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

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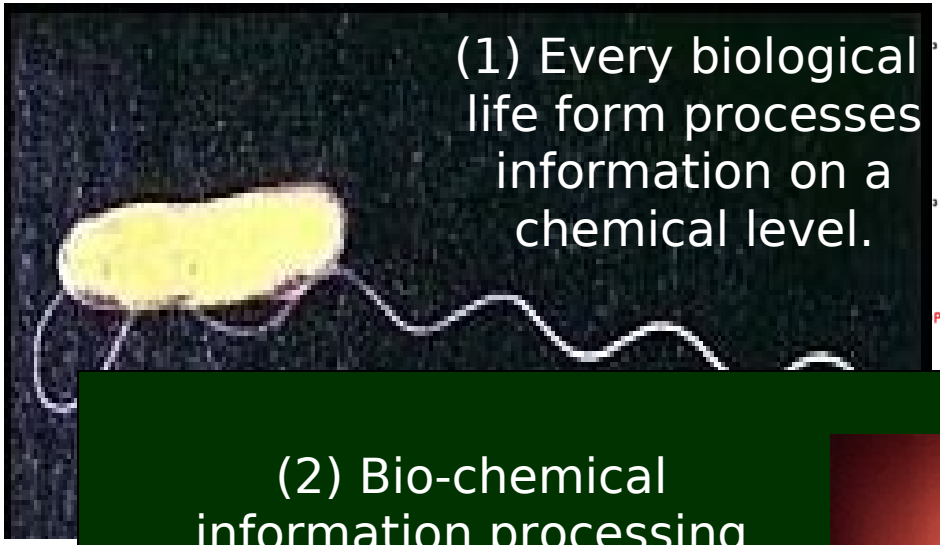
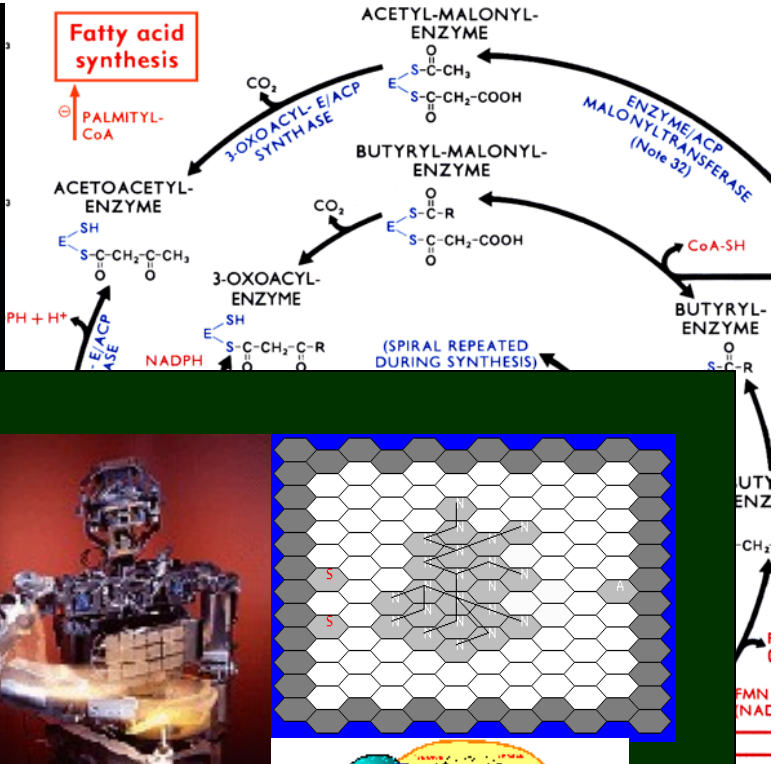
DFG Grant No. Di 852/4-1 and Di 852/4-2

Motivation



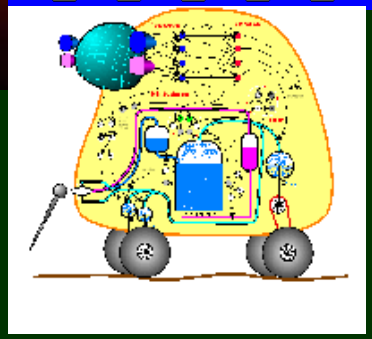
(1) Every biological life form processes information on a chemical level.



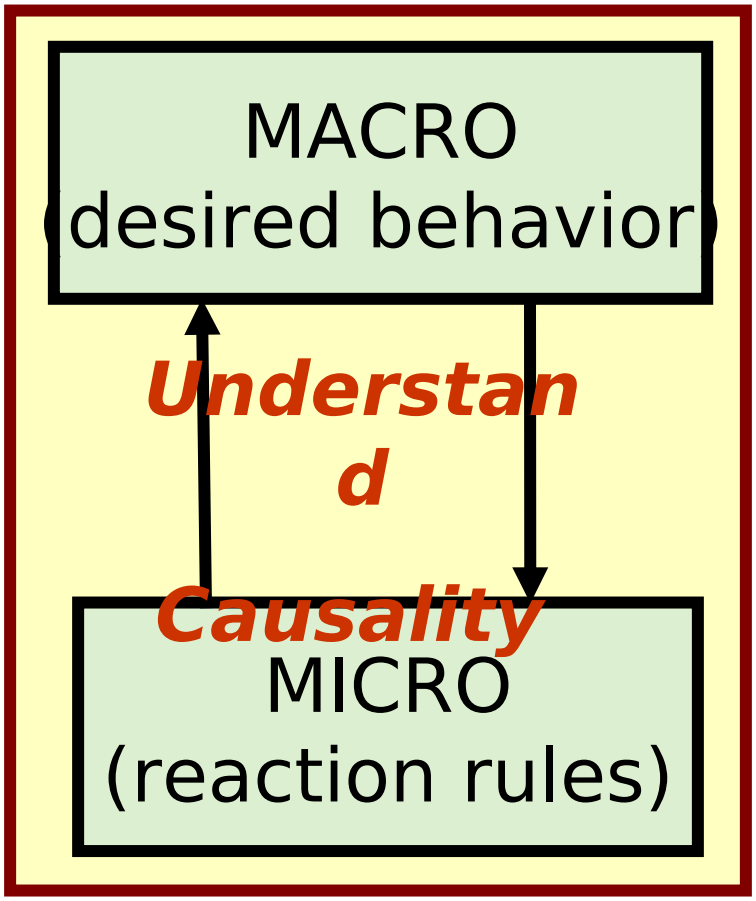
(2) Bio-chemical information processing posses a series of valuable self-x properties

(3) Chemical programming appears to be difficult.

CHemical Abstract Machine



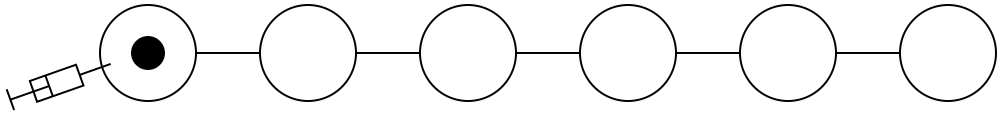
Challenge



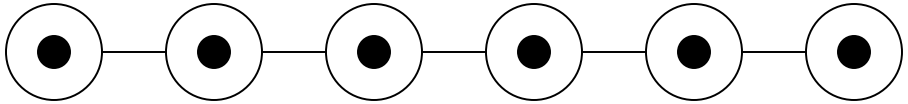
[12] Peter Dittrich.
Chemical Computing. In J.-P. Banatre, J.-L. Giavitto, P. Fradet, and O. Michel (Eds.), Unconventional Programming Paradigms (UPP 2004), *LNCS*, 3566: 19-32. Springer, Berlin, **2005**

Sketch of an Example Application

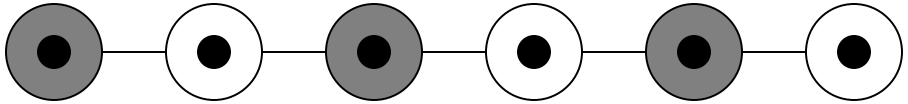
1. Inject molecules



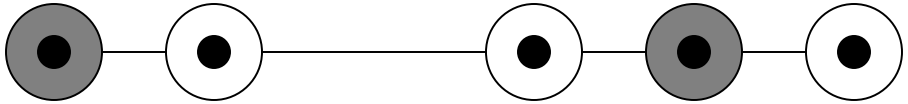
2. Molecules distribute



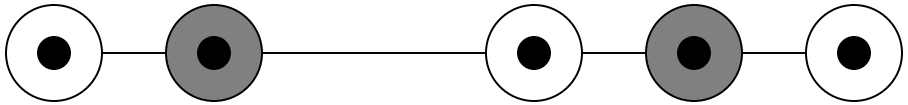
. Cells differentiate (self-organize)



4. A cell is removed



5. Reorganize



Aim

How to program chemical-like systems?

Results

1. Chemical Programming Paradigm
2. Programming Environment
3. Case Studies and Evaluation

1. Chemical Programming Paradigm

"Organization Oriented Programming"

Computation should appear as a movement within the set of organizations.

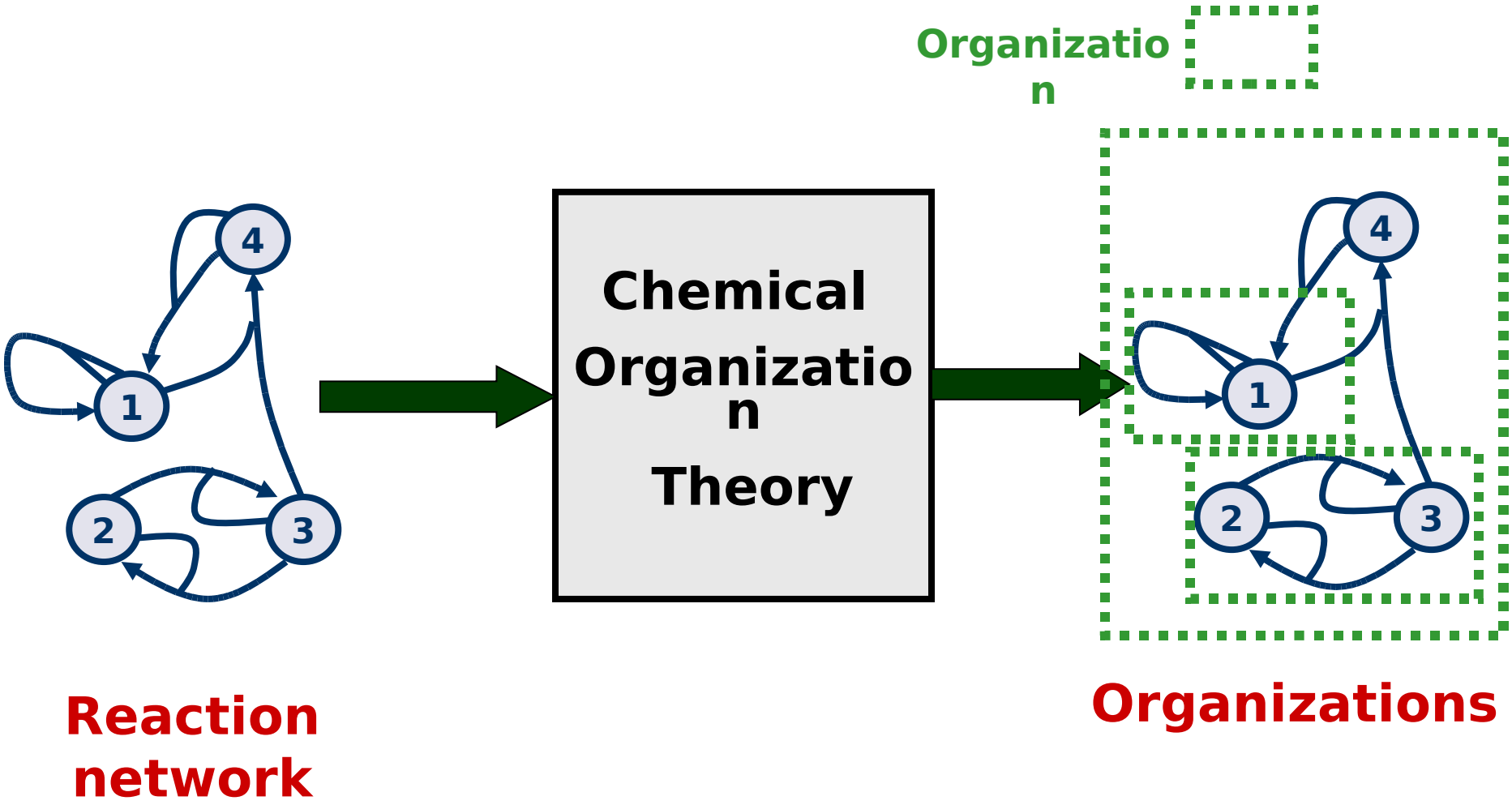
[5] P. Dittrich, N. Matsumaru,
Organization-Oriented Chemical Programming, In: Proc. of 7th International Conference on Hybrid Intelligent Systems (HIS 2007), IEEE DL, 6 pages, **2007**, (in print)

[2] N. Matsumaru, T. Lenser, T. Hinze, and P. Dittrich.
Designing a Chemical Program using Chemical Organization Theory.
BMC Systems Biology, 1(Suppl 1):P26, **2007**, (extended abstract)

[11] Peter Dittrich.
The Bio-Chemical Information Processing Metaphor as a Programming
Paradigm for Organic Computing. In U. Brinkschulte, J. Becker, C. Hochberger, T. Martinetz, C. Mueller-Schloer, H. Schmeck, T. Ungerer, and R. Wuertz, editors, ARCS '05 - 18th International Conference on Architecture of Computing Systems 2005, pages 96-100. VDE Verlag, Berlin, **2005**

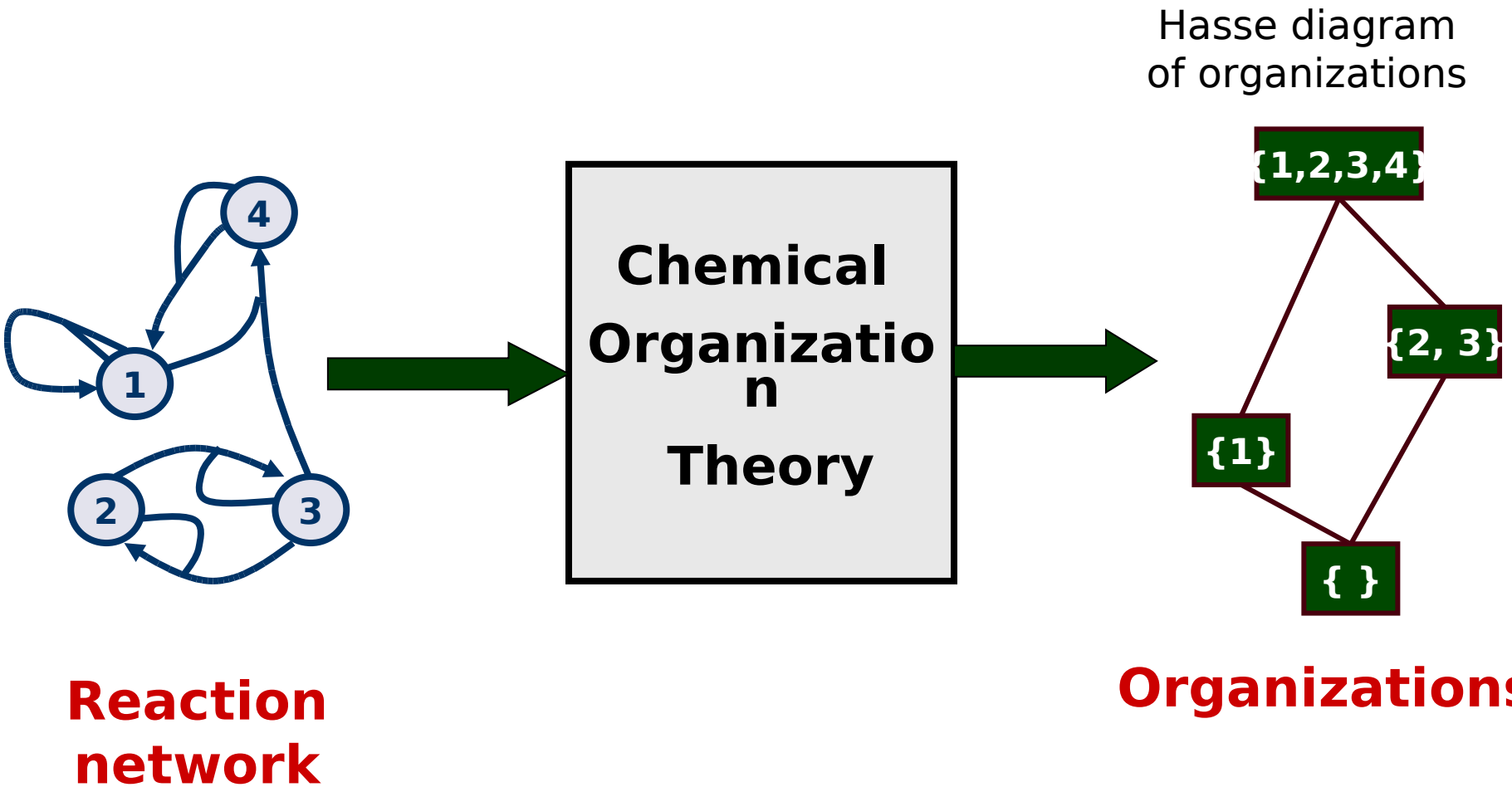
[12] Peter Dittrich.
Chemical Computing. In J.-P. Banatre, J.-L. Giavitto, P. Fradet, and O. Michel (Eds.), Unconventional Programming Paradigms (UPP 2004), *LNCS*, 3566: 19-32. Springer, Berlin, **2005**

Practical View



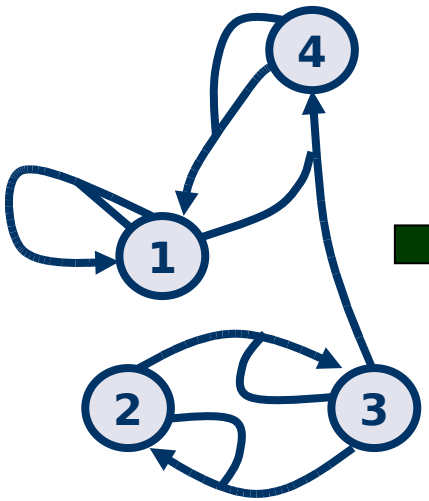
[P. Dittrich, P. Speroni di Fenizi, Chemical Organization Theory, *Bull. Math. Biol.*, 2007]

Practical View



[P. Dittrich, P. Speroni di Fenizi, Chemical Organization Theory, *Bull. Math. Biol.*, 2007]

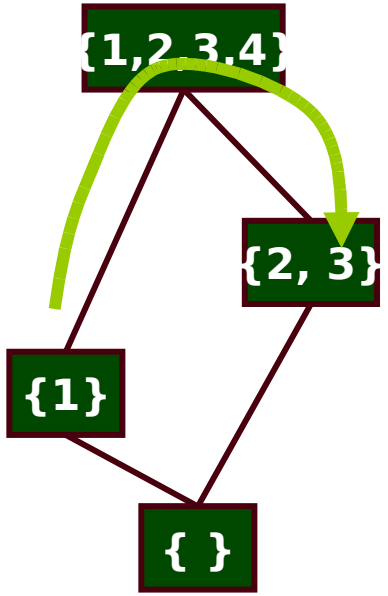
Practical View



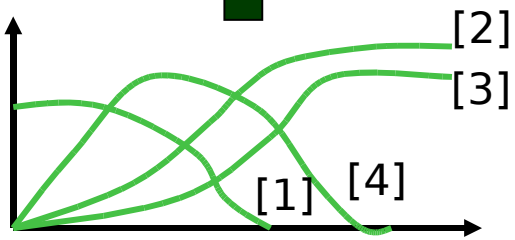
Reaction network

Chemical Organization Theory

Hasse diagram of organizations



Organizations



Dynamics

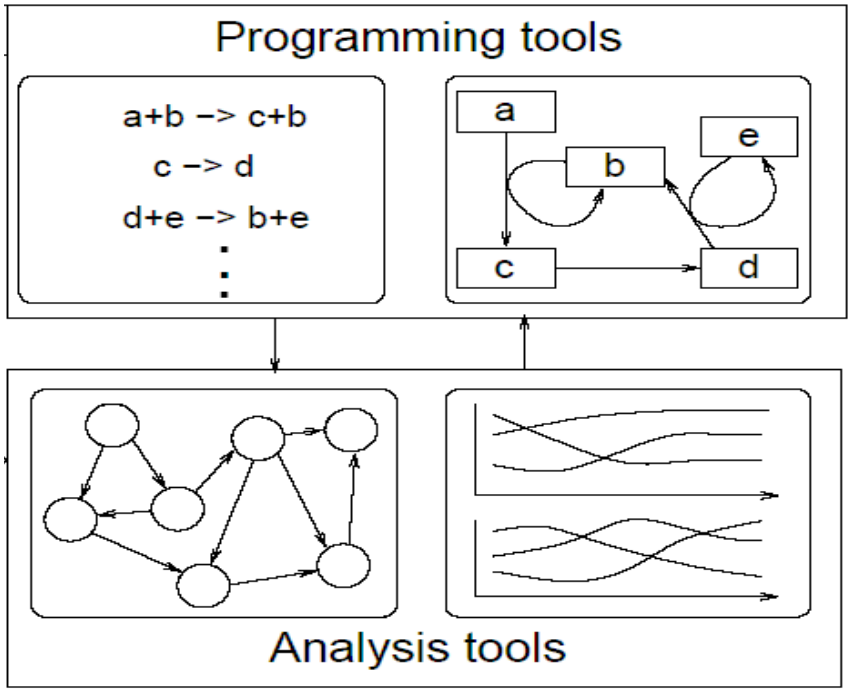
[P. Dittrich, P. Speroni di Fenizi, Chemical Organization Theory, *Bull. Math. Biol.*, 2007]

Organization Oriented Design Principles

1. For each solution there must be (at least) one organization containing the desired output molecules.
2. Eliminate as many other organizations as possible.
3. There must be a pathway from the input set to the desired organization.
4. The set of input molecules must generate an organization containing the target organization.
5. Make sure that the target organization is stable from a stoichiometric point of view.

[5] P. Dittrich, N. Matsumaru, Organization-Oriented Chemical Programming, In: Proc. of 7th International Conference on Hybrid Intelligent Systems (HIS 2007), IEEE DL, 6 pages, **2007**, (in print)

2. Programming Environment



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

N. Matsumaru, P. Dittrich,
CHEMORG I, Project Report, FSU Jena, 2007

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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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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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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

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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

OrgAnalysis

File Analysis SBW

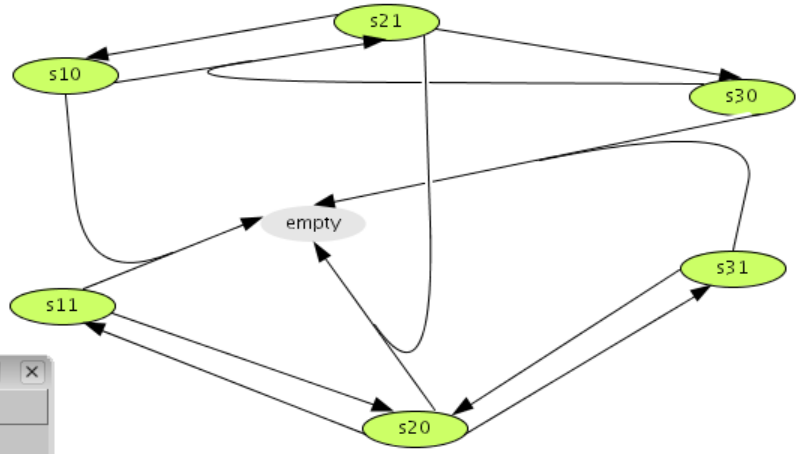
Metabolites | Reactions | Network Analysis | Log

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

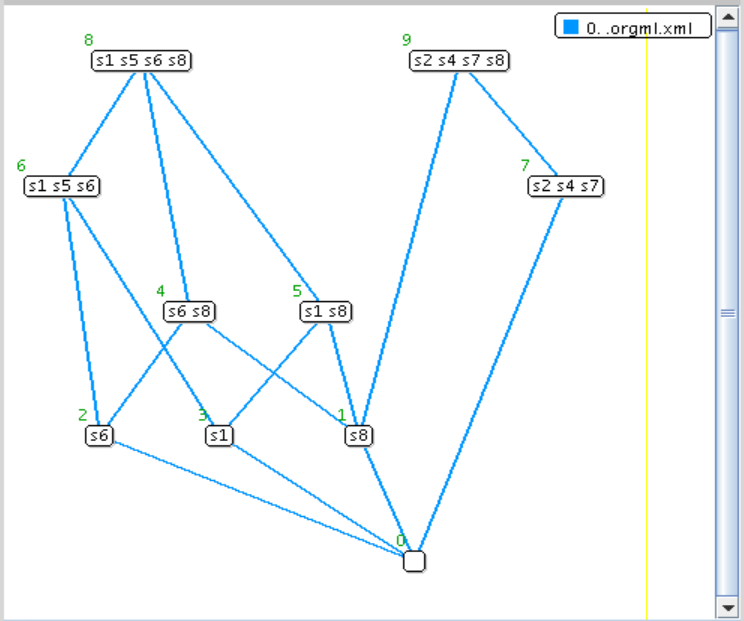
class	positionT	id	name
SIMPLE_M	inside	s1	s10
SIMPLE_M	inside	s2	s11
SIMPLE_M	inside	s4	s20
SIMPLE_M	inside	s5	s21
SIMPLE_M	inside	s6	s30
SIMPLE_M	inside	s7	s31
UNKNOWN	inside	s8	empty

Edit Notes | Edit Protein Notes

orgView - visualized Organizations

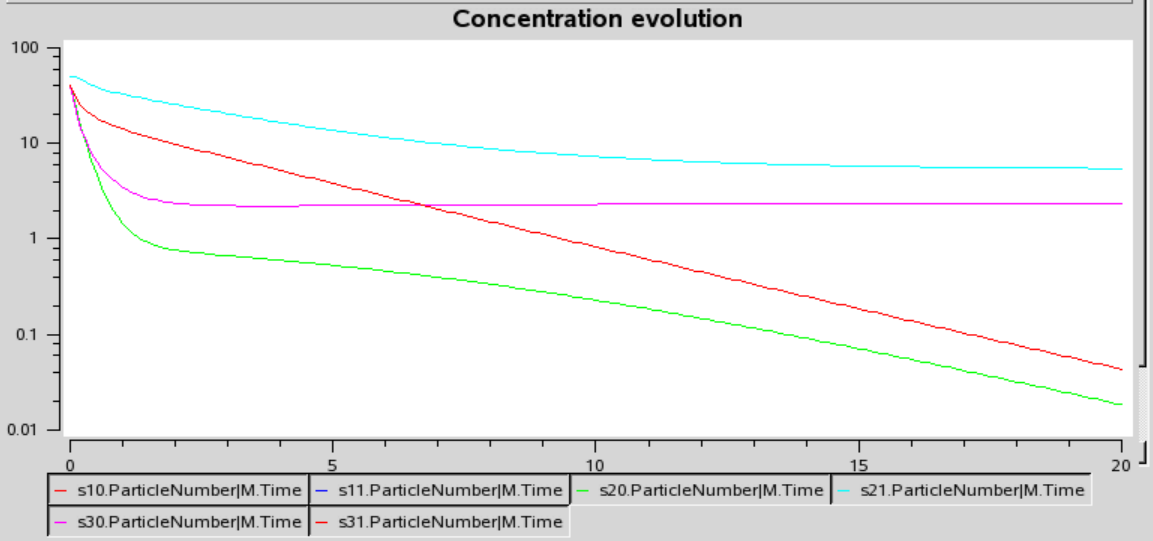
File View Tools Windows Exit SBW

Zoom: 9% FontZoom: 28%



Copasi Plot: Concentration evolution

Print Save data...



3. Evaluation and Case Studies

- Logic gates
  (e.g., chemical xor)
- Boolean networks
  (e.g., chemical flip-flop)
- Maximum independent set

[1] N. Matsumaru, F. Centler, P. Speroni di Fenizio, and P. Dittrich.
Chemical Organization Theory as a Theoretical Base for Chemical Computing.
International Journal on Unconventional Computing, 28 pages, **2007**, (in print)

[4] N. Matsumaru, T. Lenser, T. Hinze, P. Dittrich,
Toward Organization-Oriented Chemical Programming: a case study with the maximal independent set problem. In F. Dressler and I. Carreras (Eds.), Advances in Biologically Inspired Information Systems, SCI, 69: 147-163, Springer, Berlin, **2007**

[6] N. Matsumaru and P. Dittrich.
Organization-oriented chemical programming for the organic design of distributed computing systems. In Proc.of Bionetics, Cavalese, Italy, December 11-13, 7 pages, IEEE, **2006**.

[9] N. Matsumaru, F. Centler, and P. Dittrich.
Chemical Organization Theory as a Theoretical Base for Chemical Computing.
In C. Teuscher and A. Adamatzky, editors, Workshop on Unconventional Computing, p. 71-82. Luniver Press, Beckington, **2005**

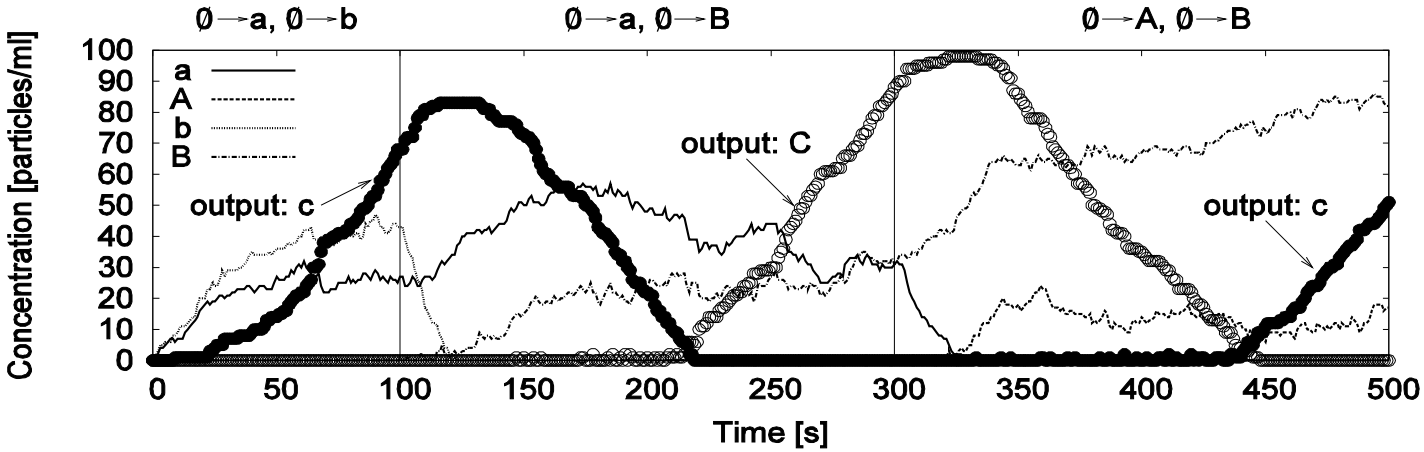
Chemical XOR

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

$$a+b\rightarrow c \qquad a+A\rightarrow 0$$
$$a+B\rightarrow C \qquad b+B\rightarrow 0$$
$$A+b\rightarrow C \qquad c+C\rightarrow 0$$
$$A+B\rightarrow c$$

a : **a == 0**

A : **a == 1**



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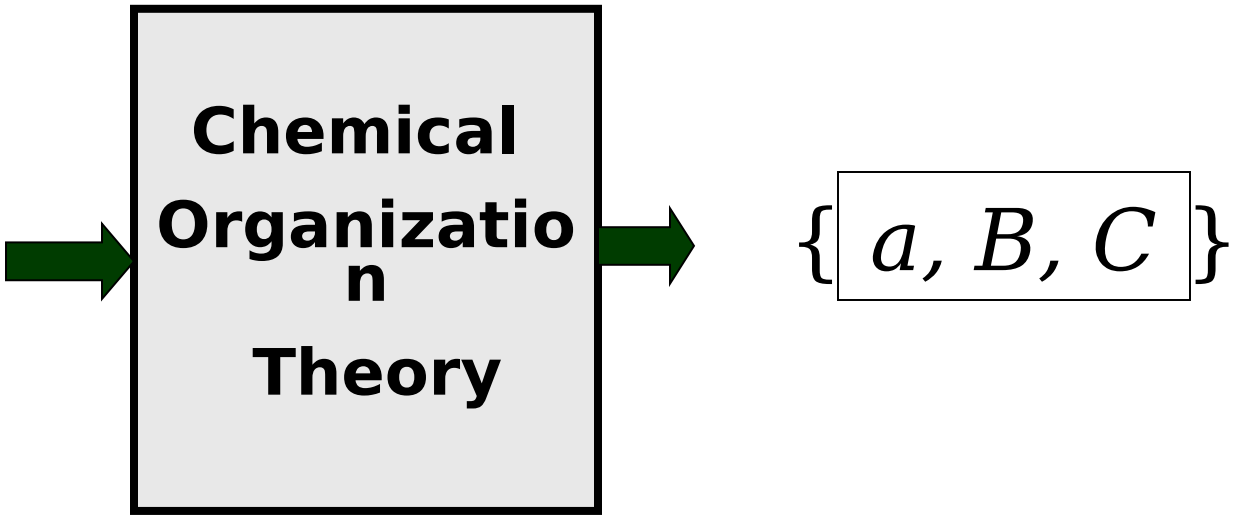
Chemical Organization Theory as a Theoretical Base for Chemical Computing.
In C. Teuscher and A. Adamatzky, editors, Workshop on Unconventional Computing, p. 71-82. Luniver Press, Beckington, **2005**

Chemical XOR (two inputs)

$$a + b \rightarrow c$$
$$a + B \rightarrow C$$
$$A + b \rightarrow C$$
$$A + B \rightarrow c$$
$$a + A \rightarrow 0$$
$$b + B \rightarrow 0$$
$$c + C \rightarrow 0$$



Organizations

$0 \rightarrow a \quad 0 \rightarrow B$ *64 possible sets of molecular species*

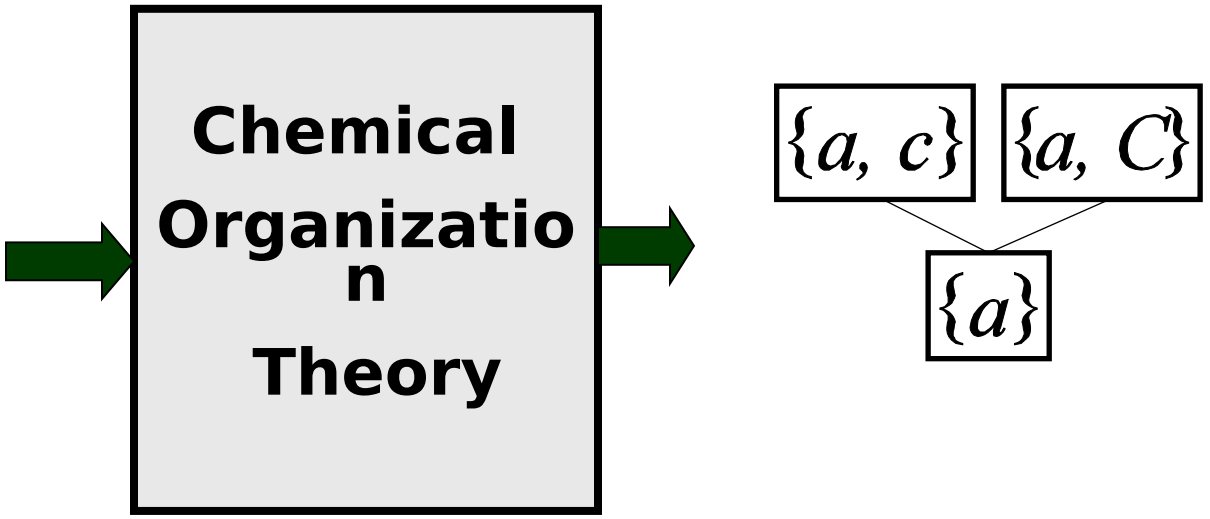
1 is an organization

[1] Matsumaru, N. et al. *Int. J. Unconv. Comp.*, 2007 (in print)

Chemical XOR (with one input)

$$a + b \rightarrow c$$
$$a + B \rightarrow C$$
$$A + b \rightarrow C$$
$$A + B \rightarrow c$$
$$a + A \rightarrow 0$$
$$b + B \rightarrow 0$$
$$c + C \rightarrow 0$$
$$0 \rightarrow a$$

Reaction network

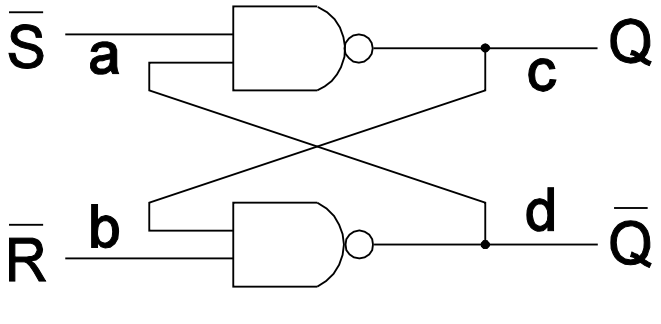


Organizations

64 possible sets of molecular species
3 are an organization

[1] Matsumaru, N. et al. *Int. J. Unconv. Comp.*, 2007 (in print)

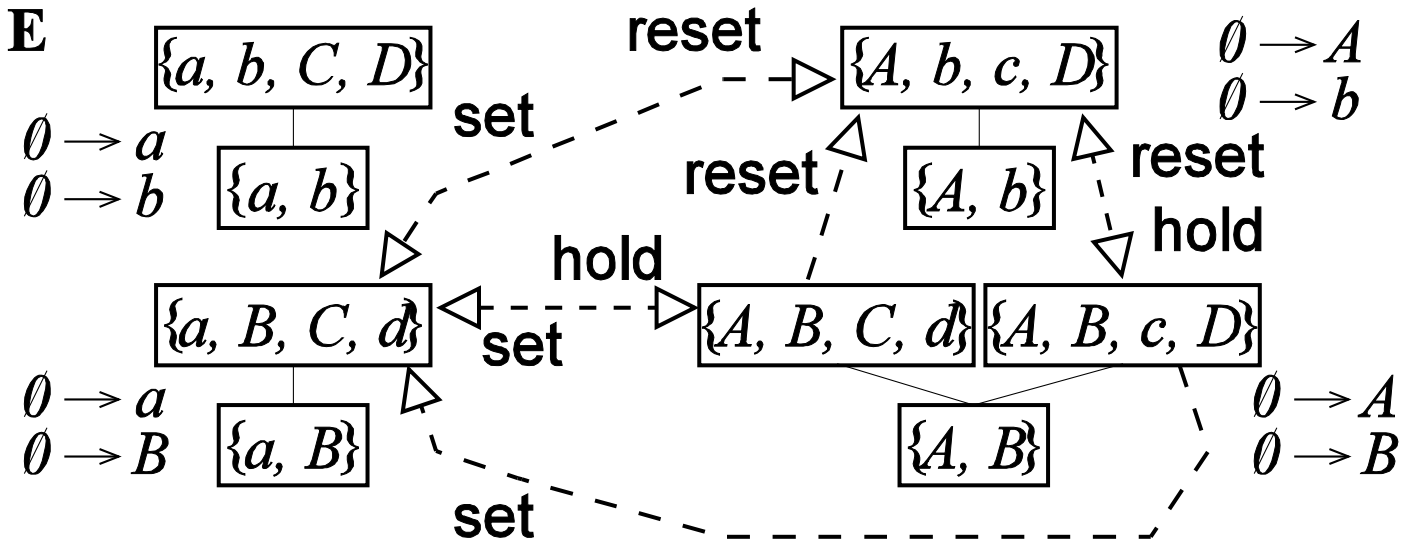
Chemical Flip-Flop (with two inputs)



A

B

$\bar{S}$	$\bar{R}$	Q_{t+1}	$\bar{Q}_{t+1}$	
0	0	1	1	—
0	1	1	0	set
1	0	0	1	reset
1	1	Q_t	$\bar{Q}_t$	hold



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In C. Teuscher and A. Adamatzky, editors, Workshop on Unconventional Computing, p. 71-82. Luniver Press, Beckington, **2005**

Maximal Independent Set

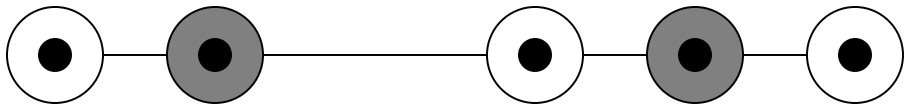
- *Def.* ***[Independent set]***

  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
$I \leftarrow I \cup \{v\} \mid v \in V$
$V \leftarrow V - (\{v\} - \mathrm{Neigh}(v))$
end

- Distributed system [Shukla, et al. 1995]

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

Algebraic Chemistry for MIS problem

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

Membership to the inde-pendent set

Vertex ID

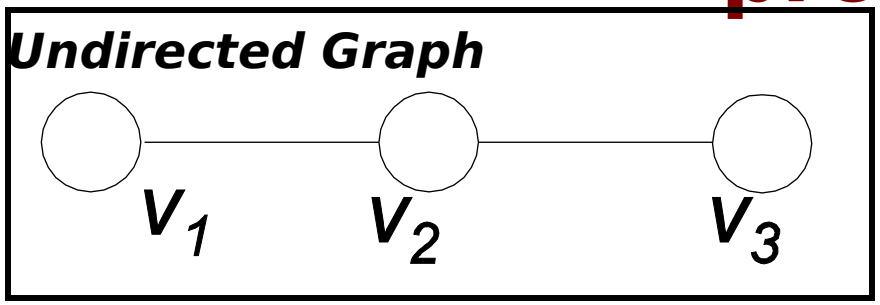
$$R=\bigcup_{i=1}^{N} R^i$$

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

[4] N. Matsumaru, T. Lenser, T. Hinze, P. Dittrich, SCI , 69:147-163, Springer, Berlin, 2007

[6] N. Matsumaru and P. Dittrich., Proc.of Bionetics, **2006**.

Algebraic Chemistry for MIS problem

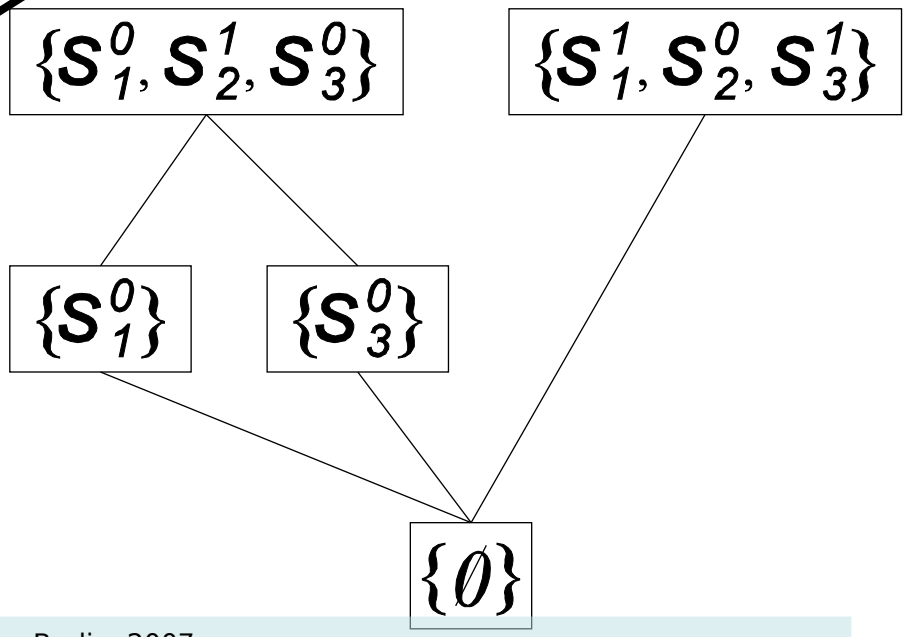


Reaction Network

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

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

Organizational structure



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[6] N. Matsumaru and P. Dittrich., Proc.of Bionetics, **2006**.

„Chemical Organization“

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

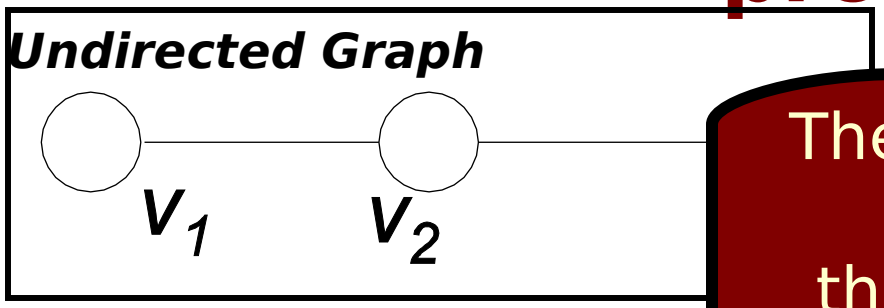
Organization :

a set of molecules t[illegible]is (algebraically) closed and self-maintaining

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

[P. Dittrich, P. Speroni di Fenizi, Chemical Organization Theory, *Bull. Math. Biol.*, 2007]

Algebraic Chemistry for MIS problem



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

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

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

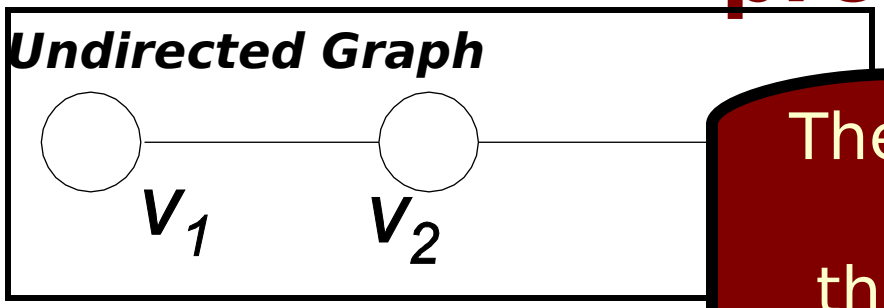
Organ[illegible]ional structure

$\{s_2^1\}$

[4] N. Matsumaru, T. Lenser, T. Hinze, P. Dittrich, SCI , 69:147-163, Springer, Berlin, 2007

[6] N. Matsumaru and P. Dittrich., Proc.of Bionetics, **2006**.

Algebraic Chemistry for MIS problem



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

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

Organ… …ional structure

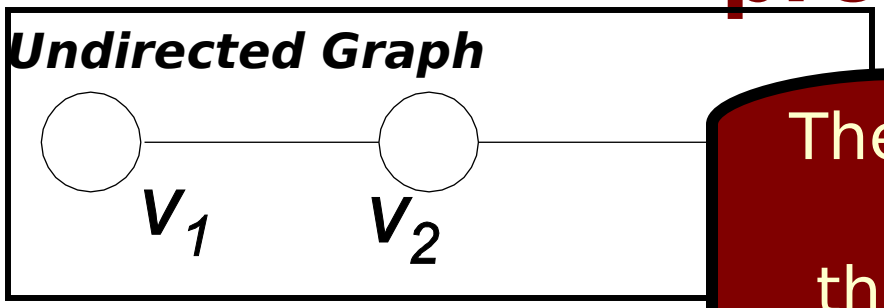
$$\{ s_2^1 \quad s_3^0 \}$$

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

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

[4] N. Matsumaru, T. Lenser, T. Hinze, P. Dittrich, SCI , 69:147-163, Springer, Berlin, 2007
[6] N. Matsumaru and P. Dittrich., Proc.of Bionetics, **2006**.

Algebraic Chemistry for MIS problem



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

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

o_I

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

$$s_1^0 + s_1^1 \to \emptyset$$
$$s_2^0 + s_2^1 \to \emptyset$$
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Within the set, all molecules consumed by a reaction can be reproduced by a reaction.

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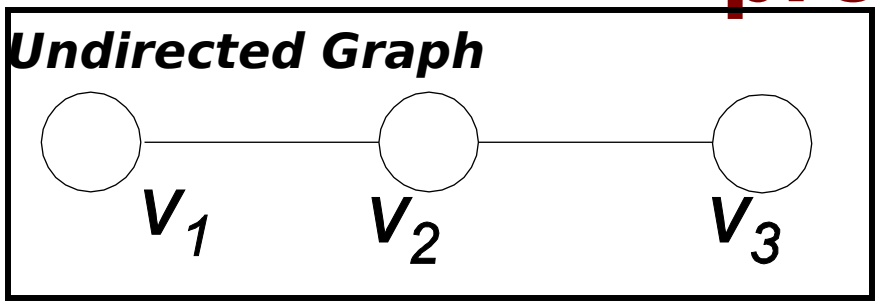
Algebraic Chemistry for MIS problem

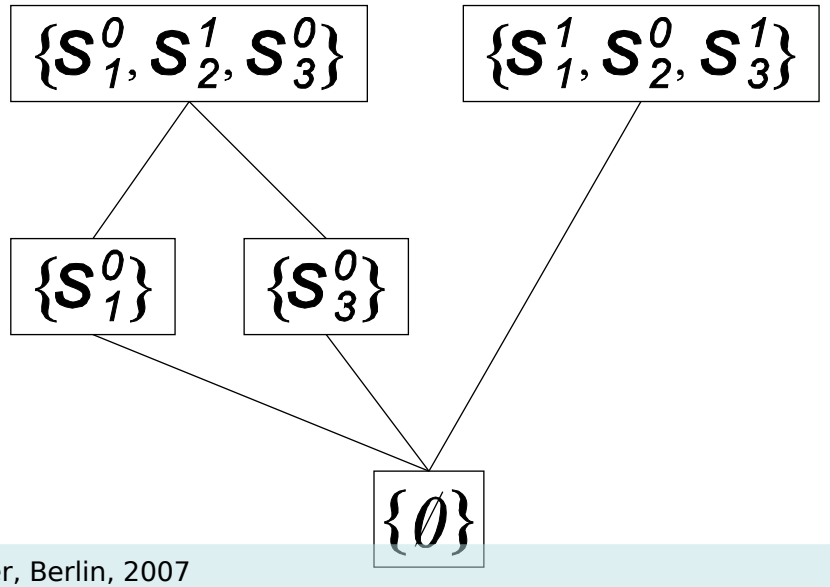


Reaction Network

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

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

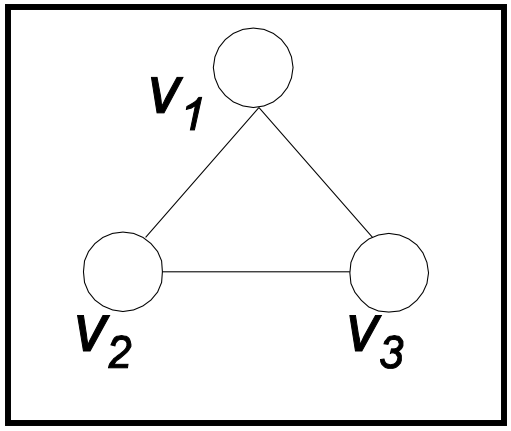
Organizational structure



[4] N. Matsumaru, T. Lenser, T. Hinze, P. Dittrich, SCI , 69:147-163, Springer, Berlin, 2007

[6] N. Matsumaru and P. Dittrich., Proc.of Bionetics, **2006**.

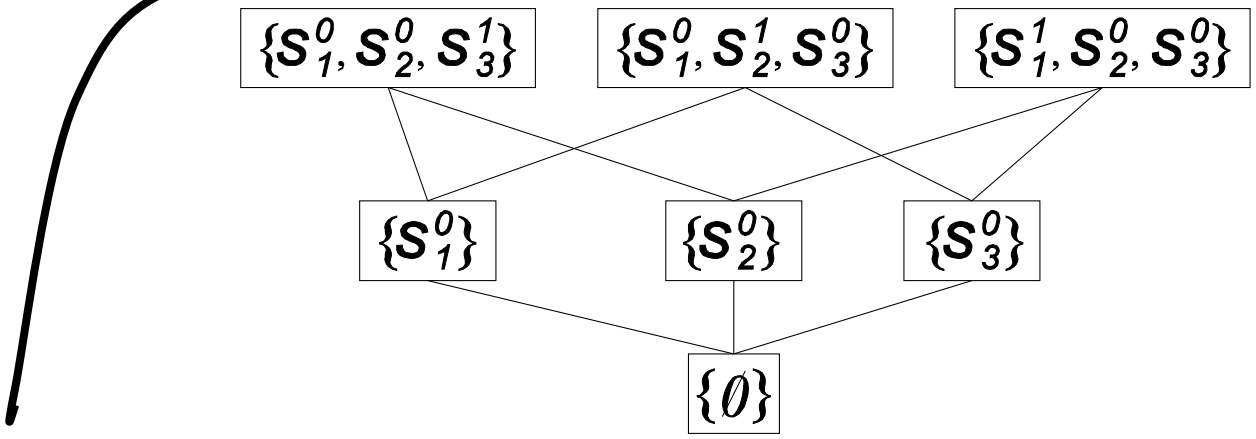
Algebraic Chemistry for MIS problem



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

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

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

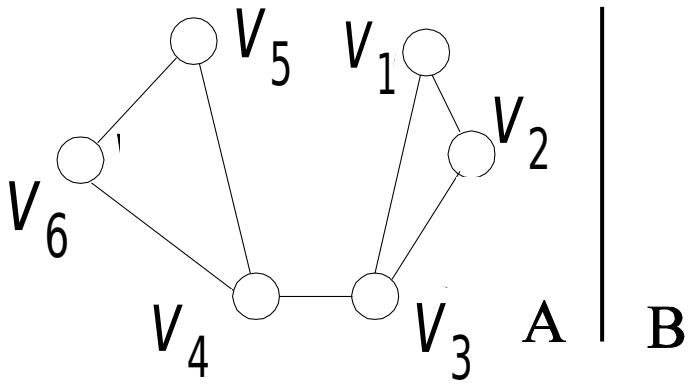


[4] N. Matsumaru, T. Lenser, T. Hinze, P. Dittrich, SCI , 69:147-163, Springer, Berlin, 2007

[6] N. Matsumaru and P. Dittrich., Proc.of Bionetics, **2006**.

Algebraic Chemistry for MIS problem

Undirected graph



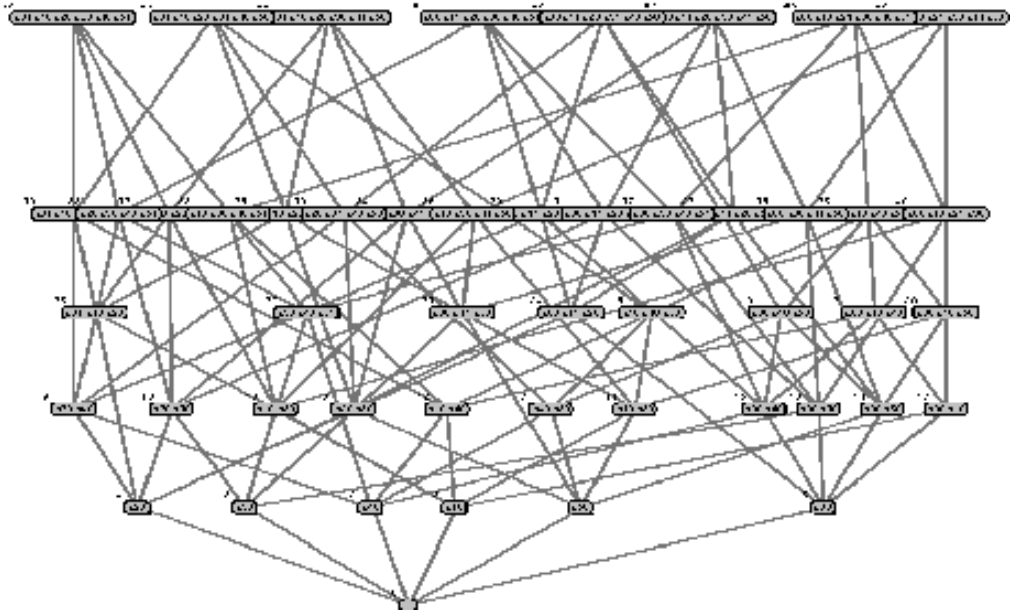
Organizational structure

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

Reaction network

M:12 molecular species

R:32 reaction rules



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Current and Future Work

1. Structured Molecules

3. Quantitative Evaluation

5. Demonstrator (sensor network scenario)

7. Intrinsic vs. Extrinsic Self-Organization

1. Structured Molecules

Example: implicitly defined molecules

M = { 0, 1, 2, 3, …, }

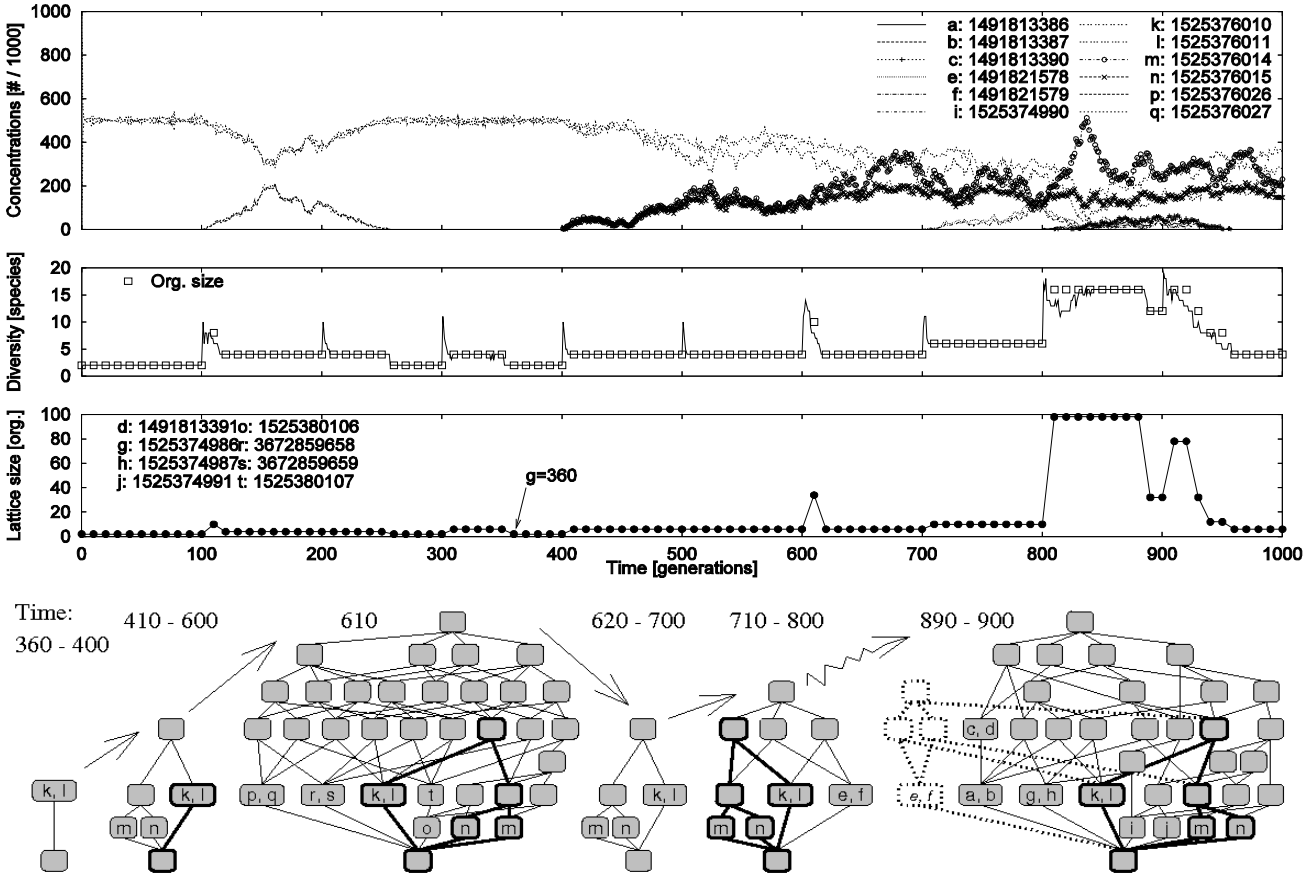
Example: implicitily defined reaction rules

a + b → c with c = a + b mod 4711

1. Candidates to be evaluated

- Bit strings and Boolean expressions
- Patter matching
- Interacting finite state machines
- Scheme
- String-based P-systems
- Fraglets

1. Preliminary Study of 32-bit-Sized Interacting Machines



[8] N. Matsumaru, P. Speroni di Fenizio, F. Centler, and P. Dittrich.
On the Evolution of Chemical Organizations. In S. Artmann and P. Dittrich (Eds.), Proc. of the 7th German Workshop of Articial Life, p.135-146, IOS Press, Amstterdam, **2006**

1. Structured Molecules: Fraglets

```
a[matchp:p_produce:newname:p_request]
a[p_produce]
a[newname:p_request]
a[match:newname:nn1:PAYLOAD]
a[nn1:PAYLOAD:p_request]
a[matchp:nn1:split:match:nn2:*:exch:nn2]
a[split:match:nn2:*:exch:nn2:PAYLOAD:p_request]
a[exch:nn2:PAYLOAD:p_request]
a[match:nn2]
a[nn2:p_request:PAYLOAD]
```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[29] C. Tschudin and L. Yamamoto. A metabolic approach to protocol resilence. In *Proc. WAC'04*, volume 3457 of *LNCS*, pages 191–206. Springer, Berlin, 2004.

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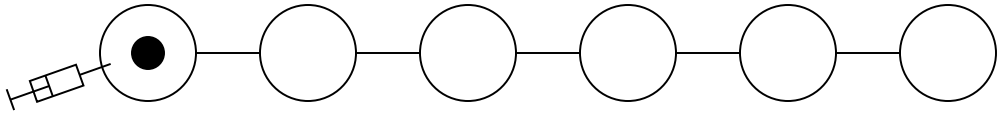
2. Quantitative Evaluation

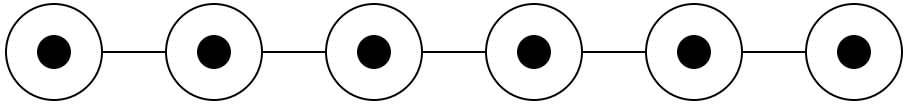
- Robustness
  e.g., probability of failure after perturbation
- Efficiency of self-organization
  e.g., transient time until desired result appears
- Scalability
  How do robustness and efficiency scale with system/problem size?

2. Benchmark Problem

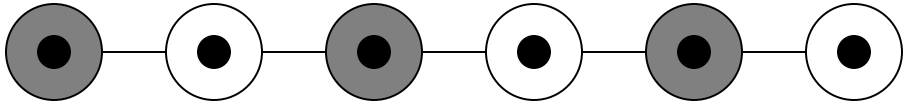
1. Inject molecules



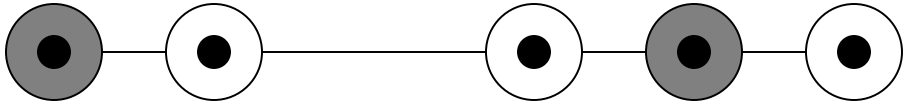
2. Molecules distribute



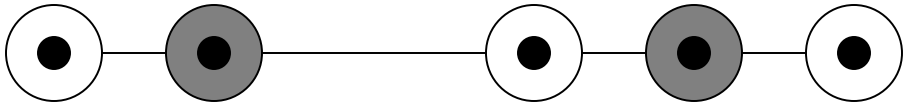
. Cells differentiate (self-organize)



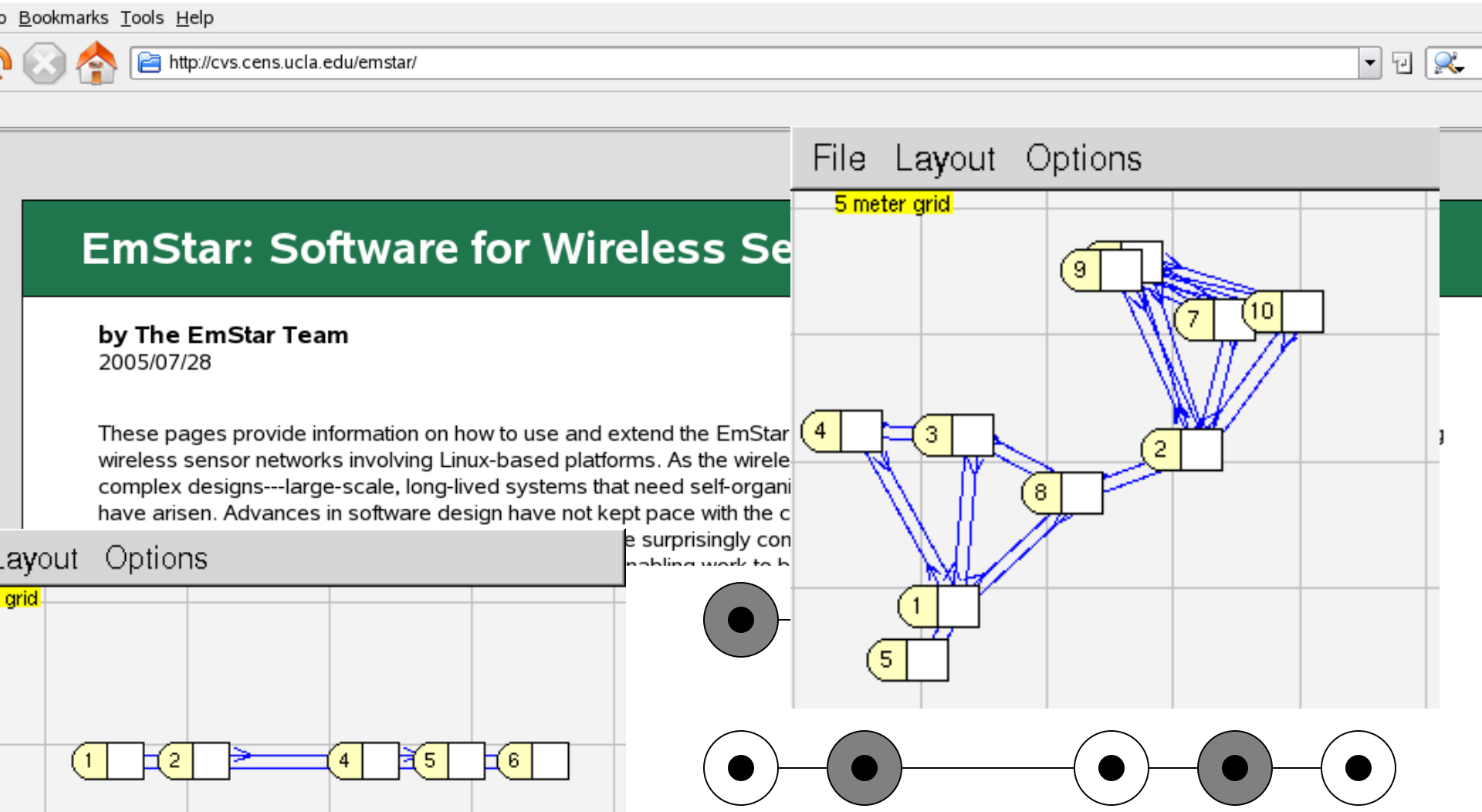
4. A cell is removed



5. Reorganize



Benchmark Problem



3. Demonstrator

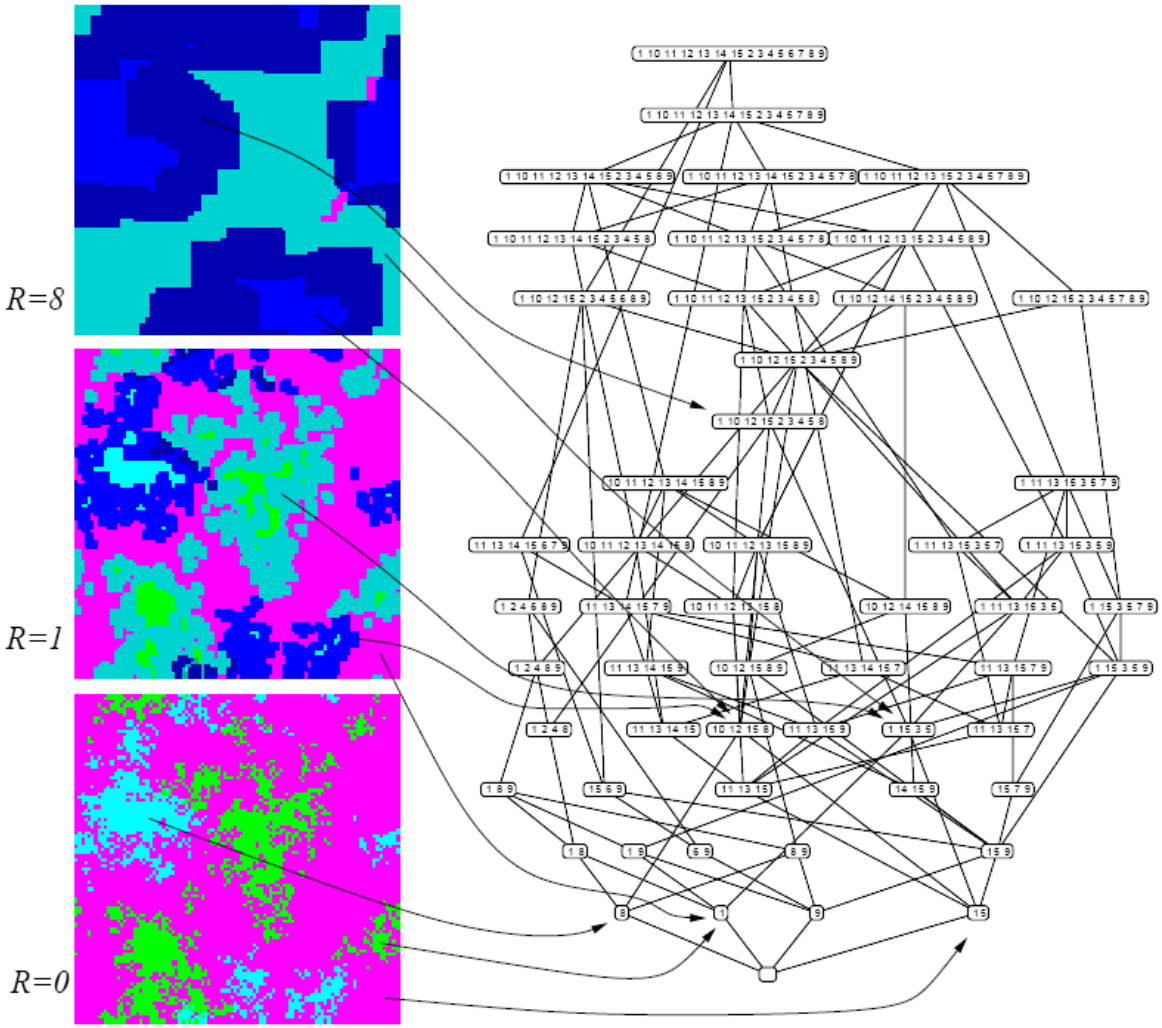
- Real sensor network

4. Intrinsic vs. Extrinsic Self-Organization

- Focus so far: How to *program?*

- In this WP: How to *control*?

Space

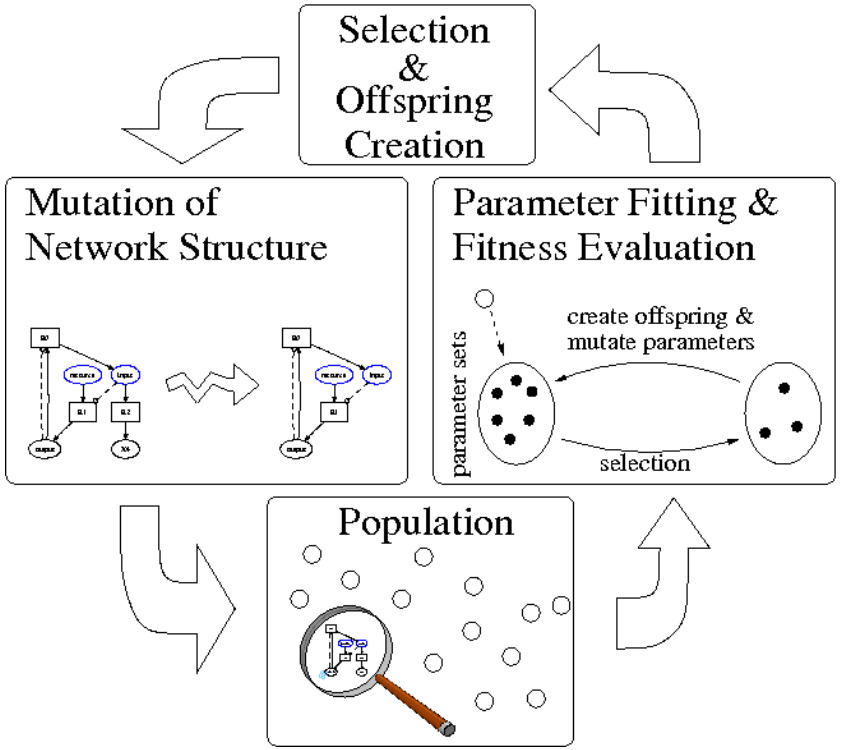


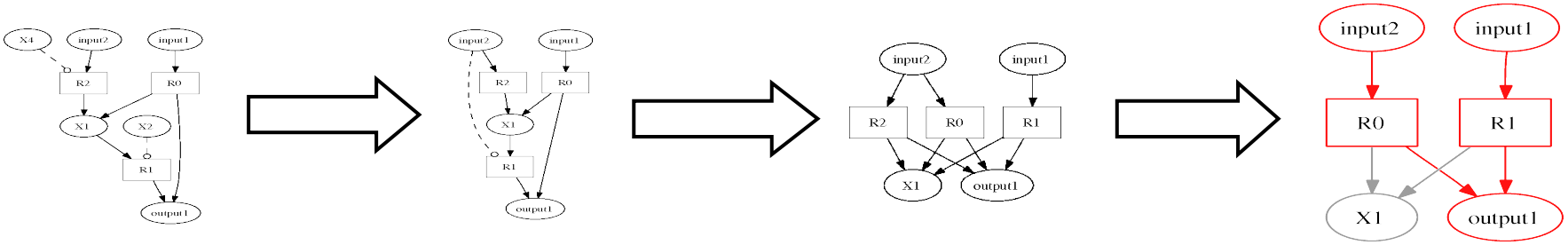
[P. Speroni di Fenizi, P. Dittrich, Chemical Organizations at Different Spatial Scales, *LNCS*, Springer, 2007]

Evolutionary Design

ESIGNET

http://www.esignet.net





[T. Lenser, T. Hinze, P. Dittrich, *LNCS*, Springer, 2007]

Final Remarks

- Mini-Workshop on chemical-like/particle based organic computing approaches.

References & Acknowledgement

Refereed Journal:

[1] N. Matsumaru, F. Centler, P. Speroni di Fenizio, and P. Dittrich. Chemical Organization Theory as a Theoretical Base for Chemical Computing.
International Journal on Unconventional Computing, 28 pages, **2007**, (in print)

[2] N. Matsumaru, T. Lenser, T. Hinze, and P. Dittrich. Designing a Chemical Program using Chemical Organization Theory. *BMC Systems Biology*, 1(Suppl 1):P26, **2007**, (extended abstract)

[3] N. Matsumaru, F. Centler, P. Speroni di Fenizio, and P. Dittrich, Chemical organization theory applied to virus dynamics
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Refereed Proceedings:

[4] N. Matsumaru, T. Lenser, T. Hinze, P. Dittrich, Toward Organization-Oriented Chemical Programming: a case study with the maximal independent set problem. In F. Dressler and I. Carreras (Eds.), Advances in Biologically Inspired Information Systems, SCI, 69: 147-163, Springer, Berlin, **2007**

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Funding: DFG Grant No. Di 852/4-1

Story

1. Introduction
2. Organization Oriented Programming
3. Framework for Chemical Programming
4. Case Studies
   - Boolean Logic
   - Boolean Networks flip-flop
   - Maximum independent set problem
5. Structured molecules
   - Pre-liminary study with artificial chemistry
   - New methods for representation and analysis needed
   - Case studies for evaluation
   - Candidates for molecular structures (fraglets)
6. Quantitative evaluation
   - Build on maximum independent set problem
   - Connect to other projects
- Demonstrator
- Some theory: Intrinsically vs. Extrinsically self-organizing systems
- Evolving networks, ESIGNET, Modularization?
- Summary of Publications