The Bio-chemical Information Processing Metaphor as a Programming Paradigm for Organic Computing (CHEMORG III)

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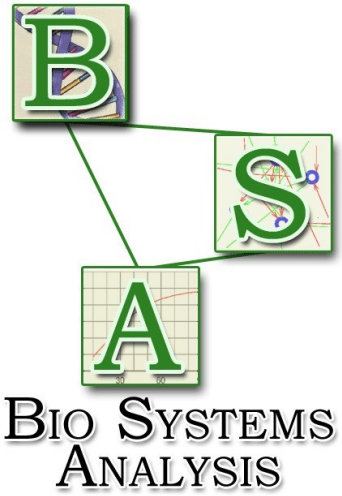
15. September 2011



Overview

- Summary

New Results

1. Space: Reaction Flow Artificial Chemistries
2. Structured Molecules: „Embodied“ Evolution
3. Theory: Decomposition Theorem and Stochastic Organizations

Outlook

- Apoptosis

Aim

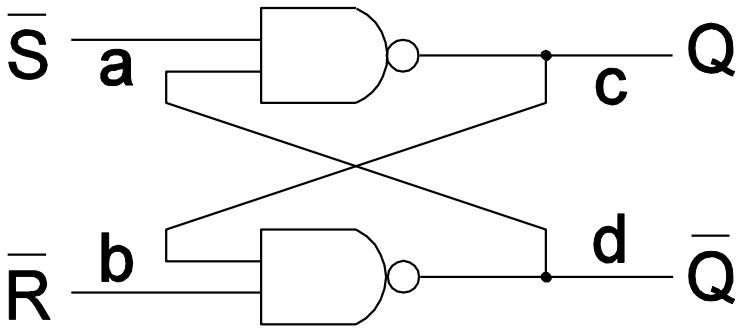
- Employ the (bio-)chemical principles of information processing as a programming approach for Organic Computing.
- How to program chemical-like systems?
- Current state: 45% of Phase III.

Main Results

- Organization-oriented chemical programing

  N. Matsumaru, F. Centler, P. Speroni d. F., P. Dittrich. Chemical Organization Theory as a Theoretical Base for Chemical Computing. *Int. J. Unconv. Comput*., 3(4), 285-309, 2007

Organizations for different inflows



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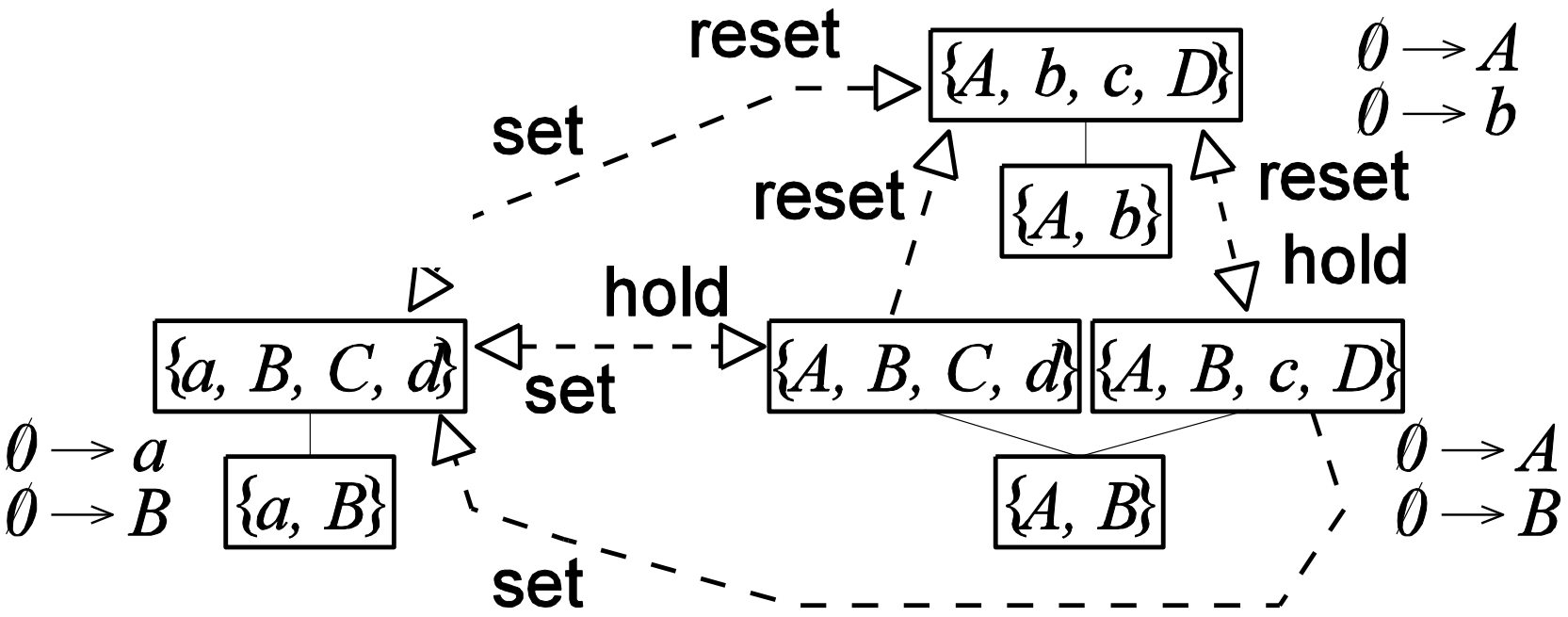

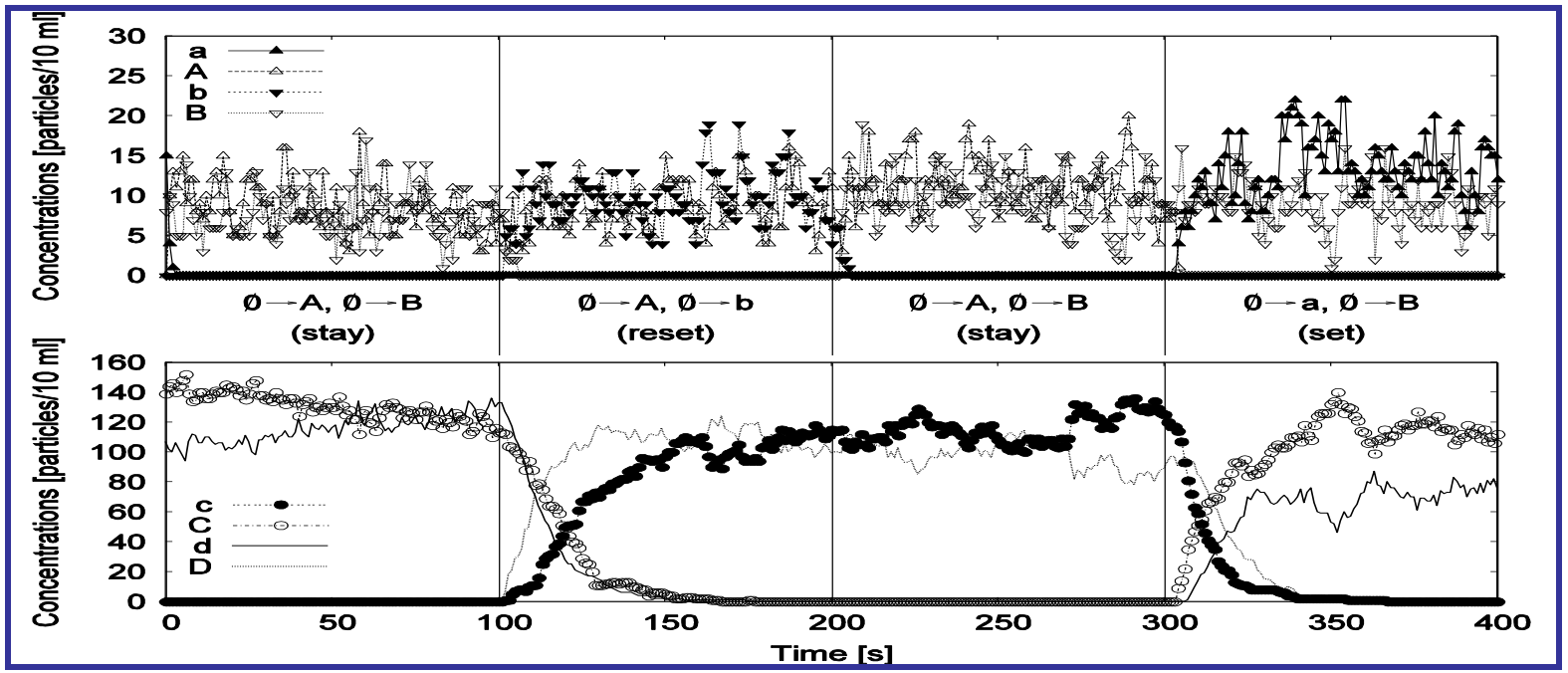
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A
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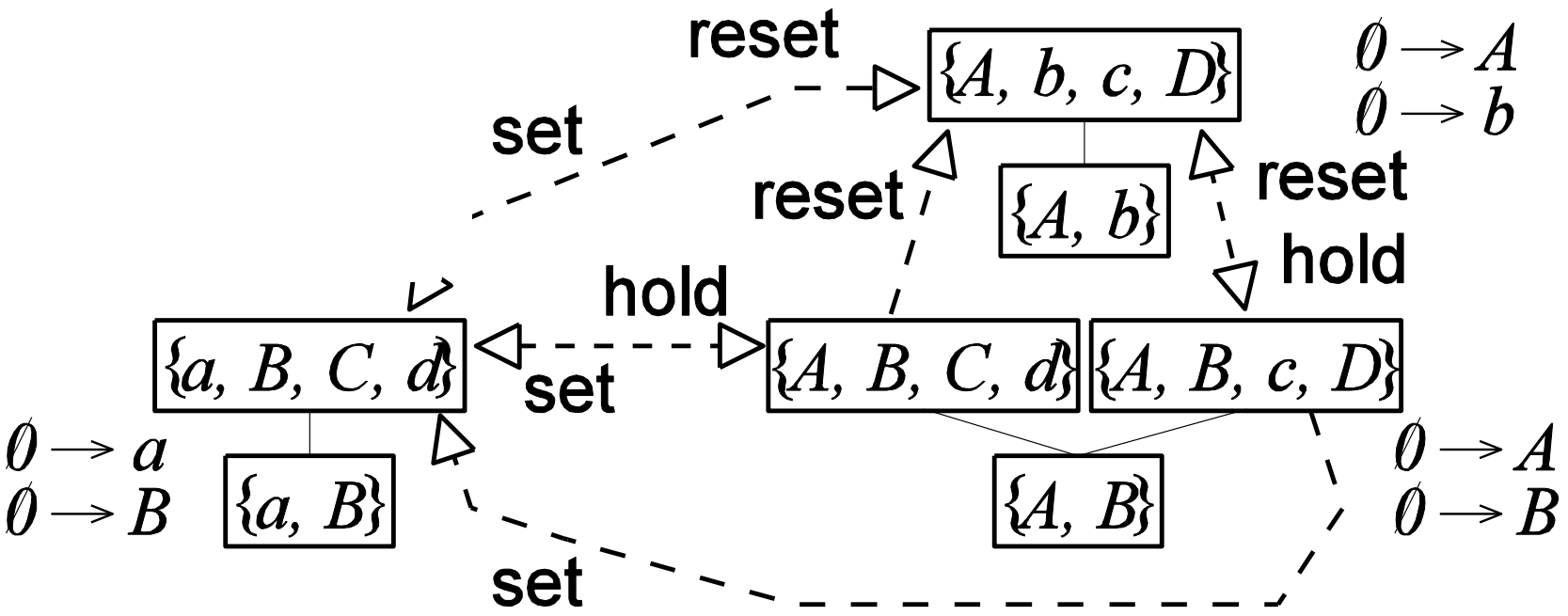
Ø → A, Ø → B
(stay)
Ø → A, Ø → b
(reset)
Ø → A, Ø → B
(stay)
Ø → a, Ø → B
(set)
c
C
d
D
Time [s]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Ø → A
Ø → b
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hold
{a, B, C, d}
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{A, B, c, D}
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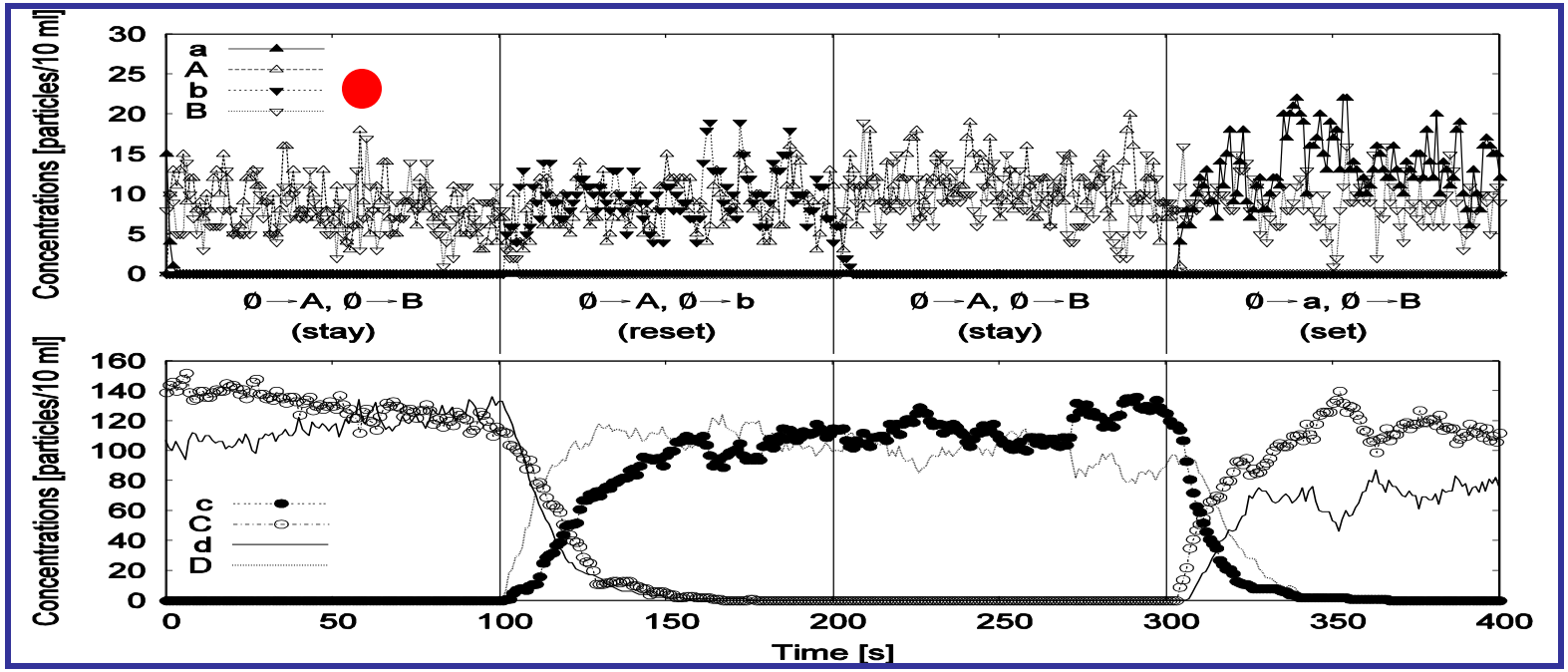
{a, B}
{A, B}
Ø → A
Ø → B
set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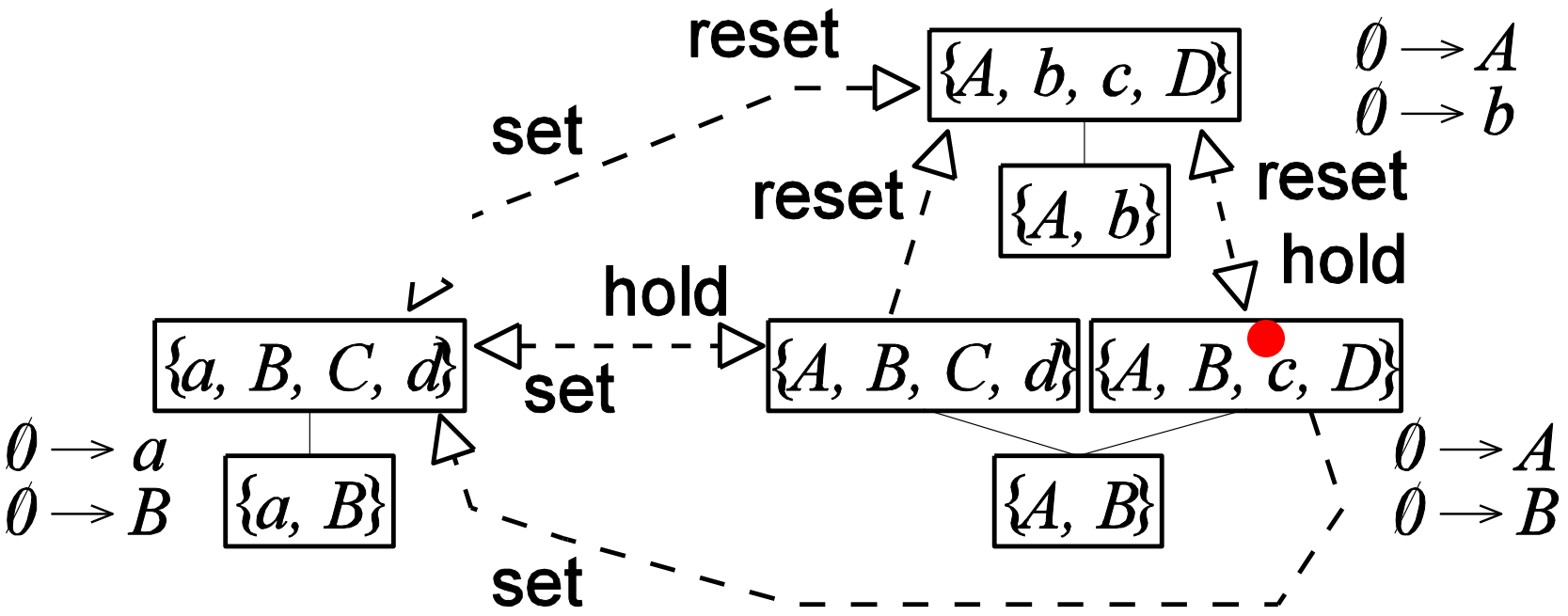
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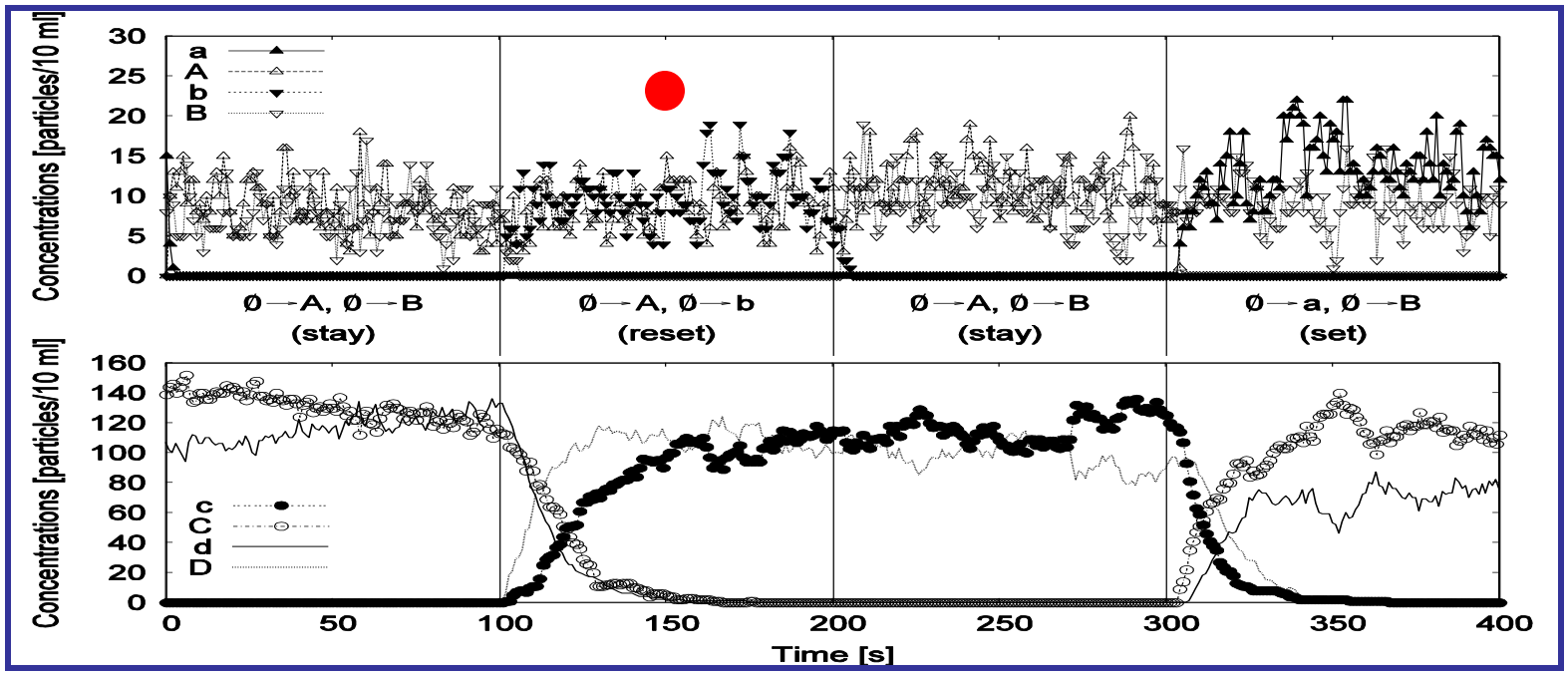
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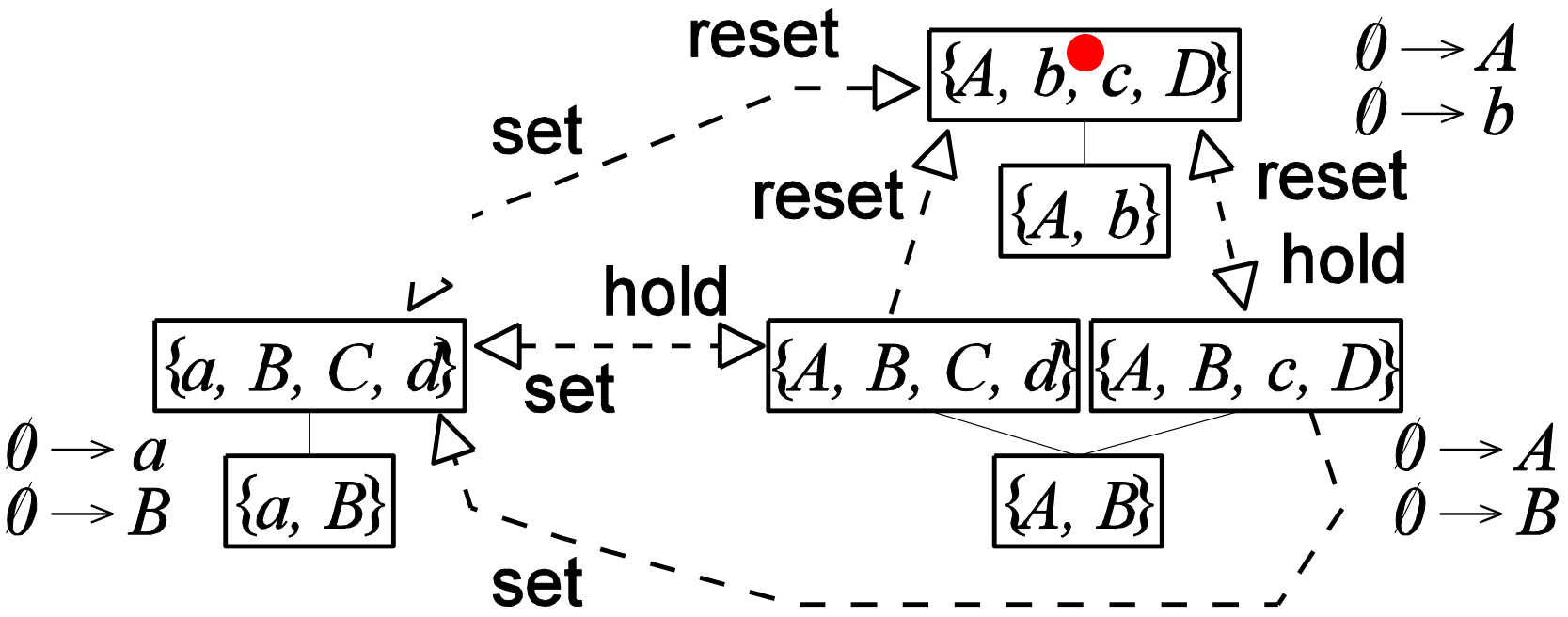
Time [s]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{a, B}
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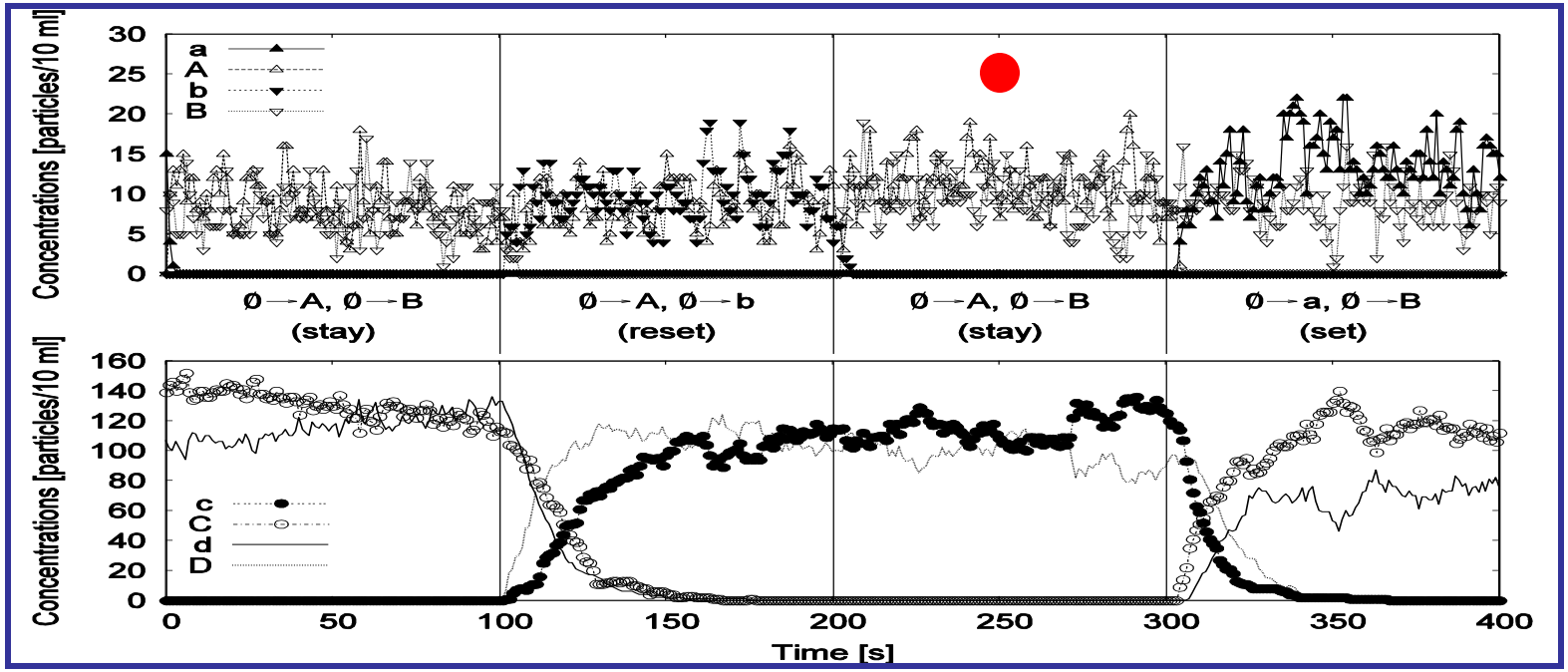
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(stay)
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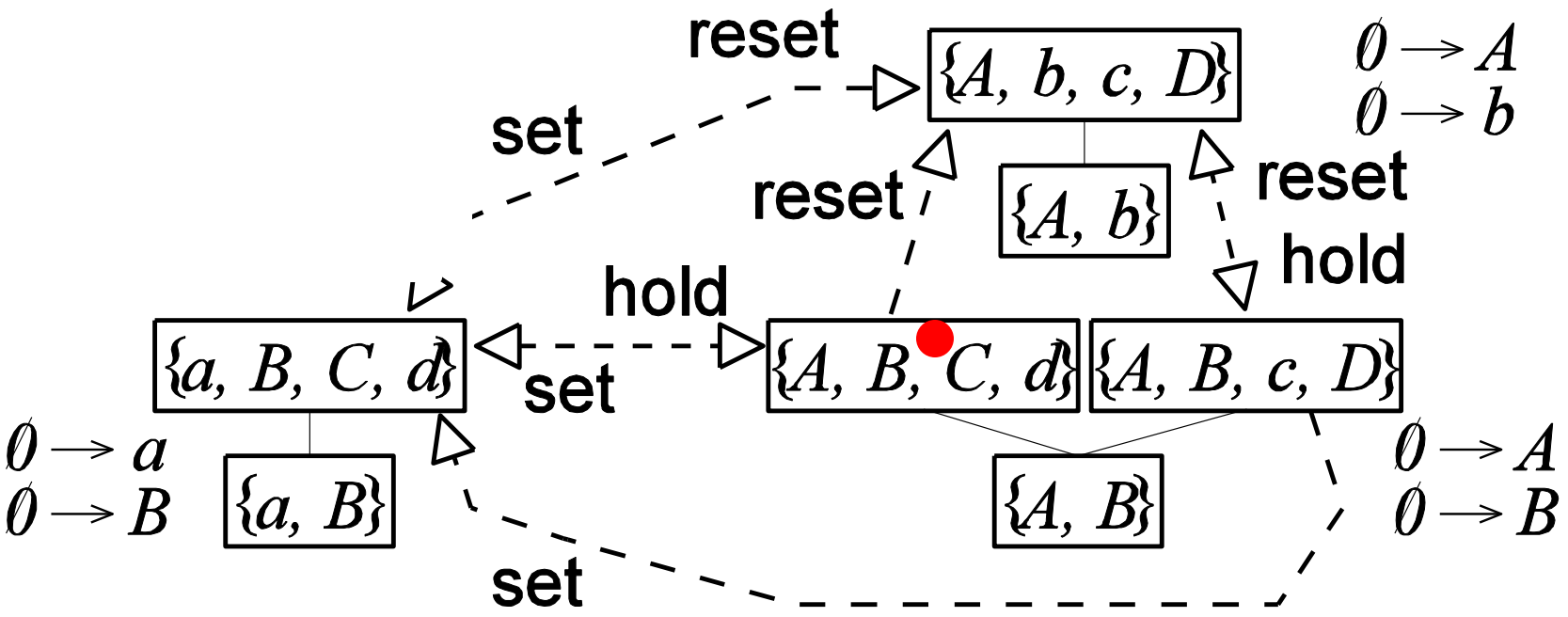
Time [s]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Ø → A
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{A, b}
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hold
{a, B, C, d}
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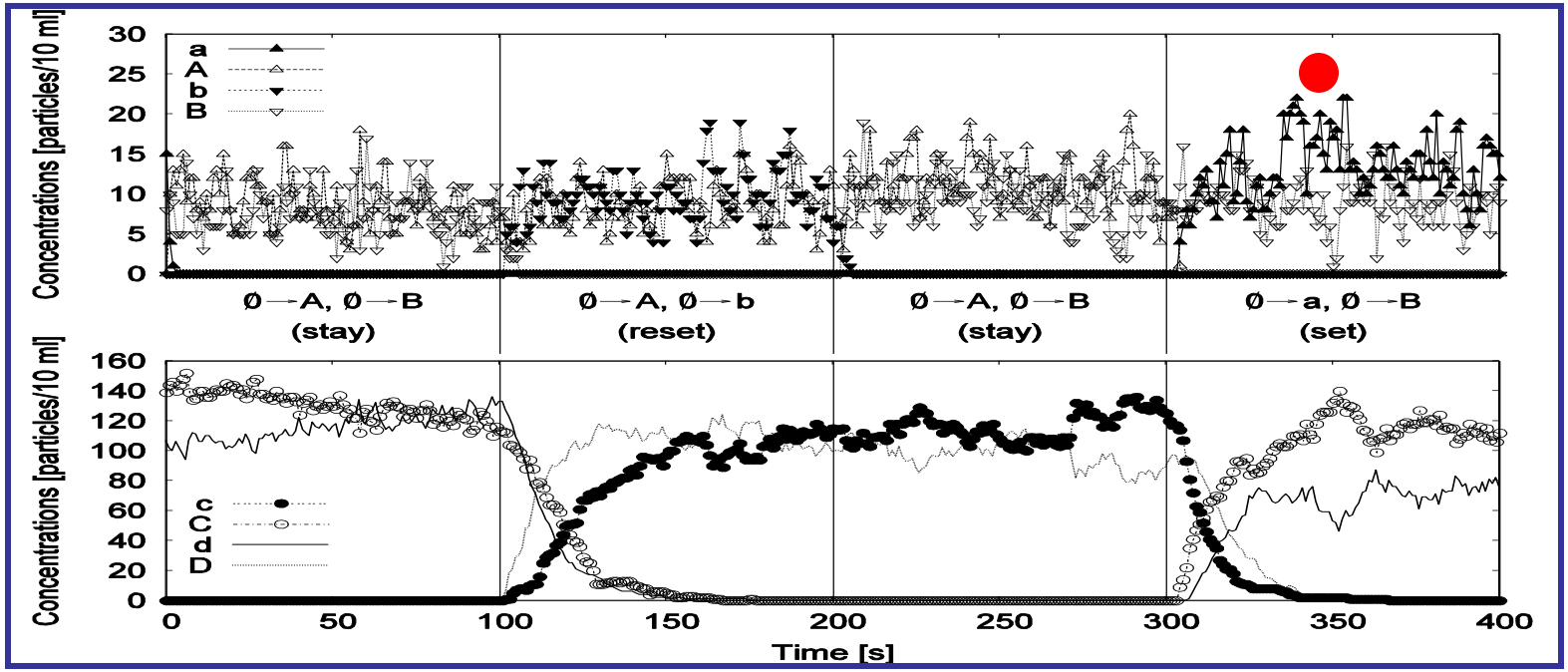
{a, B}
{A, B}
Ø → A
Ø → B
set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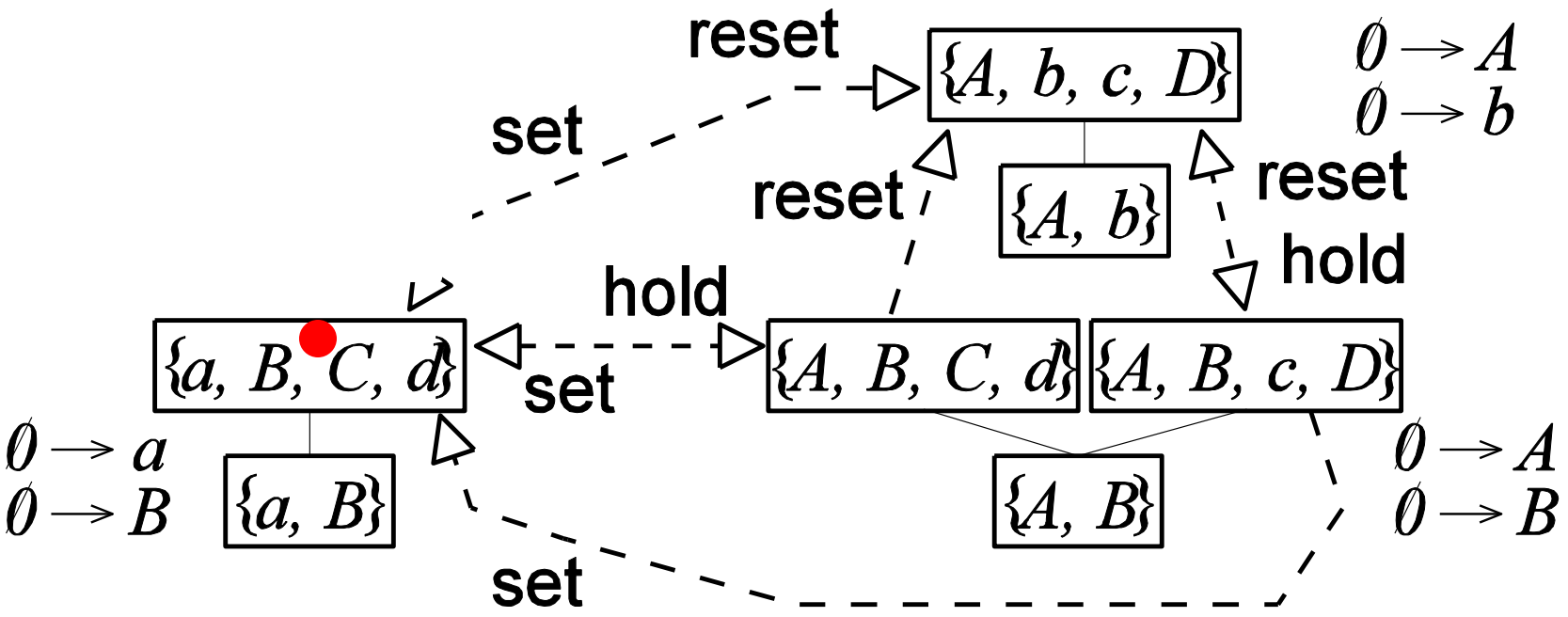
Time [s]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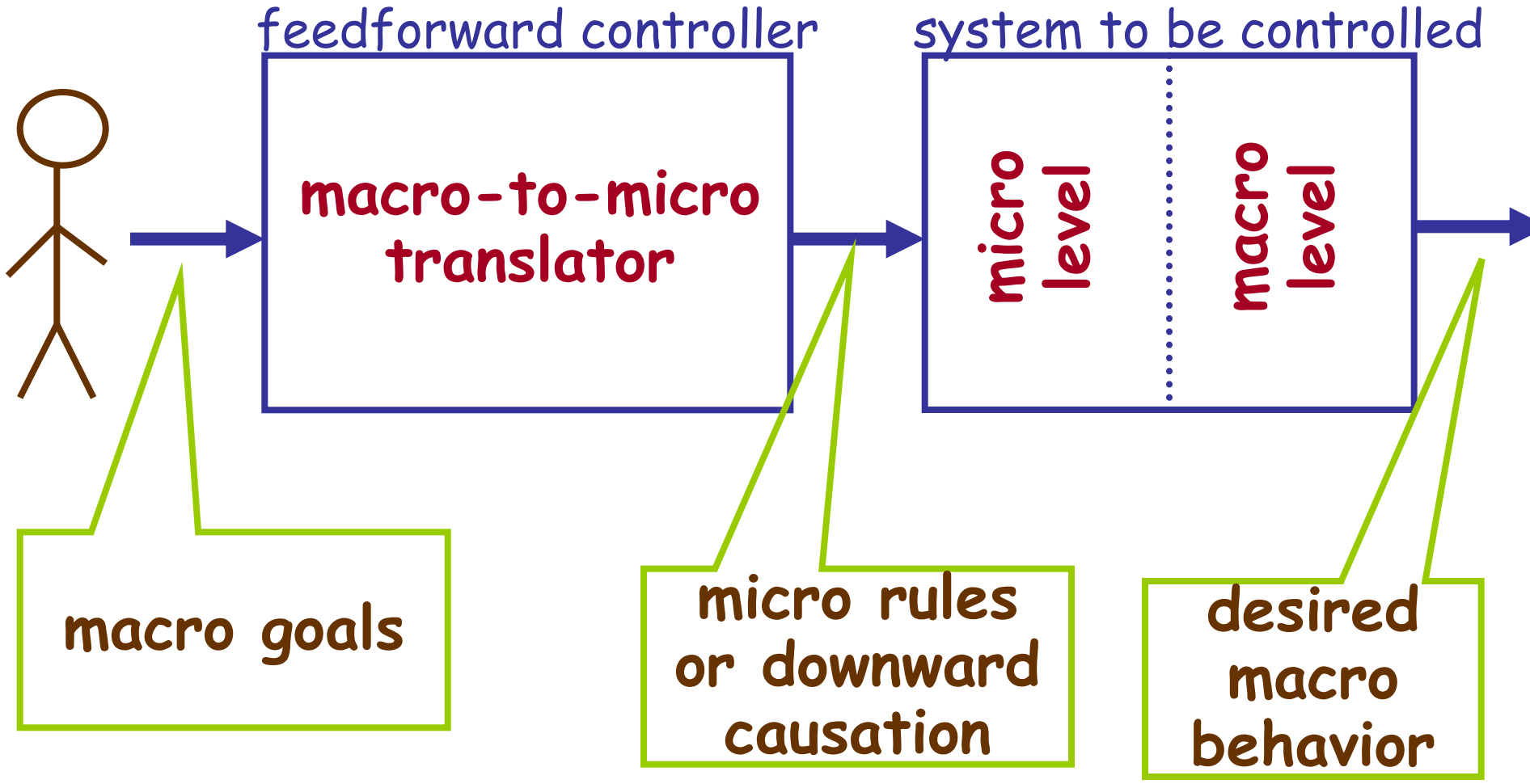
{A, B, C, d}
{A, B, c, D}
Ø → a
Ø → B
{a, B}
{A, B}
Ø → A
Ø → B
set

Main Results

- Organization-oriented chemical programing
  N. Matsumaru, F. Centler, P. Speroni d. F., P. Dittrich. Chemical Organization Theory as a Theoretical Base for Chemical Computing. *Int. J. Unconv. Comput.*, 3(4), 285-309, 2007
- Analysis
  - Simulation various examples
    N. Matsumaru, T. Hinze, P. Dittrich. Organization-Oriented Chemical Programming of Distributed Artefacts. *Int. J. Nanotechnol. Mol. Comp.*, 1(4), 1-19, 2009
  - Compared with evolutionary design
- Theory
  S. Peter, P. Dittrich. On the Relation between Organizations and Limit Sets in Chemical Reaction Systems, *Adv. Complex Syst.*, 14(1): 77-96, 2011
- Tools
  F . Centler, C. Kaleta, P. Speroni di Fenizio, P. Dittrich. Computing Chemical Organizations in Biological Networks, *Bioinformatics*, 24(14), 1611 – 1618, 2008 (& 2010)
- Concept: Emergent Control
  P. Dittrich,P. Kreyssig. Emergent Control. In: C. Muller-Schloer, H. Schmeck, T. Ungerer (Eds.), Organic Computing A Paradigm Shift for Complex Systems, Autonomic Systems, Volume 1, Part 1, 67-78, Springer, Basel, 2011

Architecture for Emergent Control



P. Dittrich,P. Kreyssig. Emergent Control. In: C. Muller-Schloer, H. Schmeck, T. Ungerer (Eds.), Organic Computing A Paradigm Shift for Complex Systems, Autonomic Systems, Volume 1, Part 1, 67-78, Springer, Basel, 2011

Considering space:

Reaction Flow Artificial Chemistry

[P. Kreyssig and P. Dittrich. *Reaction flow artificial chemistries*. In: T. Lenaerts et al. (Eds.), Proc. of ECAL 2011, MIT Press, Boston, MA, p. 431-37, 2011]

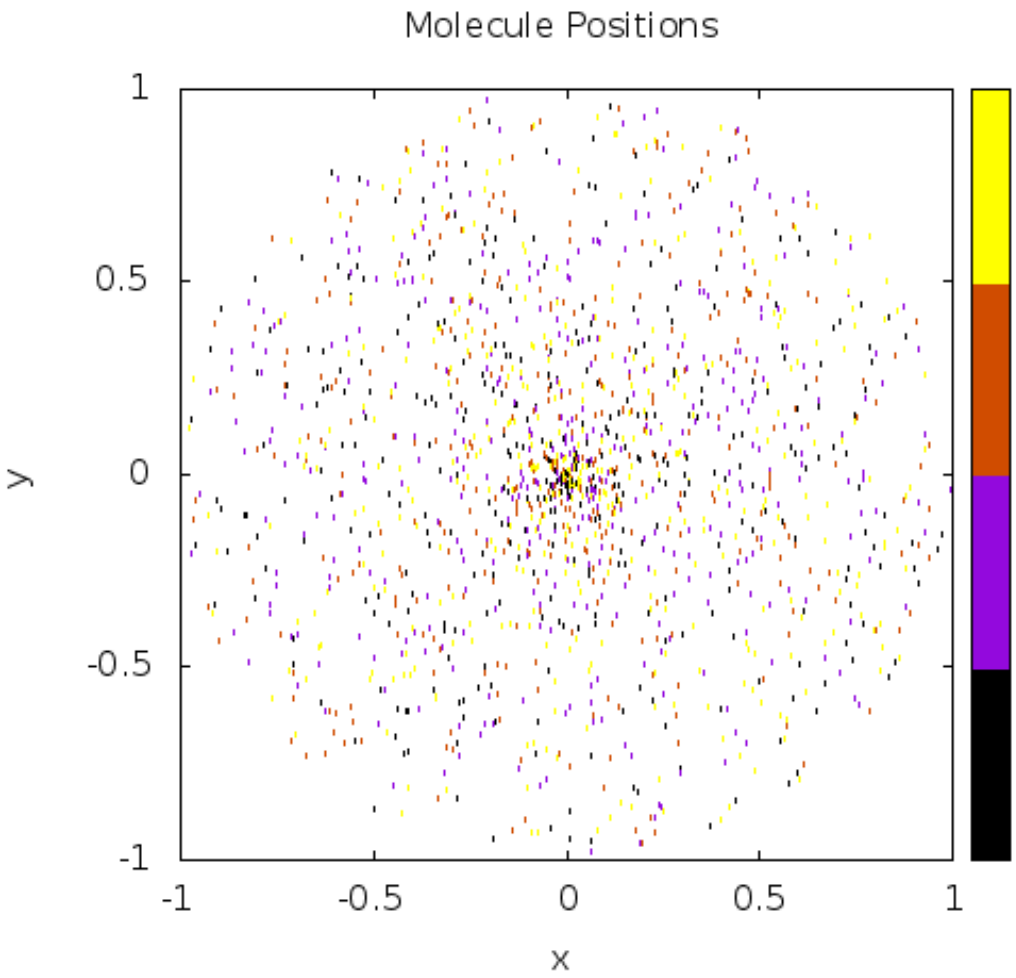
Reaction Flow Artificial Chemistries

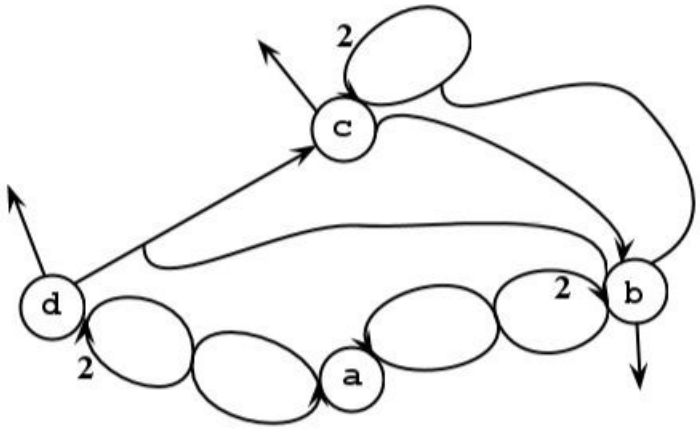
- spatial distribution of molecules given by a flow.

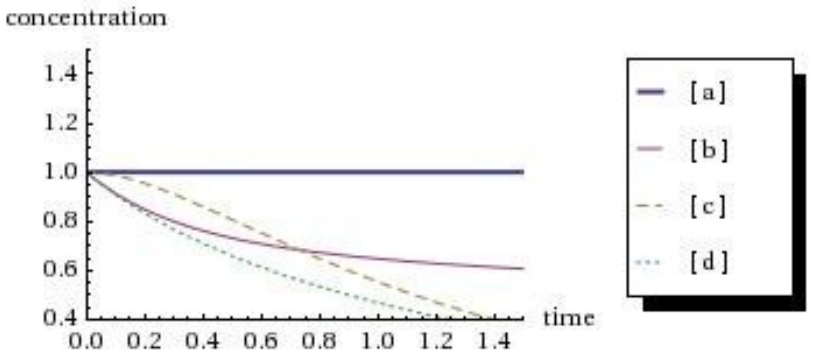
→ Get additional parameters to control and program the artificial chemistry.

[P. Kreyssig and P. Dittrich. *Reaction flow artificial chemistries*. In: T. Lenaerts et al. (Eds.), Proc. of ECAL 2011, MIT Press, Boston, MA, p. 431-37, 2011]

RFAC - Example







[P. Kreyssig and P. Dittrich. *Reaction flow artificial chemistries*. In: T. Lenaerts et al. (Eds.), Proc. of ECAL 2011, MIT Press, Boston, MA, p. 431-37, 2011]

RFAC – Differential Model

Let the species be $M = \{m_1, ..., m_{|M|}\}$.

Concentration of a species is $[m_i](x, y, t)$, so $[m_i] : R \times R \times R^+ \rightarrow R$.

$$\frac{\partial [m_i]}{\partial t} = -\frac{1}{\|V\|} \left\langle \nabla([m_i] \cdot \|V\|), V \right\rangle + R_{k,i}([m_1], ..., [m_{|M|}])$$

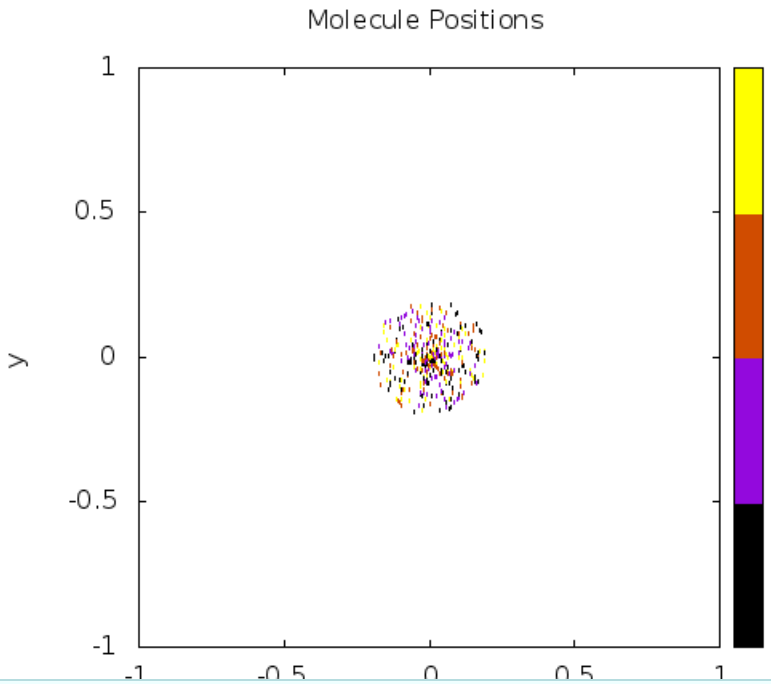
The change of molecule concentration due to movement is the directional derivative of $[m_i] \cdot \|V\|$ in the direction of V.

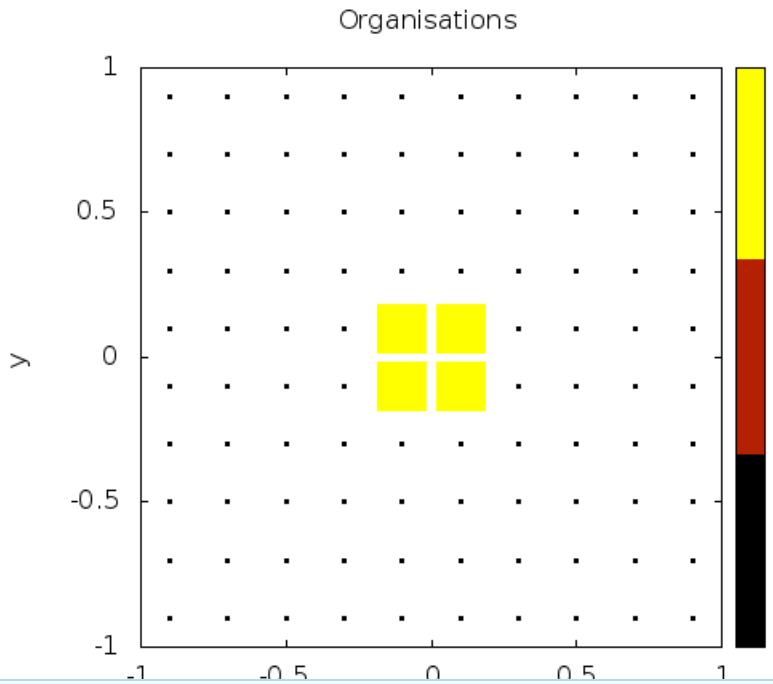
The change caused by the reactions appears in the reaction terms $R_{k,i}$, with constant reaction rates $k \in R^{\#reactions}$.

[P. Kreyssig and P. Dittrich. *Reaction flow artificial chemistries*. In: T. Lenaerts et al. (Eds.), Proc. of ECAL 2011, MIT Press, Boston, MA, p. 431-37, 2011]

RFAC – Analysis via Organizations

- Chemical organizations at different spatial scales.
- Functional units should be an organization.





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RFAC - Conclusion

- Spatial flow dynamics adds another level to influence the behavior
- Potential for a new programing mechanism for chemical information processing.
- Spatial chemical organizations helps in understanding spatial chemical computing.

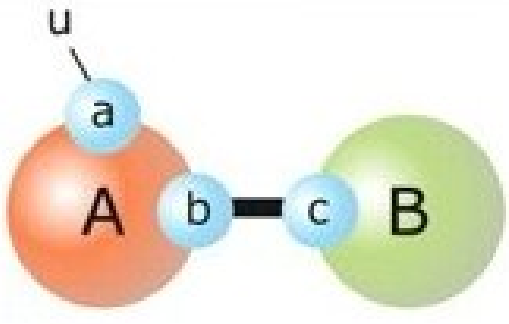
[P. Kreyssig and P. Dittrich. *Reaction flow artificial chemistries*. In: T. Lenaerts et al. (Eds.), Proc. of ECAL 2011, MIT Press, Boston, MA, p. 431-37, 2011]

Structured Molecules

"embodied" evolution

[G. Gruenert, G. Escuela, P. Dittrich, T. Hinze. *Morphological Algorithms: Membrane Receptor-ligand Interactions and Rule-based Molecule Graph Evolution for Exact Set Cover Problem*. In Proc. of 12th Conf. on Membrane Computing, LNCS, Springer, Berlin, 2011]

Structured Molecules Studied



K−expression

- inspired by biology
- of arbitrary size
- still want to describe and analyze it

[J. Feret, V. Danos, J. Krivine, R. Harmer, and W. Fontana. *Internal coarse-graining of molecular systems*. PNAS 2009]

```
[matchp f1 s0]
[matchp s1 split s1
   * send seg0 n2 f1]
[f1]     [s1]
```

four different fraglets

- inspired by computer sciences
- interesting for implementing our algorithms

[C. Tschudin. *Fraglets-a metabolistic execution model for communication protocols.* AINS 2003]

Structured Molecules: Molecular EA

- Embodied evolution: Using molecules as substrate for Evolutionary Algorithms
- Rule-based implementation (even Selection and Reproduction)

```
T(x~a,t!1).Trans(f!1~a,t!11~a,t!12~b,t!13~c,t,dock~p1).T(x~a,t!11).T(x~b,t!12).T(x~c,t!13)          30
T(x~b,t!1).Trans(f!1~b,t!11~d,t!12~e,t!13~f,t,dock~p1).T(x~d,t!11).T(x~e,t!12).T(x~f,t!13)
T(x~c,t!1).Trans(f!1~c,t!11~g,t!12~h,t,t,dock~p1).T(x~g,t!11).T(x~h,t!12)                          3
T(x~d,t!1).Trans(f!1~d,t!11~i,t!12~j,t,t,dock~p1).T(x~i,t!11).T(x~j,t!12)                         30
T(x~e,t!1).Trans(f!1~e,t!11~a,t,t,t,dock~p1).T(x~a,t!11)                                  30
T(x~f,t!1).Trans(f!1~f,t!11~d,t,t,t,dock~p1).T(x~d,t!11)                                  30


1  Sol(test~ok,t~a,eval!+)  +  T(x~a,t!5).Trans(f!5,dock~p1)   ->   Sol(test~ok,t~a!1,eval!+).T(x~a
1  Sol(test~ok,t~b,eval!+)  +  T(x~b,t!5).Trans(f!5,dock~p1)   ->   Sol(test~ok,t~b!1,eval!+).T(x~b
1  Sol(test~ok,t~c,eval!+)  +  T(x~c,t!5).Trans(f!5,dock~p1)   ->   Sol(test~ok,t~c!1,eval!+).T(x~c
1  Sol(test~ok,t~d,eval!+)  +  T(x~d,t!5).Trans(f!5,dock~p1)   ->   Sol(test~ok,t~d!1,eval!+).T(x~d
1  Sol(test~ok,t~e,eval!+)  +  T(x~e,t!5).Trans(f!5,dock~p1)   ->   Sol(test~ok,t~e!1,eval!+).T(x~e
# dissociate, if dock~bad
1  Sol(t!1).T(x!1,t!5).Trans(f!5,dock~bad)  ->  Sol(t) + T(x,t!5).Trans(f!5,dock~bad)          kTDis


# bind evaluation components:  (if not bound to copyTo)
2  Sol(test~ok,eval!2).Eval(t~a,sol!2)  + T(x~a,t!5).Trans(t!5,dock~p1)   ->   Sol(test~ok,eval!2).E
2  Sol(test~ok,eval!2).Eval(t~b,sol!2)  + T(x~b,t!5).Trans(t!5,dock~p1)   ->   Sol(test~ok,eval!2).E
2  Sol(test~ok,eval!2).Eval(t~c,sol!2)  + T(x~c,t!5).Trans(t!5,dock~p1)   ->   Sol(test~ok,eval!2).E
2  Sol(test~ok,eval!2).Eval(t~d,sol!2)  + T(x~d,t!5).Trans(t!5,dock~p1)   ->   Sol(test~ok,eval!2).E
2  Sol(test~ok,eval!2).Eval(t~e,sol!2)  + T(x~e,t!5).Trans(t!5,dock~p1)   ->   Sol(test~ok,eval!2).E
2  Sol(test~ok,eval!2).Eval(t~f,sol!2)  + T(x~f,t!5).Trans(t!5,dock~p1)   ->   Sol(test~ok,eval!2).Ev
# dissociate if dock~bad
2  Eval(t!1).T(x!1,t!5).Trans(t!5,dock~bad)  ->  Eval(t) + T(x,t!5).Trans(t!5,dock~bad)          kTDi
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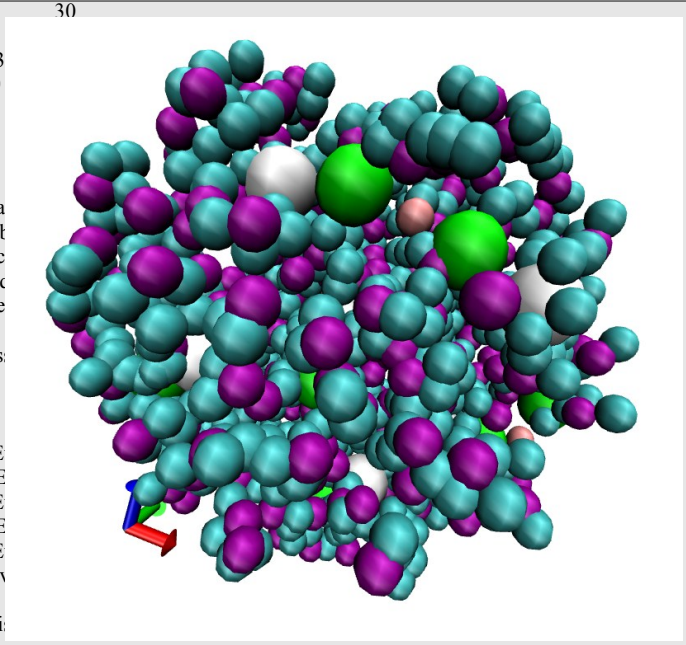
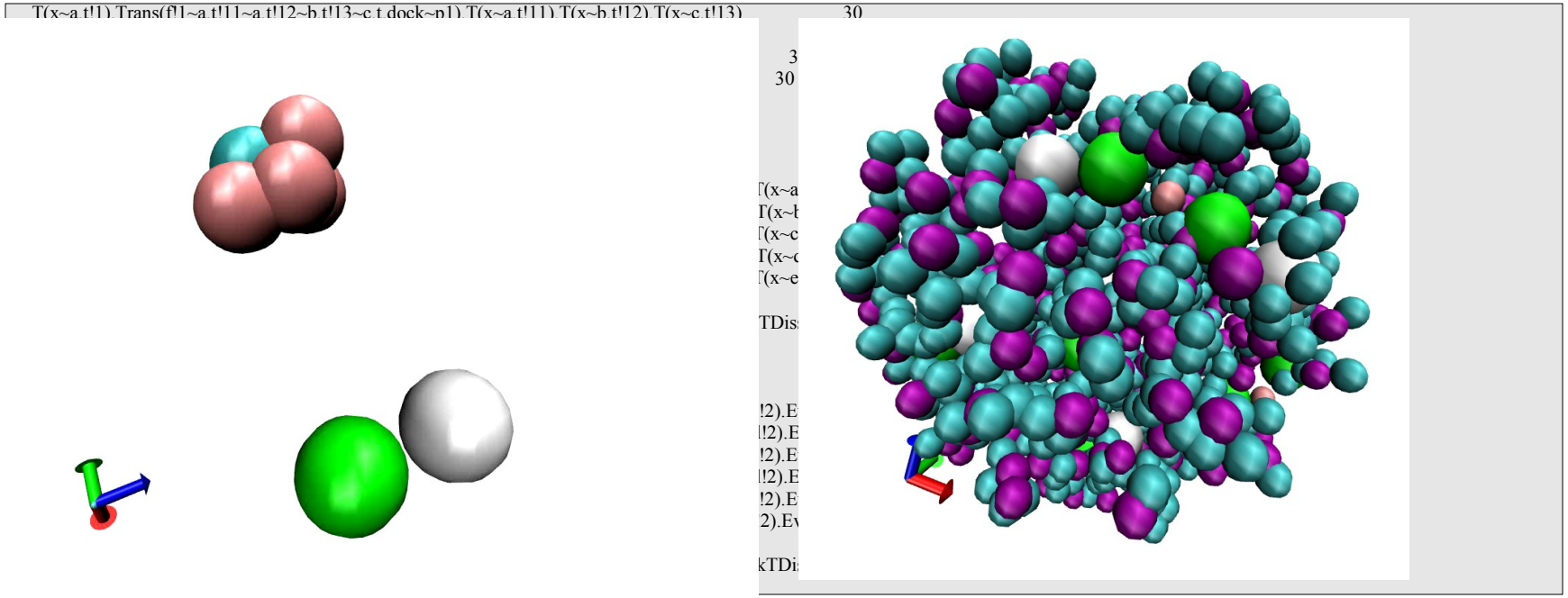


[G. Gruenert, G. Escuela, P. Dittrich, T. Hinze. *Morphological Algorithms: Membrane Receptor-ligand Interactions and Rule-based Molecule Graph Evolution for Exact Set Cover Problem*. CMC 2011]

Structured Molecules: Molecular EA

- Embodied evolution: Using molecules as substrate for Evolutionary Algorithms
- Rule-based implementation (even Selection and Reproduction)



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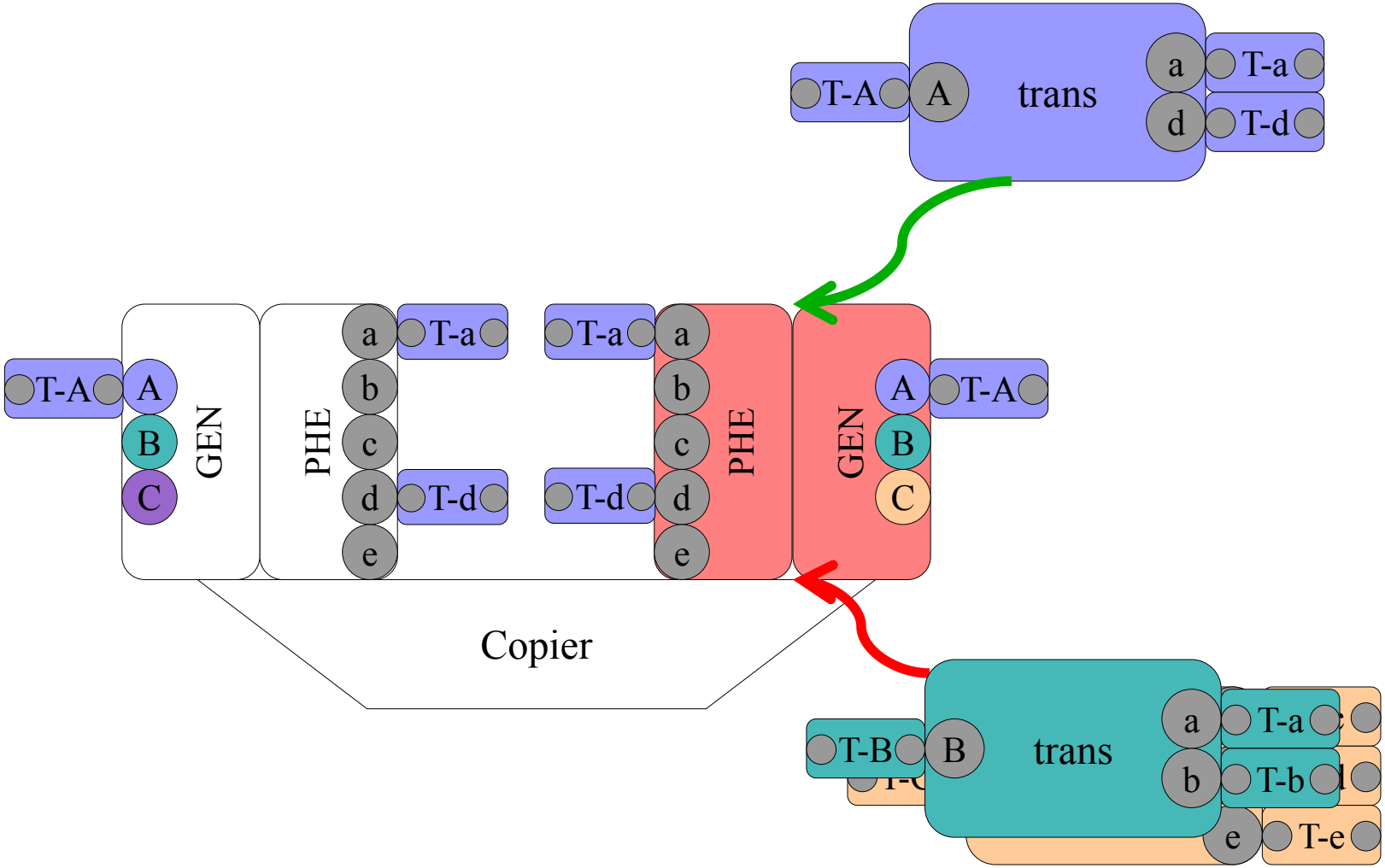
Structured Molecules - EAs



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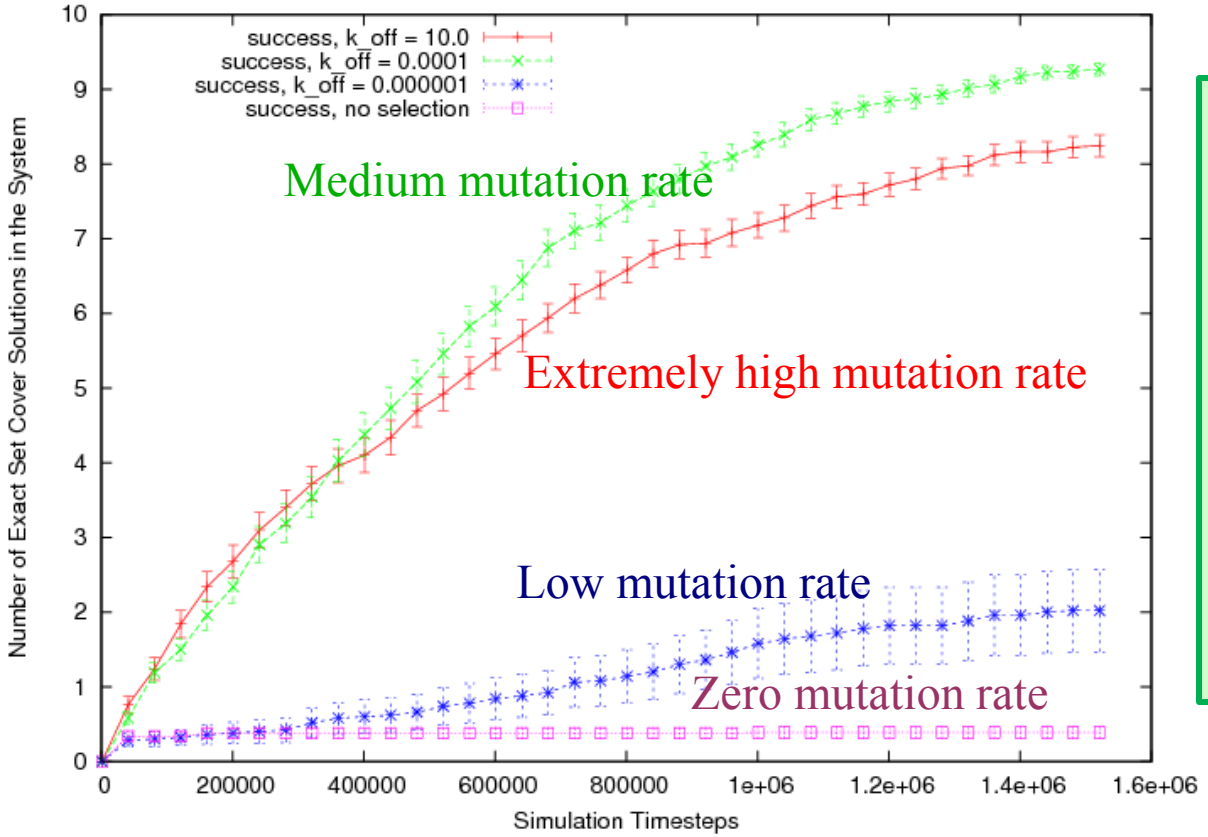
Structured Molecules - EAs



- ✓Only local rules
- ✓ Asynchronous
- ✓ Dynamic optimisation
- ✓ Large populations
- ✓ Space

[G. Gruenert, G. Escuela, P. Dittrich, T. Hinze. *Morphological Algorithms: Membrane Receptor-ligand Interactions and Rule-based Molecule Graph Evolution for Exact Set Cover Problem*. CMC 2011]

Theory

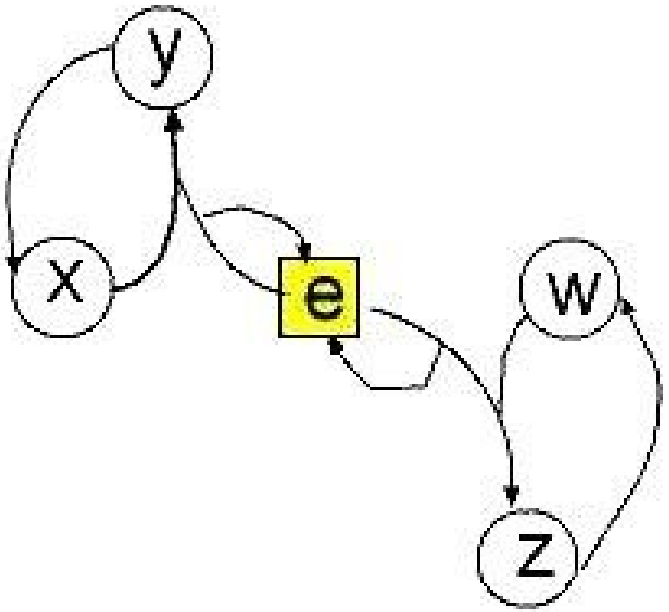
- Decomposition theorem of chemical organizations
- Stochastic systems

[T. Veloz, B. Reynaert, D. Rojas-Camaggi and P. Dittrich. *A Decomposition Theorem in Chemical Organizations*. T. Lenaerts et al (Eds.), Proc. of ECAL 2011, MIT Press, Boston, MA, 2011]

[C. Wozar, S. Peter, P. Kreyssig and P. Dittrich.
Chemical Organization Theory in Discrete Systems. (in preparation)]

Decomposition Theorem - Example

$A = N + E + F + C_1 + C_2 + \ldots + C_l$



1. Non-reactive molecules
   $N = \{ n \}$

2. (pure) Catalysts
   $E = \{ e \}$

3. Overproduced molecules
   $F = \{ o \}$

4. (pure) Cycle molecules C
   $C = M - (E+F+N) = \{ x, y, w, z \}$
   $C = C_1 + C_2 + \ldots + C_l = \{x, y\} + \{w, z\}$

[T. Veloz, B. Reynaert, D. Rojas-Camaggi and P. Dittrich. *A Decomposition Theorem in Chemical Organizations*. T. Lenaerts et al (Eds.), Proc. of ECAL 2011, MIT Press, Boston, MA, 2011]

Decomposition Theorem - Conclusion

→ better algorithms

→ better understanding

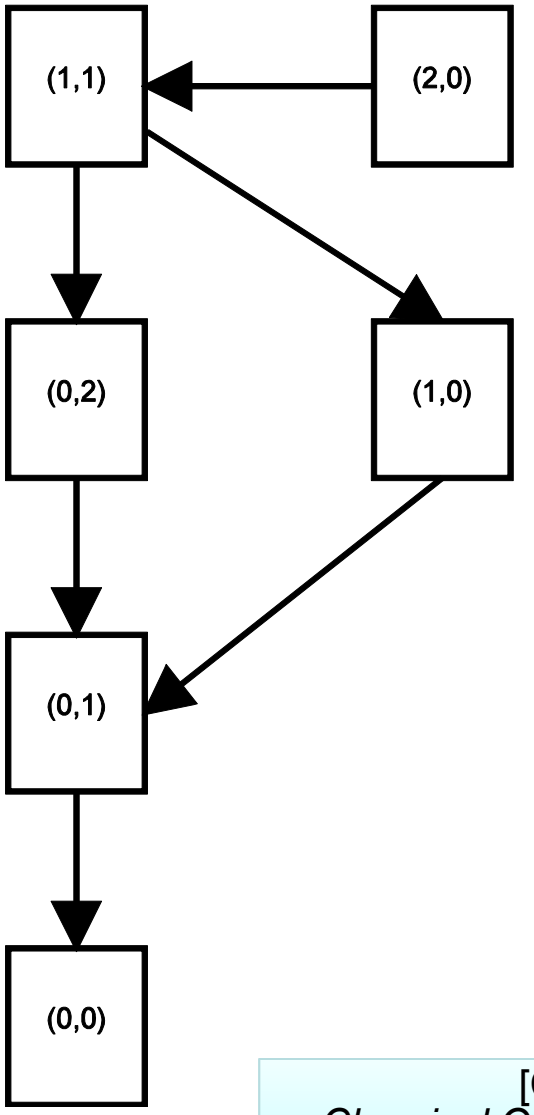
[T. Veloz, B. Reynaert, D. Rojas-Camaggi and P. Dittrich. *A Decomposition Theorem in Chemical Organizations*. T. Lenaerts et al (Eds.), Proc. of ECAL 2011, MIT Press, Boston, MA, 2011]

Theory II: Stochastic Organizations

- Link discrete stochastic dynamic models of (artificial) chemical systems to the theory of organizations.
- Markov chain

[C. Wozar, S. Peter, P. Kreyssig and P. Dittrich.
Chemical Organization Theory in Discrete Systems. (in preparation)]

Stochastic Organizations - Example



$$M = \{A, B\}$$

$$R = \{A \rightarrow B, B \rightarrow \phi\}$$

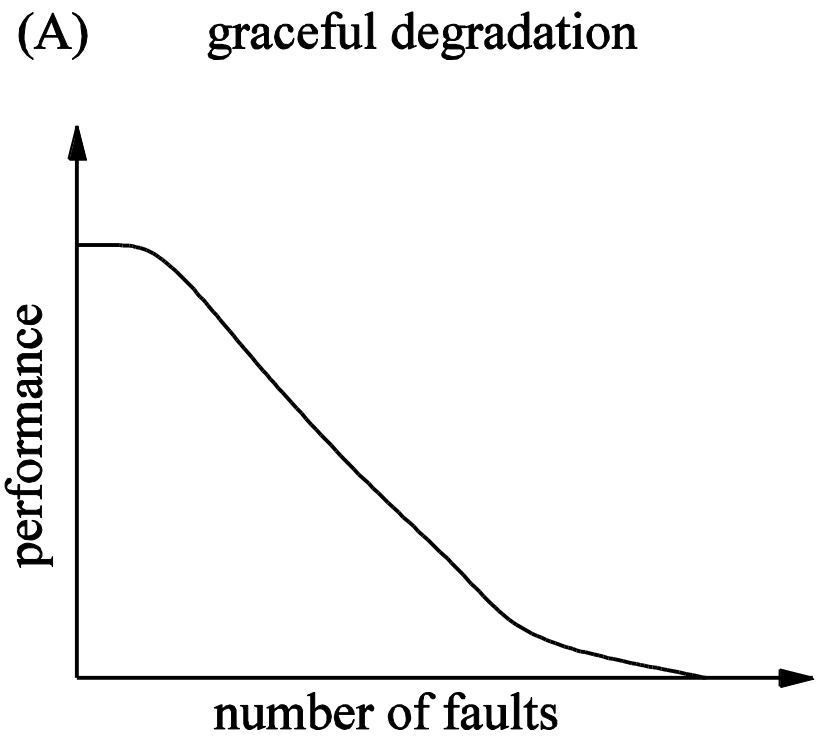
- Organizational part := set of strongly connected states such that no transition leaves the set from inside.

[C. Wozar, S. Peter, P. Kreyssig and P. Dittrich.
Chemical Organization Theory in Discrete Systems. (in preparation)]

Outlook

Artificial Apoptosis

Apoptosis vs Graceful Degradation

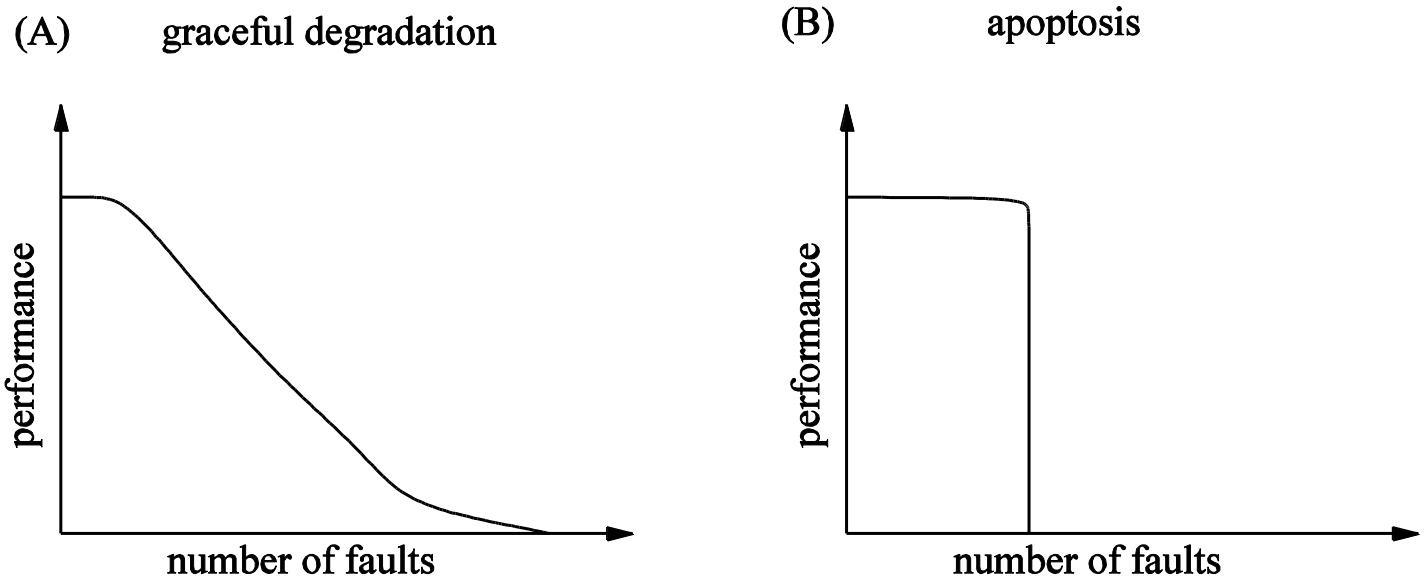


Apoptosis - Biology

- Apoptosis denotes the programmed cell death unlike the premature death of cells (necrosis).
- Can already be found in colonies of cells (not only in multi-cellular organisms) and in plants.
- Three functional units:
  - Signaling pathways which can be activated from the inside or via receptors from the outside by other cells to induce the cell death.
  - Apoptosis mechanism which breaks down the cell in small chunks (controlled demolition) without an inflammation (unlike necrosis).
  - Notification of other cells of own death.

Apoptosis vs Graceful Degradation

- First purposes of apoptosis is protection from further damage if cell is dysfunctional or could spread diseases.
- Different from graceful degradation which is prevalent in most technical systems.



Apoptosis for Morphogenesis

- Second purposes of apoptosis is the shaping of an organism (morphogenesis).
- Artificial development uses it for homeostasis rather than for giving form to the organism.
- Olsen *et.al.* showed the importance of the feedback (notification) before cell death in cancer growth simulations.

[M.M. Olsen, N. Siegelmann-Danieli, H.T. Siegelmann. *Dynamic Computational Model Suggests that Cellular Citizenship is Fundamental for Selective Tumor Apoptosis*. PLoS One 2010]

Apoptosis in AIS

- Artificial Immune Systems (AIS) for Wireless Sensor Networks use apoptosis.
- Switch-off nodes which are malicious and disturbing other nodes.

Artificial Apoptosis

Artificial Apoptosis

Artificial Apoptosis

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