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

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Project Aim

- Employ the (bio-)chemical principles of information processing as a programming approach for organic computing.

- How to program chemical-like systems?

Overview

I. Result of Phase II

II. Outlook for Phase III

I. Results of Phase II

I. Results of Phase II

1. Organization-oriented chemical programming
2. Organization analysis of chemical computing in space
3. Evolutionary design vs. manual Design
4. Simulator for quantitative evaluation of distributed chemical computing
5. Chemical control in artificial development
6. Emergent control

Primary Publications (Phase II)

Refereed Journal:

[1] N. Matsumaru, T. Hinze, and P. Dittrich.
Organization-oriented chemical programming for Distributed Artifacts
International Journal of Nanotechnology and Molecular Computation (2009, minor revision)

Refereed Proceedings:

[2] T. Lenser, N. Matsumaru, T. Hinze, P. Dittrich. Tracking the Evolution of Chemical Computing Networks. In S. Bullock, J. Noble, R. Watson, M.A. Bedau (Eds.), Proceedings of the Eleventh International Conference on the Simulation and Synthesis of Living Systems (Artificial Life XI), pp. 343-350, MIT Press, 2008
[3] N. Matsumaru, T. Lenser, F. Centler, P. Speroni di Fenizio, T. Hinze, and P. Dittrich,
Common organizational structures within two chemical flip-flop, Proceeding of International Workshop on Natural Computing, 2008
[4] P. Speroni di Fenizio, N. Matsumaru, P. Dittrich (2009),
Flying Over Mount Improbable, Proc ECAL 2009, LNCS, Springer, Berlin, 2009 (in print)

Dissertation:

[5] N. Matsumaru

Chemical Programming to Exploit Chemical Reaction Systems for Computation, Friedrich-Schiller-University Jena, 2009

Secondary Publications (Phase II)

Refereed Journal:

[7]. C. Kaleta, F. Centler, P Speroni di Fenizio, P. Dittrich : Phenotype prediction in regulated metabolic networks, *BMC Systems Biology* 2008, 2:37 (25 April 2008)

[8] B. Ibrahim , S. Diekmann, E. Schmidt, P. Dittrich : In--Silico Modling of the Mitotic Spindle Assembly Check point, *PLoS ONE* 3(2):e 1555, 2008

[9]. F. Centler, C. Kaleta, P. Speroni di Fenizio, P. Dittrich : Computing Chemical Organizations in Biological Networks *Bioinformatics*, 24: 1611-1618, 2008

Refereed Proceedings:

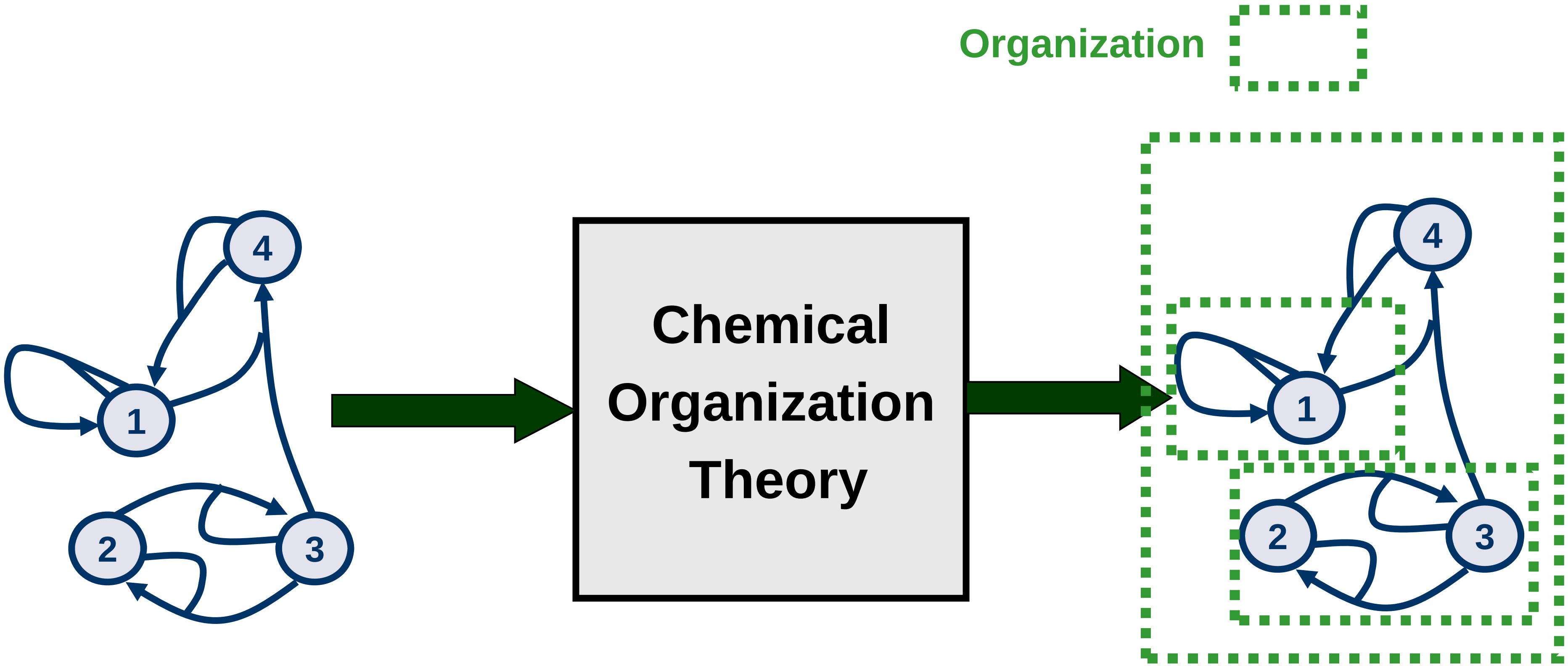
[10] T. Hinze, R. Fassler, T. Lenser, N. Matsumaru, P. Dittrich. Event-Driven Metamorphoses of P Systems. In P. Frisco, D.W. Corne, G. Paun (Eds.), Prel. Proceedings Ninth International Workshop on Membrane Computing (WMC9), pp. 209-225, Heriot-Watt University, also in LNCS, Springer, 2009

[11] T. Hinze, S. Hayat, T. Lenser, N. Matsumaru, P. Dittrich : Biosignal--Based Computing by AHHL Induced Synthetic Gene Regulatory Networks. In *Proc. of the First International Conference on Bio-Inspired Systems and Signal Processing (BIOSIGNALS2008)*, Vol. 1, pp. 162-169 , IEEE Engineering in Medicine and Biology Society, Institute for Systems and Technologies of Information Control and Communication, INSTICC press, 2008

1. Organization-Oriented Chemical Programming

- Basic: Computation should be understood as a transition between organizations.

Practical View



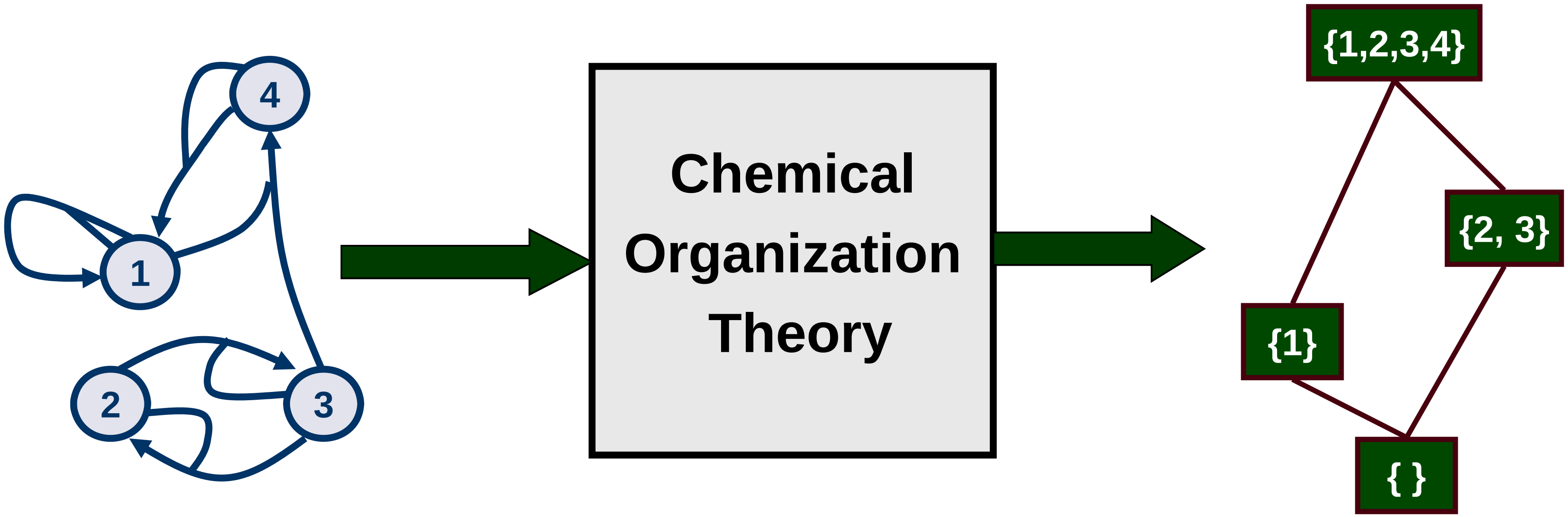
Reaction network

Organizations

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

Practical View

Hasse diagram of organizations



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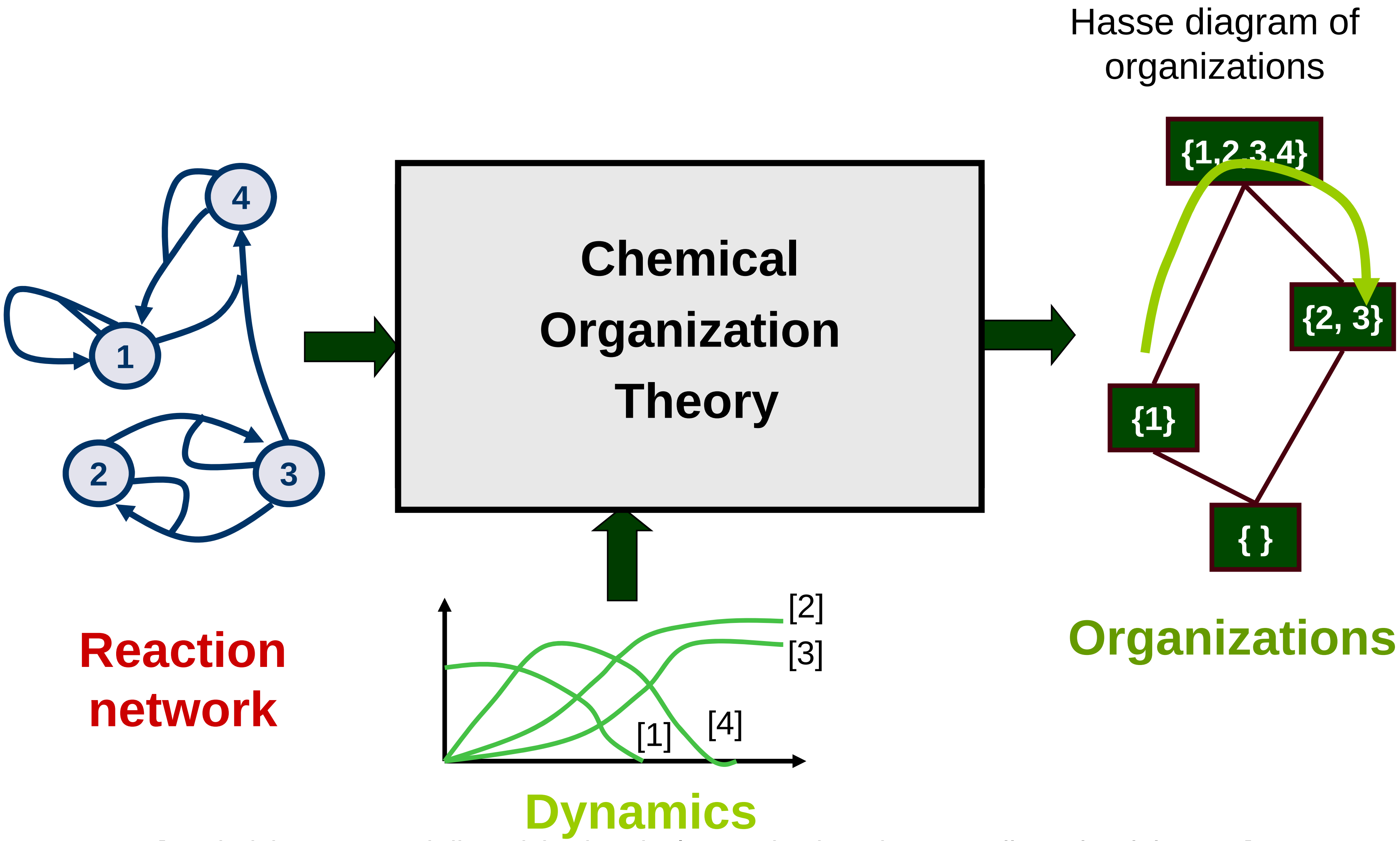

[P. Dittrich, P. Speroni di Fenizi, Chemical Organization Theory, *Bull. Math. Biol.*, 2007]

1. Seven Principles for Organization-Oriented Chemical Programming

P1: There should be one organization for each output behavior class

P2: The result should be in the closure of the input.

P3: The the input should generate the organization representing the desired output

P4: Eliminate organizations not representing a desired output

P5: An output organization should have no organization below

P6: Assure, if possible, stoichiometrically the stability of an output organization

P7: Use kinetic laws for fine tuning

[1] N. Matsumaru, T. Hinze, and P. Dittrich. Organization-oriented chemical programming for Distributed Artifacts *International Journal of Nanotechnology and Molecular Computation (submitted)*

1. Example: Maximum Independent Set Problem (MIS)

- New chemical algorithm
  - only four species
  - no distinction of neighbors required

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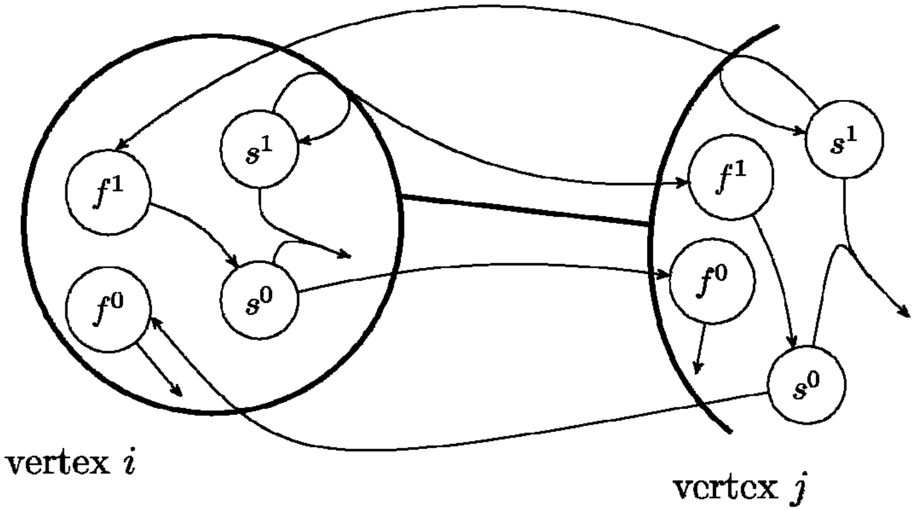
1. Example: MIS chemistry



$\mathcal{R}_i$
$s^1 + s^1 \rightarrow \emptyset$
$f^0 \rightarrow \emptyset$
$f^1 \rightarrow s^0$

$\mathcal{T}_{ij} : v_i \rightsquigarrow v_j$
$s_i^1 \rightarrow s_i^1 + f_j^1$
$s_i^0 \rightarrow f_j^0$

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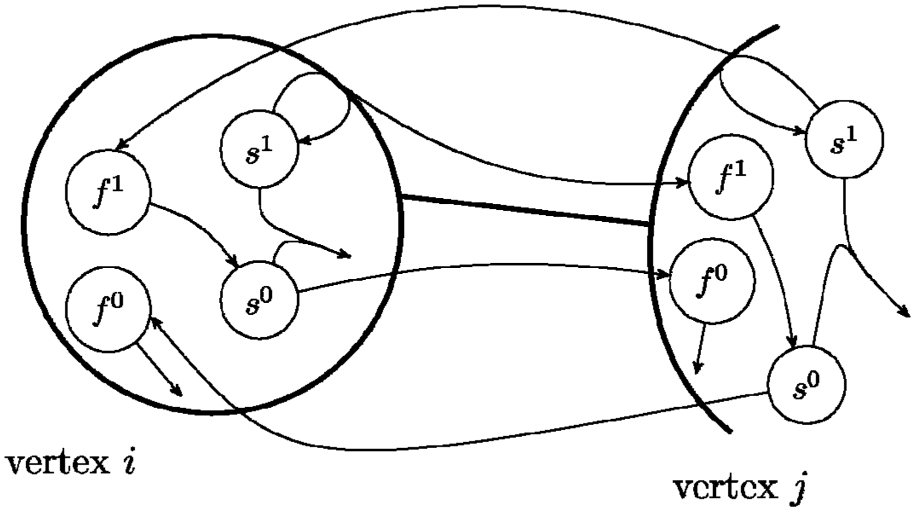

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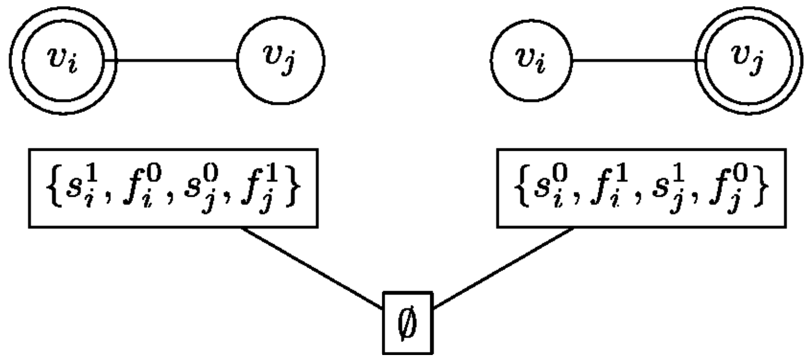

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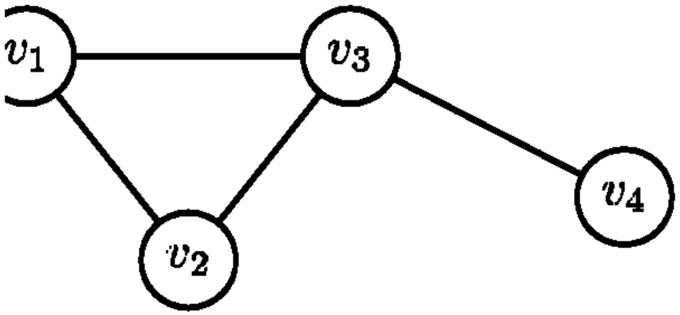

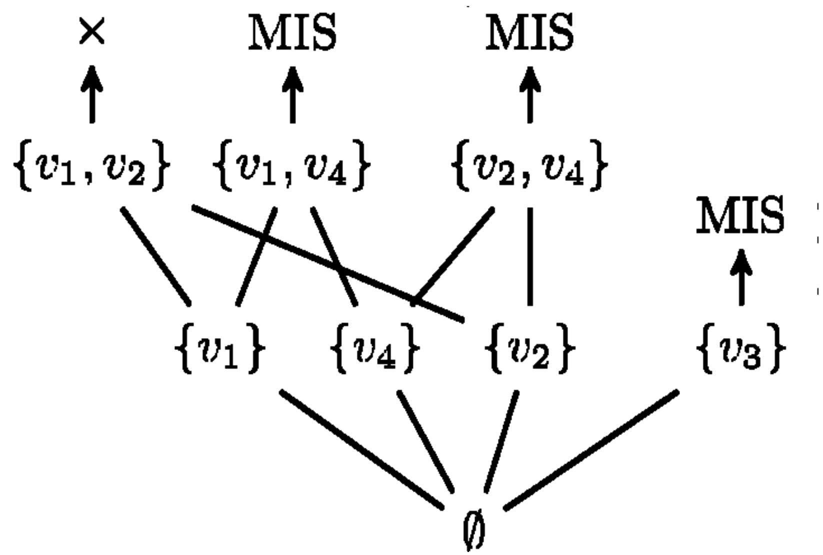

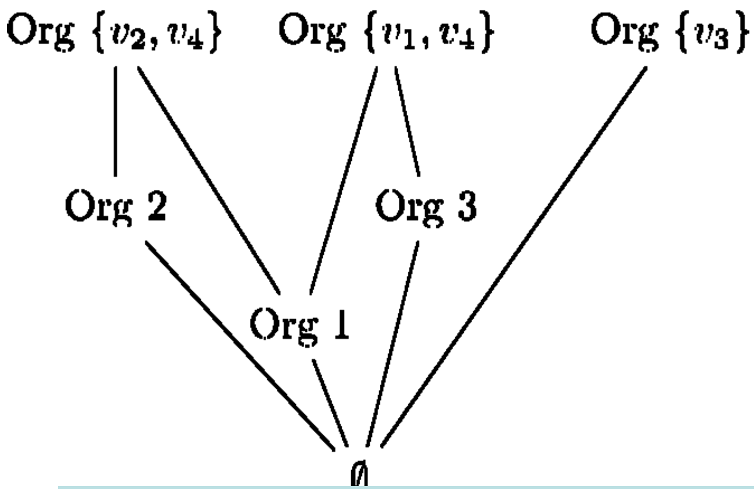

Org 1 : $\{f_1^0, f_2^0, s_3^0, f_3^1, s_4^1, f_4^0\}$

Org 2 : $\{s_1^0, f_1^1, f_1^0, s_2^1, f_2^0, s_3^0, f_3^1, f_3^0, f_4^0\}$

Org 3 : $\{s_1^1, f_1^0, s_2^0, f_2^1, f_2^0, s_3^0, f_3^1, f_3^0, f_4^0\}$

Org $\{v_2, v_4\}$: $\{s_1^0, f_1^1, f_1^0, s_2^1, f_2^0, s_3^0, f_3^1, f_3^0, s_4^1, f_4^0\}$

Org $\{v_1, v_4\}$: $\{s_1^1, f_1^0, s_2^0, f_2^1, f_2^0, s_3^0, f_3^1, f_3^0, s_4^1, f_4^0\}$

Org $\{v_3\}$: $\{s_1^0, f_1^1, f_1^0, s_2^0, f_2^1, f_2^0, s_3^1, f_3^0, s_4^0, f_4^1\}$

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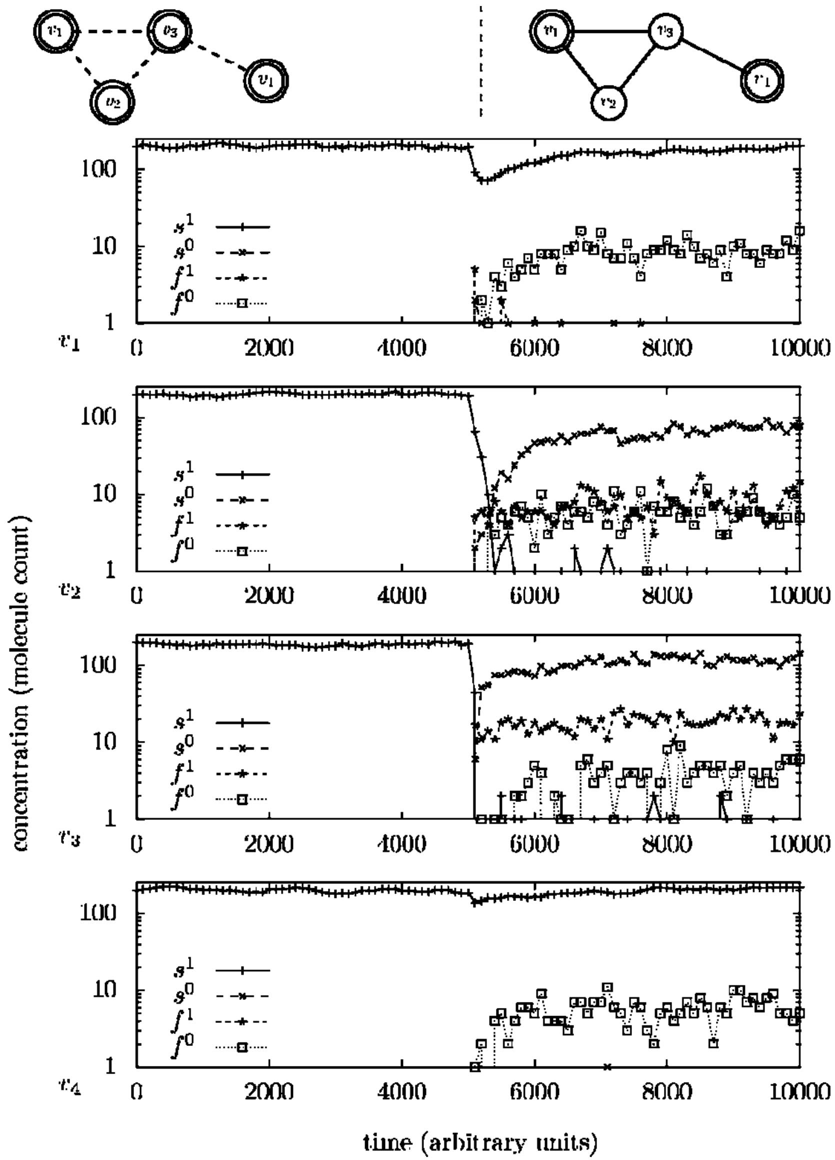
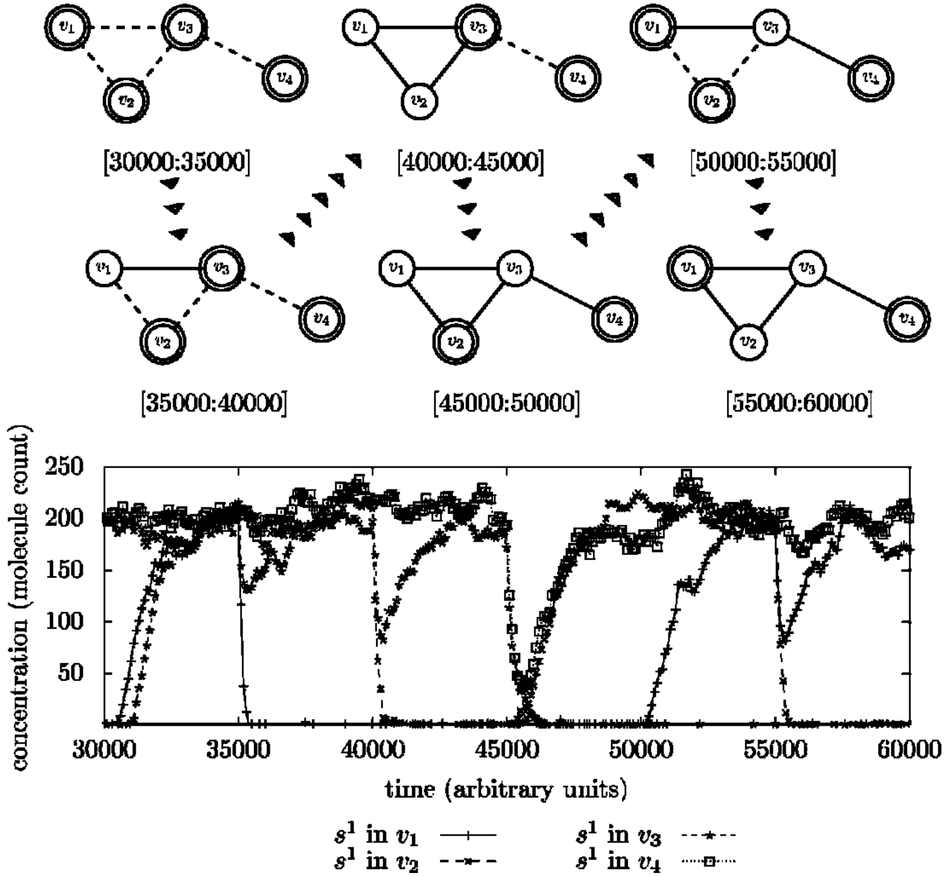
1. Example: MIS simulation





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2. Organizational Analysis in Space

a. "Spatial Organization"
- previous work
- no diffusion and no communication

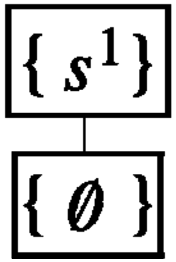
b. Global Analysis
- considers a concrete global topology

c. Local Analysis
- all possible local environments are represented by inflow and outflow reactions.

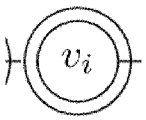
[1] N. Matsumaru, T. Hinze, and P. Dittrich. Organization-oriented chemical programming for Distributed Artifacts *International Journal of Nanotechnology and Molecular Computation (submitted)*

2.c Local Analysis

$$\langle M_{local}, R_{local} \rangle$$



no neighbors



- local environment is modeled by inflow and outflow

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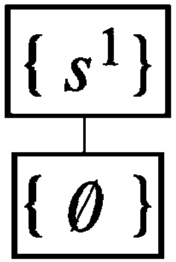
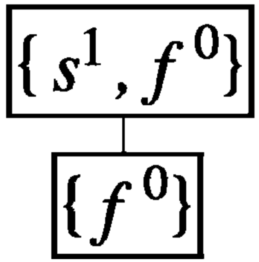
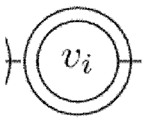
2.c Local Analysis

$\langle M_{local}, R_{local} \rangle$ $\langle M_{local}, (R_{local} \cup \{\emptyset \to f^0\}) \rangle$

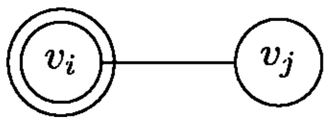




no neighbors



one “0” neighbors



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2.c Local Analysis

$$\langle M_{local}, R_{local} \rangle \qquad \langle M_{local}, (R_{local} \cup \{\emptyset \rightarrow f^0\}) \rangle$$

$\{s^1\}$ — $\{\emptyset\}$ $\qquad$ $\{s^1, f^0\}$ — $\{f^0\}$

$$\langle M_{local}, (R_{local} \cup \{\emptyset \rightarrow f^1\}) \rangle \qquad \langle M_{local}, (R_{local} \cup \{\emptyset \rightarrow f^0, \emptyset \rightarrow f^1\}) \rangle$$

$\{s^0, f^1\}$ $\qquad$ $\{s^0, f^0, f^1\}$

- local environment is modeled by inflow and outflow

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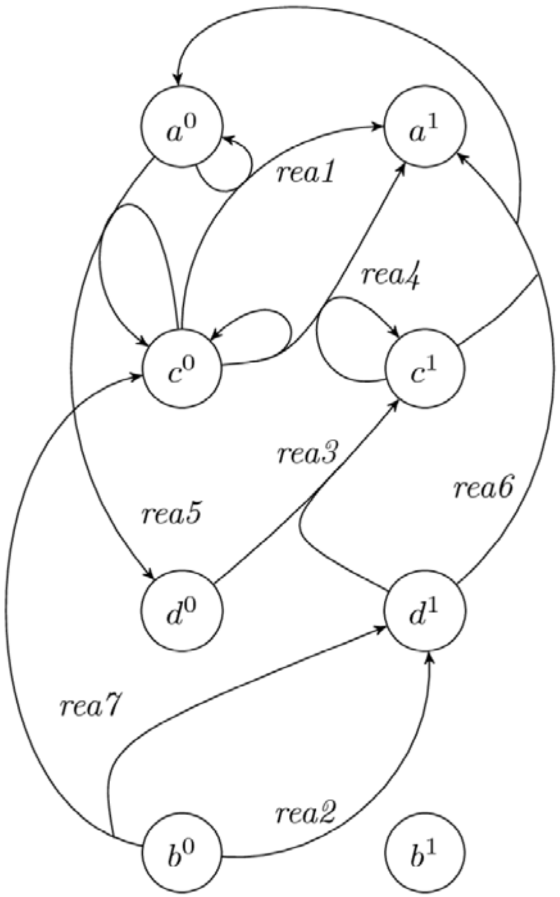
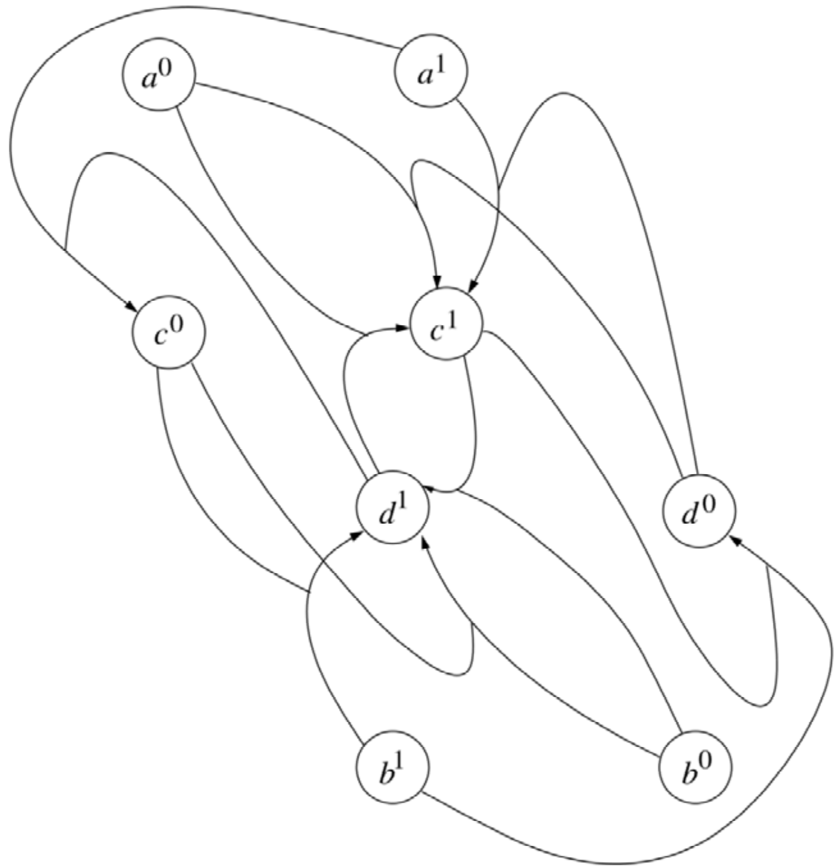
3. Evolution vs. manual design



evolved



manually designed

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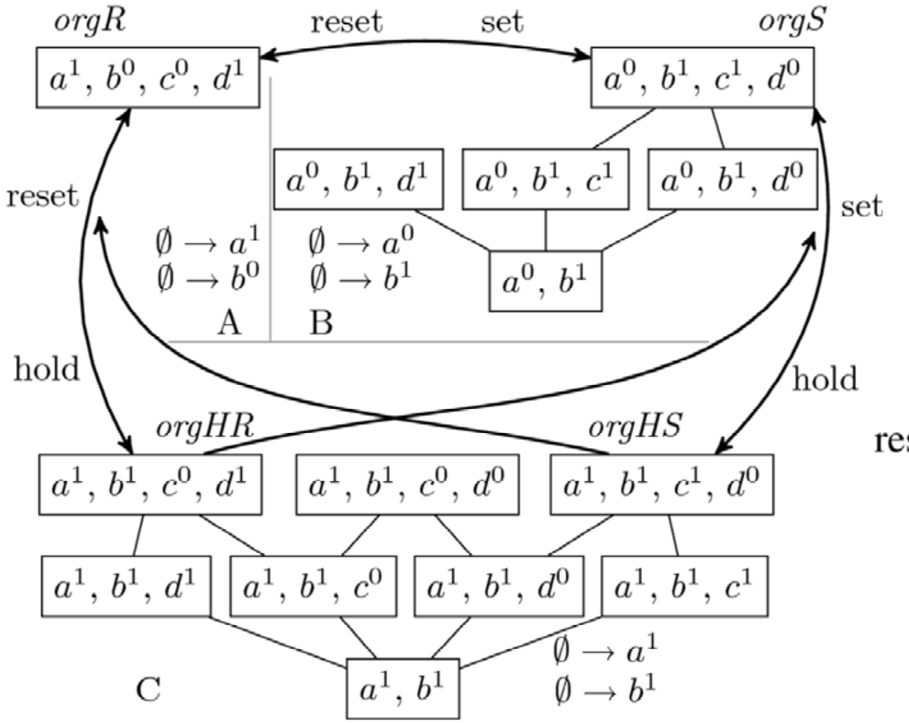
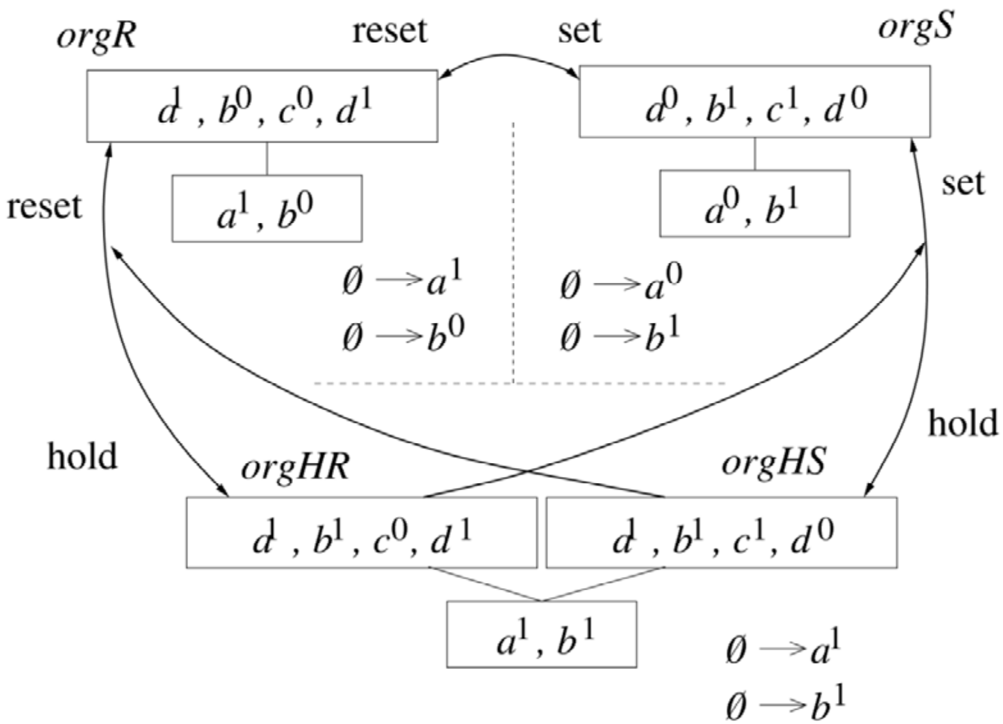


evolved



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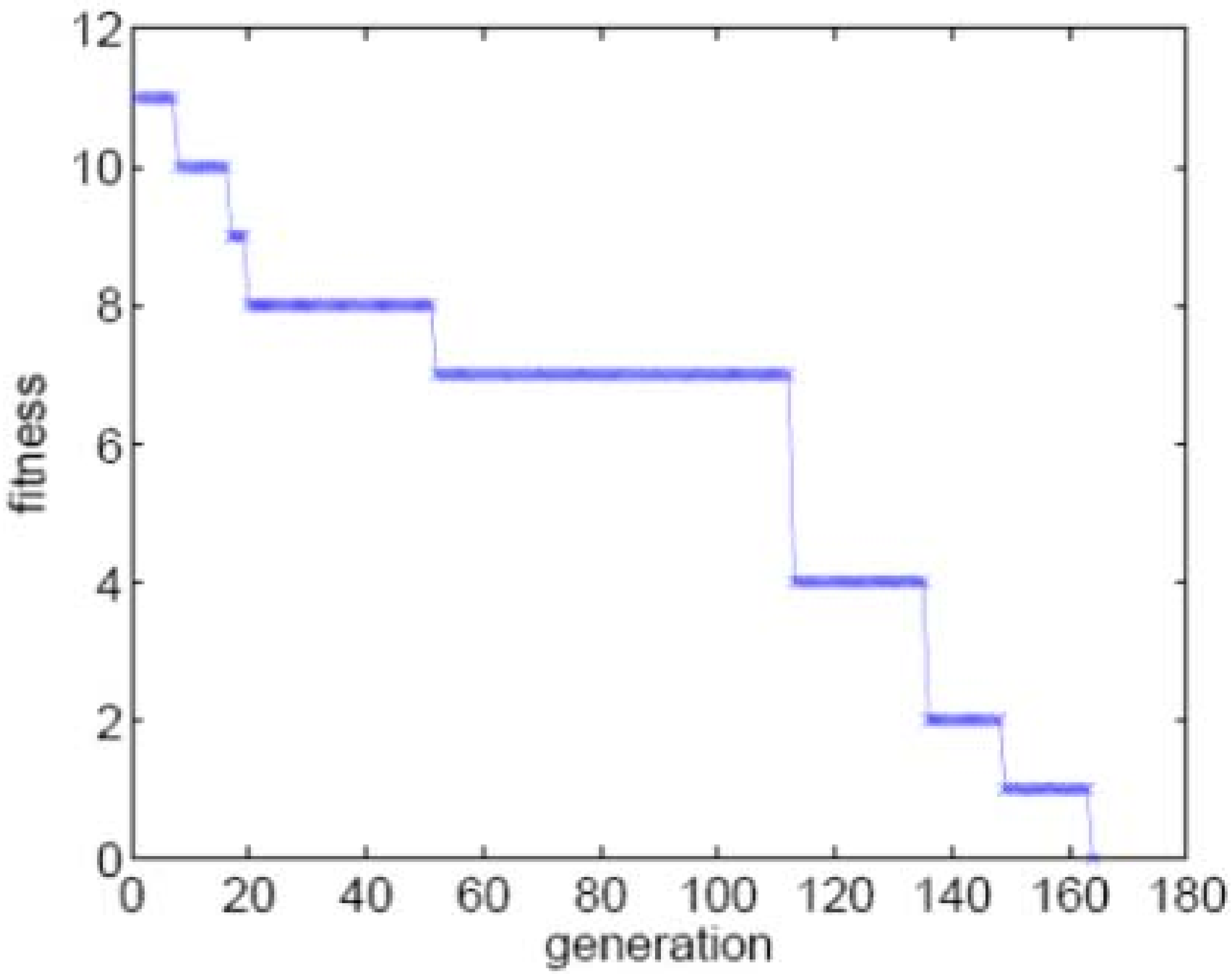
3. Evolutionary Process: Fitness



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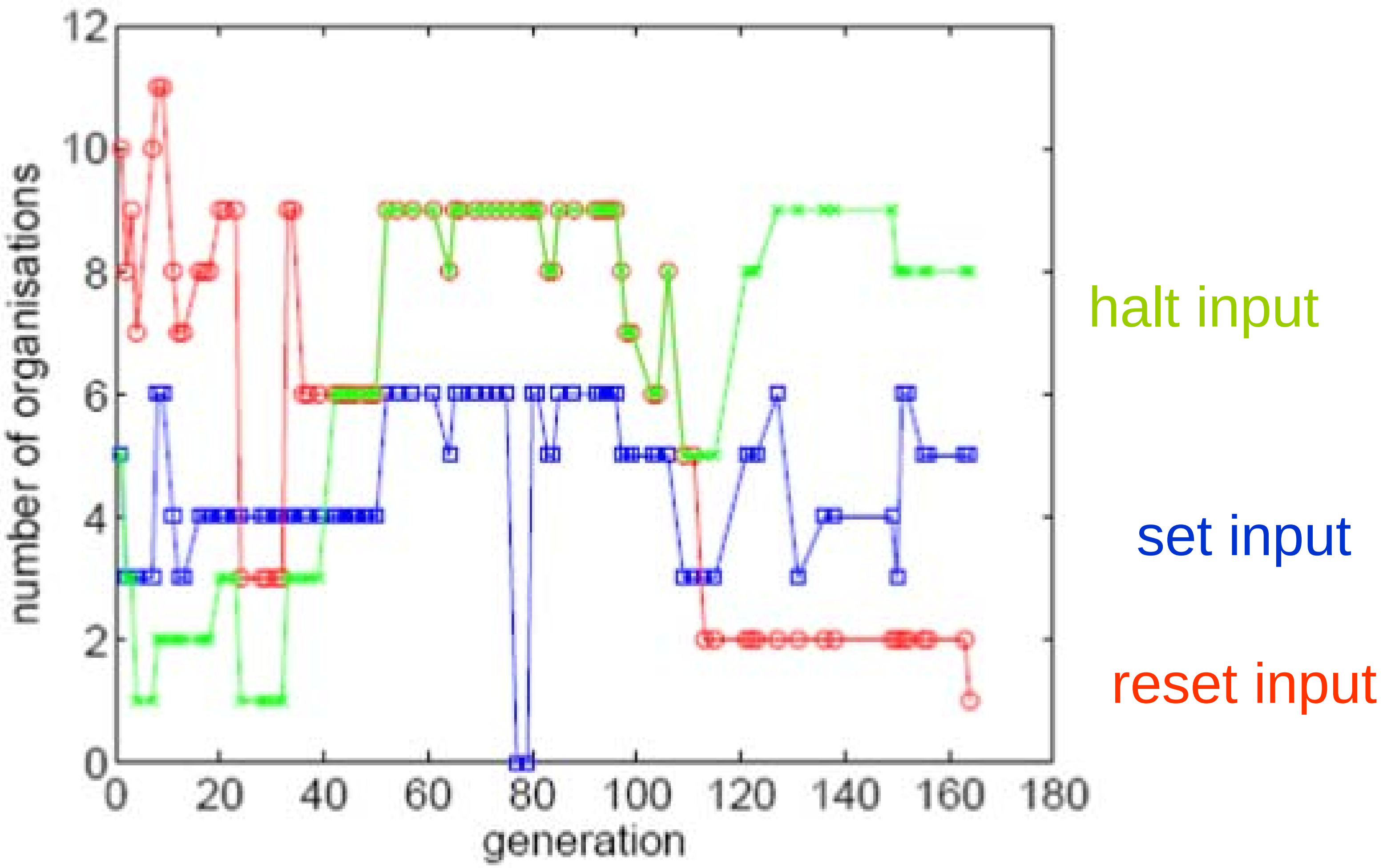
3. Evolutionary Process: Number of Organizations



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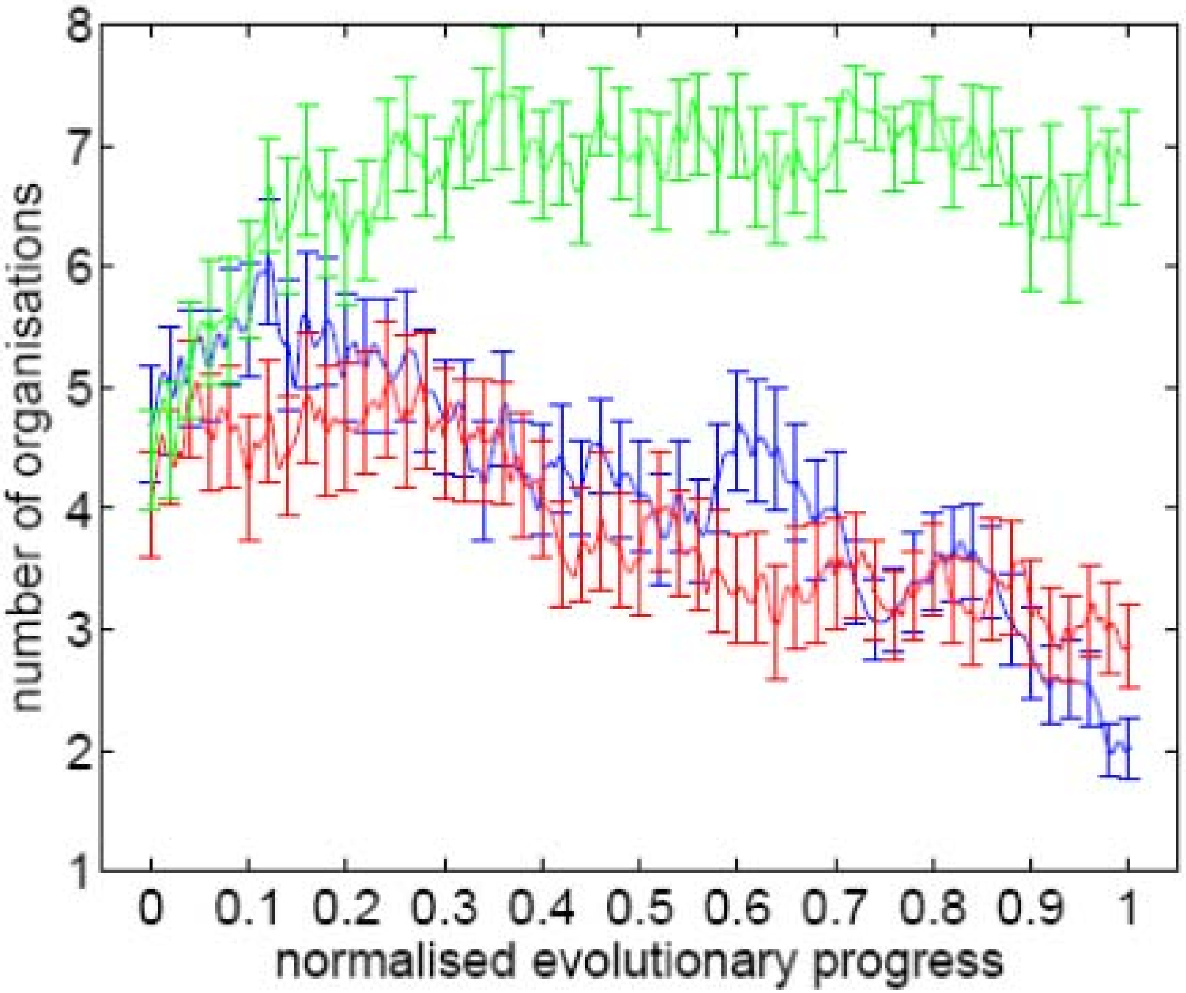
3. Evolutionary Process: Average Number of Organizations



halt input

reset input
set input

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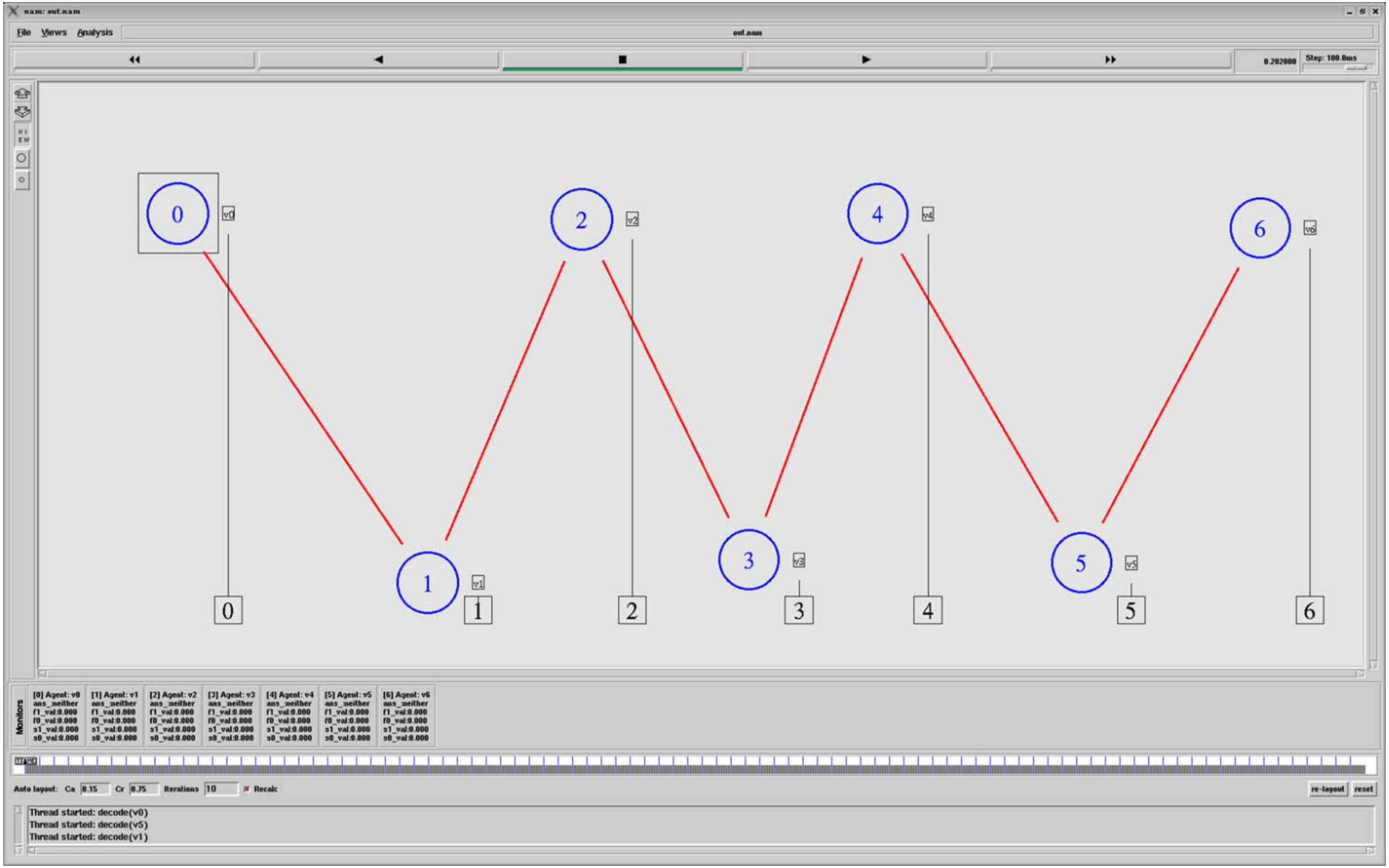
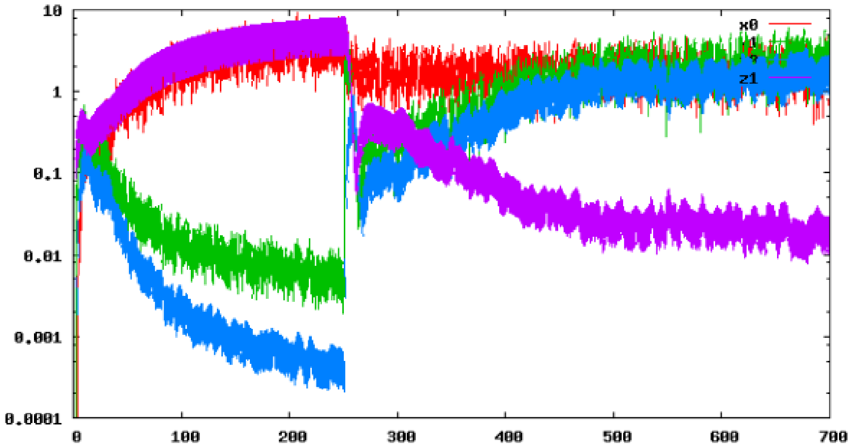
4. Simulator for Quantitative Evaluation of Distributed Chemical Computing

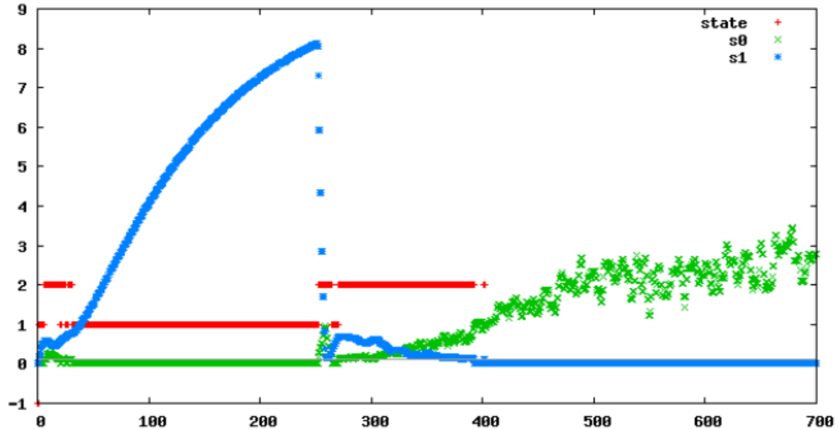
- Specify chemical program by a set of explicit reaction rules
- Specify topology by a graph
- Run stochastic simulation
- Visualize dynamics

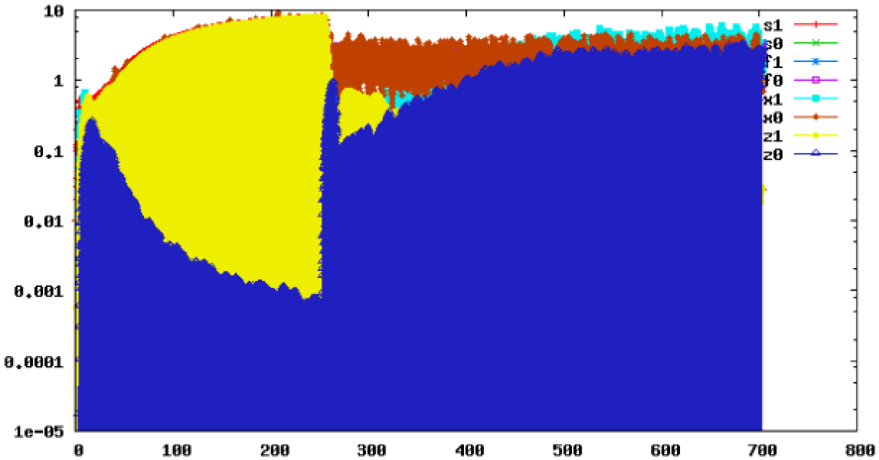
4. Simulator for Quantitative Evaluation of OC

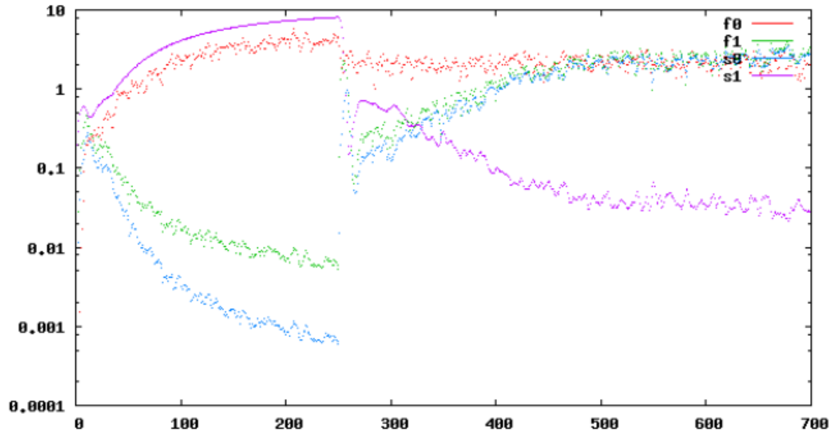


4. Looking at the dynamics of one node (V2)









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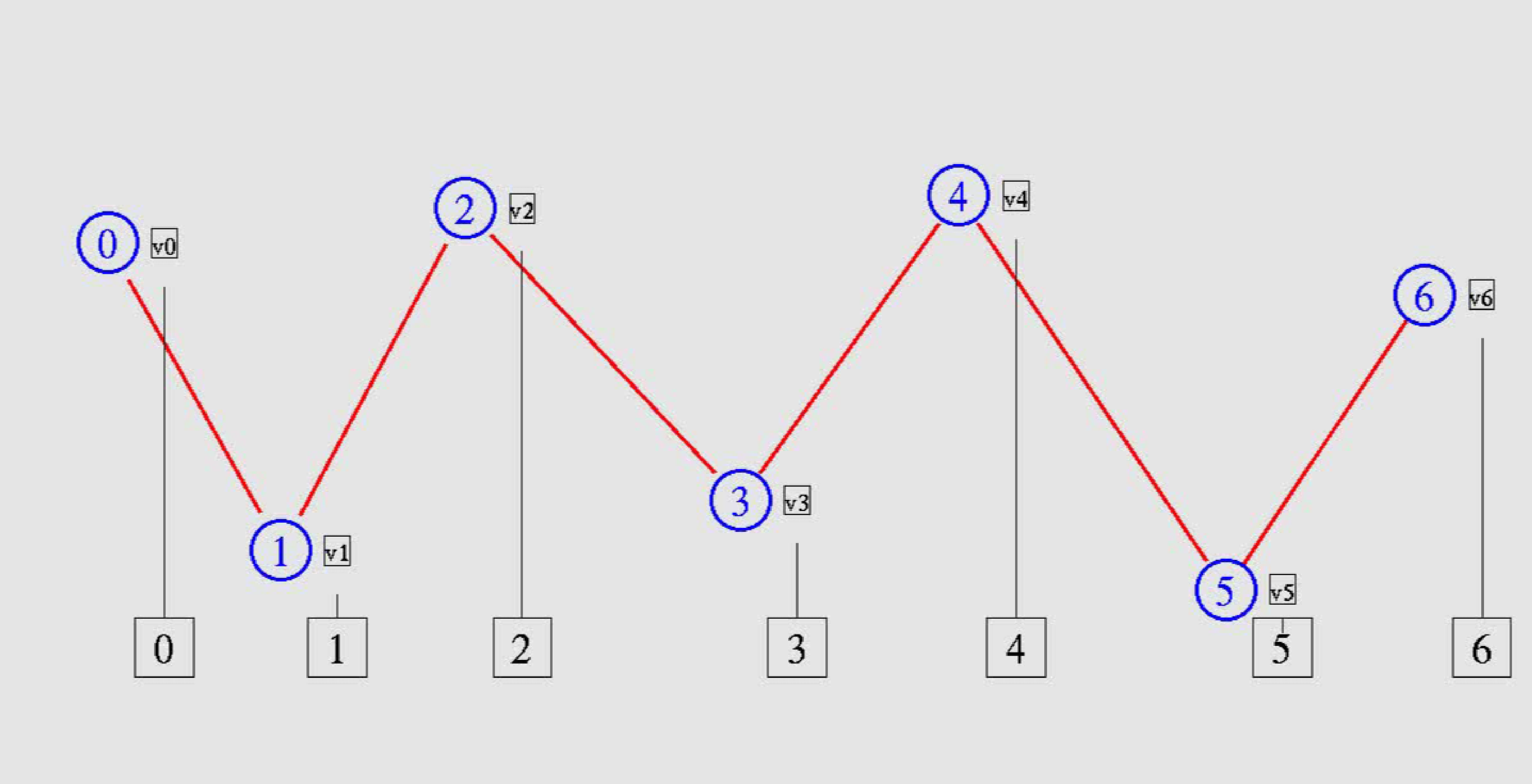


5. Organization Oriented Chemical Computing for Artificial Development

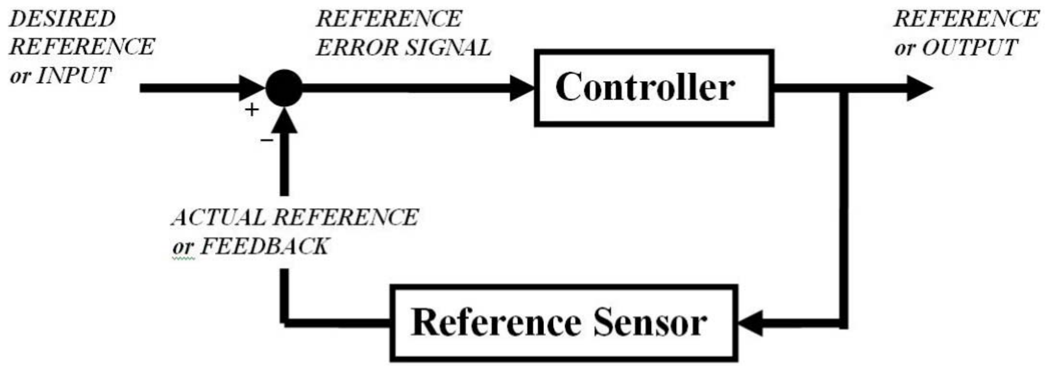
- OO-ChemProg applied to cell differentiation / morphogenesis
- Differentiation can be understood as a transition between organizations

-> might be useful in
Artificial Development + Evolution

6. Emergent Control

(manuscript in preparation)

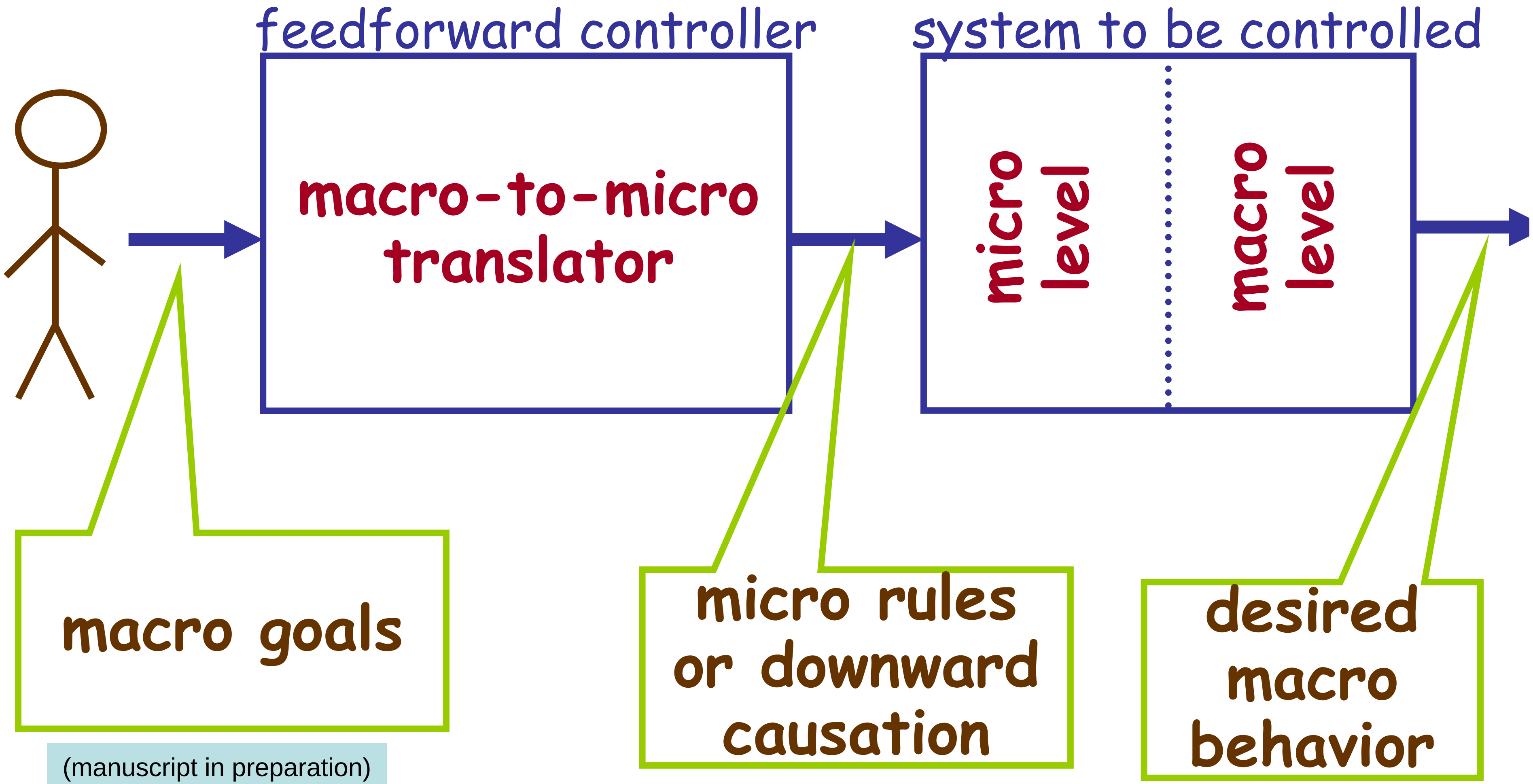
6. Feed back control is everywhere



Source: http://upload.wikimedia.org/wikipedia/en/4/40/Feedback_loop.JPG

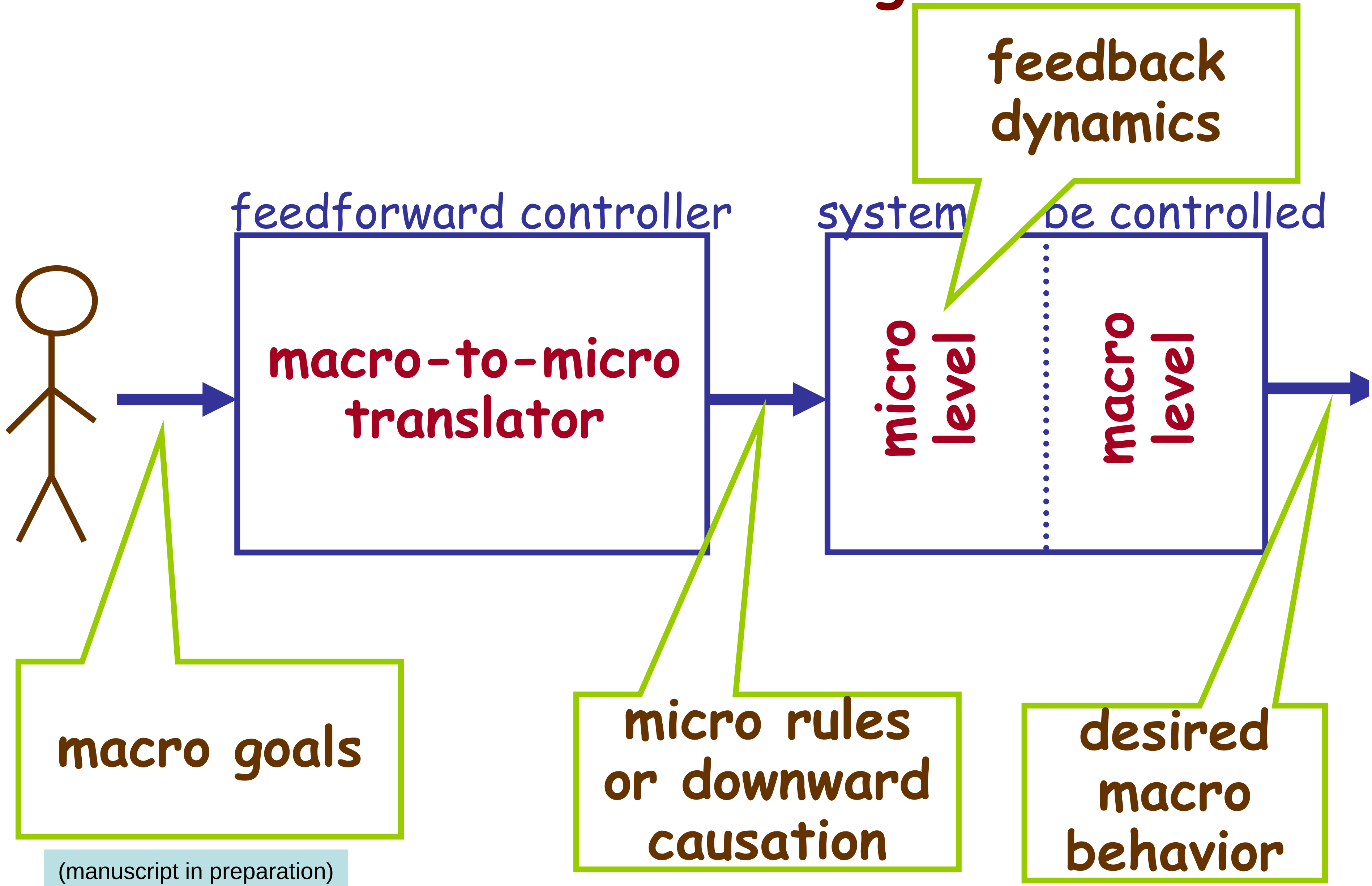
6. Emergent Control

6. Architecture for Emergent Control



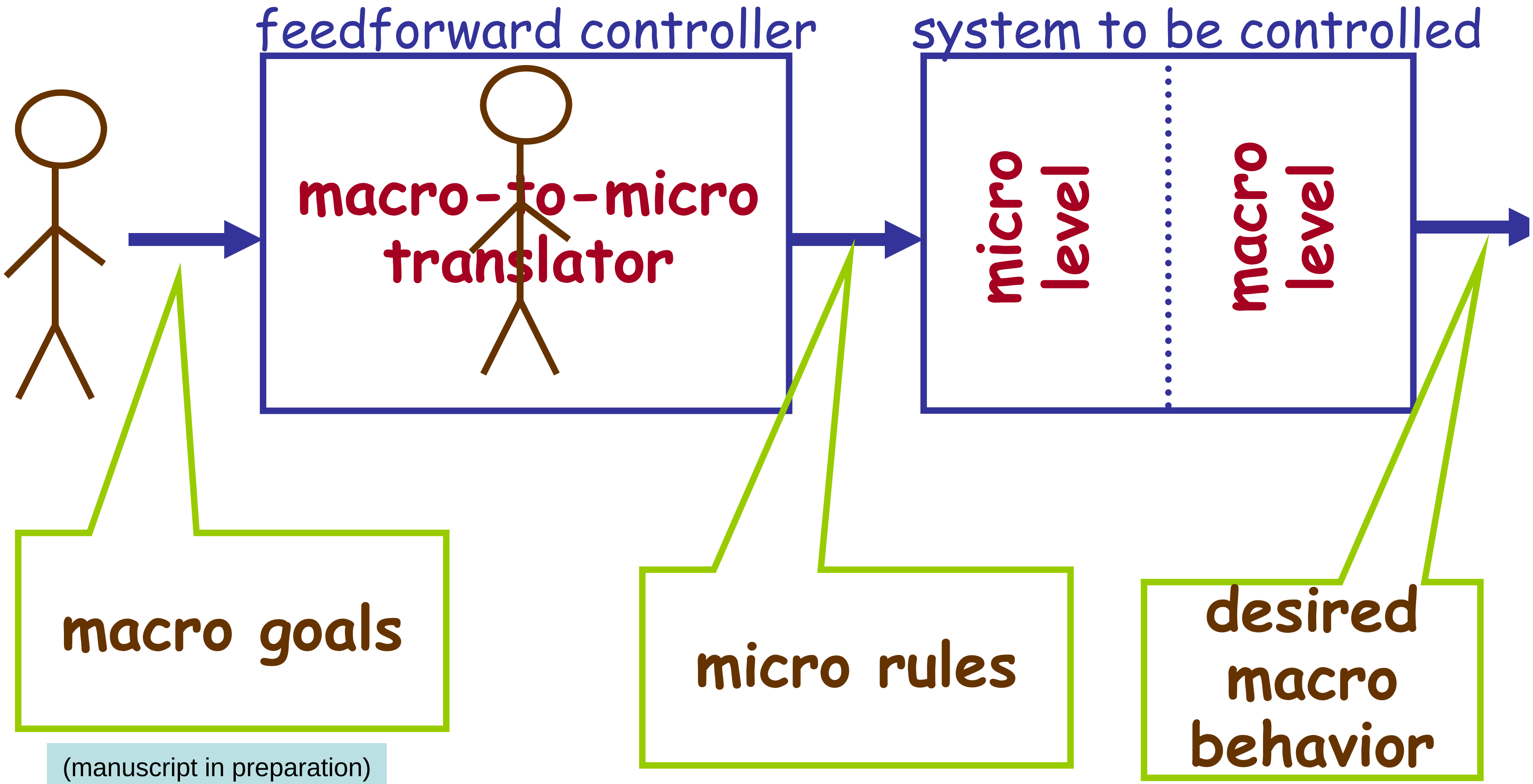
(manuscript in preparation)

6. Architecture for Emergent Control



(manuscript in preparation)

6. Current Situation



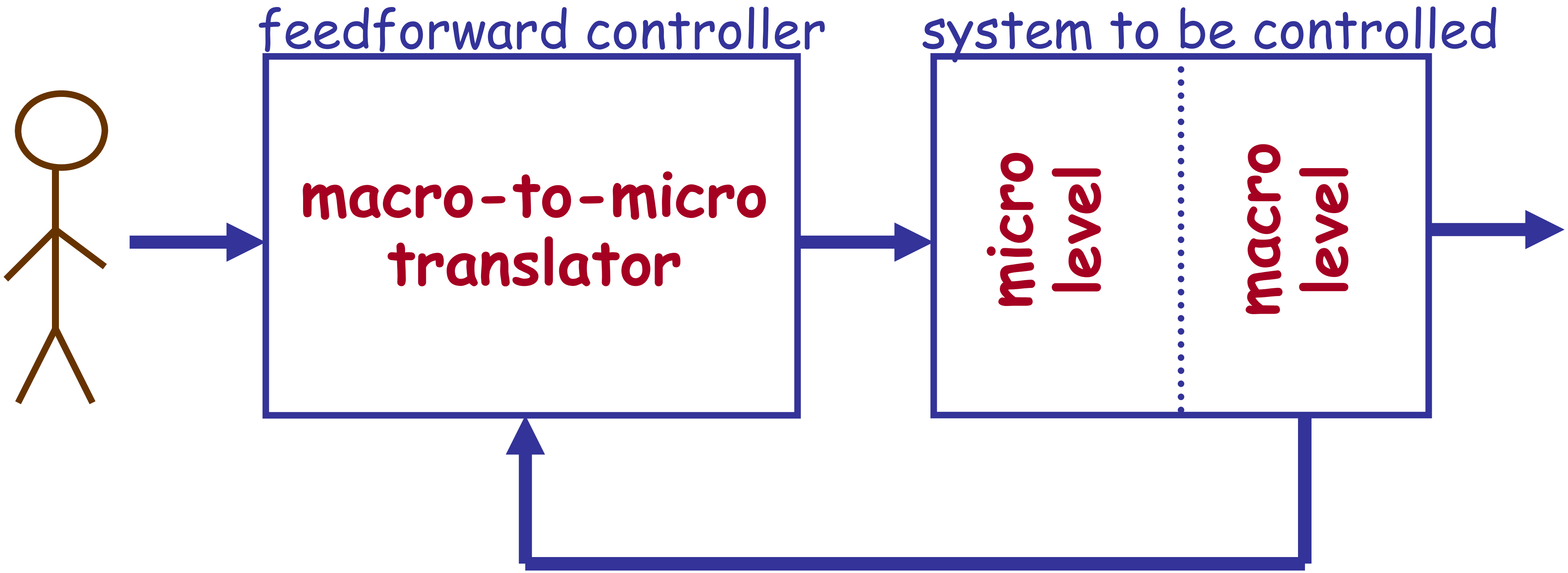
(manuscript in preparation)

6. Strategies for Building a Macro-to-Micro Translator

- Manual "intelligent" design, Policies
- Evolution (optimization, playing, etc)
- Theory
- Mimicking
- Compiling
- Experiment and numerical inversion

(manuscript in preparation)

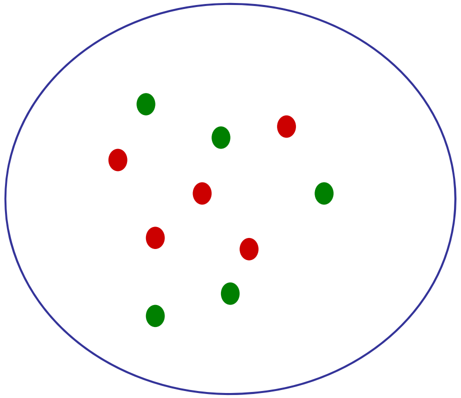
6. In practical applications, emergent control will often be combined with feedback control.



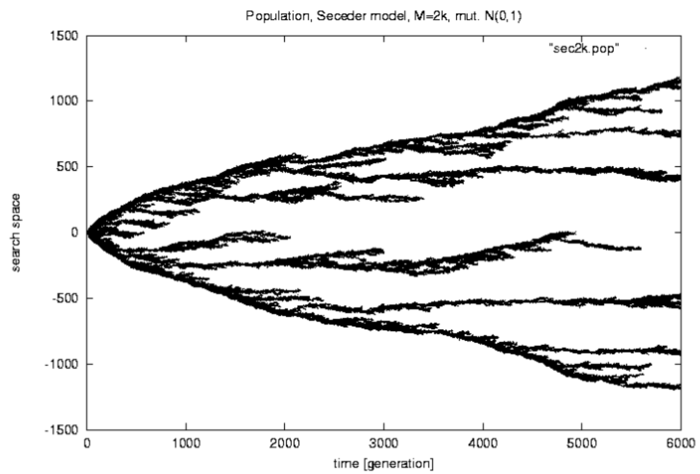
(manuscript in preparation)

6. Emergent Control Examples Studied

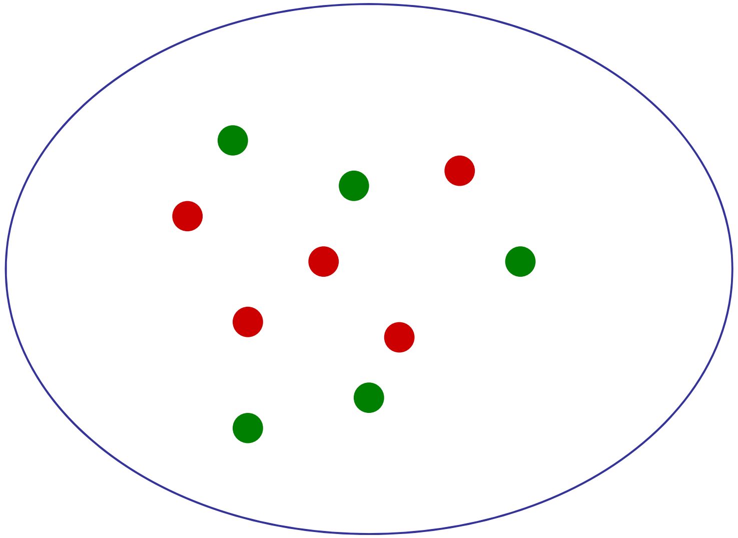
a. Balance the number of particles of two types



b. Control the number of clusters in a population of evolving entities.

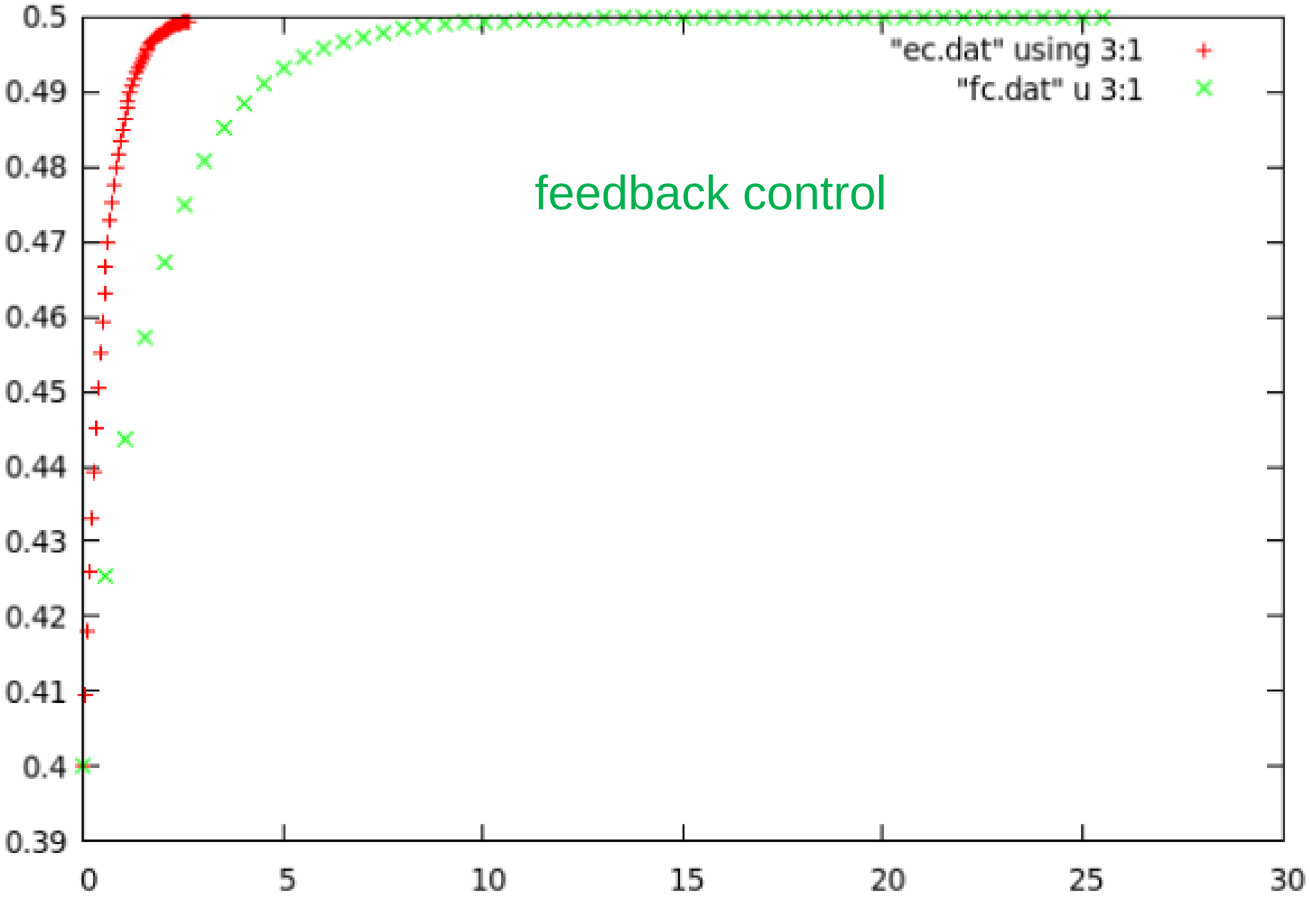


6.A Example: Balance the number of particles of two types



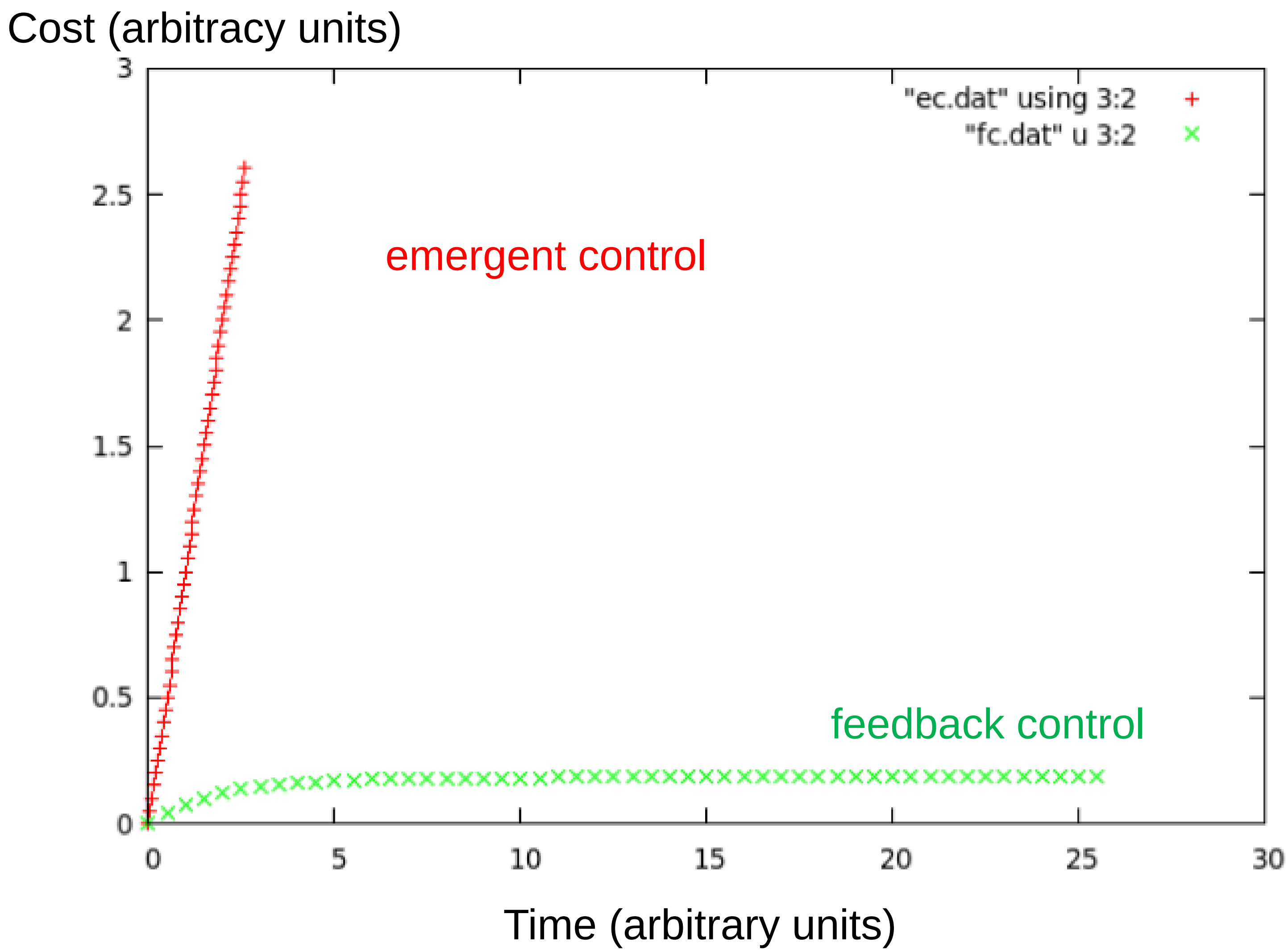
6.A Example: Recovery Time

emergent control



Time (arbitrary units)

6.A Example: Cost



6. Emergent Control Conclusions

- Emergent control is fundamentally different from feedback control.
- In emergent control it is more difficult to consider the user's demands.
  - There are various approaches, but no satisfying (i.e. general enough) macro-to-micro translators yet.
- Emergent control appears to be more costly.
- Macro-level models of the dynamics are not enough for quantitative evaluation.
- ➔ a powerful abstraction of emergent (self-organizing) control is needed.

II. Outlook Phase III

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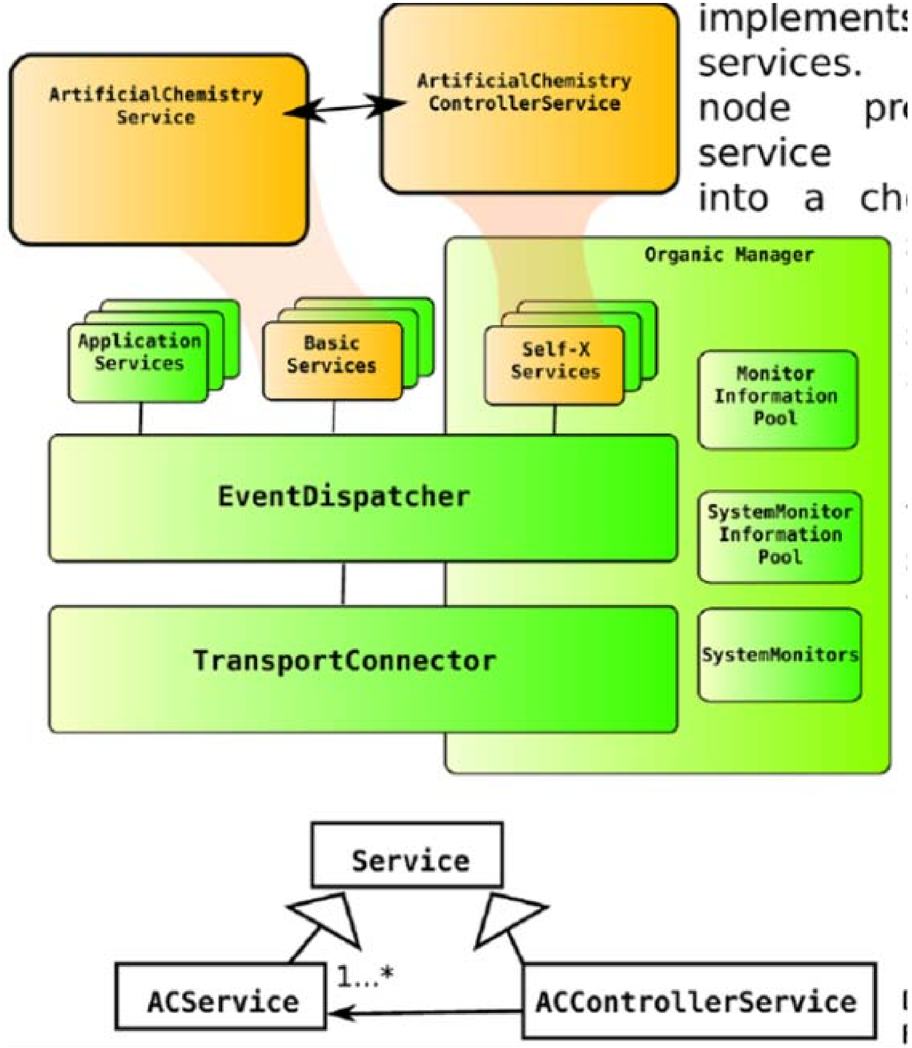
1. Controlled emergent control
2. Structured molecules
3. Application scenarios:
   "chemical" middleware and sensor net

Towards a Chemical Middleware (with Augsburg)



II. Outlook Phase III

1. Controlled emergent control
2. Structured molecules
3. Application scenarios:
   “chemical” middleware and sensor net
4. Bringing European community of
   “chemical-like OC” together.
   → European Mini Workshop (April 2010)
   - very focused, in-silico only
   - How to design/program?
   - Quantitative evaluation?

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