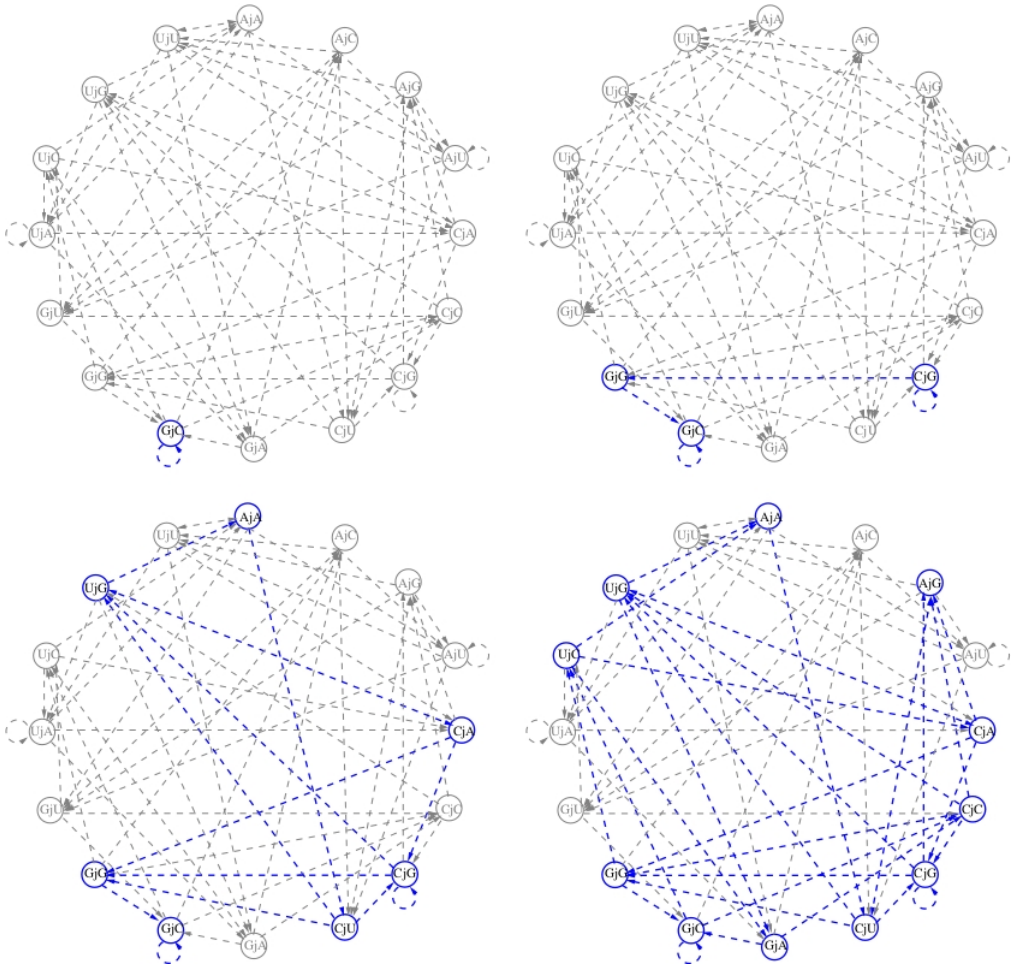
A Formal Framework for Autocatalytic Sets

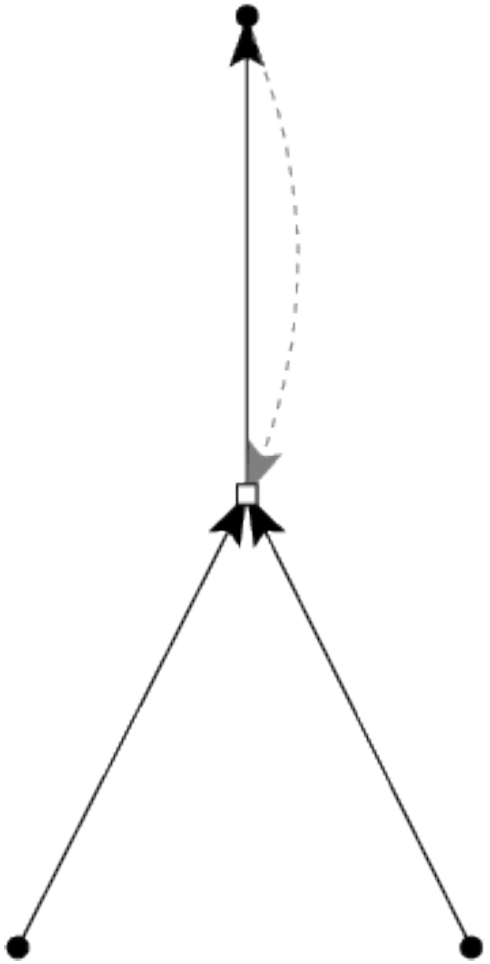


Wim Hordijk & Mike Steel

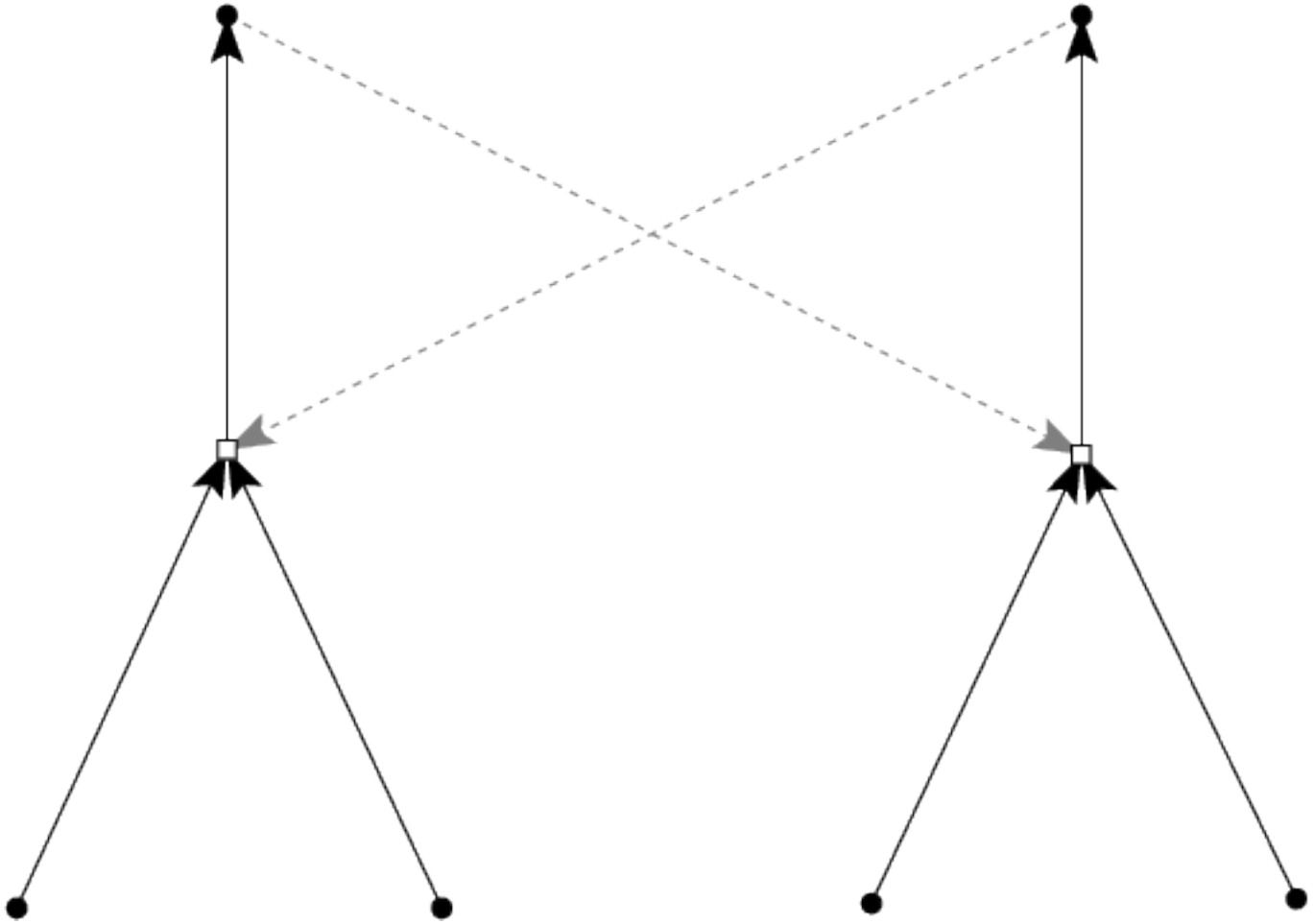
Introduction

- The idea of autocatalytic sets is more than 40 years old (Kauffman, 1971).
- Autocatalytic sets are believed to have played an important role in the origin of life.
- Development of a formal framework for studying the emergence & evolution of autocatalytic sets.

Autocatalytic Reaction



Autocatalytic Set



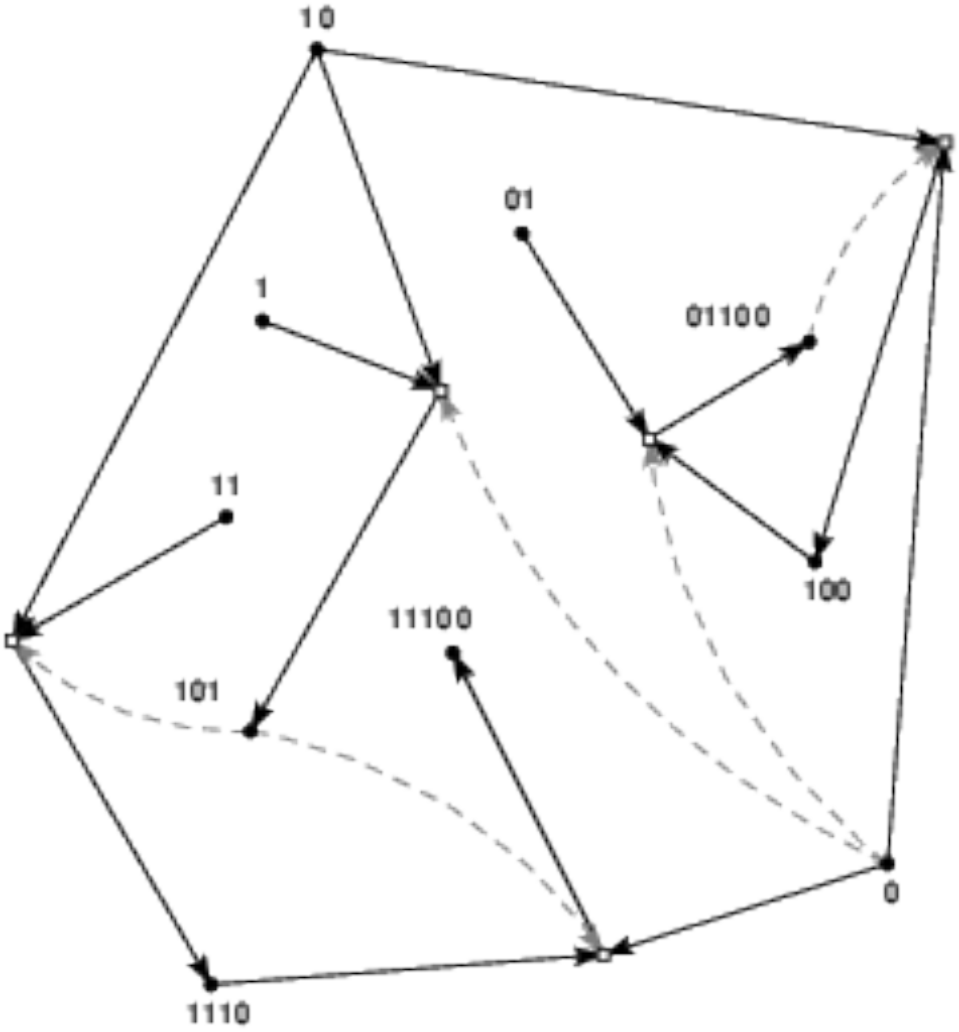
Autocatalytic (RAF) Set

- An autocatalytic (RAF) set is a set of reactions and associated molecules, which is:
  - Reflexively autocatalytic (RA): all reactions in the set are catalyzed by at least one molecule from the set itself.
  - Food-generated (F): all molecules in the set can be produced starting from a “food set” and using only reactions from the set itself.

The Binary Polymer Model

- A set of molecules represented by bit strings up to length n, with food molecules up to length t (with $t << n$).
- A set of reactions of two types:
  - ligation: 000+111→000111
  - cleavage: 0101010→0101+010
- Randomly assigned catalysis:
  - Pr[m catalyzes r] = p

RAF Set Example



n=5

t =2

p=0.0045

Original Claim

"*The formation of autocatalytic sets of polypeptide catalysts is an expected emergent collective property of sufficiently complex sets of polypeptides, amino acids, and other small molecules.*"

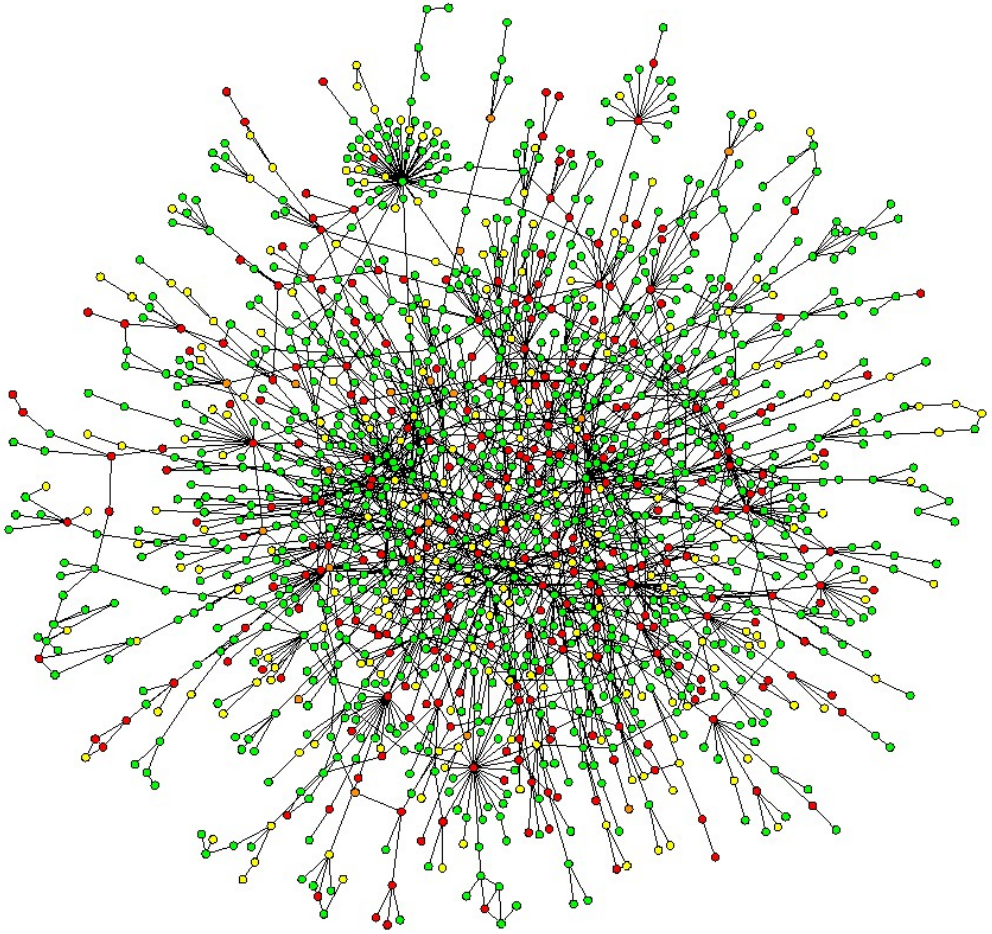
(Kauffman, 1986)

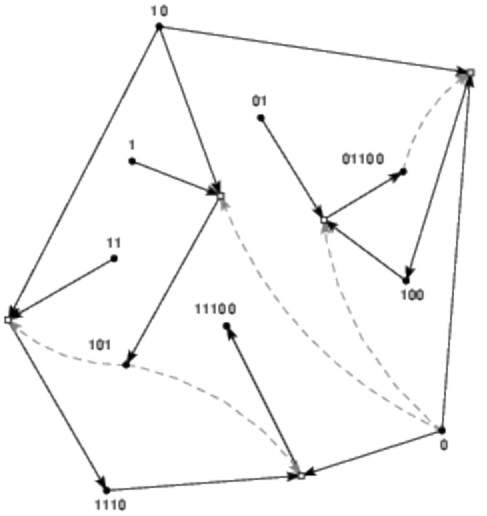
Basic idea: Given a fixed probability of catalysis *p* and increasing *n*, at some point there is a phase transition where the entire reaction graph becomes an autocatalytic set, similar to giant connected components appearing in random graphs.

RAF Algorithm

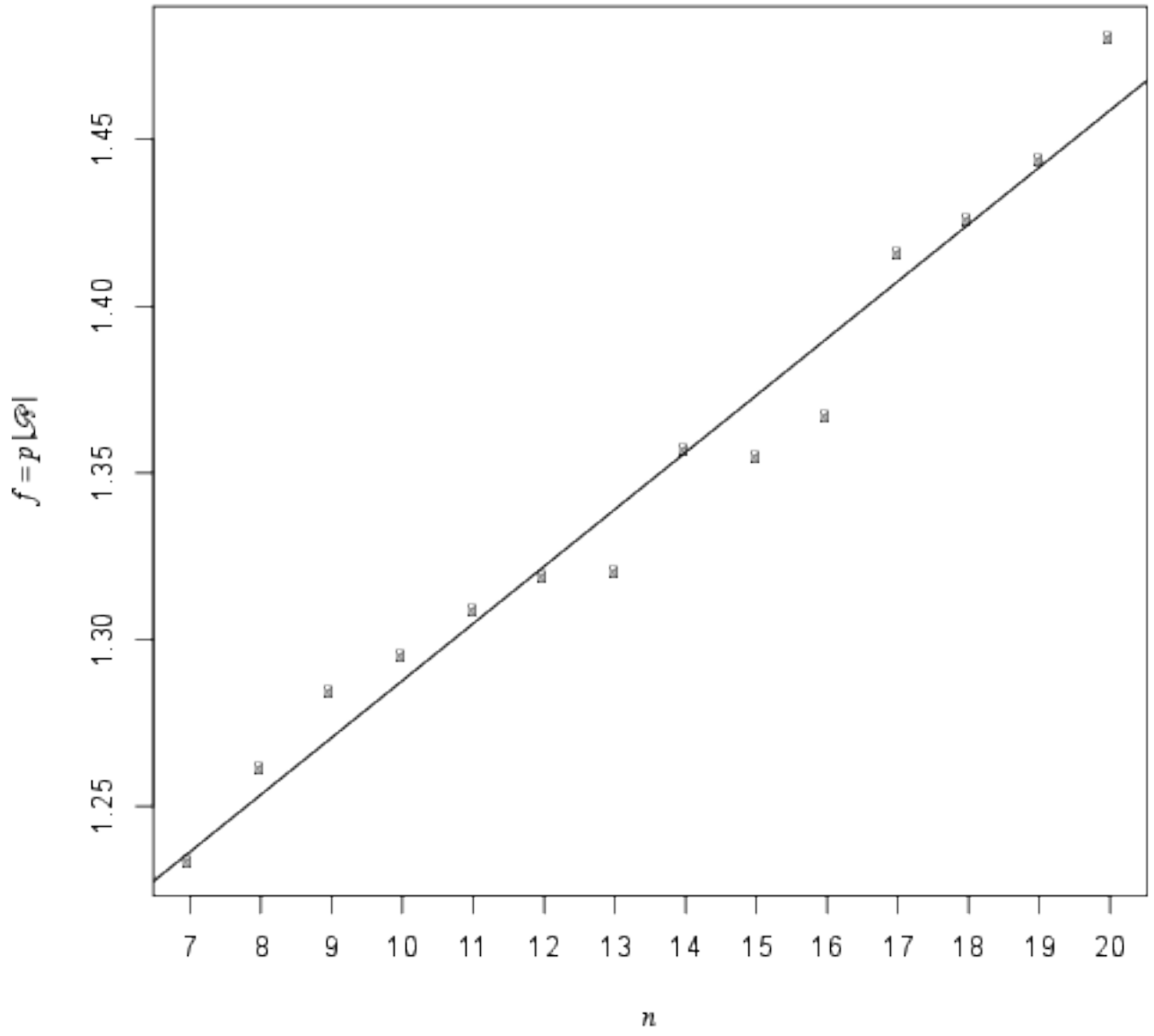
- Given a chemical reaction system (CRS), decide whether there exists a subset of reactions and molecules that forms an RAF set.
- Returns:
  - the maximal RAF set within the given CRS, or
  - the empty set.
- Polynomial running time in the size of the CRS.

RAF Algorithm

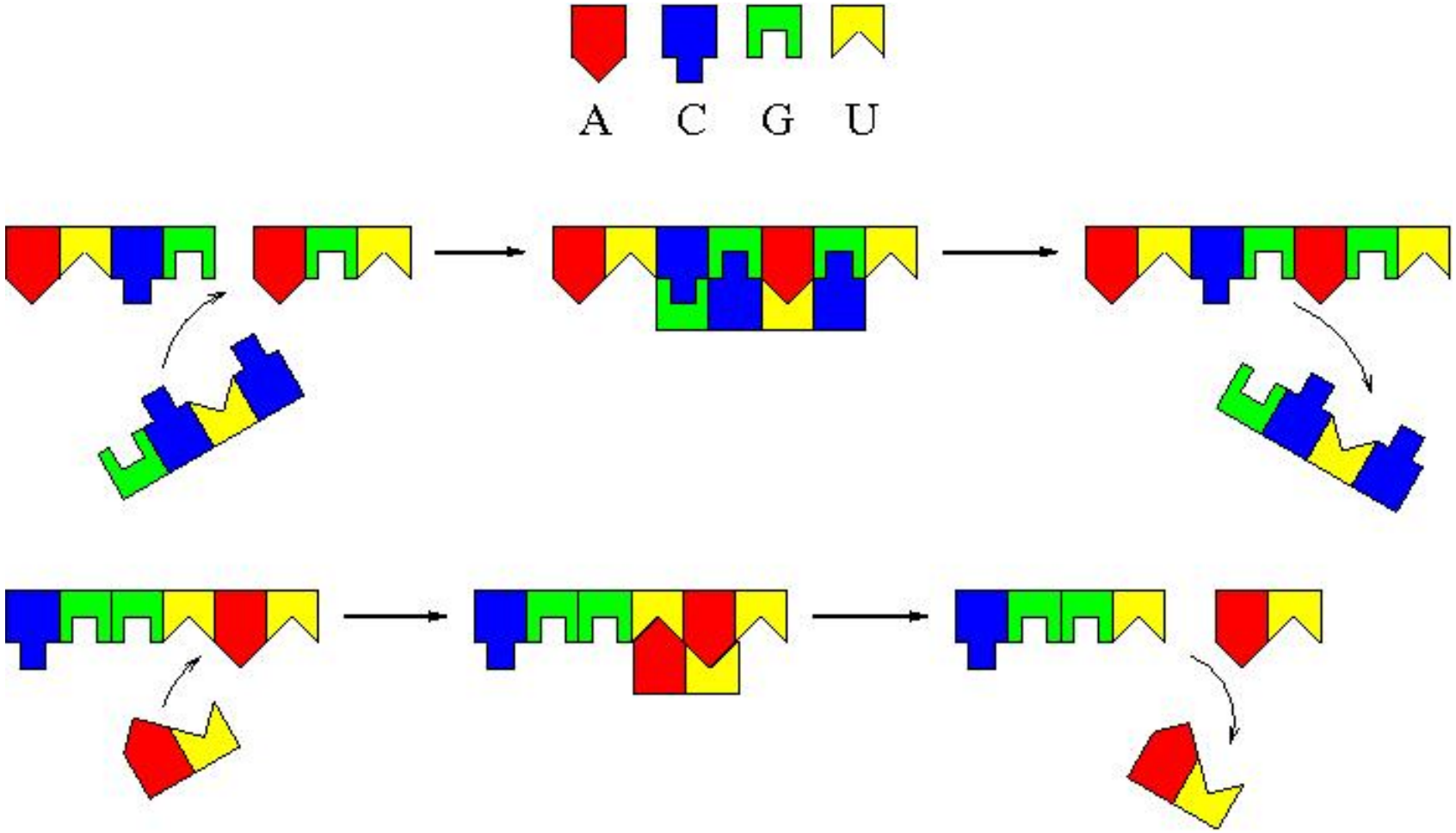




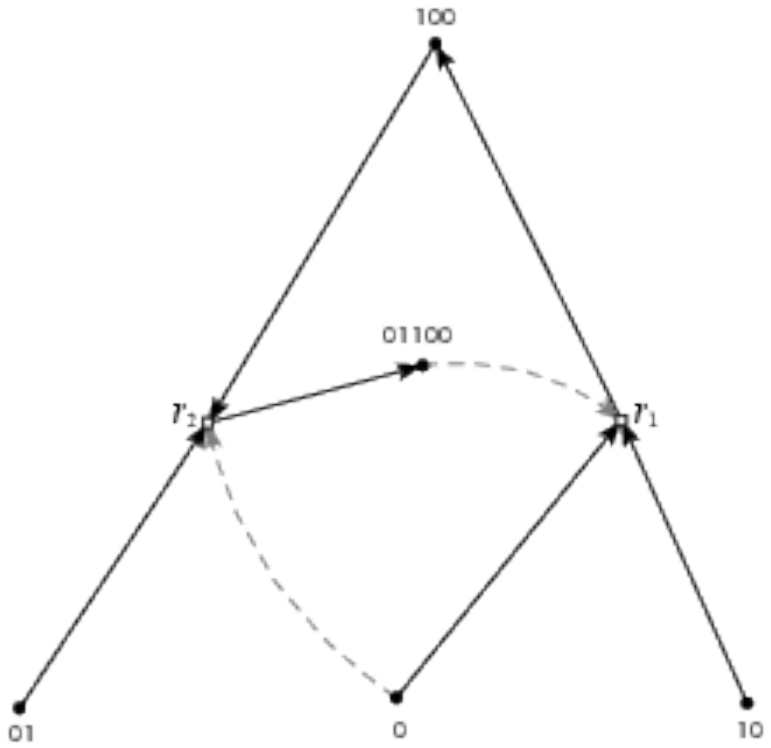
Growth Rate in Level of Catalysis

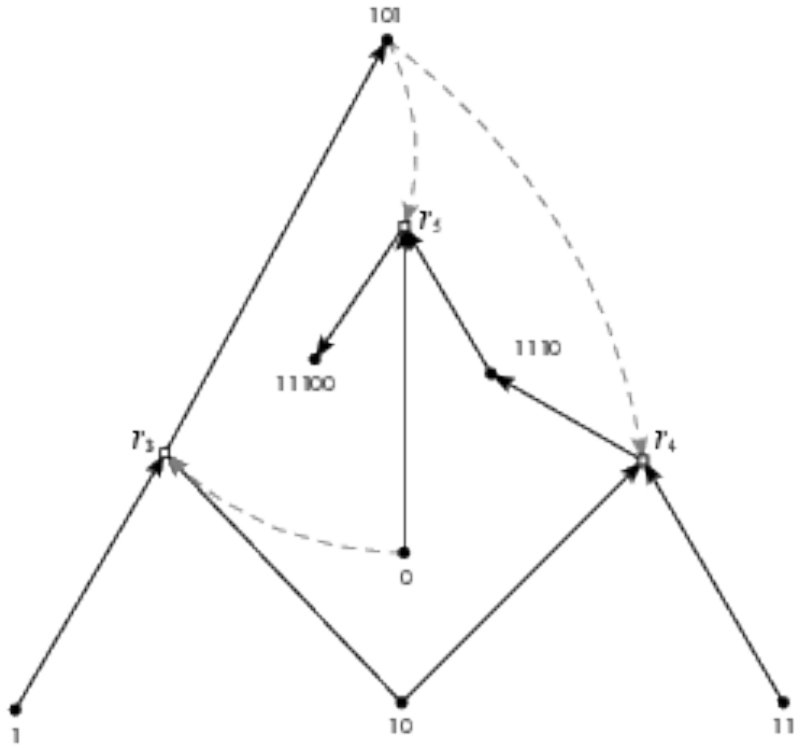


Template-based Catalysis

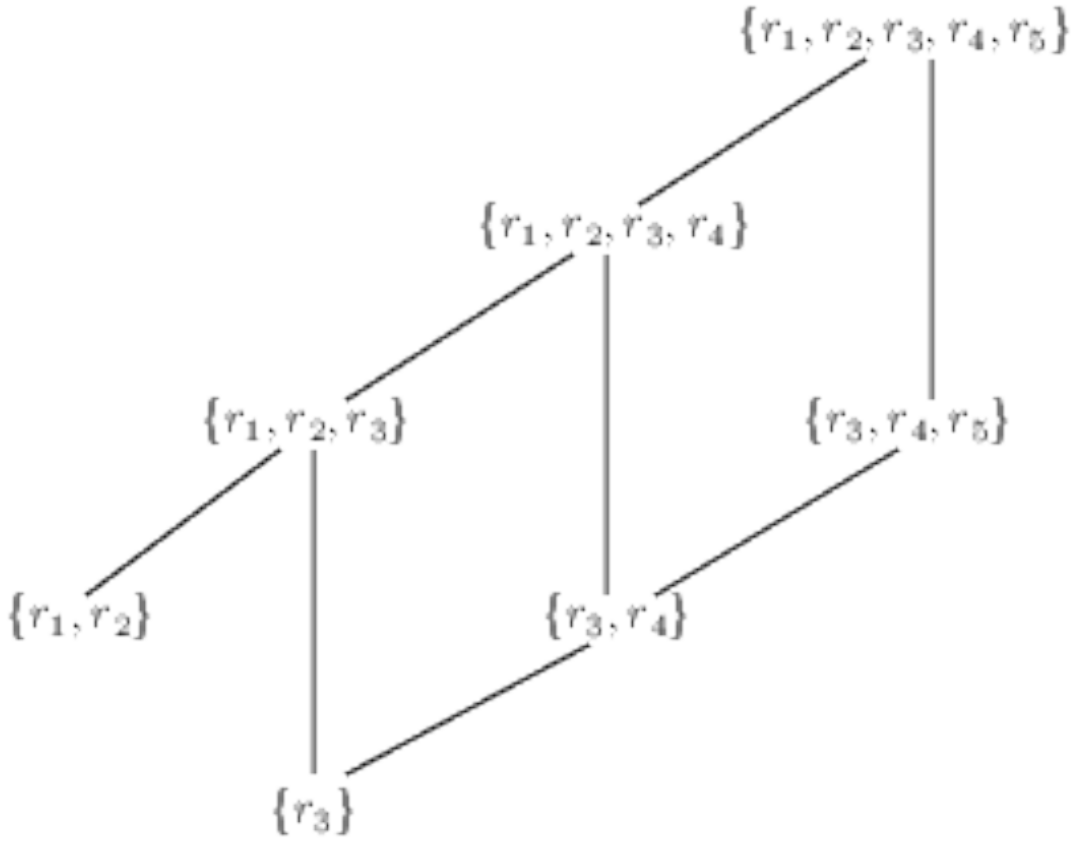


SubRAFs & Irreducible RAFs





Poset of subRAFs



Modeling Experimental Systems

ARTICLE

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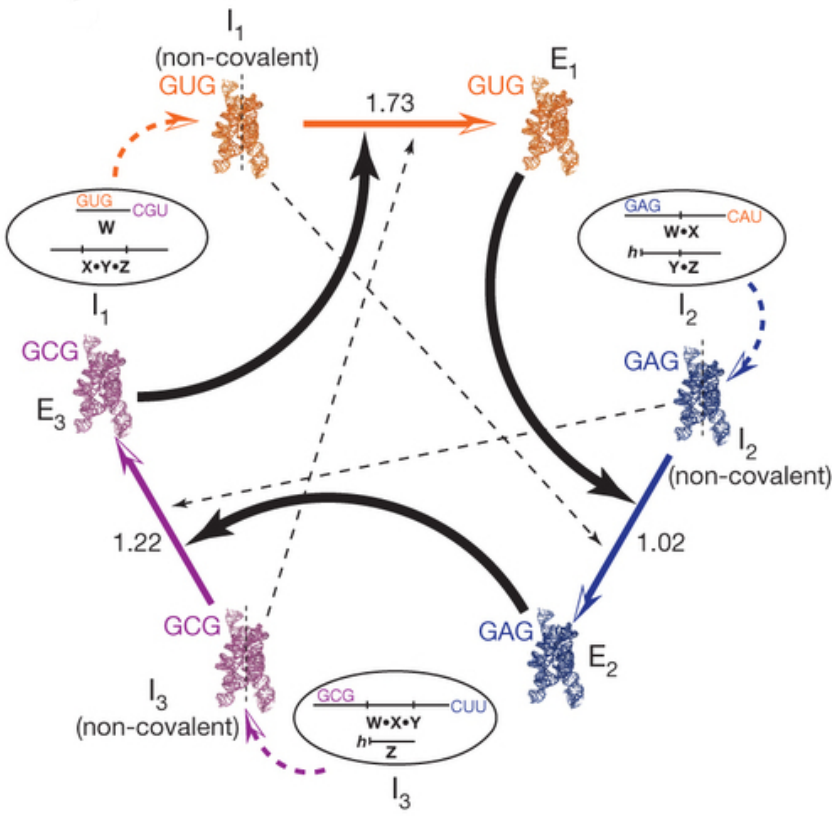
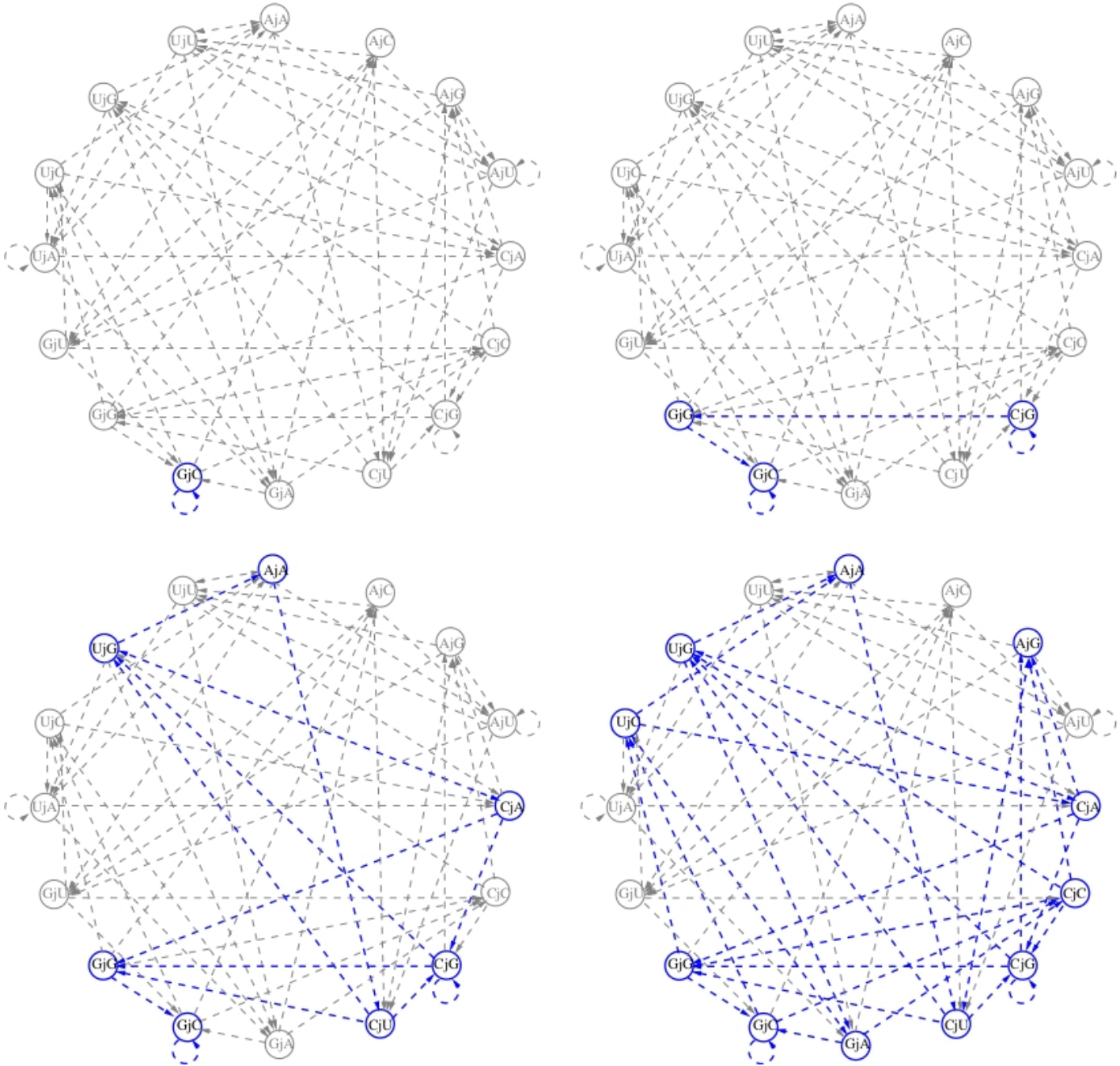
Spontaneous network formation among cooperative RNA replicators

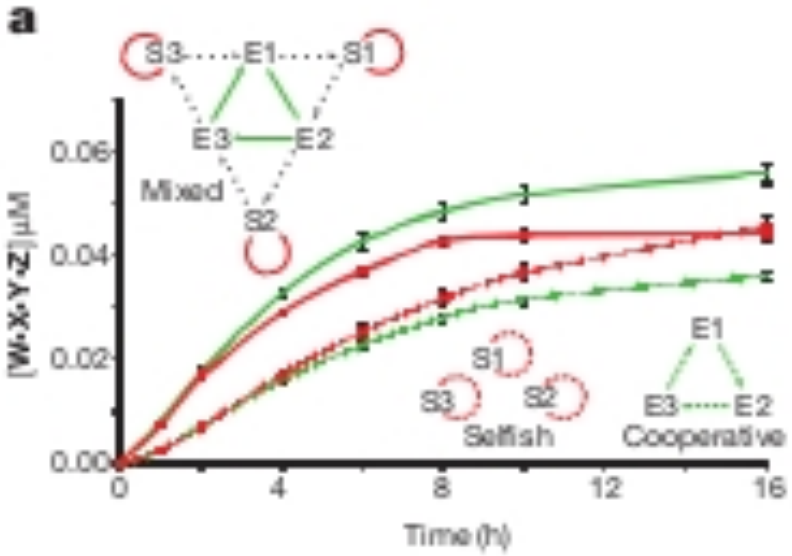
Nilesh Vaidya[1], Michael L. Manapat[2], Irene A. Chen[3]†, Ramon Xulvi-Brunet[3], Eric J. Hayden[4] & Niles Lehman[1]

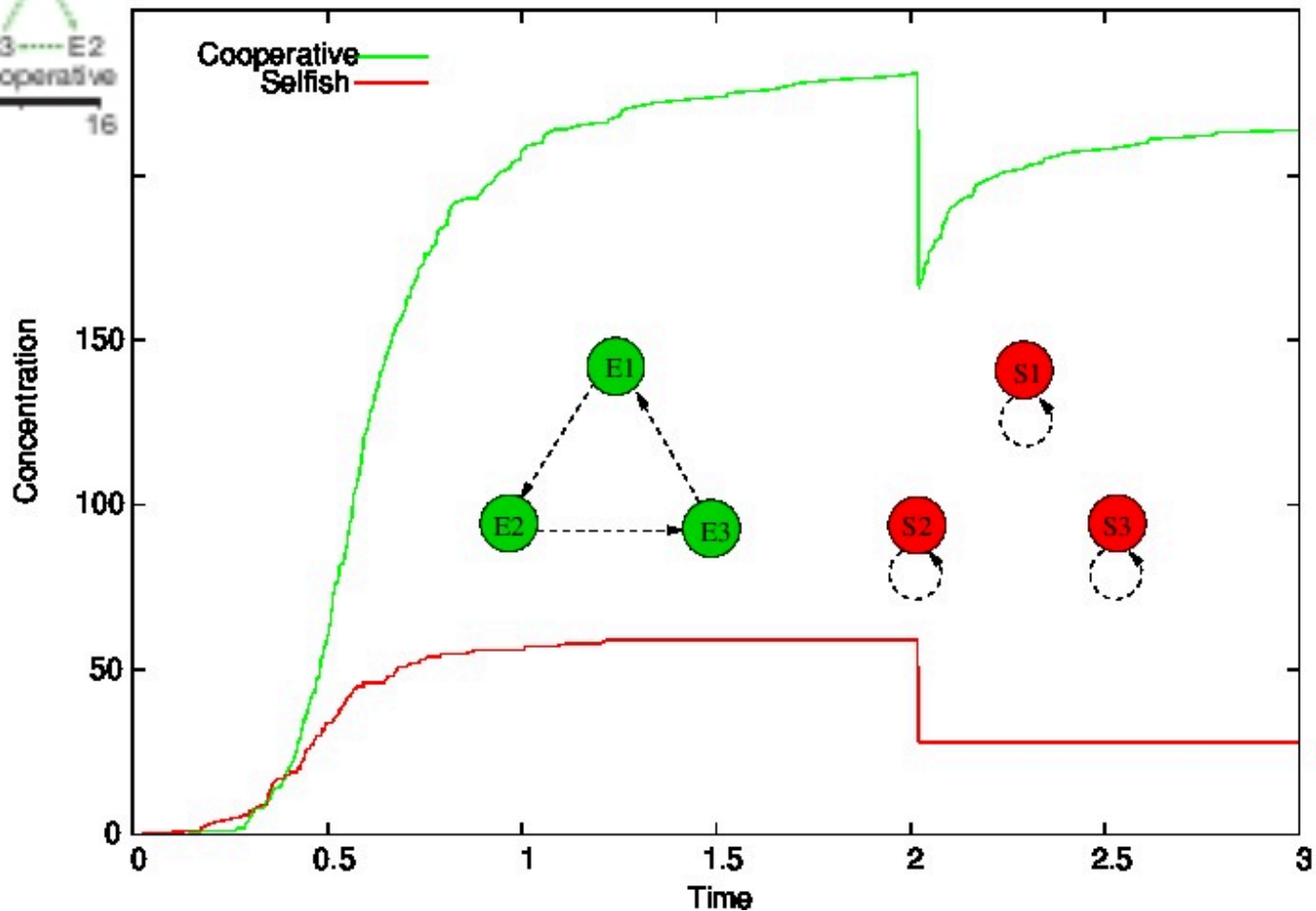


RAFs in the RNA Replicator System



Cooperation vs. Selfishness





Conclusions

- Formal framework for autocatalytic (RAF) sets.
- Efficient algorithm for finding RAF sets.
- High probability of RAF sets in binary polymer model with moderate level of catalysis (linear bound).
- Realistic extensions like template-based catalysis.
- Evolvability from hierarchical structure of subRAFs.
- Applicable to real chemical networks.

Autocatalytic Collaboration

Mike Steel

W. Hordijk & M. Steel. **A formal model of autocatalytic sets emerging in an RNA replicator system**. *Journal of Systems Chemistry* 4:3, 2013.

The Origin of Life