SimSoup Project - www.simsoup.info

Non-Template Molecules Designed For Open-Ended Evolution

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Abstract

- There are two main views of the Origin of Life:
  - Template Replication First (eg based on RNA)
  - Metabolism First (no template molecules like RNA)
- Can metabolic systems support open-ended evolution?
- Earlier work on the SimSoup project demonstrated that artificial chemical systems can have memory; an essential requirement for evolution
- Here, a 'proof of concept' approach to the question is taken. The following are shown:-
  - An artificial chemical network forming a 'memory bank' with many possible states
  - The link between chemical network structure and molecular structure
  - A design for a set of artificial molecular species for the memory bank network
- Preliminary simulation results confirm the operation of an initial set of memory units
- This supports the view that open-ended evolution can begin without highly complex template molecules

Proposition And Proof Of Concept Approach

Proposition

- Early organisms were metabolic systems that transmitted inherited information without using template replicating molecules such as DNA and RNA
- They would not need the very complex and prebiotically implausible mechanisms required for accurate replication of template molecules
- They were individuals capable of growth and reproduction. Variation in fitness would drive evolution

Proof Of Concept Approach: Network And Molecule Design

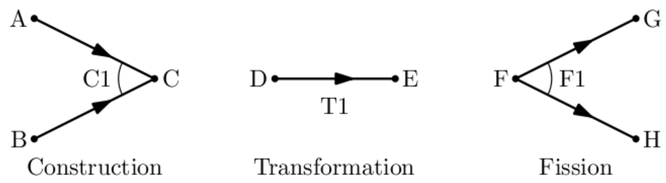
- Requirements for workability of the proposal:-
  - Successful variations must be retained and inherited
  - To be effective, evolution must be open-ended, with a large number of possible variations in metabolism
- Approach: *Design* an artificial chemical network and molecular structures for open-ended evolution
- If the molecules are not too complex, then molecules with similar capabilities are prebiotically plausible

Memory In Chemical Networks

A Network Oriented View Of Chemistry

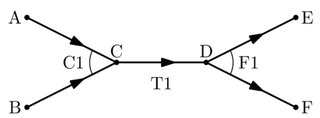
Network Components

- Chemistry involves particles and elementary reactions
- In SimSoup, particles are *Molecule Types* and elementary reactions are *Interaction Types*
- From a network point of view,there are only three forms of elementary reaction:

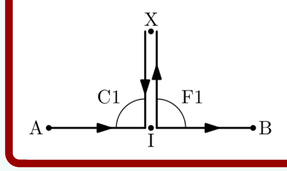


Compound Interactions

- Interaction Types can be combined
- The following shows a Compound Interaction with overall scheme A + B → E + F



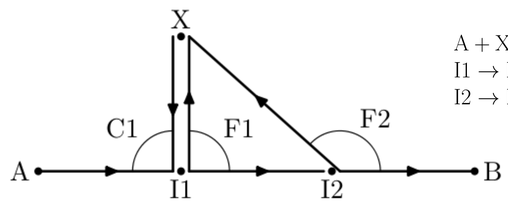
Catalysis



- 'Catalyst' is not a type of Molecule. It is a *role*
- X plays the role of catalyst

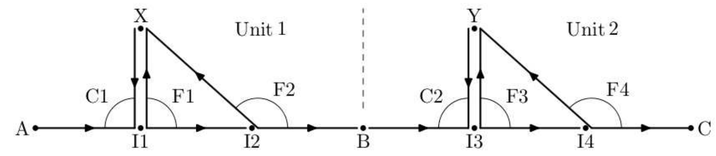
Network Memory And Exploration

A Two State Memory Unit



- The figure shows an artificial chemistry consisting of three Interaction Types: C1, F1 and F2
- A is abundantly available 'food'; initially no other Molecules are present and no reactions occur
- If a single Molecule of X is introduced, the reactions proceed and continue due to excess production of X
- The network has two states and therefore constitutes a memory unit with an information capacity of 1 bit

Network Exploration



- The figure shows two memory units connected in series
- There are three possible persistent states: i) neither unit active, ii) only unit 1 active, iii) both active
- In a large network a process of 'exploration' occurs. A perturbation (eg addition of a single X or Y molecule) can cause new sub-networks to become accessible