Artificial Chemistries

Steps towards understanding the essences of living systems

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CPSC 601.73 — Biological Computation, Winter 2003

Source material:

- Peter Dittrich: *Artificial Chemistries*
  http://ls11-www.cs.uni-dortmund.de/achem
- Peter Dittrich, Jens Ziegler, and Wolfgang Banzhaf:
  Artificial Chemistries—A Review
  Artificial Life 7 (2001), pp. 225-275.

Artificial Life and Artificial Chemistry

Understanding the origin and nature of life.

Impressive collection of data about the processes of life.

The informational perspective—not yet considered by biology in order to understand the issue of life's essence.

Artificial Life research:

- □ abstracts from specific examples of life processes,
- □ integrates different approaches to extract the first principles of life.

ALife Working Hypothesis

> Biotic phenomena can be modeled using complex systems of many interacting components.

Emergence

The complex systems approach employs *emergence* as a central concept.

Global properties of a system are deduced from local interactions between its subsystems.

The local interactions may follow simple effective rules that

- ○ cause global behavior of the system to emerge,
- ○ but cannot be predicted by simply analyzing the subsystems and their components.

> "The whole is bigger than the sum of its parts."

A system has certain properties not due to the properties of its constituents, but due to

- ○ their *organization* and
- ○ their mutual *function* in the whole.

Important Consequence

Natural systems, such as organism or social structures (consisting of truly different matter and components), might follow the same organizational principles.

Hypothesis: Living organisms are alive not because of the properties of their constituents but because of their organization.

Example: *Evolution*

- Principle of random variation and competitive selection
- Also valid on the level of
  - replicating molecules,
  - immune systems,
  - social systems, or
  - cultural systems.

What the Theory of Evolution does not explain ...

Questions relating to the

- *evolutionary units* and
- their *origin*.

- How do the entities that are varied and selected come into being?
- How did new evolutionary mechanism emerge qualitatively?
  - sexual recombination
  - regulation of mutation rates
  - genetic code
  - ...

Artificial Chemistries: "The Right Stuff"

- AC as a subfield of ALife
- Abstracting from natural molecular processes.
- AC deals with
  - combinatorial elements that change or maintain themselves,
  - especially, systems that construct new components,
  - forms of organization,
  - self-maintenance,
  - self-construction,
  - conditions for those structures to arise.

> Artificial chemistries are "the right stuff" to study when trying to uncover the basic mechanisms of life, and more generally, the origin and evolution of organizations.

Three Main AC Dimensions

Modeling

Artificial chemistry modeling systems in different domains:

- biological systems
- evolutionary systems
- social systems
- parallel processing systems

- ...

Metaphor of colliding molecules as their common relation to chemistry.

Information Processing

Many instances of chemical processes in nature can be interpreted as performing computations.

- Chemical reaction networks controling the movement of bacteria
- Neural information processing
- Gene regulation
- Transcription and translation
- Genome splicing
- Mutations, recombinations, ...
- Immune system
- Control of developmental processes

Computational properties of chemical systems can be studied through

- real chemical computing: use real molecules for computing (e.g., DNA computing)
- artificial chemical computing: chemical metaphors as design paradigms for new hardware and software architectures.

Chemical systems as information processors.

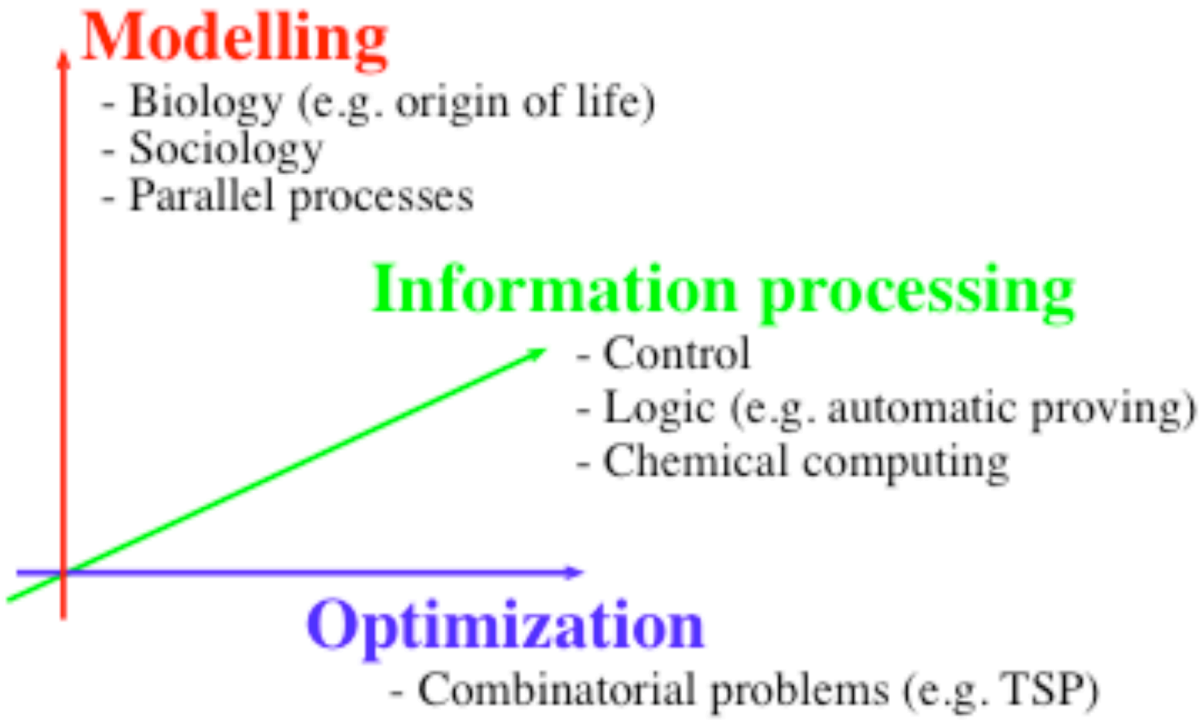
Optimization

Use the AC paradigm to help find solutions for "difficult", mostly combinatorial problems.

Closely related to evolutionary computing.

Evolutionary algorithms can be seen as artificial chemical systems.

Modeling, Info. Processing, and Optimization



Basic Concepts

What is an Artificial Chemistry (AC)?

Very general:

An artificial chemistry system is a man-made system that is similar to a real chemical system.

More formally:

An *artificial chemistry* is defined as a triple $(\mathcal{S}, \mathcal{R}, \mathcal{A})$, where

- $\mathcal{S}$ is the set of all possible objects (called *molecules*),
- $\mathcal{R}$ is the set of interaction rules (called *collision* or *reaction* rules),

  representing the interaction among the molecules
- $\mathcal{A}$ is an algorithm defining the population dynamics,

  by describing the reaction vessel or domain and how the rules are applied to the molecules inside the vessel.

What is an AC? (II)

1. Objects

abstract symbols, numbers, λ-expressions, binary strings, proofs, character sequences, abstract data structures, ...

2. Reaction Rules

string maching, string concatenation, λ-calculus, abstract finite-state machines, Turing machines, matrix manipulation, simple arithmetic operation, cellular automata, boolean networks, electronic hardware, ...

3. Dynamics

ordinary differential equation (ODE), difference equation, meta-dynamics, explicit collision simulation, cellular automaton, well-stirred reactor, 3D Euclidean space, self-organizing topology, ...

What is an AC? (III)

The Set of Objects / Molecules $\mathcal{S}$

Real chemistry:

- What kind of atomic configurations form stable molecules?
- How do these molecules appear?

The *set of molecules* $\mathcal{S} = \{s_1, \ldots, s_i, \ldots, s_n\}$, where n might be infinite, describes all valid molecules that may appear in an AC.

The Set of Rules $\mathcal{R}$

The set of reaction rules $\mathcal{R}$ describes the interactions between molecules $s_i \in S$.

A rule $r \in \mathcal{R}$ can be written according to the chemical notation of reaction rules:

$$s_1 + s_2 + \ldots + s_n \longrightarrow \bar{s}_1 + \bar{s}_2 + \ldots + \bar{s}_m$$

A reaction rule determines the n components on the left-hand side that can react and subsequently be replaced by the m components on the right-hand side.

Note: The "+" sign is not an operator, but only separates the components on either side.

Alternative notation

$$f[s_1, s_2, \ldots, s_n] \xrightarrow{r} g[\bar{s}_1, \bar{s}_2, \ldots, \bar{s}_m]$$

Dynamics / Reactor Algorithm $\mathcal{A}$

An algorithm $\mathcal{A}$ determines how the set of rules is applied to a collection of molecules $\mathcal{P}$, called the *reactor*, *soup*, *reaction vessel*, or *population*.

Note: $\mathcal{P}$ is generally not identical to $\mathcal{S}$,

- as not all molecules need to be present in $\mathcal{P}$,

- some molecules in $\mathcal{P}$ might occur in more than a single copy
  (→ multisets).

Algorithm $\mathcal{A}$ depends on the representation of $\mathcal{P}$.

With no spatial structure in $\mathcal{P}$, the population can be represented

- as a multiset (explicit) or
- as a concentration vector (implicit).

Example: A Constructive Number-Division Chemistry

Every molecule is explicitly simulated.

The population is represented as a multiset $\mathcal{P}$.

A Typical Algorithm:

- Draw a sample of molecules randomly from the population $\mathcal{P}$.
- Check whether a rule $r \in \mathcal{R}$ can be applied.
  If so, the molecules are replaced by the right-hand-side molecules given by r.
  If more than one rule can apply, a decision has to be made as to which rule to employ.
- If no rule can be applied, a new random drawing is initialized.

Example algorithm with second-order reactions:

$$\begin{array}{l}\underline{\text{while}}\ \neg \mathit{terminate}()\ \underline{\text{do}} \\ \quad s_1 := \mathit{draw}(\mathcal{P}); \\ \quad s_2 := \mathit{draw}(\mathcal{P}); \\ \quad \underline{\text{if}}\ \exists\, (s_1 + s_2 \longrightarrow \bar{s}_1 + \bar{s}_2 + \ldots + \bar{s}_m) \in \mathcal{R} \\ \quad\quad \underline{\text{then}} \\ \quad\quad\quad \mathcal{P} := \mathit{remove}(\mathcal{P}, s_1, s_2);\end{array}$$

$\mathcal{P} := insert(\mathcal{P}, \bar{s}_1, \bar{s}_2, \ldots, \bar{s}_m);$

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od

Implemented Example: Number-Division Chemistry

1. Objects

$\mathcal{S} = \{2, 3, 4, \ldots\}$

2. Reaction Rules

$$s_1 + s_2 \longrightarrow s_1 + s_3 \text{ with } s_3 = \begin{cases} s_2 / s_1 & \text{if } s_2 \bmod s_1 = 0 \\ s_2 & \text{otherwise} \end{cases}$$

3. Dynamics

Population: $\mathcal{P}[1], \mathcal{P}[2], \ldots, \mathcal{P}[M]$

while $\neg terminate()$ do

$s_1 := draw(\mathcal{P});$

$s_2 := draw(\mathcal{P});$

$s_3 := reaction(s_1, s_2);$

if $s_3 \neq 0$ then $\mathcal{P}[i_2] := s_3;$

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Dynamical Simulation

Constructive Dynamical Systems

○ New components can appear.

- Dynamics of the system may change.
- Components are not given explicitly at the beginning.
- Weekly constructive: New components are generated randomly.
- Strongly constructive: New components are generated through action of other components.

[Fontana, 1992; Fontana et al., 1994]

Explicit or Implicit Populations (I)

Explicit Population

e.g., as an array $\mathcal{P}[]$:

$\mathcal{P}[1] = 1$
$\mathcal{P}[2] = 1$
$\mathcal{P}[3] = 2$
$\mathcal{P}[4] = 2$
$\mathcal{P}[5] = 1$

Implicit Population

e.g., as an array $\mathcal{N}[]$:

$\mathcal{N}[1] = 3$
$\mathcal{N}[2] = 2$

Explicit or Implicit Populations (II)

Explicit Population

+ concentration proportional selection: $\mathcal{O}(1)$

– concentration of type i: $\mathcal{O}(\mathrm{M})$

+ finite populations with high diversity

+ easy to implement

+ flexible (e.g., space)

+ easy to distribute on a parallel machine

Implicit Population

– concentration proportional selection: $O(\log(M))$

+ concentration of type i: $O(\log(M))$

+ large/infinite populations with low diversity

+ memory efficient

+ easy monitoring

Methods for Dynamical Simulation — Overview

(1) Stochastic molecular collisions

e.g. [Fontana and Buss, 1996]

(2) Continuous differential or discrete equations

e.g., [Segr and Lancet, 1998; Banzhaf, 1994]

(3) Metadynamics

e.g. [Bagley and Farmer, 1992]

(4) Mixed approaches

e.g., [Zauner and Conrad, 1998]

(5) Symbolic analysis of the equations

e.g., [Farmer et al., 1986]

Approaches

Rewriting or Production Systems

The Chemical Abstract Machine (CHAM)

The Chemical Rewriting System on Multisets (ARMS)

The Chemical Casting Model (CCM)

Lambda-Calculus (AlChemy)

Arithmetic Operations

Simple Arithmetic Operators

Natural number chemistry [Berry and Boudol, 1992; Banzhaf et al., 1996]

Matrix-Multiplication Chemistry

[Banzhaf, 1993]

Abstract Automata

Turing machine like

RNA motivated [McCaskill, 1988; Thürk, 1993]

Machine-Tape Interaction

[Ikegami and Hashimoto, 1995]

Finite state machine

abstract [Dittrich, 1995; Dittrich and Banzhaff, 1998]

Artificial Molecular Machines

Polymers as Turing Machines

Machine-Tape Interaction

Automata Reaction

Lattice Molecular Systems

Autopoietic System

Autopoiesis is a process whereby a system produces itw own organization and maintains and constitutes itself in a space.

[Varela et al., 1974; McMullin and Varela, 1997]

Lattice Polymer Automaton

[Rasmussen and Smith, 1994]

Lattice Molecular Automaton (LMA)

[Mayer and Rasmussen, 1998]

Self-Replicating Cell

[Ono and Ikegami, 1999]

Assembler Automata and Core-Wars-like Systems

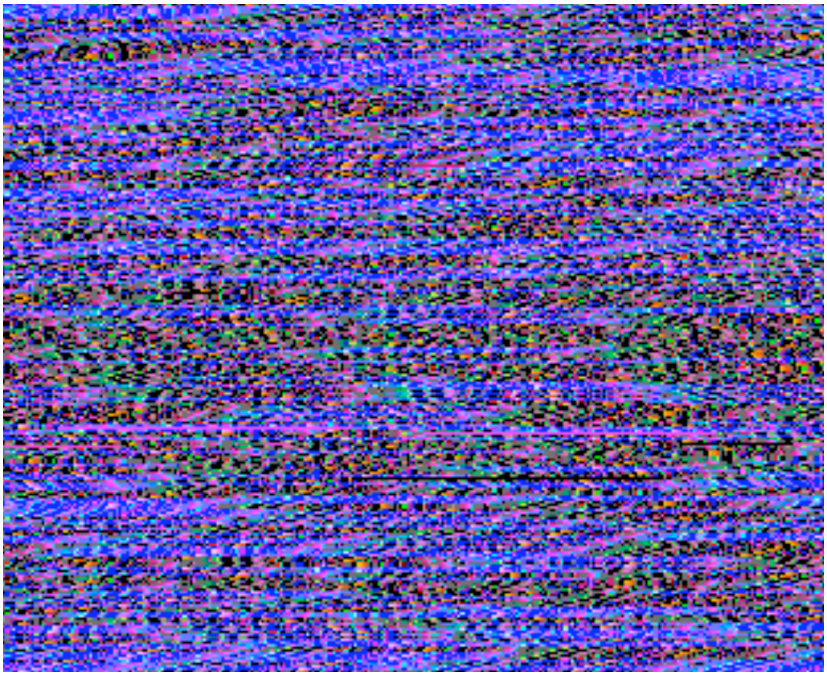
Core Wars

[Dewdney, 1984]

Coreworld

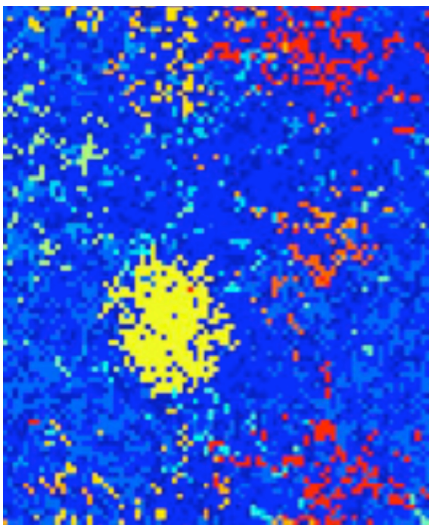
primordial [Rasmussen et al., 1990]

Tierra



species diversification, cambrian explosion [Ray, 1992]

Avida



spatial auto-catalytic self-replication [Adami, 1998]

Spontaneous generation of self-replicators

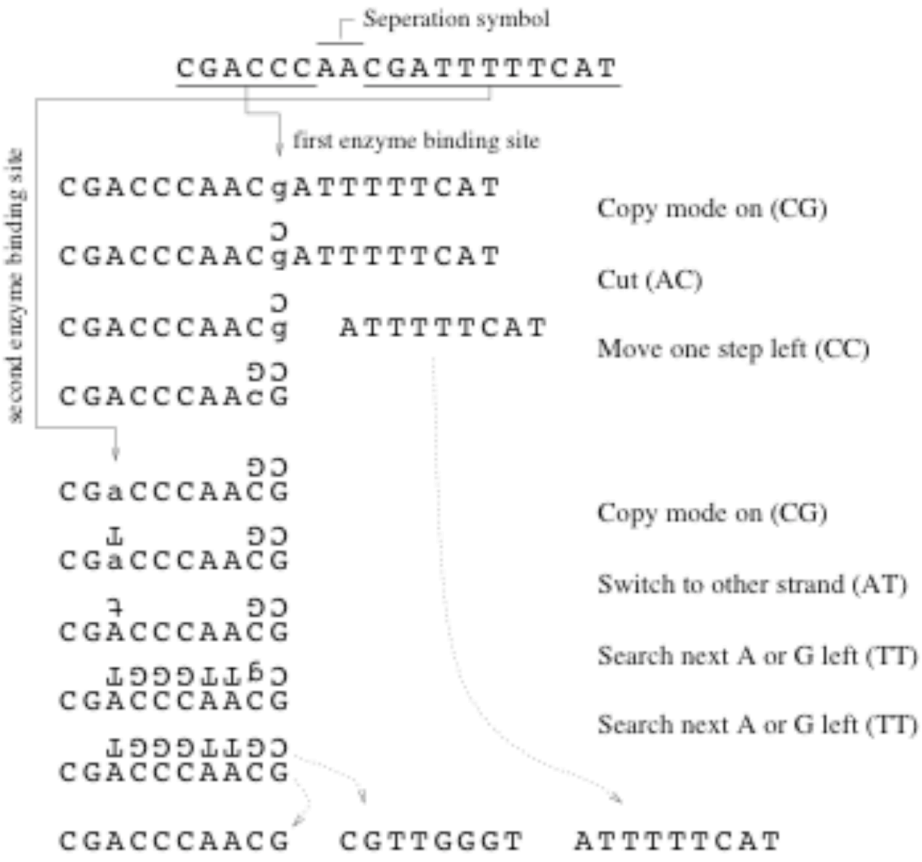
[Pargellis, 1996]

COSMOS

[Taylor and Hallam, 1998]

Other Approaches

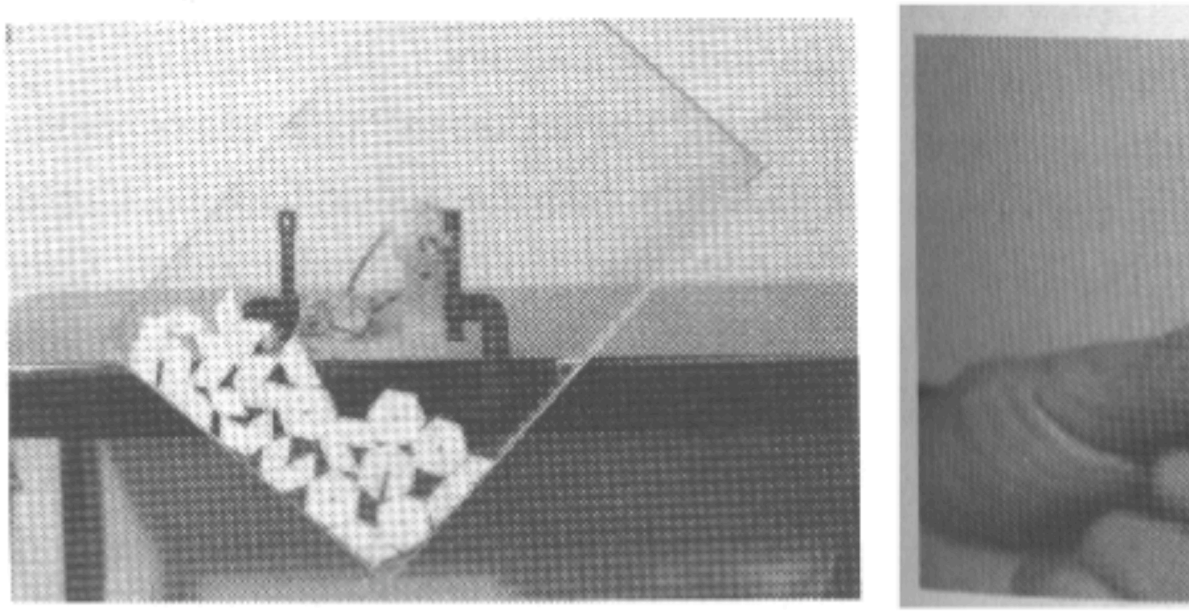
Typogenetics (Notebook)



[Hofstadter, 1979; Morris, 1989; Varetto, 1993]

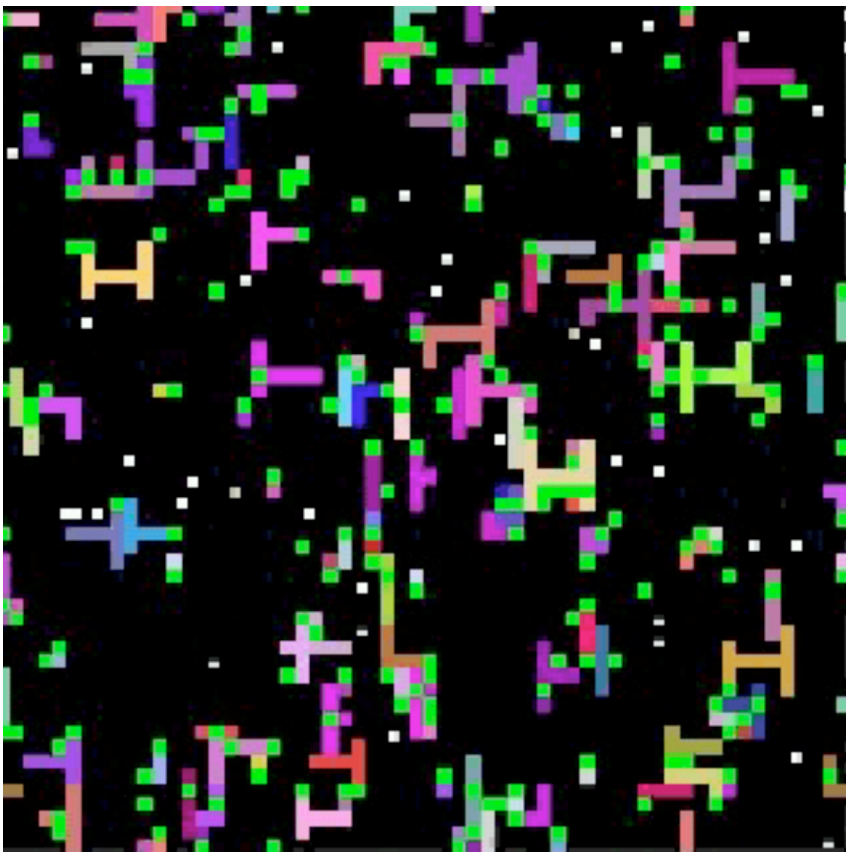
Self-Assembling Systems

Physical Self-Assembling Systems



[Hosokawa et al., 1994]

Simulated 2D Self-Assembly



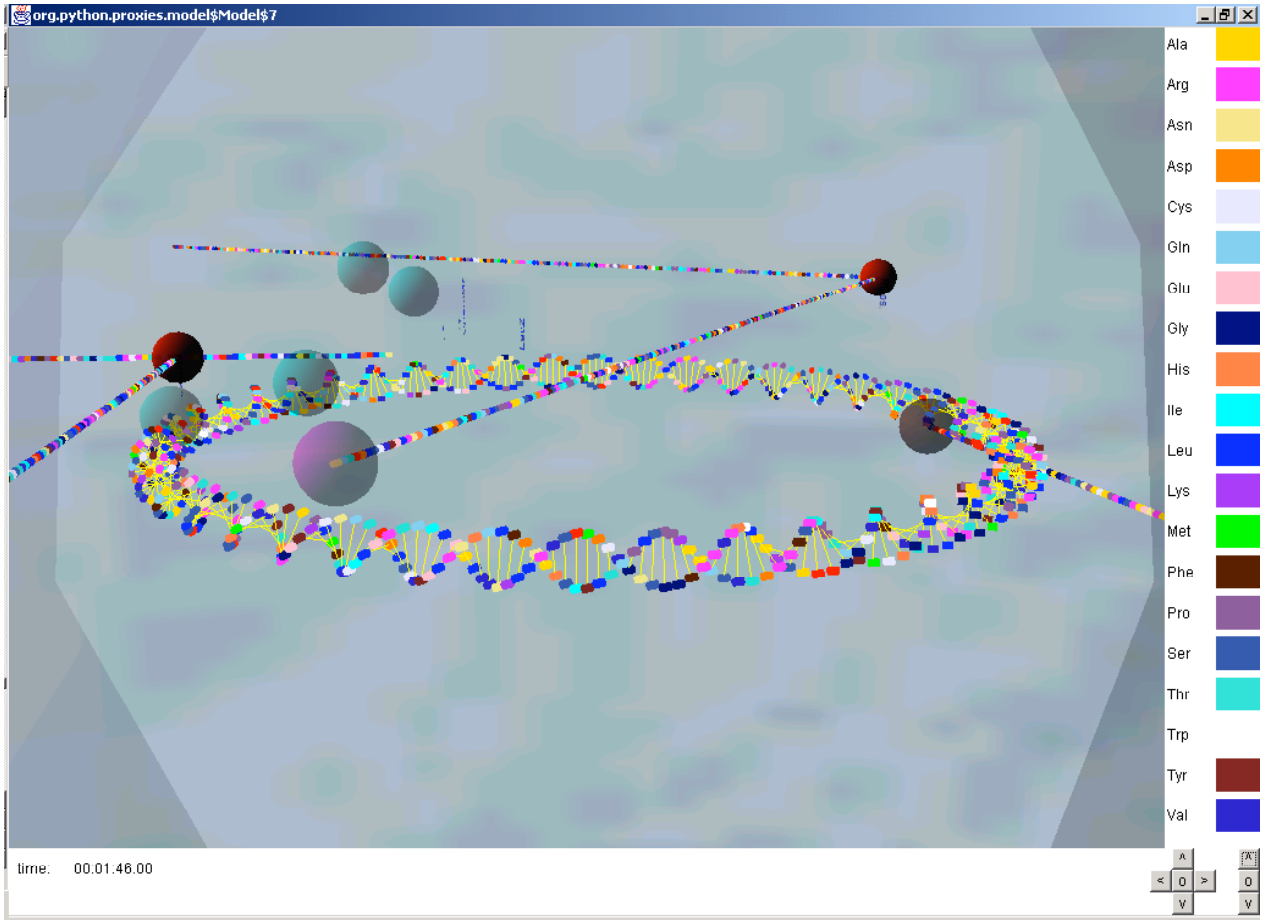
Henry Kwong, 2001

Self-modifying genetic programming

[Koza, 1994]

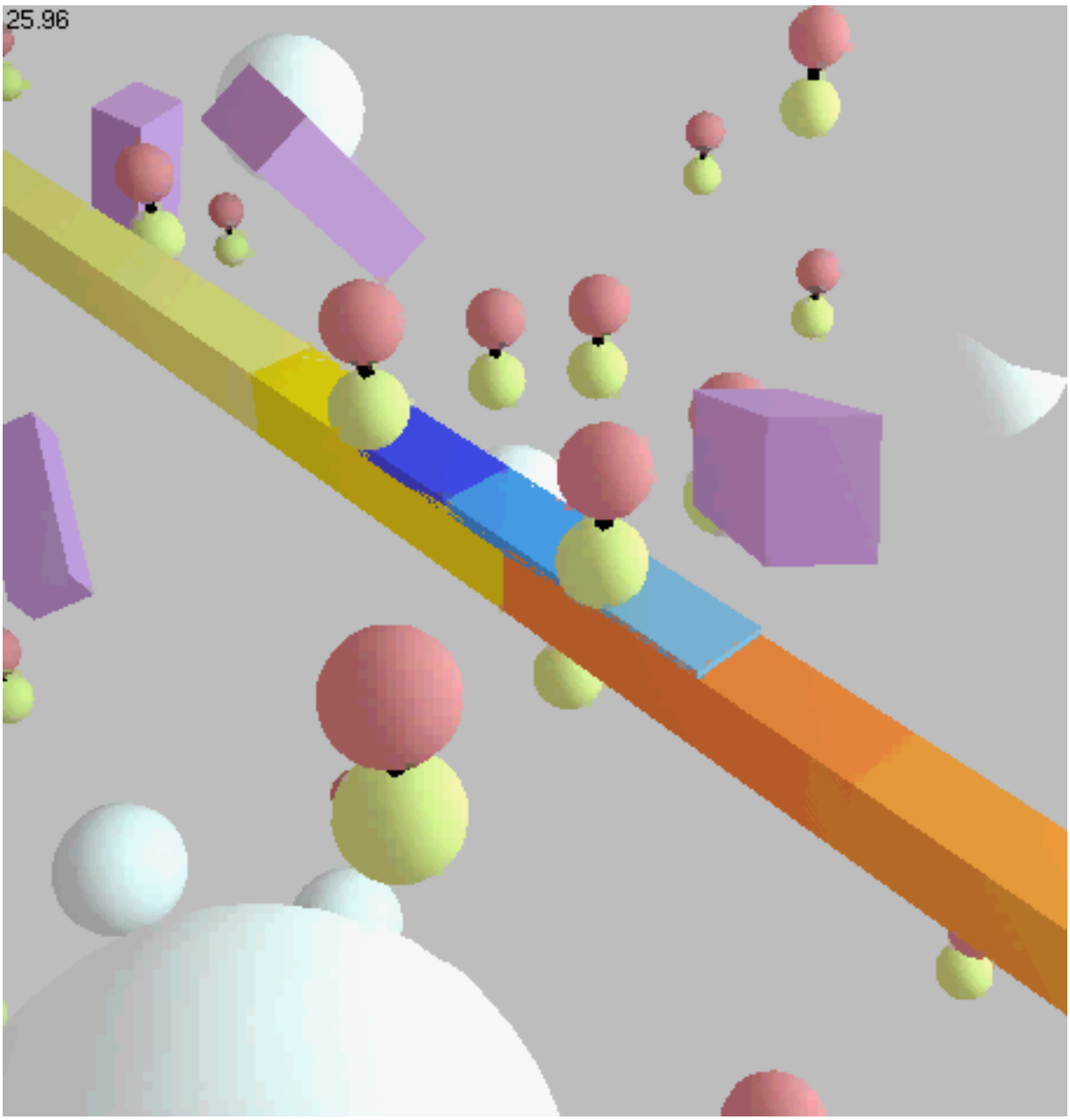
Explicit 3-D simulation of complex macro-molecular dynamics

Lactose Operon



Ian Burleigh, Garret Suen, and Julie Andreotti, 2002

Lambda Switch



Glorious Tsui, 2003

Parallel reconfigurable hardware

[McCaskill et al., 1994]

Chemical Casting Model

[Kanada and Hirokawa, 1994]

Cellular automata and boolean networks

[Dittrich, 1995]

Application of Chemical Computing

Artificial Chemical Computing

- Cell growth in ANN [Astor and Adami, 1998]
- Chemical communication among cells, "neural gas" [Husbands, 1998]
- Hormone system [Brooks, 1996] (Creatures)
- Subsystem in ecological/agent simulations
- Robust low-level control

Real Chemical Computing

- Enzyme kinetics
- DNA computing
- Conformational-driven computing
- Chemo-optical computing

Outlook, Challenges

1. Theory for constructive dynamical systems

2. Phenomenology of artificial chemistries

3. Methods of obversation and analysis

4. Conditions of emergent and self-improving hierarchical organizations

5. Potential for applications

Modeling

Modeling (Bio)chemical Systems

Evolution and Self-assembly

Ecological Modeling with Artificial Chemistries

Social Modeling with Artificial Chemistries

Information Processing

Artificial Chemical Computing

Real Chemical Computing

Optimization