Artificial Chemistries

Autonomic Computer Systems
University of Basel
Yvonne Mathis

Motivation

Chemical program evolution rather than design

- Chemical system quickly become complex
- Exploit emergent properties (self-organization, self-healing, robustness)
- Bottum-up approach
- From Pre-Programmed to Emergent Chemical Programs

Chemistry not only as a metaphor for **parallel** computation, but also **emergent** computation, c.f. Section 5

Contents

- Classification & Definition of AC
- Motivation & Goal of AC
- Artificial Chemical Computing
- Dynamics
- Emergent Computation
- Evolutionary Dynamics
- Algorithmic Chemistry
- Chemical Organization Theory
- Examples in Fraglets

1. Classification & Definition of AC

- A branch of Artificial Life (ALife), dedicated to the study of chemical processes related to life and organizations in general [1]
- AC is on the level of **molecules**, molecules as information carriers and processors. It is about chemistry, biochemistry, prebiotic evolution.
- AC can be defined by a **triple** (S, R, A), where S is the set of all possible molecules, R is a set of collision rules representing the interaction among the molecules si ϵ S, and A is an algorithm describing the reaction vessel or domain and how much the rules are applied to the molecules inside the vessel. [1]

2. Motivation & Goal of AC

- Simulate (bio-)chemical processes, e.g. origin of life from primordial soup of molecules
- Explore alternative computation models: **chemical computing,** c.f. section 3
- Understand **emerging/self-maintaining structures**, e.g. chemical organization theory [2], c.f. sections 5, 8
- ***Terminology***: *Molecular species, Multiset, (well-stirred) Vessel, Concentration, Chemical reaction*

3. Artificial Chemical Computing

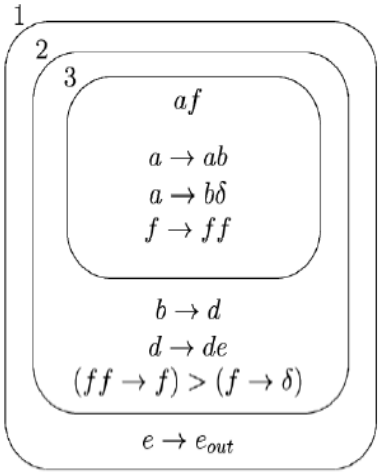
- Program (= set of molecules) is executed (= molecules are consumed and produced in chemical reactions) until no more reactions can take place
- Examples:

Formal models:
  - Computing with rules in a multiset (Gamma)
  - Computing with hierarchical multisets (Membrane Computing (P Systems))

-> result is within molecule

  - **Computing with Concentrations** (algebraic functions, also with real chemistry)

-> result is reflected by the **concentration**



P Systems

4. Dynamics

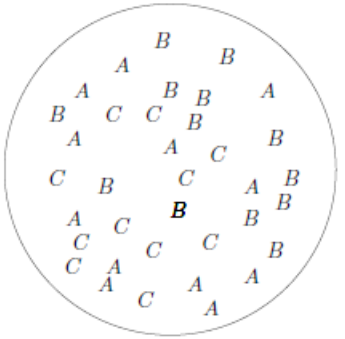
$$r : 2A + 3B \xrightarrow{k} C$$

- **Concentration levels** convey information about **dynamics**. **Computation** is used to assess changes in concentration. The Result is ready when the system reaches **equilibrium**. Concentration dynamics are describes by a system of **ODEs**:

$$d\vec{x}/dt = \mathrm{M}\vec{v}$$

- **Terminology**: *law of mass action,* $v = k[A]^2[B]^3$ $v = k\prod_{i=1}^{n}[S_i]^{\alpha_i}$ *reaction networks, equilibrium:* $d\vec{x}/dt = \vec{0}$ *simulation algorithms: deterministic vs stochastic*

4. Dynamics



$|A| = 12 \;\; |B| = 13 \;\; |C| = 11$

$a_1 = c_1|A||B|$
$a_1 = 1 \cdot 12 \cdot 13 = 156$

$a_2 = c_2|C|$
$a_2 = 10 \cdot 11 = 110$

(1) $a_0 = a_1 + a_2 = 266$

(2) $\mathrm{E}[\tau] = \frac{1}{a_0} = 3.76 \cdot 10^{-3}$

Stochastic simulation:
Gillespie's Algorithm (1977)

calculates **which** reaction occurs **when**

- Advantages:
  - Realistic for small numbers of molecules
  - Can easily deal with the dynamic creation of new species
- Shortcomings: not scalable to large numbers of molecules, or large numbers of possible reactions

4. Dynamics

Chemical reactions network emerge from an initial population and seem to stabilize -> emergence of **organizations** (c.f. section 8, Chemical Org. Theory)

Dynamics can be analyzed by the following methods:

- **Perturbation analysis**: equilibrium and stability (steady-state analysis)
- **Simulation algorithms**: deterministic vs stochastic

Problem: The analysis doesn't include the creation of new species (c.f. section 7, Algorithmic Chemistry)

4. Dynamics

- Dynamics control which of the parallel execution paths is processed at which speed
- Under selective pressure, the growth rate of a set of molecules determines its fitness (see Evolutionary Dynamics)

5. Emergent Computation

- **Creation/Selection process** from an **evolutionary dynamics** (c.f. Section 6) perspective
- **Molecules** with **structure** (program, data) instead of simple atoms
- Reaction rules defined by the molecular structure instead of being fixed and predefined
- **Advantages**: more robust and efficient, more flexible in the face of complex and dynamic environments, do not need to foresee all contingencies, better model for complex natural processes
- ***Terminology: Emergent phenomena*** *(unexpected global behavior or pattern arising from the interaction of parts in a complex system)* ***Self-organization*** *(process by which the system is able organize itself from the inside, out of a disordered state),* ***Complex System***

6. Evolutionary Dynamics

Terminology:

- Replication (autocatalytic reaction) and Death (decay reaction) $X \xrightarrow{b} 2X$ $X \xrightarrow{d}$.
- Selection and Fitness (=rate of reproduction)
- Growth laws $\dot{x}_i = f_i x_i^c$, for varying c
- Variation (e.g. mutations), induced external/passive or internal/active, Reproduction = Replication + Variation, quasispecies
- Interactions (Random catalytic reaction networks with Catalytic Reaction Equation:)

$$\frac{dx_k}{dt} = \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{ij}^k x_i x_j - x_k \phi(t)|$$

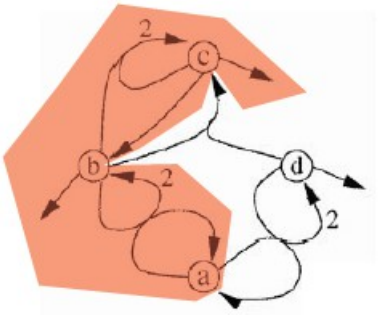
7. Algorithmic Chemistry

- A Constructive system: A set of molecules may generate **new molecule species**, which again influence the reaction dynamics
- Considers molecule structure:
  - Molecules are λ-expressions from λ-calculus
  - All molecules represent **functions** (programs in functional programming)
  - Functions operate on functions to produce other functions: $f + g \rightarrow f + g + f(g($

Precursor of chemical organization theory

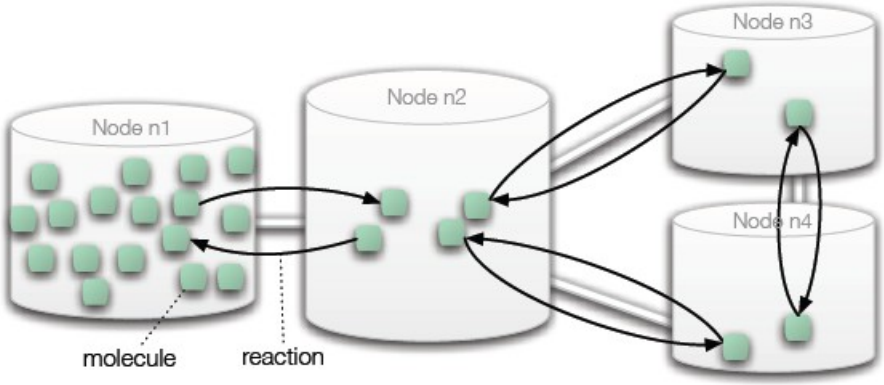
8. Chemical Organization Theory

- Identify organizations (stable set of molecules) and the transition between them
- **Definition: An organization is a set of molecule species that is closed and self-maintaining**
- Chemical Organization Theory determines the stability of the set of molecule species and analyzes then dynamic fixpoints (= instances of organizations)
- The set of organizations form a lattice
- **Mutations** cause molecule species to come and go
- Down- and upward movement

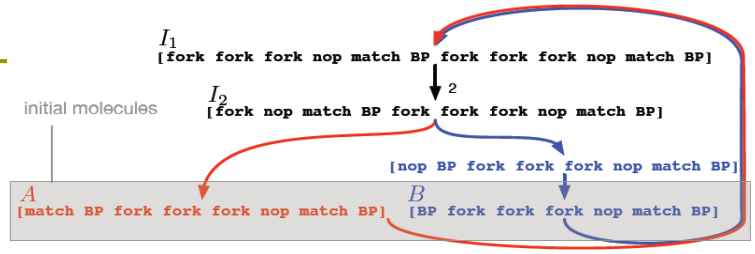


9. Examples in Fraglets

- Distributed Averaging
  - Distributed calculation as an **emergent phenomena**
  - Make use of the chemical equilibrium
  - Reaction network is distributed among the whole network
  - System strives to equilibrium where solution is presented



9. Examples in Fraglets



- Self-Healing Programs
  - Autocatalytic reaction
  - Two molecules species form an organization
  - population grows hyperbolically -> introduce limitation (total number of molecules) -> survival of the common (first program).
  - The resulting program is robust to invasion from other programs and code deletion -> **inherent self-healing emerges**

Application: Self-Healing link load balancing protocol

References

- P. Dittrich, J. Ziegler, and W. Banzhaf. “Artificial Chemistries – A Review”. Artificial Life, 7(3):225–275, 2001.
- P. Dittrich and P. Speroni di Fenizio. *“Chemical Organization Theory”*. Bulletin of Matematical Biology, 69(4):1199–1231, 2007.