SimSoup Project - www.simsoup.info

Evolution Without Smart Molecules

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Introduction

Origin Of Life Issues and Views

Origin of Evolution: How did the first organisms transfer inherited information?

- **Genetic View:** They used template replicating molecules like RNA[a]
- **Metabolic View:** They used metabolic networks

Trophic Method: What were the first organisms built from (what did they eat)?

- **Heterotrophic View:** Organic molecules synthesised in a 'primordial soup'
- **Autotrophic View:** Small readily available inorganic molecules

[a]Some theories envisage organic templates smaller than RNA. Cairns-Smith envisages templates based on clay crystals.

Smart Molecules Or Networks?

Smart Molecules Don't Explain Everything: Template replicating molecules, and complex enzymes can be called **'smart' molecules**. Life cannot be explained solely in terms of such molecules[a]

SimSoup Investigates Evolution Of Networks: The aim is to show that a chemical network of 'dumb' molecules can carry inherited information

[a]The popular misconception that the DNA code 'causes' life has been called 'DNA-mania' by André Pichot

SimSoup Model

Conceptual Background

Metabolic View Theories: Oparin, Kauffman, Dyson, and the Lipid World and GARD model of Doron Lancet's group

Network Theory: Jain and Krishna

Wächtershäuser: Iron-Sulphur World

Model Highlights

Represents Structure Of Chemical Network: Network elements correspond to the elementary (unimolecular or bimolecular) reactions of chemistry

Catalysis Is Not 'Built In': It results from network structure

No Assumption Of Constant Reactant Concentration

Mass Is Conserved: And each Molecule Type has a defined mass

Energy Is Conserved: And each Molecule Type has a defined potential energy

Interaction Rates Based On Energy: The model is thermodynamically realistic

Heterotrophic Or Autotrophic: SimSoup is applicable in either case[a]

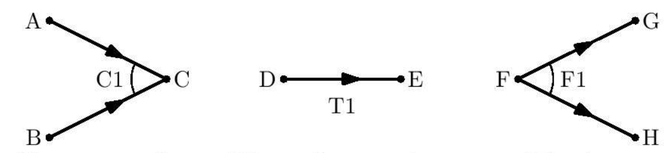
A Reactor: In which interactions occur

Each Molecule Is An Object: Detailed behaviour in the Reactor can be monitored. Eg cycles and cycle rates

[a]The name 'SimSoup' does not imply an *organic* soup. "You can have a soup of anything" (Wächtershäuser)

The Basic Model

Three Forms Of Interaction:-



Construction $A + B \rightarrow C$, $Rate = k_f ab - k_r c$

Transformation $D \rightarrow E$, $Rate = k_f d - k_r e$

Fission $F \rightarrow G + H$, $Rate = k_f f - k_r gh$

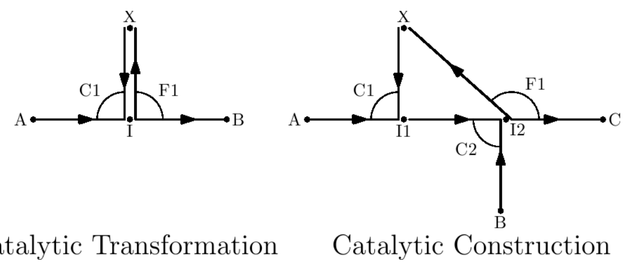
Generality: Covers any chemical network[a]

Molecule Types: Each node represents a type of Molecule. Lower case letters (a, b etc.) represent the concentrations of the corresponding (upper case) Molecule Types

Rate Constants: k_f and k_r are the forward and reverse rate constants

[a]The three basic elements can be combined in Compound Interactions to represent any chemical network of arbitrary complexity. Exception: Trimolecular reactions not covered, but are rare

Compound Interactions



Catalytic Transformation Catalytic Construction

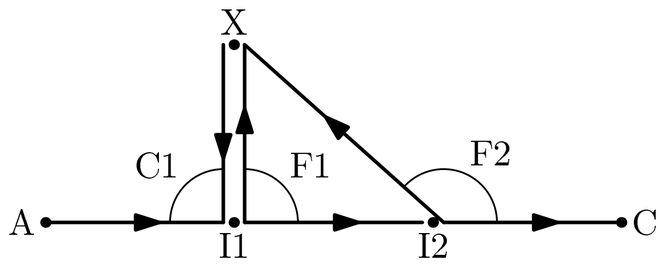
Compound Interactions Can Be Catalytic: X is a catalyst in both cases above

Catalysis Entails Cycling: Catalytic Transformation has an order 2 cycle. Catalytic Construction has an order 3 cycle

SimSoup Models The True Structure Of Chemical Networks: Some models would represent each of the above as a single link from catalyst to the final Product[a]

[a]This is equivalent to assuming constant concentrations of 'food' molecules and intermediates

A Mechanism For Memory



Perturbation Is Remembered:-

- Two stable states, 'Off' and 'On'
- Off: X absent - reaction cannot proceed
- On: Once X is introduced it is maintained as long as there is a supply of A

Reactor Composition

Reactor Composition, R: Number of Molecules of each type present. r_i is the (integer) number of Molecules of type i

Dynamic Behaviour, $\mathbf{R}(t_j)$: Reactor Composition at the j_{th} timestep. r_{ji} is the number of Molecules of type i at time t_j

Measuring Change In Reactor Composition

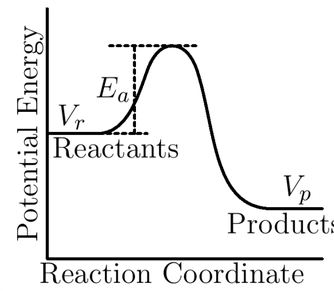
Manhattan Distance:-

- **R** may be static or changing
- Manhattan Distance between Reactor Compositions at times t_1 and t_2 is:-

$$D(\mathbf{R}(t_1), \mathbf{R}(t_2)) = \Sigma_i |r_{1i} - r_{2i}|$$

Thermodynamics In SimSoup

Reaction Profile



Rate constants are based on Arrenhius' equation $k \approx Ae^{\frac{-E_a}{RT}}$. Heat release is $dQ = V_r - V_p$. Entropy production = $\frac{dQ}{T}$

Trackers and Cycle Detection

Trackers: Are attached to Molecules, and are passed from Reactant(s) to Product(s)

Cycle Detection: Tracker paths are monitored. Cycle completions are detected

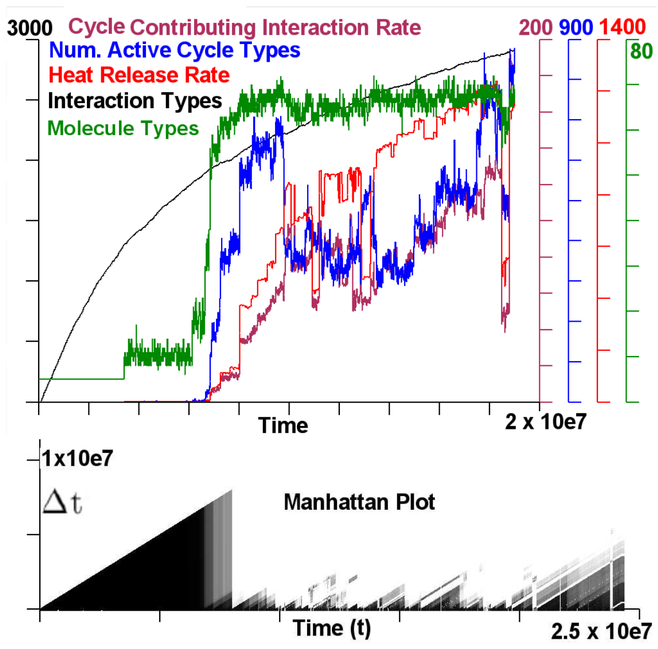
Network Evolution

Model Setup

Initial Conditions: 100 Molecule Types, 5 'food' Molecule Types, slow leakage. No Interaction Types (no network connections)

Evolution: Periodically modify network and select for high heat release

Results



- Tone of each point in Manhattan Plot shows $D(\mathbf{R}(t), \mathbf{R}(t - \Delta t))$
- Triangles indicate near constant **R**. Right hand edge of each triangle indicates sudden change in Reactor Composition

Conclusions

- Realistic model of chemical networks
- Catalysis is a property of network, not of 'smart' molecules
- High activity networks with many cycles develop
- 'Side reactions' do not destroy network activity. Material leaving one cycle supports others?
- Evolution leads to sharp rises in activity, and crashes like those of Jain and Krishna
- Stable and distinct Reactor Compositions persist over long periods, even in the face of regular mutations...
- A metabilising network with no 'smart' molecules can maintain its identity as a 'species'
- Mutations can lead to new 'species'
- The unit of evolution is the entire network