CHEMORG

The Bio-Chemical Information Processing Metaphor as a Programming Paradigm for Organic Computing

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Friedrich-Schiller-University Jena

CHEMORG

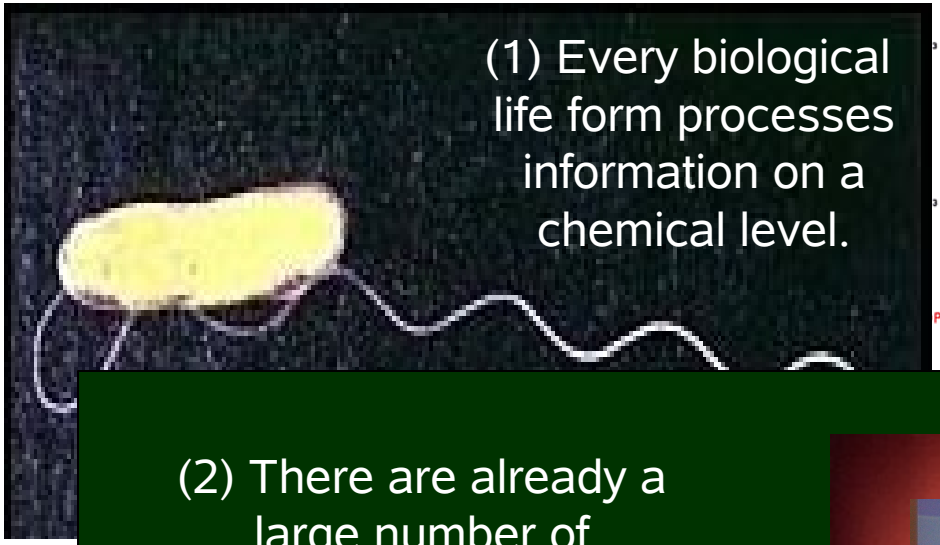
The Bio-Chemical Information Processing Metaphor as a Programming Paradigm for Organic Computing

Utilize bio-chemical information processing metaphor for organic system

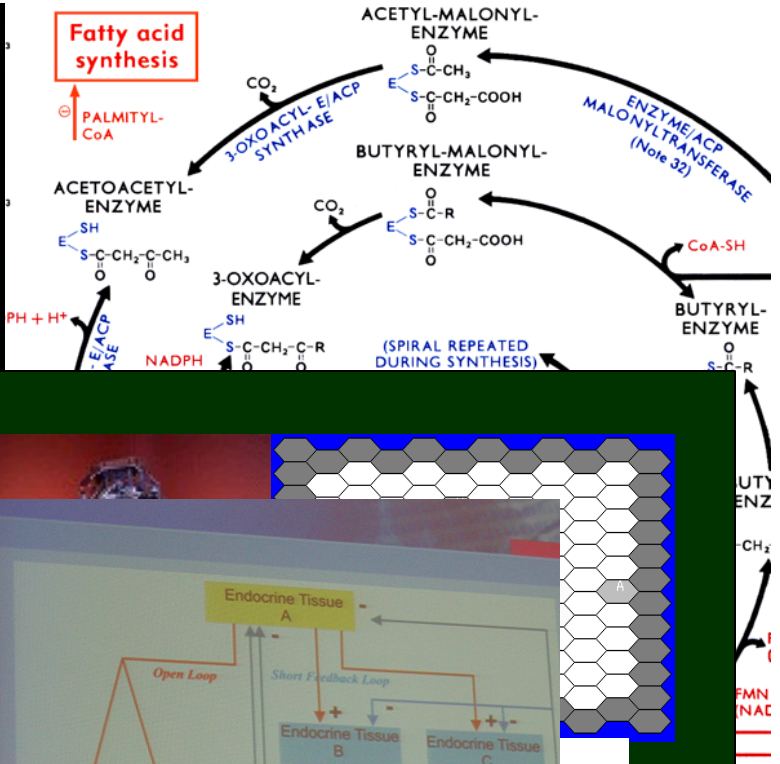
Utilize chemical reactions for organic system

• Dittrich, P. The Chemical Information Processing Metaphor as a Programming Paradigm for Organic Computing.
In: Proc of the Workshop Self-Organization and Emergence, ARCS ´05, VDE Verlag, 95-100, 2005
• Dittrich, P. Chemical Computing. LNCS 3566, 19-32, 2005

Motivation

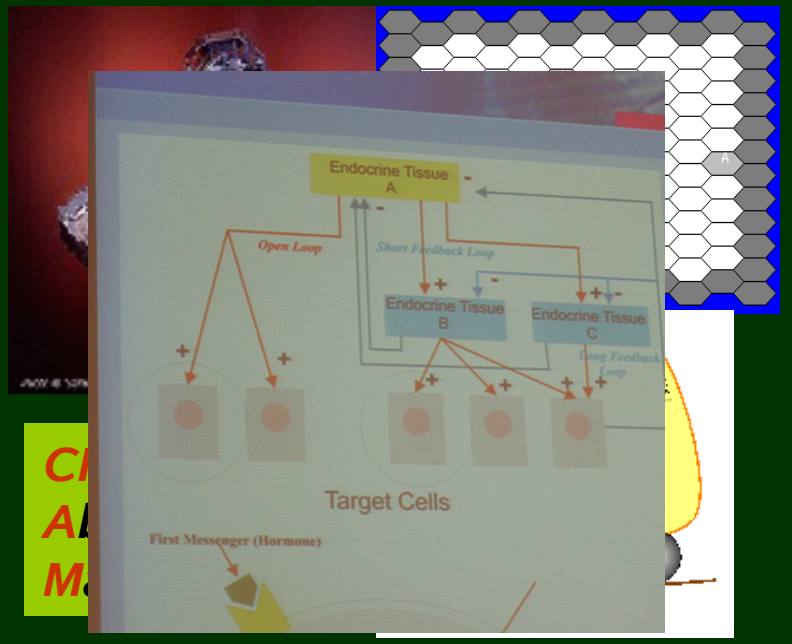


(1) Every biological life form processes information on a chemical level.

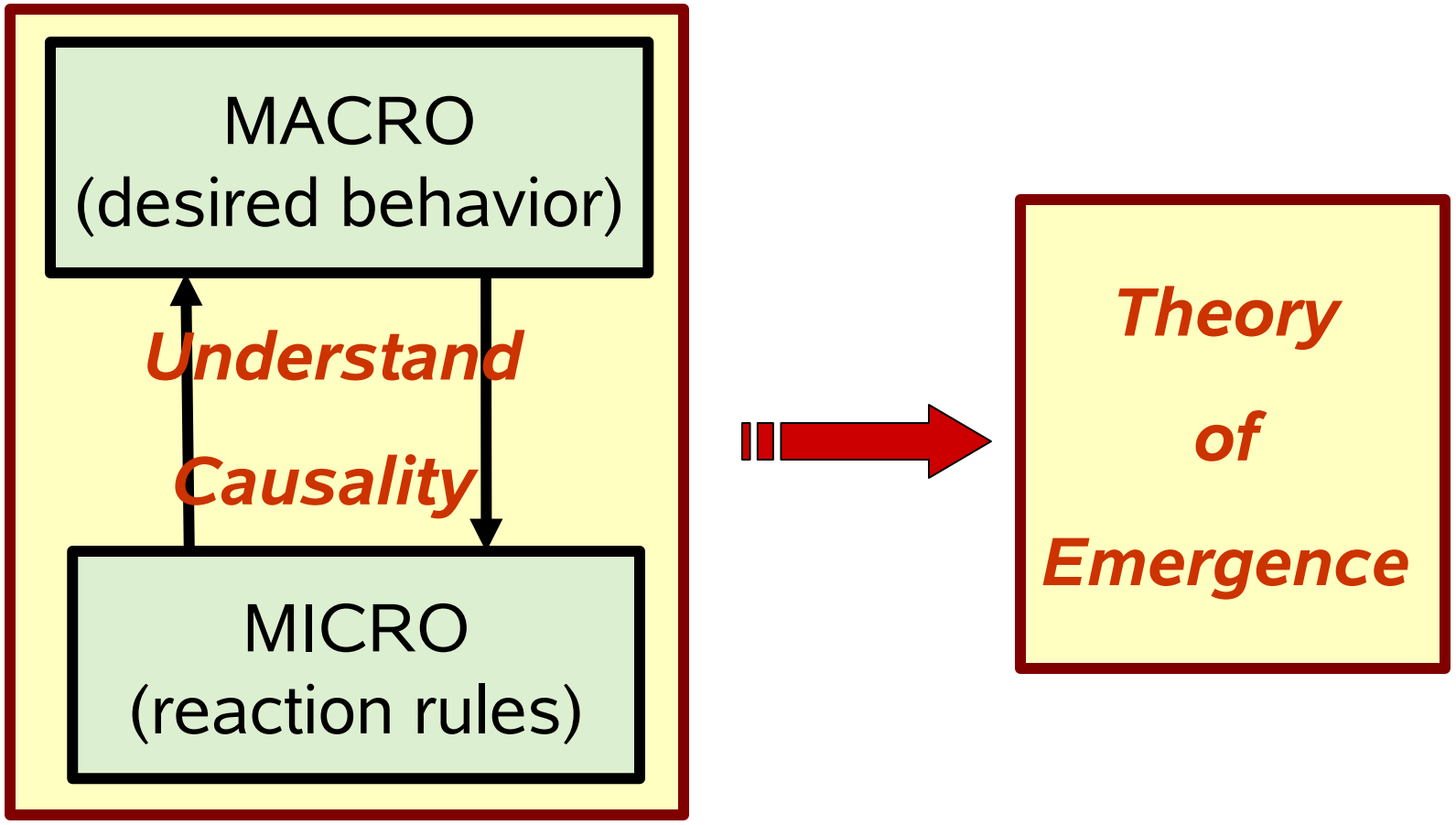


(2) There are already a large number of technical approaches inspired by bio-chemical principles.

(3) In order to program them we have to bridge the micro-macro gap.



Challenge


MACRO
(desired behavior)
Understand
Causality
MICRO
(reaction rules)
Theory
of
Emergence

Mission

1. Develop programming techniques for chemical-like computational systems

2. Evaluate such systems
   - qualitatively
   - quantitatively

Results previously shown

1. Develop programming techniques for chemical-like computational systems

- Programming principle:
  Organization Oriented Programming
- Recipe for mapping boolean networks to chemical systems
- Demonstrating for various circuits
  (XOR, FLIP-FLOP, oscillator, etc.)

• Matsumaru, N., F. Centler, P. Dittrich. Chemical Organization Theory as a Theoretical Base for Chemical Computing. In: Teuscher, C. and A. Adamtzky. Proc. of. Unconvntional Computing 2005, Luniver Press, p.75-88, 2005
• Matsumaru, N., P. Speroni di Fenizio, F. Centler, P. Dittrich. Chemical Organization Theory as a Theoretical Base for Chemical Computing, *Int. J. Unconv. Comp.*, 2006 (in print)

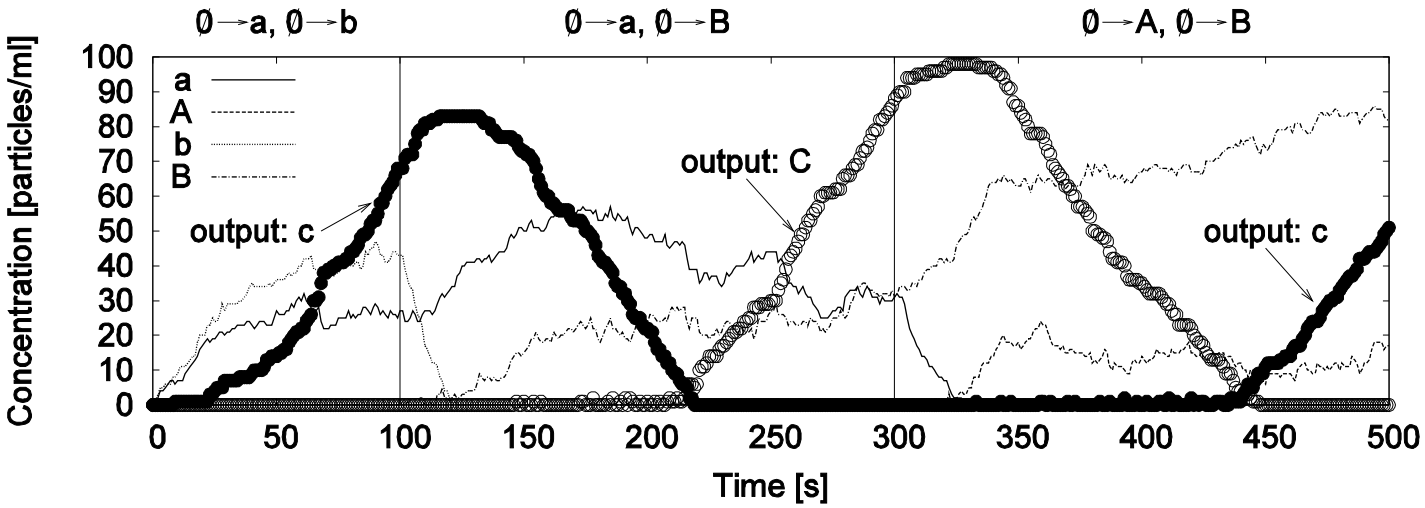
Chemical XOR

a	b	c
0	0	0
0	1	1
1	0	1
1	1	0

$$a + b \rightarrow c \qquad a + A \rightarrow \emptyset$$
$$a + B \rightarrow C \qquad b + B \rightarrow \emptyset$$
$$A + b \rightarrow C \qquad c + C \rightarrow \emptyset$$
$$A + B \rightarrow c$$

a : **a == 0**

A : **a == 1**



FLIP-FLOP, oscillator, etc.

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Mission

1. Develop programming techniques for chemical-like computational systems

2. Evaluate such systems
   - qualitatively
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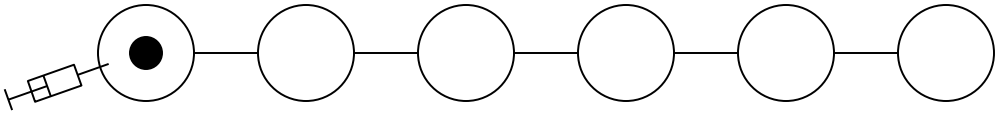
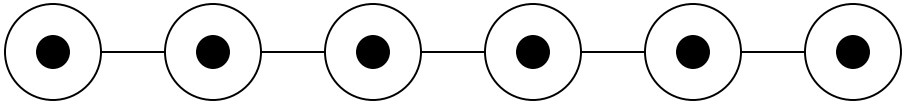
Benchmark Problem

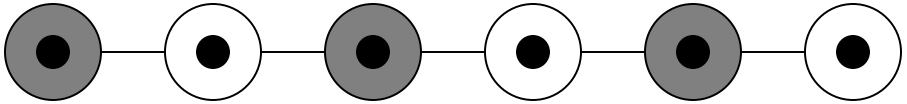
1. Inject molecules



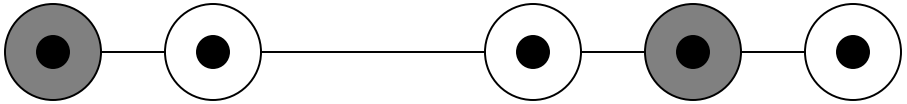
2. Molecules distribute



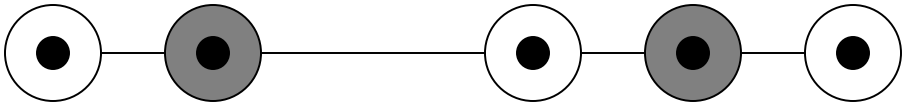
3. Cells differentiate (self-organize)



4. A cell is removed



5. Reorganize



Maximal Independent Set

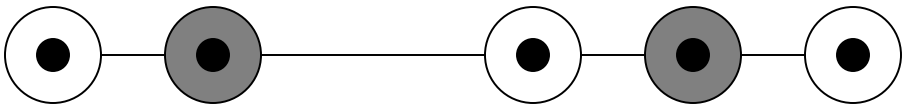
- *Def.* ***[Independent set]***

  A set of vertices no two of which are adjacent

- *Def.* ***[Maximal Independent set]***

  Given an undirected graph, an independ set is maximal if no vertex can be added to the independent set.

Note: Maximal independent set is different from maximum independent set.



There are two maximal independent sets.

The maximum independent set has the size of 3.

Algorithms for MIS problem

- Under central daemon [Luby 1985]

$G=\langle V,E\rangle, \quad I \leftarrow \emptyset$
while $V \neq \emptyset$ do
begin
$I \leftarrow I \cup \{v\} \mid v \in V$
$V \leftarrow V\text{-}(\{v\} - \mathrm{Neigh}(v))$
end

- Distributed system [Shukla, et al. 1995]

$$(\forall n \in \mathrm{Neigh}(v), n.Ind == False) \rightarrow (v.Ind := True)$$
$$(\exists n \in \mathrm{Neigh}(v), n.Ind == True) \rightarrow (v.Ind := False)$$

Algebraic Chemistry for MIS problem

$$M=\{s_i^0, s_i^1 | i=1,\cdots,N\}$$

$$s_i^{\text{bin}}$$

Membership to the inde-pendent set

Vertex ID

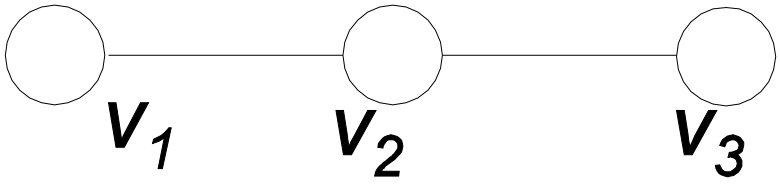
$$R=\bigcup_{i=1}^{N} R^i$$

$$\begin{cases} \underbrace{s_j^0+s_k^0+\cdots+s_l^0}_{n_i:\text{number of neighbors}} \rightarrow n_i s_i^1 \\ \{s_j^1 \rightarrow s_i^0 | (v_i, v_j) \in E\} \\ s_i^0 + s_i^1 \rightarrow \emptyset \end{cases}$$

- Matsumaru, N., P. Dittrich. Organization-oriented chemical programming for the organic design of distributed computing systems; submitted to Bionetics 2006

Algebraic Chemistry for MIS problem

Undirected Graph



Reaction Network

$$M = \{ s_1^0, s_1^1, s_2^0, s_2^1, s_3^0, s_3^1 \}$$

$$s_2^1 \to s_1^0 \qquad s_1^1 \to s_2^0 \qquad s_2^1 \to s_3^0$$

$$s_2^0 \to s_1^1 \qquad s_3^1 \to s_2^0 \qquad s_2^0 \to s_3^1$$

$$s_1^0 + s_3^0 \to 2s_2^1$$

$$s_1^0 + s_1^1 \to \emptyset$$

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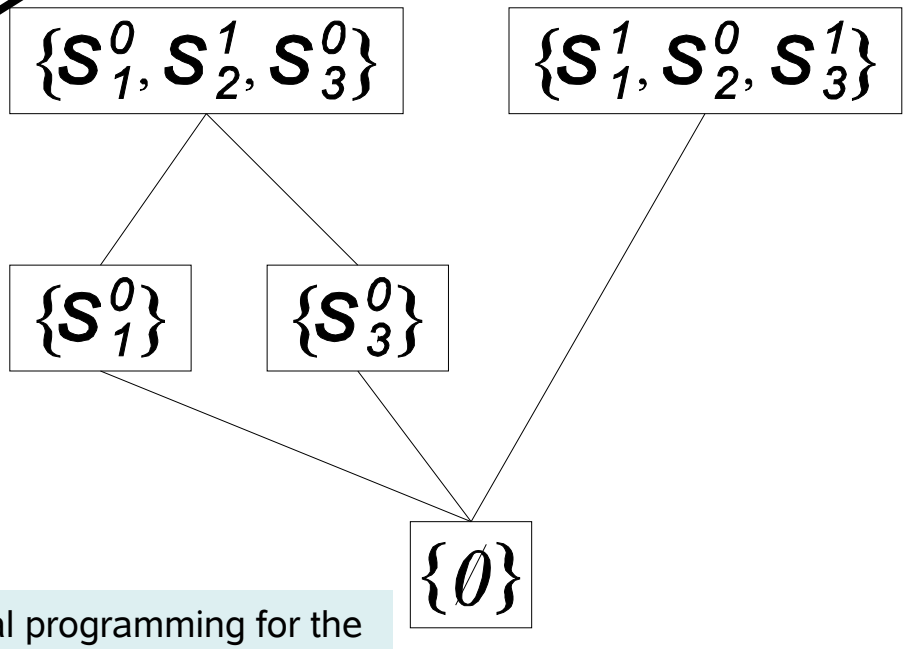
Organizational structure



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„Chemical Organization"

There is no reaction producing any other molecules than the member of the set.

Organization :=

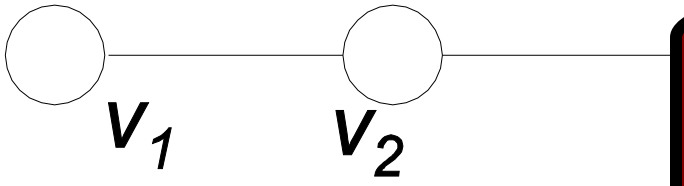
a set of molecules that is (algebraically) closed and self-maintaining

Within the set, all molecules consumed by a reaction can be reproduced by a reaction.

• Dittrich, P., P. Speroni di Fenizio. Chemical Organization Theory, *Bull. Math. Biol.*, in print, 2006

Algebraic Chemistry for MIS problem

Undirected Graph



There is no reaction producing any other molecules than the member of the set.

$$s_2^1 \rightarrow s_1^0 \qquad s_1^1 \rightarrow s_2^0 \qquad s_2^1 \rightarrow s_3^0$$

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Orga tional structure

$$\{s_2^1\}$$

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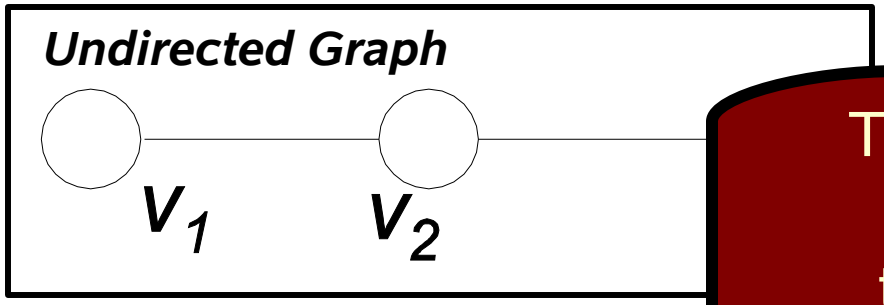
Algebraic Chemistry for MIS problem



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Orga tional structure

$$\{ s_2^1 \quad s_3^0 \}$$

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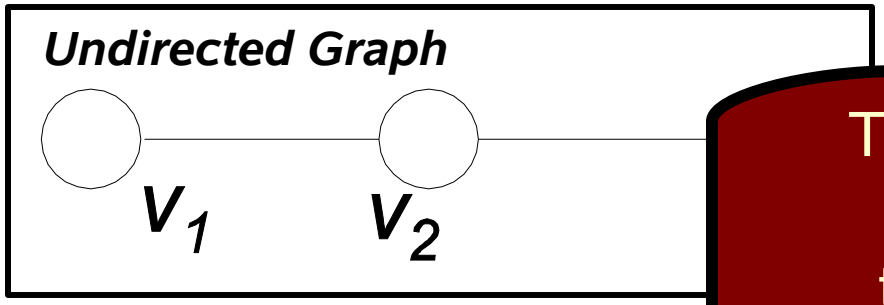

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$\{s_1^0, s_2^1, s_3^0\}$

$$s_1^0 + s_1^1 \to \emptyset$$
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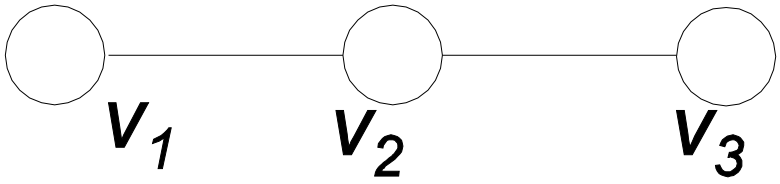

Reaction Network

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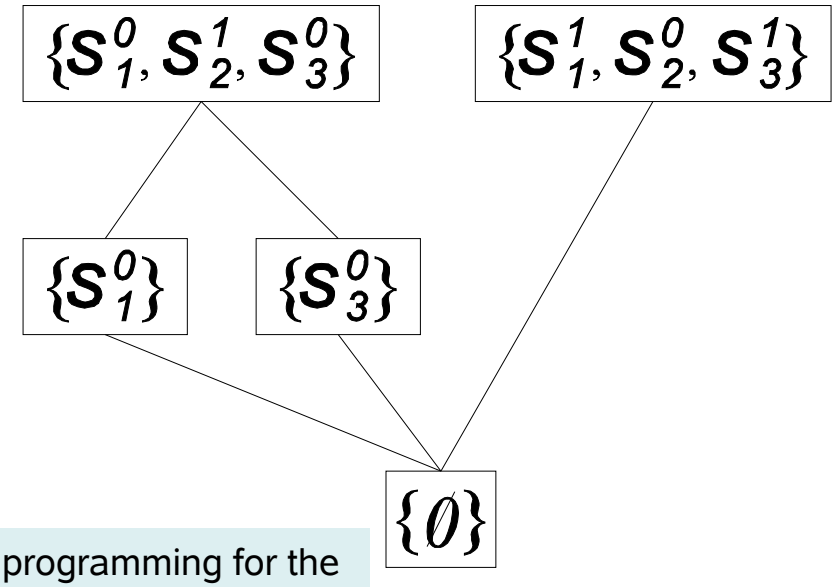
Organizational structure



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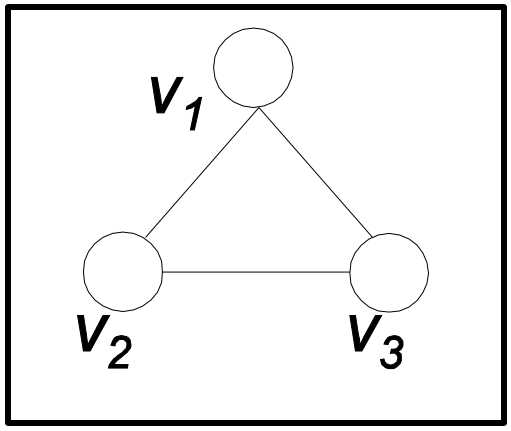

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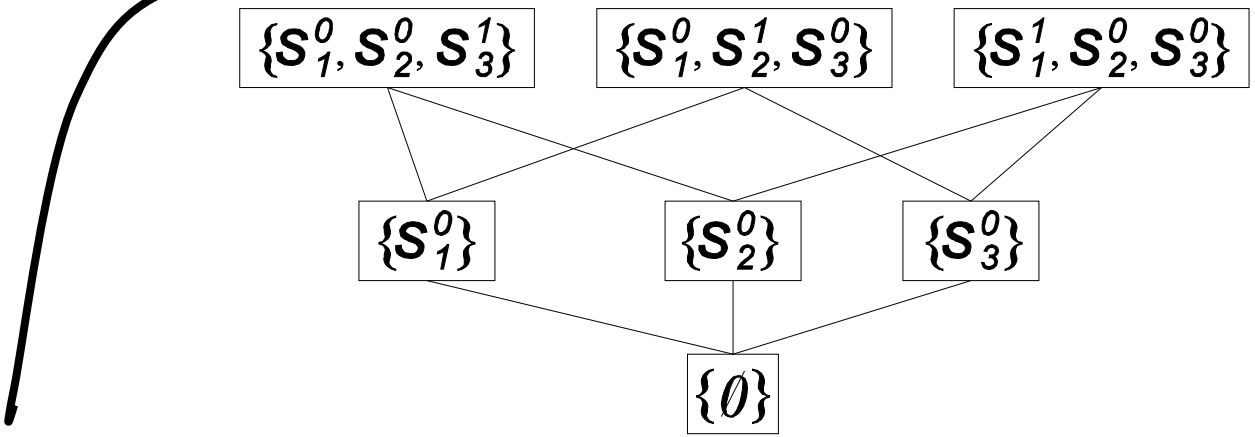

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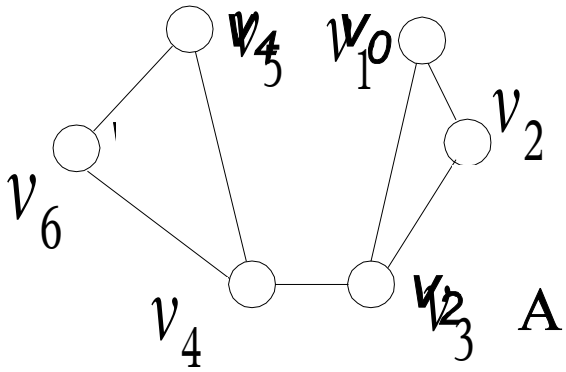
Algebraic Chemistry for MIS problem

Undirected graph



A

B

Organizational structure

$\{ s_1^1, s_2^0, s_3^0, s_4^0, s_5^0, s_6^1 \}$ $\{ s_1^0, s_2^1, s_3^0, s_4^1, s_5^0, s_6^0 \}$

$\{ s_1^1, s_2^0, s_3^0, s_4^1, s_5^0, s_6^0 \}$ $\{ s_1^0, s_2^1, s_3^0, s_4^0, s_5^1, s_6^0 \}$

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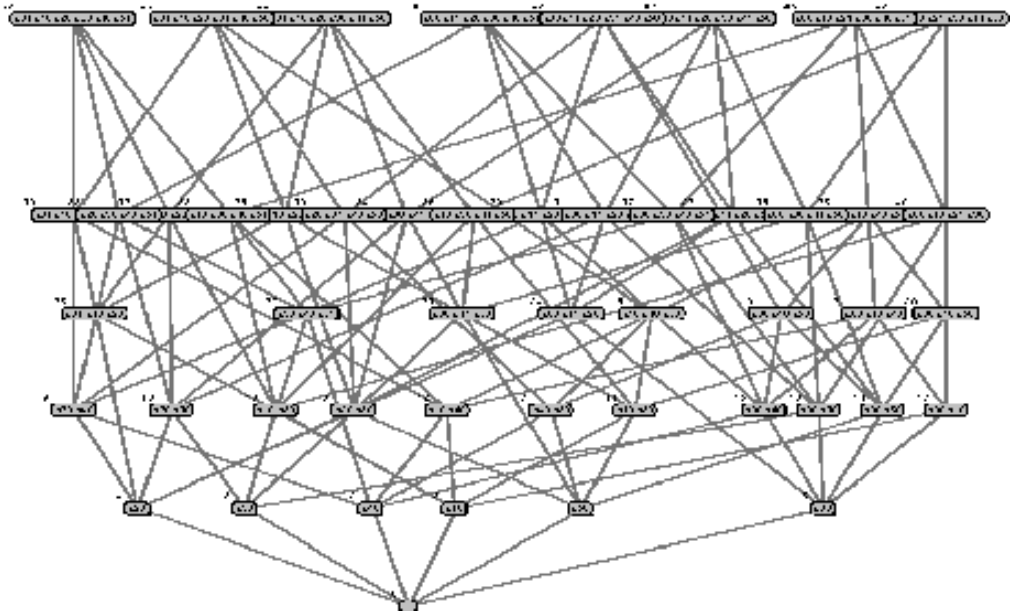
Reaction network

M :12 molecular species

R :32 reaction rules



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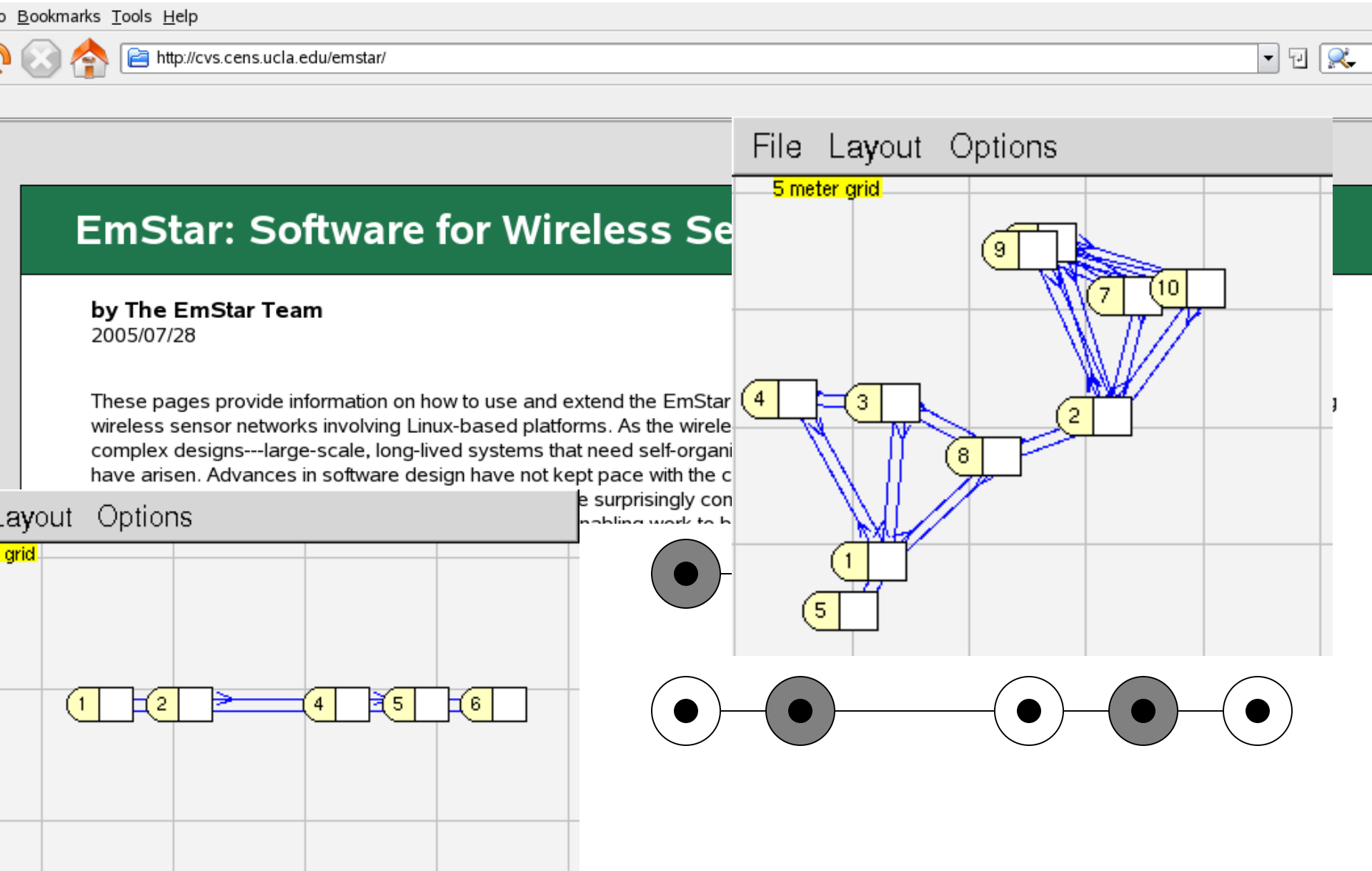
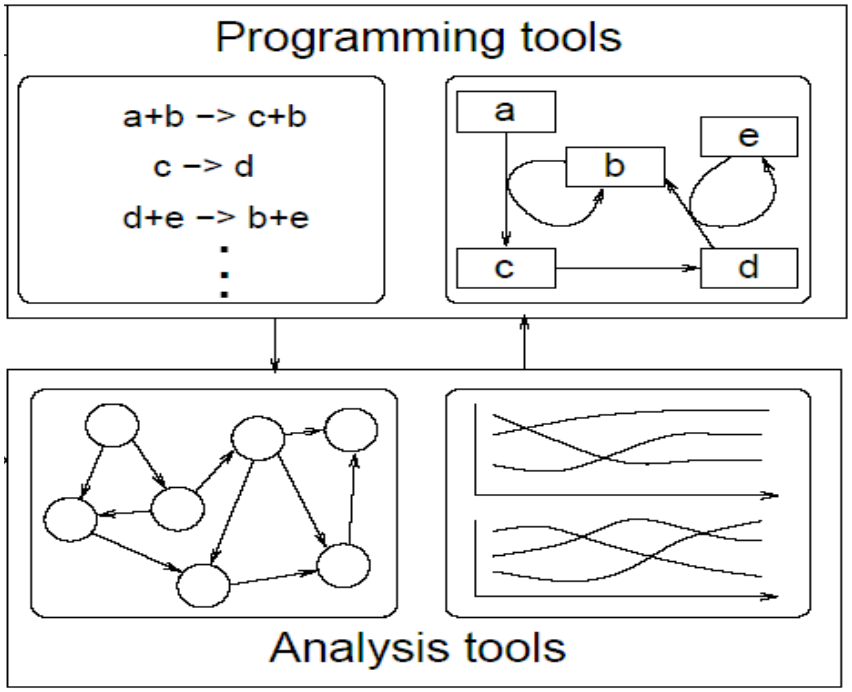
Benchmark Problem



Programming Environment



- Programming
  - List of reaction rules
    (Text editor)
  - Network structure
    (CellDesigner.org)
- Analysis
  - Static, structural
    (OrgAnalysis)
    (FluxAnalyzer)
  - Dynamical
    (ODESolver)
    (Copasi)
- Protocols
  (SBW)
  - Data format
    (SBML)

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http://sbml.org/index.psp

SBML Systems Biology Markup Language

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The Systems Biology Markup Language (SBML) is a computer-readable format for representing **models of biochemical reaction networks**. SBML is applicable to metabolic networks, cell-signaling pathways, regulatory networks, and many others.

Internationally Supported and Widely Used

SBML has been evolving since mid-2000 through the efforts of an international group of software developers and users. Today, SBML is **supported by over 100 software systems**, including the following (where '*' indicates SBML support in development):

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SBW

SB Conferences

Systems Biology Workbench

iology Workbench (SBW), an open s
. SBW is made up of two kinds of compo

lications that a user would use. We ha
d model analysis tools.
framework that allows developers to cr
lication modules to form new application

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CellDesigner.org

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l in modeling have a look at the JDesig

g interfaces. Jarnac Quickstart or Jarnac

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CellDesigner™: A

CellDesigner 3.2 R

backlinks...

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copasi

Complex Pathway Simulator

Latest version: Version 4.0 (Build 18) released June 16, 2006 (first official release)

What's new in Version 4.0 Build 18

Login

user:

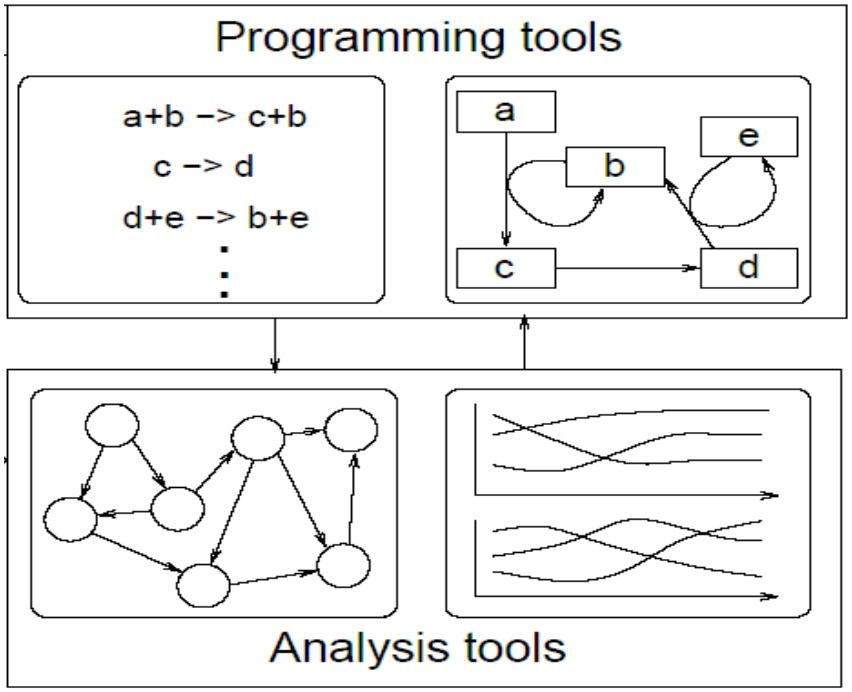
pass:

login

Remember me

I forgot my pass

Programming Environment



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    (SBML)

OrgAnalysis

File Analysis SBW

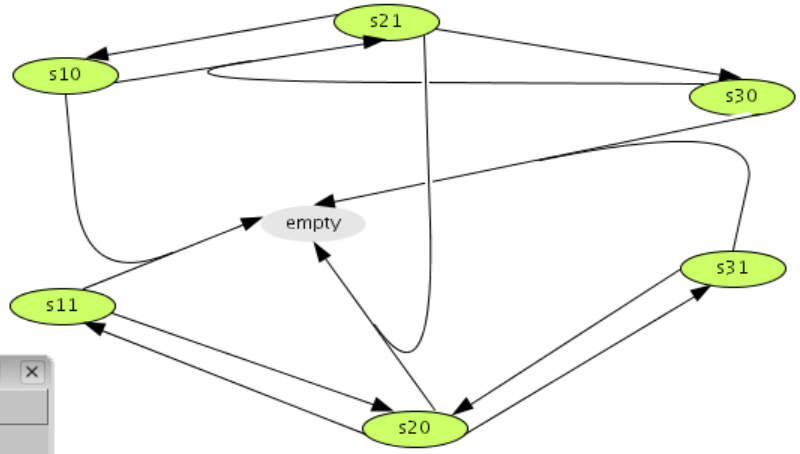
Metabolites | Reactions | Network Analysis | Log

delete reaction | add reaction | unmark all

Reactions
1.0 s4 -> 1.0 s2
1.0 s1 1.0 s6 -> 2.0 s5
1.0 s4 -> 1.0 s7
1.0 s5 -> 1.0 s1
1.0 s2 -> 1.0 s4
1.0 s7 -> 1.0 s4
1.0 s5 -> 1.0 s6
1.0 s6 1.0 s7 -> 1.0 s8
1.0 s4 1.0 s5 -> 1.0 s8
1.0 s2 1.0 s1 -> 1.0 s8

View Database Simulation Window SBW Preference Help

mis-analysis-cd-n3-line.xml *



Species | Proteins | Genes | RN

Edit

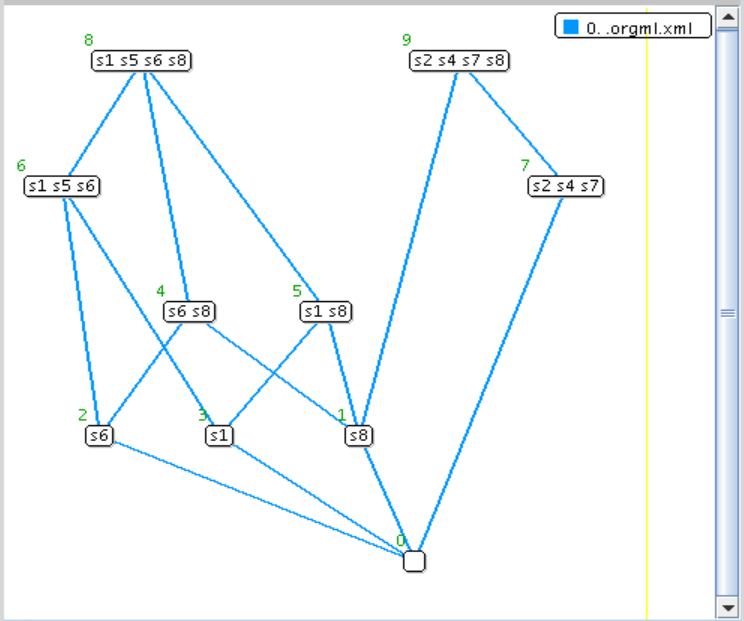
class	positionT	id	name
SIMPLE_M	inside	s1	s10
SIMPLE_M	inside	s2	s11
SIMPLE_M	inside	s4	s20
SIMPLE_M	inside	s5	s21
SIMPLE_M	inside	s6	s30
SIMPLE_M	inside	s7	s31
UNKNOWN	inside	s8	empty

Edit Notes | Edit Protein Notes

orgView - visualized Organizations

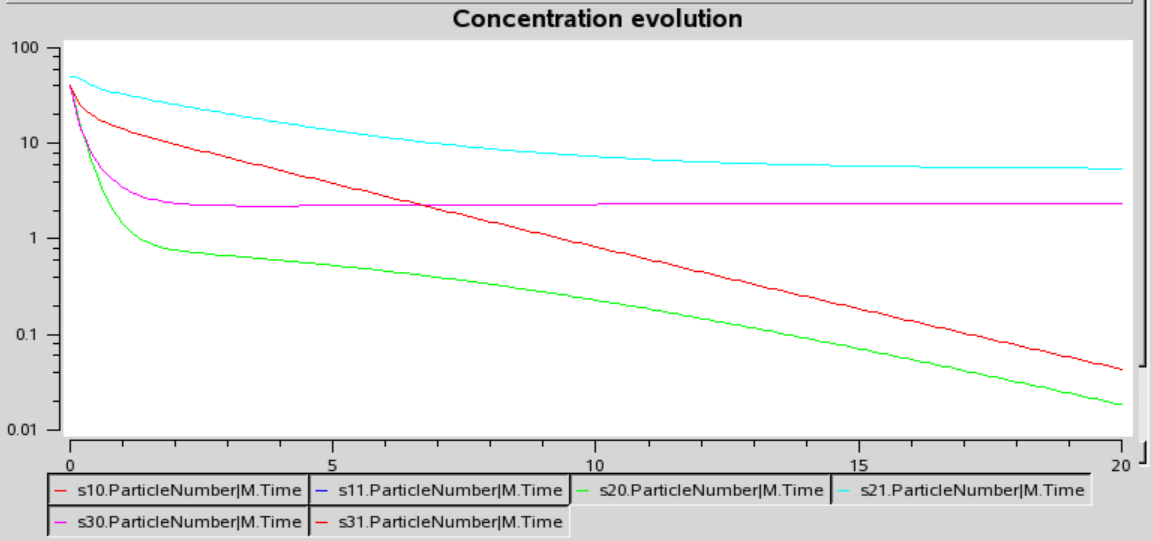
File View Tools Windows Exit SBW

Zoom: 9% FontZoom: 28%



Copasi Plot: Concentration evolution

Print Save data...



Summary of Results

(1) Basic Principles of Chemical Computing

1. Dittrich, P. The Chemical Information Processing Metaphor as a Programming Paradigm for Organic Computing In: U. Brinkschulte et al. (Eds.), Proc. W orkshop Self-Organization and Emergence, ARCS ´05, VDE Verlag, p. 95--100, 2005
2. Dittrich, P. Chemical Computing. *LNCS,* **3566**: 19--32, 2005

(2) Chemical Organization Theory as a Theoretical Base for Chemical Computing of Boolean Functions (XOR, FLIP-FLOPS, oscilator, etc.)

1. Matsumaru, N., F. Centler, P. Dittrich. Chemical Organization Theory as a Theoretical Base for Chemical Computing. In: Teuscher, C. and A. Adamtzky. Proc. of. Unconvntional Computing 2005, Luniver Press, p.75-88, 2005
2. Matsumaru, N., P. Speroni di Fenizio, F. Centler, P. Dittrich. Chemical Organization Theory as a Theoretical Base for Chemical Computing, *Int. J. Unconv. Comp*., 2006 (in print)

(3) Organization-Oriented Chemical Programming and the Independet Set Problem (sensor network senario)

1. Matsumaru, N., P. Dittrich. Organization-oriented chemical programming for the organic design of distributed computing systems. Bionetics 2006 (submitted)

(4) Programming Environment Preliminary Prototype

(ongoing)

(5) Evaluation with wireless sensor network simulation

(ongoing)

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CHEMORG

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