SimSoup Project - www.simsoup.info

SimSoup: Artificial Chemistry Meets Pauling

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Introduction and Motivation

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Theories of the Origin of Life can be categorised as 'template replication first' and 'metabolism first'. A key question for metabolism first theories is the mechanism for transfer of inherited information.

The motivation for the SimSoup project is to show that a metabolic network has sufficient information carrying properties to enable evolution to begin without the assistance of highly evolved molecules such as proteins or DNA.

Earlier work presented a mechanism based on catalytic cycles, along with supporting results from the SimSoup artificial chemistry simulator[a]. Here, an enhanced model that is more open ended and closer to real chemistry is presented. Molecules and the types of Interactions between them are constructed by the model itself using simple rules based on valence theory.

[a]The C++ source code for SimSoup is available at http://code.google.com/p/simsoup/

Conceptual Background

- Metabolic theories of Aleksandr Oparin, Stuart Kauffman, Freeman Dyson, Fernando and Rowe, and the Lipid World theory of Doron Lancet's group
- Network theory, including the work of Sanjay Jain and Sandeep Krishna
- Günter Wächtershäuser's chemo-autotrophic Iron-Sulphur World
- Chemical bond and valence theory as developed by Linus Pauling and others

SimSoup As A Network Simulator

Chemical Network

- Molecule Types (species) are represented as network nodes
- Interaction Types (reactions) are represented as connections
- Molecule Types have Mass and Potential Energy
- Interaction Types take three forms: Construction ($A + B \rightarrow C$), Fission ($A \rightarrow B + C$), and Transformation ($A \rightarrow B$)
- Rate Constants are thermodynamically realistic

Network Dynamics

- Interactions take place between Molecules in a well stirred Reactor
- Rate of a bimolecular Interaction Type (Construction) is the product of the Rate Constant and the concentrations of the two Reactants
- Rate of a unimolecular Interaction Type (Fission or Transformation) is the product of the Rate Constant and the concentration of the (single) Reactant

Compound Interactions and Catalysis

- Interaction Types can be combined in ways that have catalytic properties
- $A + X \rightarrow I$ followed by $I + B \rightarrow J$ and finally $J \rightarrow X + C$ make up a Compound Interaction with overall scheme $A + B \xrightarrow{x} C$
- X operates as a catalyst

Trackers and Cycle Detection

- Trackers follow actual reaction paths, enabling cycle detection

Reactor Composition and The Manhattan Plot

- Variability in the molecular composition of the Reactor can be plotted

SimSoup Extended As A Network Explorer

A More Open-Ended Approach - Adding Molecular Structure

- Each Molecule Type has a structure
- Molecules can Join or Split to form Molecules of different types
- Joining and Splitting occur in ways that depend on the structural properties of the Reactant(s) and are analogous to real chemistry
- The rules are conceptually simple and computationally tractable
- The open ended approach provides a vast number of opportunities for novelty, perhaps approaching the range of real chemistry

Molecular Structure in SimSoup

- Molecules are two dimensional rigid structures in a square 'Board' layout
- Bond angles are always 90° or 180°, and bond lengths are all equal

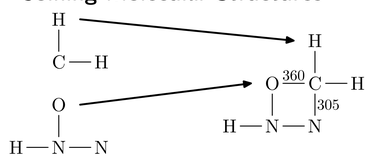
Atom Types and Maximum Possible Bonds

- Each Atom Type has a maximum number of possible bonds
- Examples include: Hydrogen - 1, Carbon - 4, Nitrogen - 3, Oxygen - 2

Bonds, Bond Order and Bond Energy

- SimSoup models single, double and triple order (covalent) bonds, so that each of the following is possible: O—H, C═O, O═C═O, C≡N
- Bond Energies are the averages for corresponding bonds in real chemistry

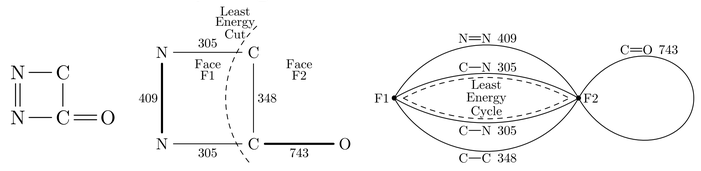
Joining Molecular Structures



Two Molecules can Join (Construction) subject to the following rules:

- Two Atoms cannot occupy the same Board position
- No Atom can exceed the maximum number of Bonds for its Atom Type
- Bond energy is maximised. If Molecules can Join in different ways, as in the above example, a Join that maximises total Bond Energy is chosen

Splitting Molecular Structures



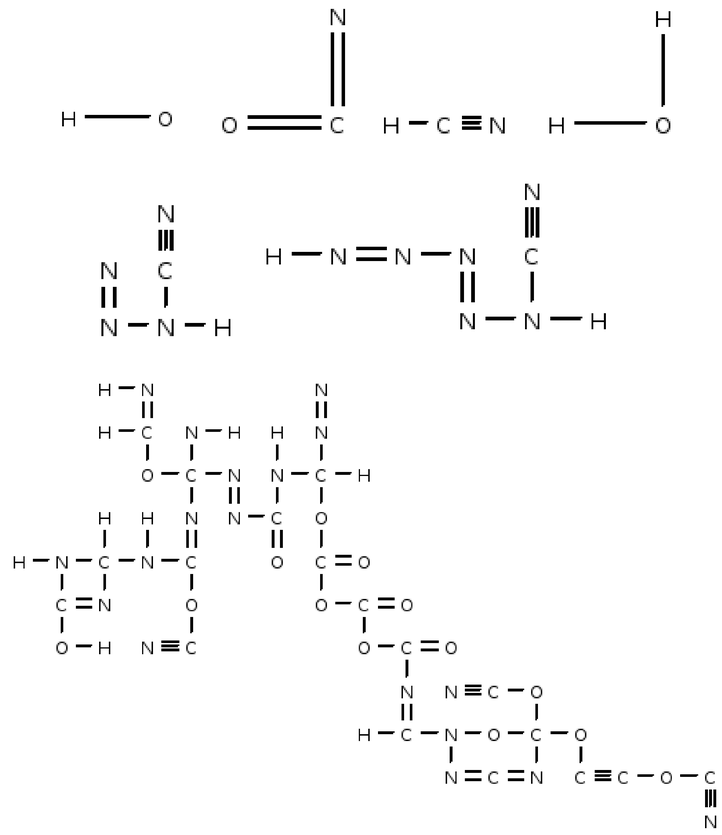
The Splitting (Fission) algorithm uses techniques of graph theory[a]. It considers alternative splits and identifies a 'Least Energy Cut'. This is a set of Bonds which, if broken, will separate the Molecule into two parts. Main steps are:

- Represent Molecule Type to be split (above left) as an 'Atom Oriented Graph' (centre). Identify faces and label edges with energy of single/multiple bonds
- Transform Atom Oriented Graph into a 'Face Oriented Graph' (above right)
- Use the Dijkstra shortest path algorithm to find a least energy cyclic path in the Face Oriented Graph. The path edges identify the Least Energy Cut

[a]The SimSoup implementation makes use of the Boost Graph Library code.

Preliminary Results

Molecules Produced By SimSoup



- Reactor was supplied with Hydrogen, Carbon, Oxygen and Nitrogen
- At 5000 timesteps, 74 Molecule Types were present, but in excess of 7000 different Molecule Types had been actualised during the run
- Most Molecules produced were small and of only a few types. There was a 'long tail' of more diverse and transient Molecules, many of them complex
- The screenshots above show a sample of the Molecules produced

Conclusions and Prospects

Conclusions

- SimSoup represents chemistry at the level of elementary reactions
- Catalysis is a property of the network
- Molecular structure and reaction mechanisms are analogous to real chemistry
- A vast space of chemical networks can be explored in a very open ended way

Prospects

Possible avenues for future investigation using SimSoup include:

- High activity networks and the role played by catalytic cycles
- The ability of such networks to 'remember' perturbations and thereby carry inherited information
- The role of molecular structure in (non template based) inheritance