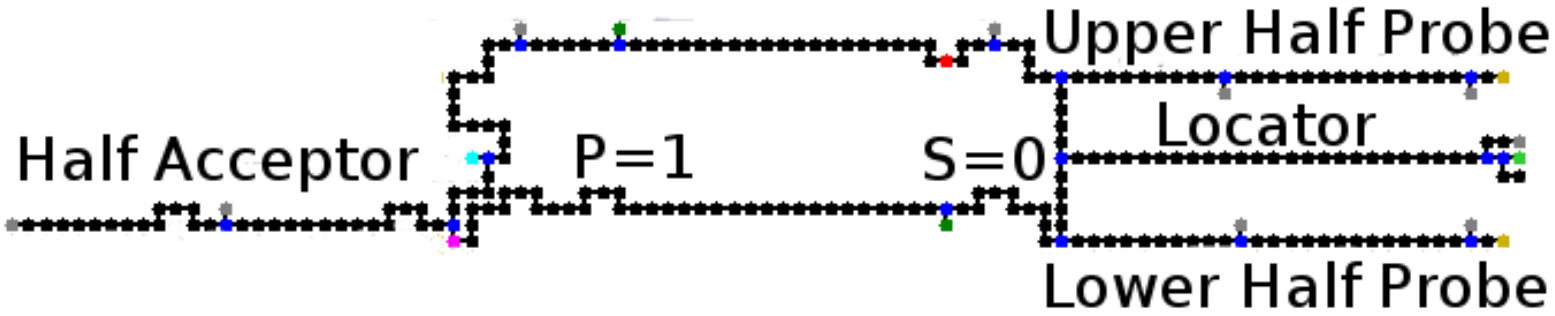
Memory Bank Network



- Each Unit:
  - Is activated by a particular Monomer. Eg U_{01} is activated by M_{01}
  - Extends a Polymer by adding a Monomer. Eg U_{02} adds M_{01} to Polymer P_{01}
  - Uses Polymers produced by its predecessor. (Except first unit in each series, which uses length 1 'Polymer' M_{s0} from food-set)
  - Splits a 'Closed Dimer' (food) to produce two activating Monomers
- The excess ensures the unit remains active
- There are 10^{10} possible states. State 4444456789 is shown

Memory Bank Design
Molecular Structures

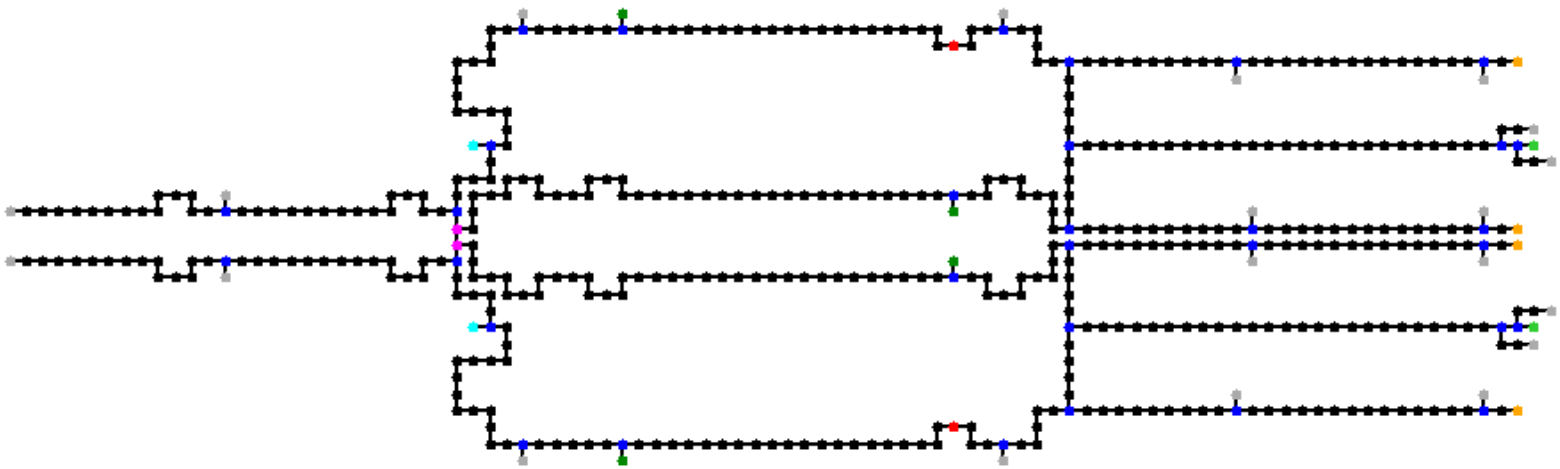
Monomer M_{01} Anatomy



- This monomer activates memory bank unit U_{01}
- The various recesses and protuberances support the 'lock and key' mechanism that ensure that Molecule Types in different memory units do not interfere

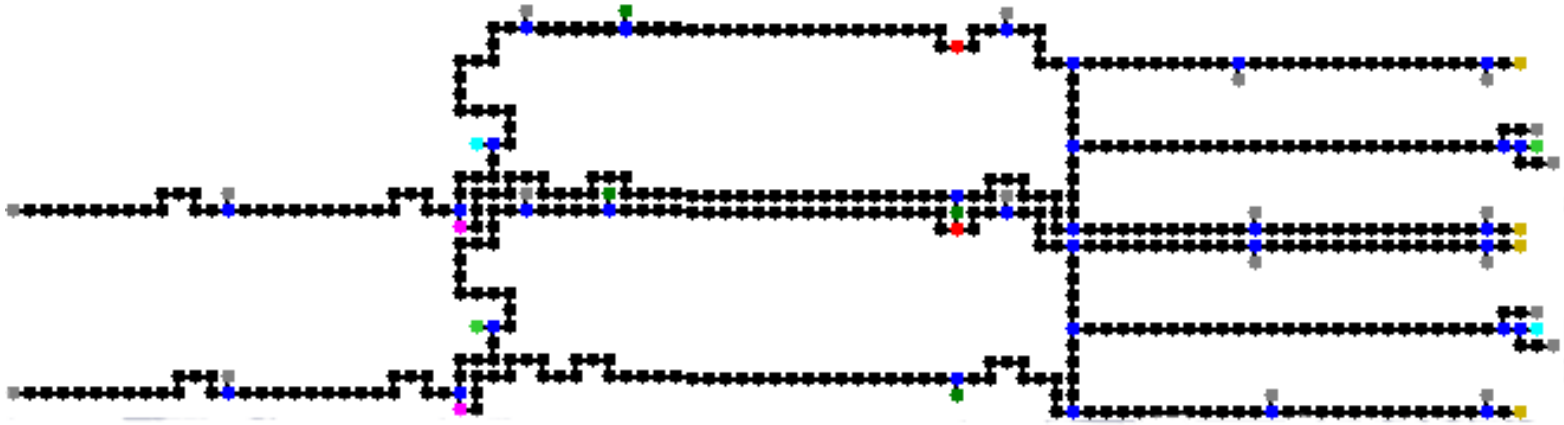
Memory Bank Design
Molecular Structures

Closed Dimer D_{01}



Memory Bank Design
Molecular Structures

Polymer P_{01}

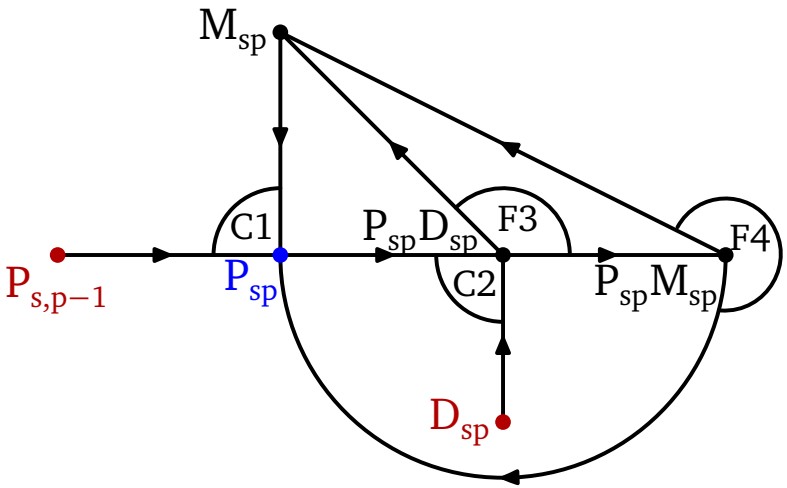


Memory Bank Design
Molecular Structures

Polymer P_{03}

Memory Bank Design
Memory Unit Sub-Network

Memory Unit Sub-Network



$$P_{s,p-1} + M_{sp} \rightarrow P_{sp} \quad \text{C1}$$
$$P_{sp} + D_{sp} \rightarrow P_{sp}D_{sp} \quad \text{C2}$$
$$P_{sp}D_{sp} \rightarrow P_{sp}M_{sp} + M_{sp} \quad \text{F3}$$
$$P_{sp}M_{sp} \rightarrow P_{sp} + M_{sp} \quad \text{F4}$$

Two State Memory Unit: Once Activated It Stays Active

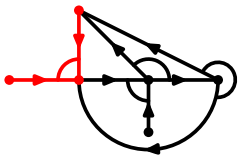
- Overall scheme: $P_{s,p-1} + D_{sp} \xrightarrow{M_{sp}} P_{sp} + M_{sp}$
- $P_{s,p-1}$ and D_{sp} are 'food'
- M_{sp} activates memory unit. Excess keeps unit active
- P_{sp} is input to next memory unit
- Limitation: This version of unit is not switchable[a]

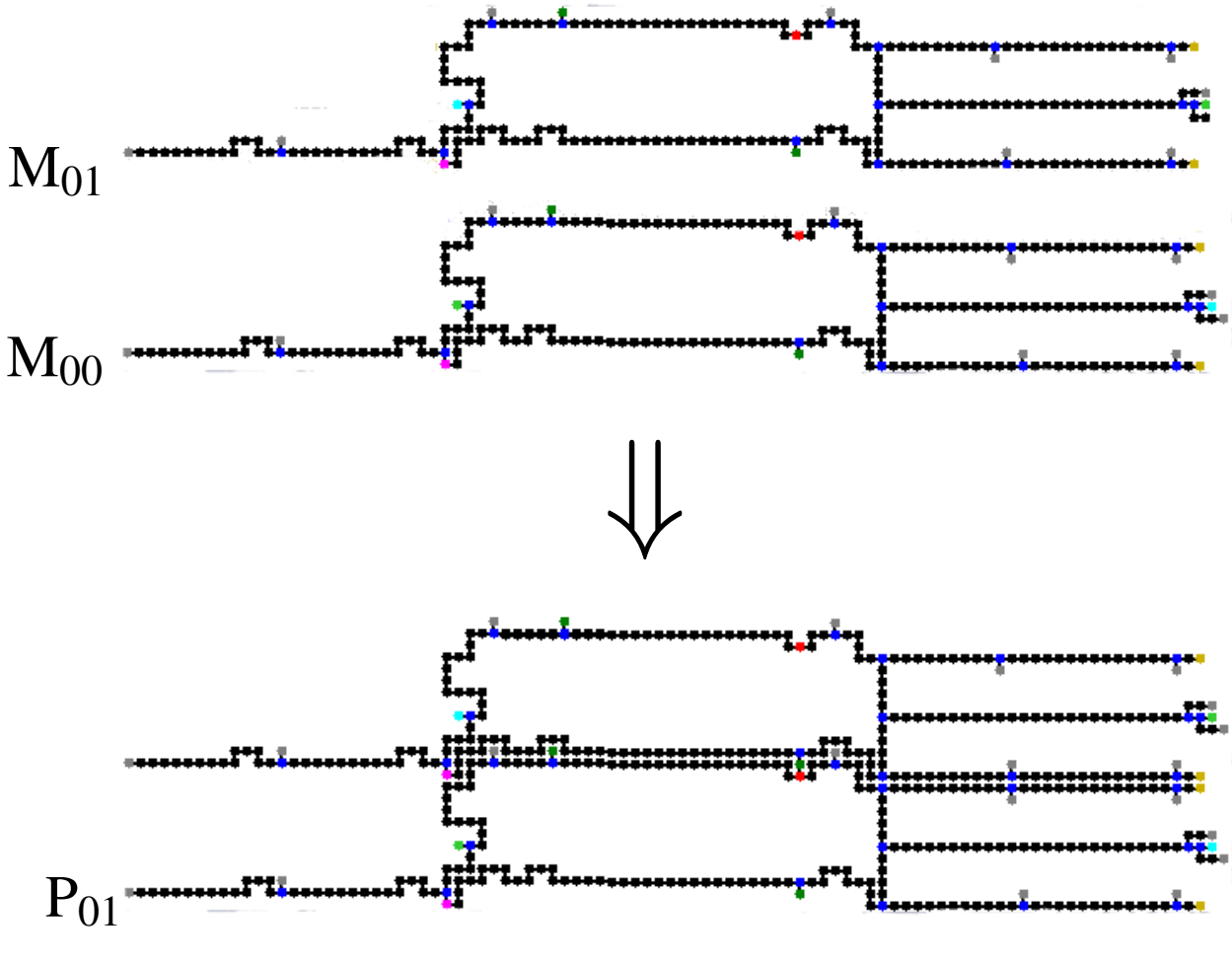
[a] but evolution *is* supported

Memory Bank Design

Memory Unit Interactions

Construction C1 - Polymerisation: $M_{00} + M_{01} \rightarrow P_{01}$

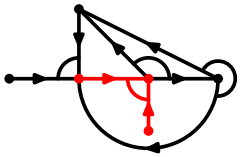


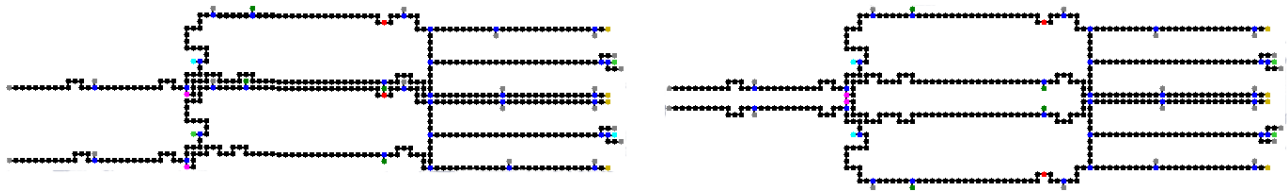


Memory Bank Design

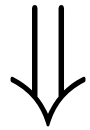
Memory Unit Interactions

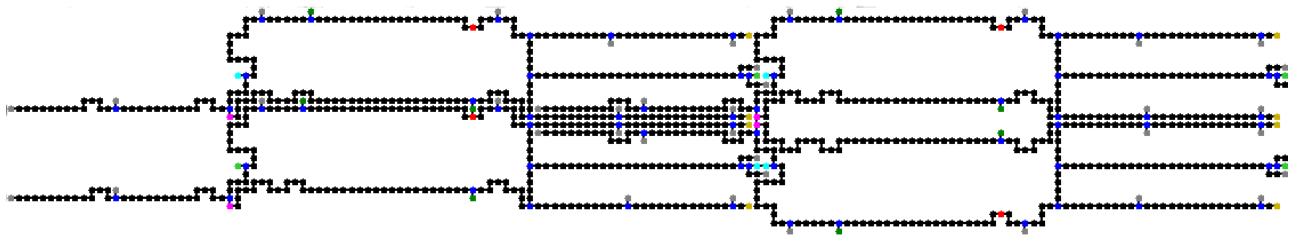
Construction C2: The Dimer Is Weakened





$P_{01} + D_{01}$

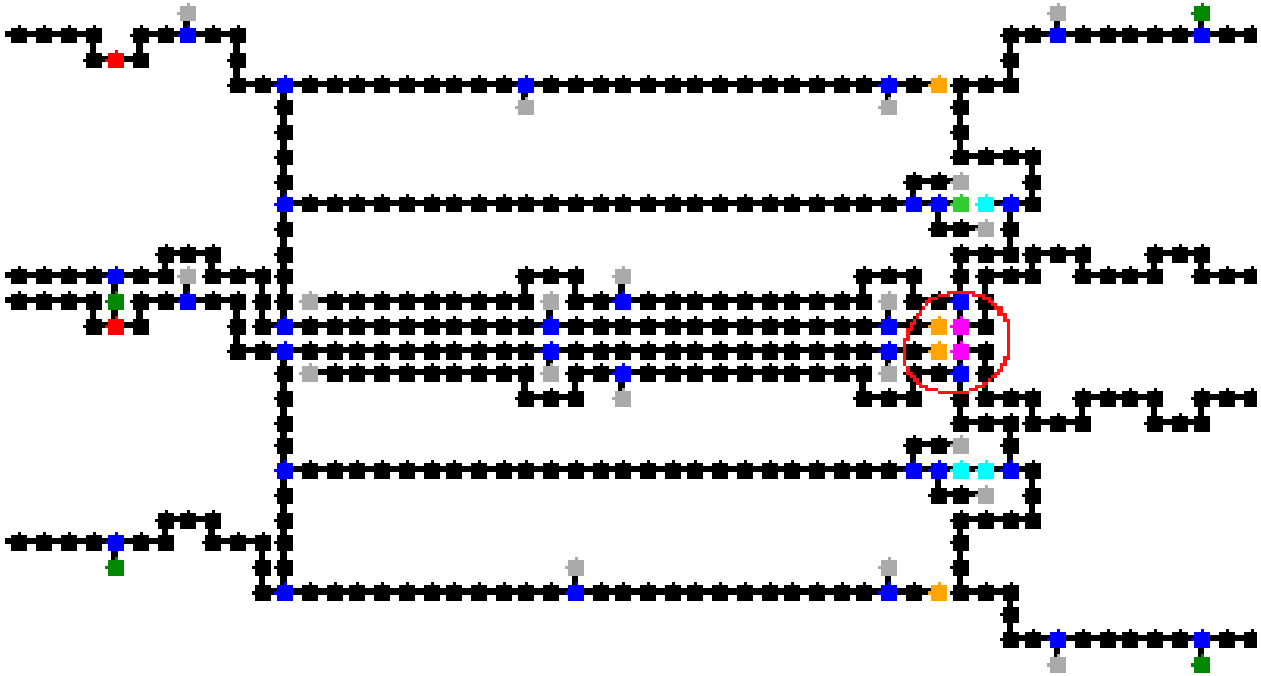




$P_{01}D_{01}$

Memory Bank Design
Memory Unit Interactions

Closeup of $P_{01}D_{01}$

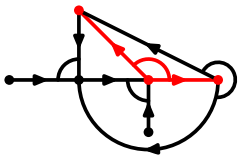


Perturbium-Perturbium bond is weakened by nearby Metal Atoms

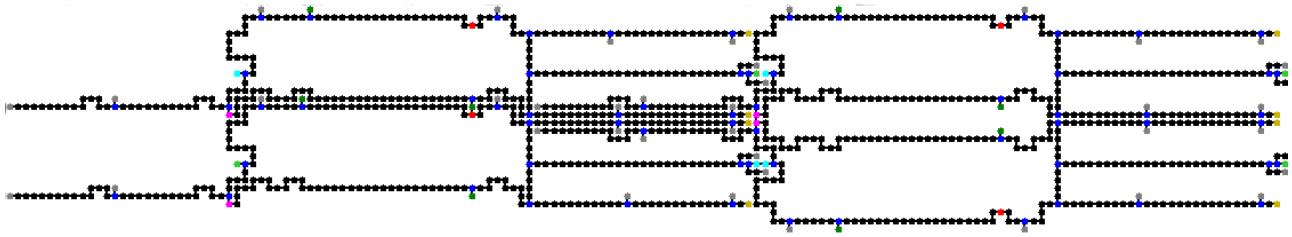
Memory Bank Design

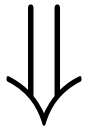
Memory Unit Interactions

Dimer Splitting



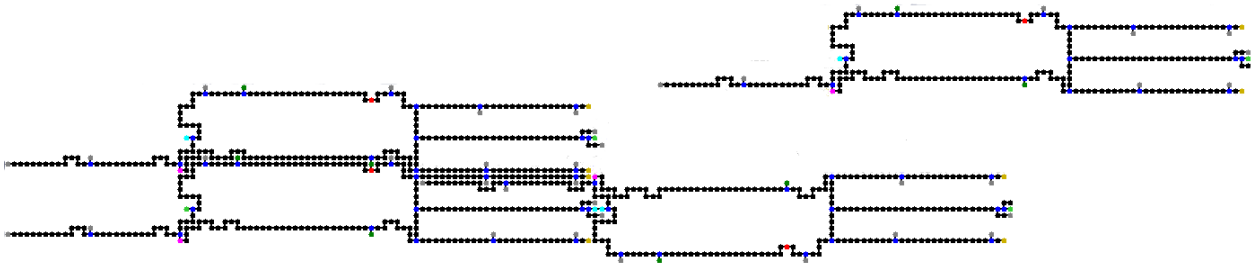
$P_{01}D_{01}$





$P_{01}M_{01}$

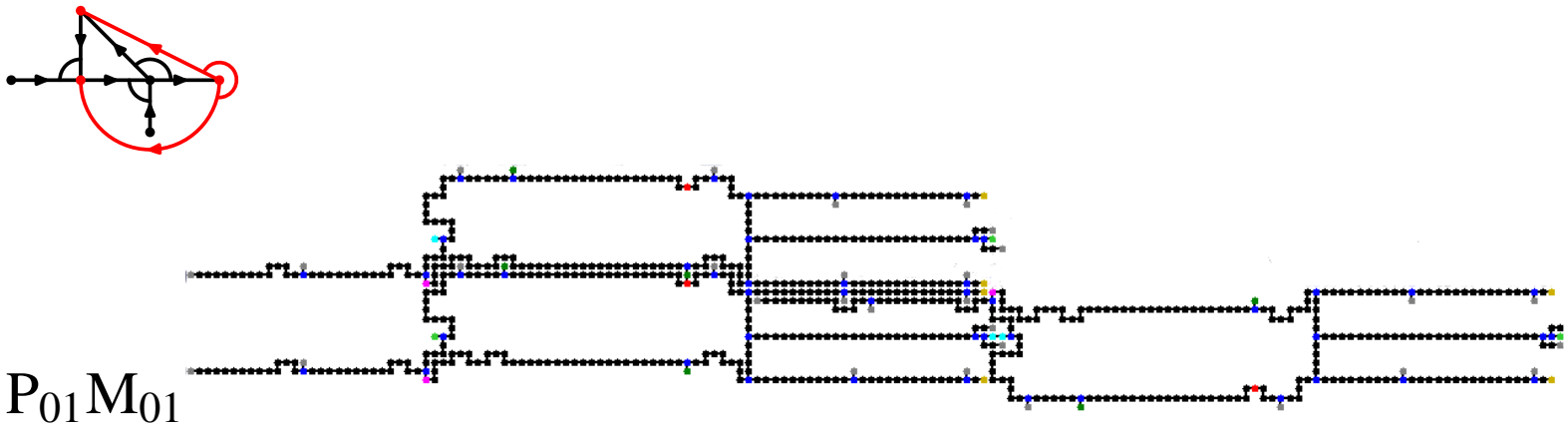
M_{01}



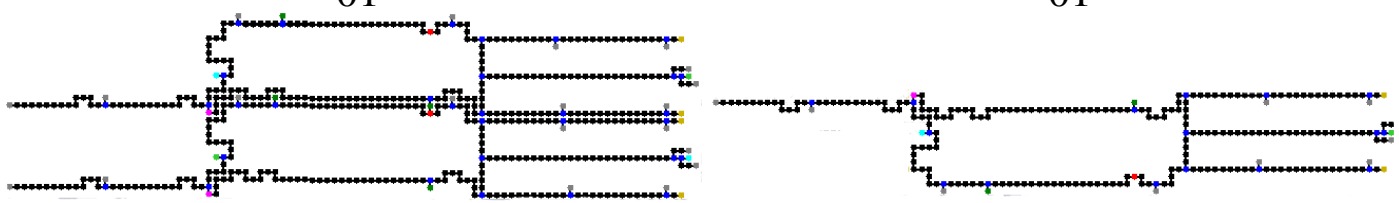
Memory Bank Design

Memory Unit Interactions

An Additional Monomer Is Released



$P_{01}M_{01}$



P_{01} M_{01}

Memory Bank Operation

In This Section...

Results of a SimSoup run demonstrating four states in Series 0 of the memory bank

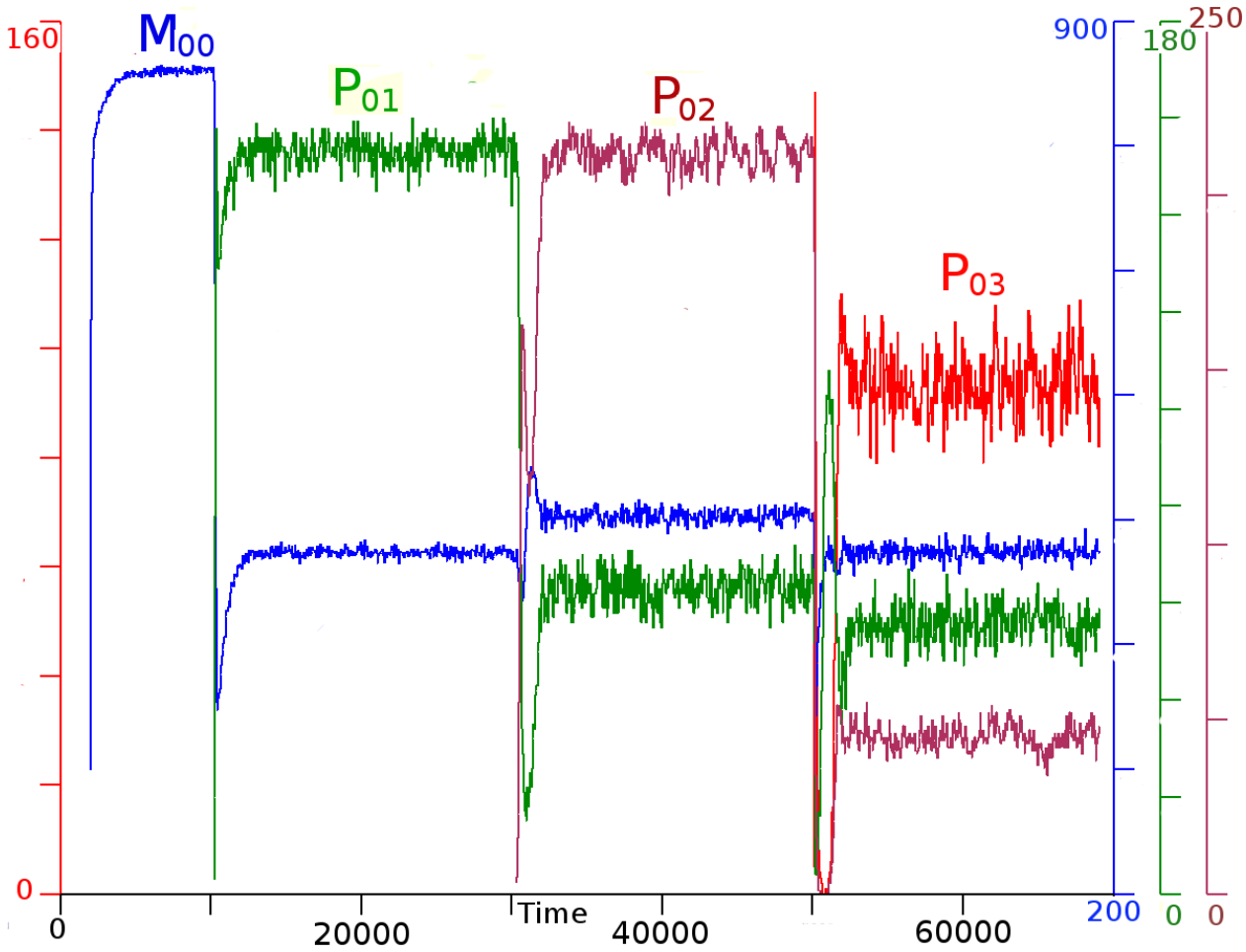
Memory Bank Operation
Model Scenario

Simulation Setup

- Food - Every 10 seconds, add:
  - 400 Molecules of M_{00}
  - 200 Molecules of each of $\mathrm{D}_{01}, \mathrm{D}_{02}$ and D_{03}
- Leakage: At each timestep, each Molecule has removal probability of 0.001
- One Molecule of each of $\mathrm{M}_{01}, \mathrm{M}_{02}$ and M_{03} is added at t = 10000, 30000, and 50000 respectively

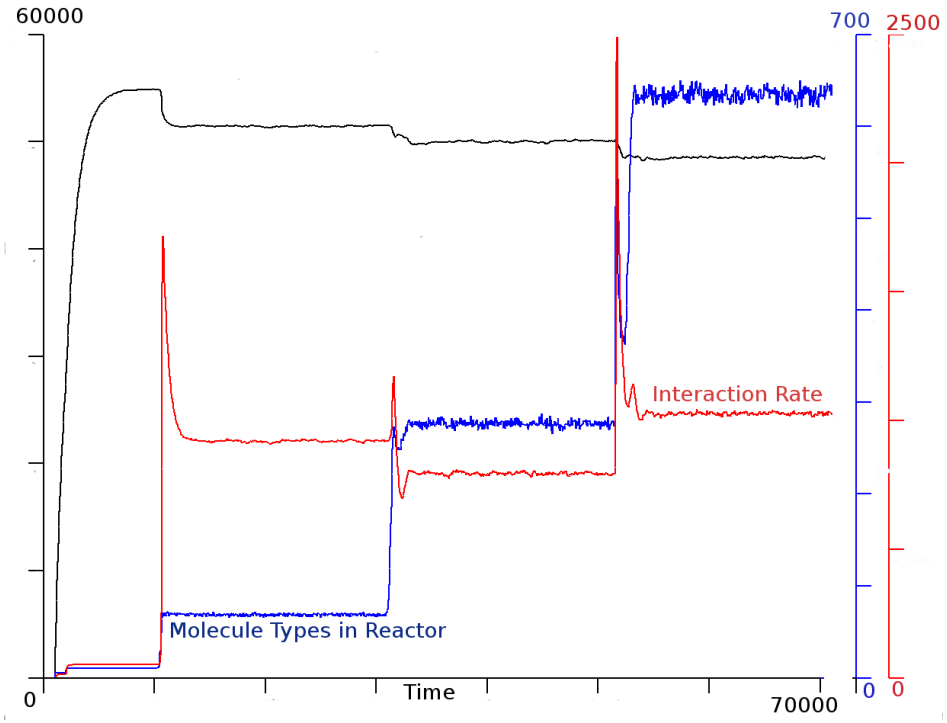
Memory Bank Operation
Results

Time Series Plots Of M_{00} and Series 0 Polymers



Memory Bank Operation
Results

Reactor Overview Plots



- In the P_{03} state, there are about 50,000 Molecules, and over 600 Molecule Types
- The network is more complex than intended ‘by design’, but this is not disrupting the operation

Conclusions And Prospects

Conclusions

- The memory bank design supports 10^{10} states
- Preliminary results demonstrate the basic operation
- Tests so far showed only a limited number of states

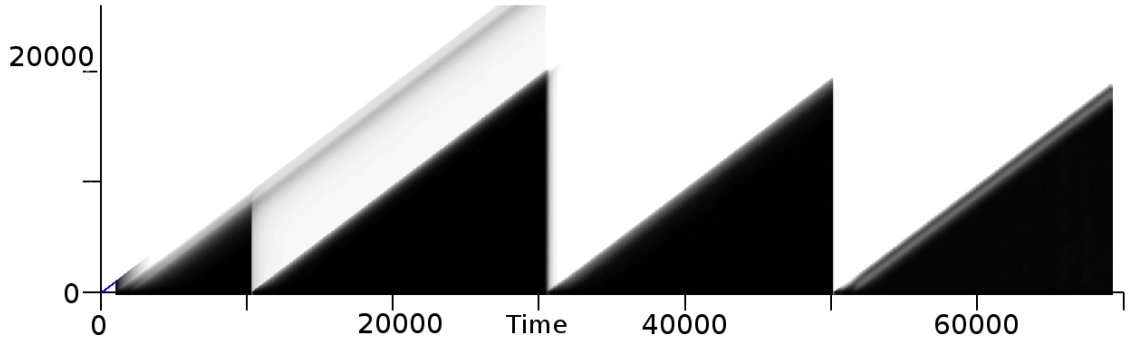
Prospects

- Extend the design to make the memory unit switchable
- Test for a large number of states
- Remove the mass limitation on Constructions
- Transfer to BioChemIT?
  - Molecular structures would probably be completely different
  - Switching would be needed

Comments / Questions?

Memory Bank Operation
Results

Manhattan Plot



Manhattan Plot

- Horizontal axis is ‘current’ time
- Vertical axis is time before current time
- A dark point indicates a time at which the composition of Molecule Types is close to that at the earlier time
- The dark triangles represent periods of stable Molecular composition