CHEMORG II

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

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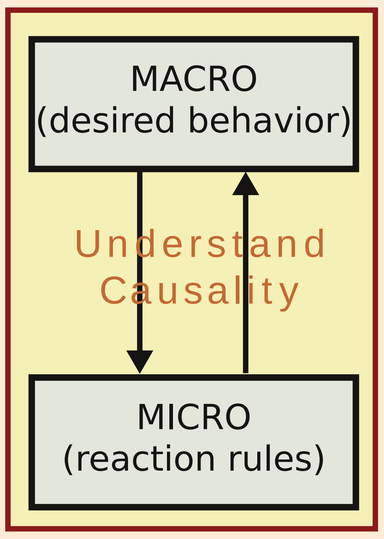
Summary

Employing a large number of entities, it becomes difficult to rationalize the systems' behavior on the global (macro) level, emerging from the interactions on the local (micro) level between entities. There is a gap betwen those two levels, and our fundamental challenges include how to establish the bridge over the gap. In our project, interactions betweem entities are restricted to those describable in the form of chemical reaction rules. In Phase I, we excercised chemical programming [7,10], and organization-oriented programming principles are derived [8]. The maximal independent set problem (MIS) is, then, tackled [1] for evaluating chemical computing quantitatively. We also discussed about an architecture for controlling those emerging behaviors, and components are arranged as a feedforward process. It neccesitates the development of *macro-to-micro translator*.

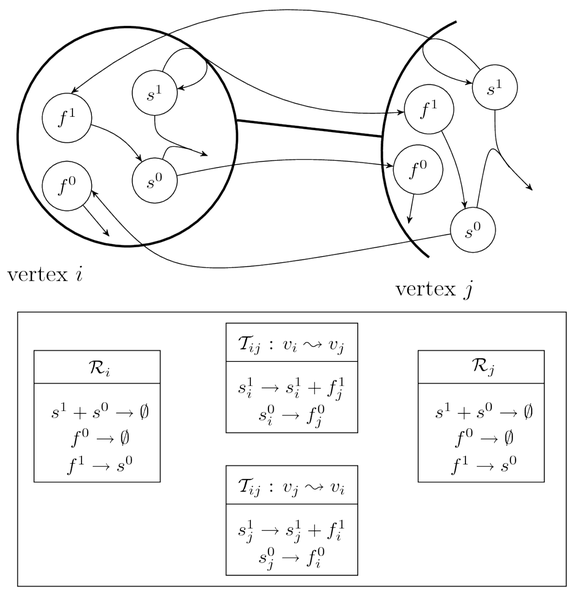


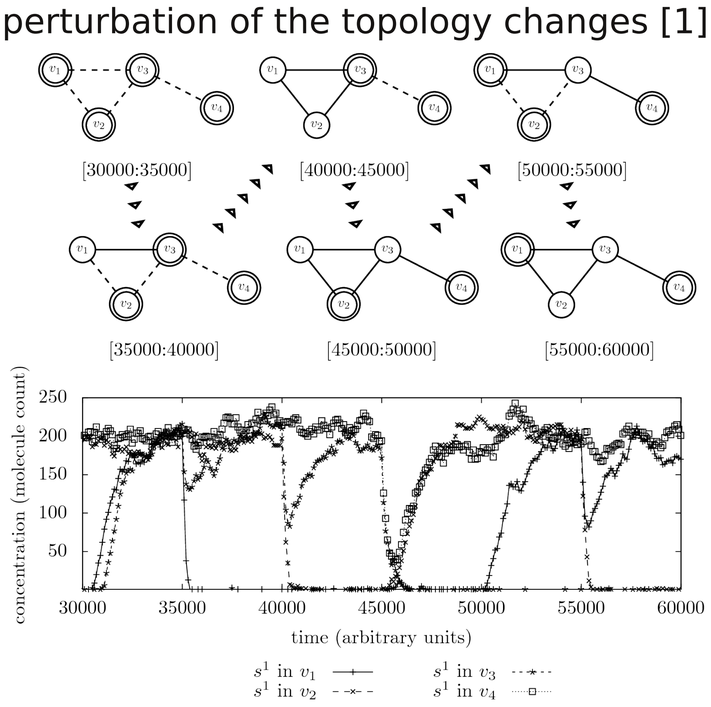
Organization-Oriented Chemical Programming Principles [1,4,8]

P1: There should be one organization for each output behavior class
P2: The result should be in the closure of the input
P3: 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

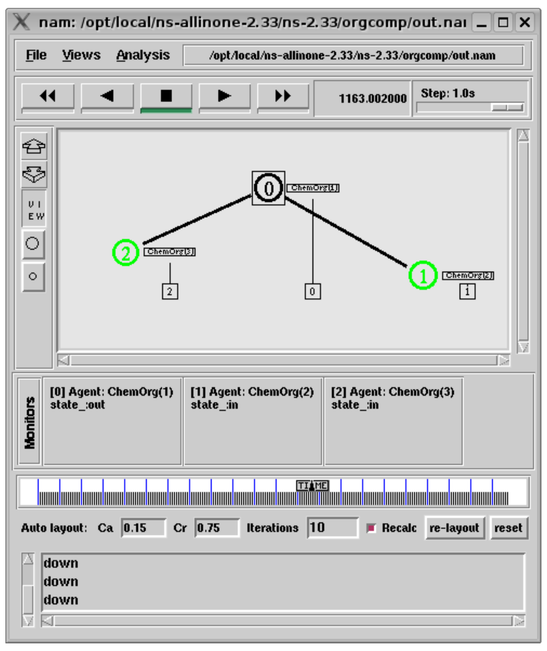
Toward quantitative evaluation

In order to evaluation quantiatively, a scenario of self-organizing and self-repairing phenomena is sketched. Given a graph, each vertex differentiates from the neighbors. This process can be interpretted as the MIS problem. A chemical reaction network is desined for this problem with the help of chemical organization theory. Dynamical simulation study using a software for reaction pathway analysis, *Copasi*, shows the self-organizing processes against perturbation of the topology changes [1].





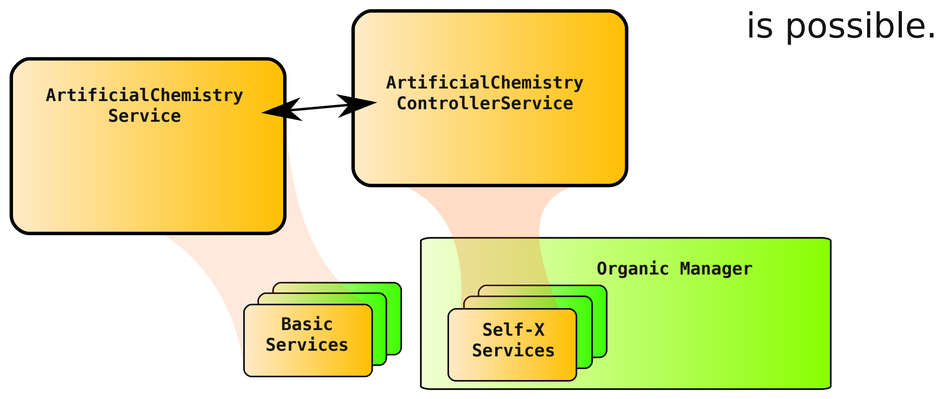
Dynamical behaviors of the graph structure and those of a chemical program for the MIS problem. The dashed lines represent no connection, and double circled vertices indicate the inclusion in the MIS. On dynamically changing topology, the chemical reaction systems compute so that the property of the MIS is always sustained.



The reaction system described above has been implemented on a network simulator ns-2 for quantitative performance evalution. The EmStar was dropped because the simulator is specialized for wireless networking and it is complex to control connection links.

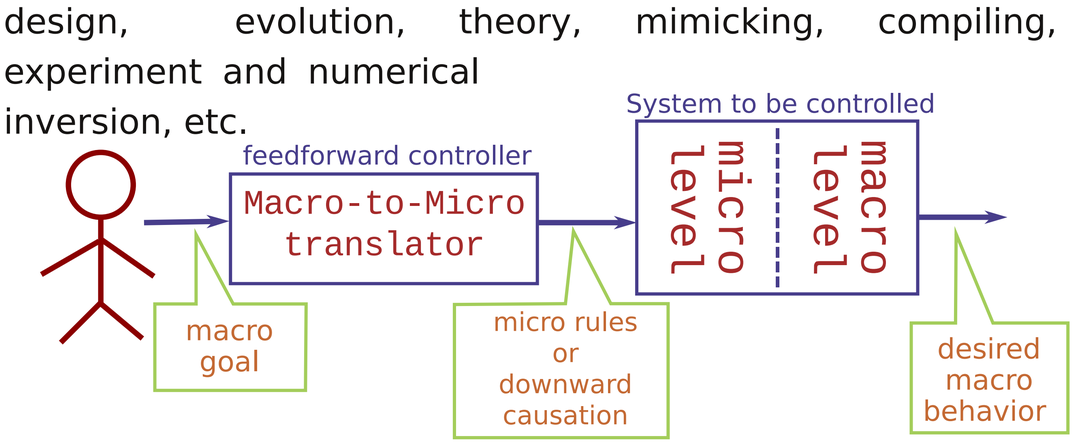
A chemical service for OCμ

In order to achieve self-configure, self-optimize, and self-healing system across a network of nodes, the OCμ framework offers a Java middleware to implement organic services. We have implemented ACservice and ACControllerService providing (artificial) chemical services. Integrations of our chemical programs into OCμ framework is possible.



Emergent Control

We conceived an architecture for controlling emerging behaviors as a feedforward process. The macro-to-micro translator converts users' demand into interactions on the local level. Feedback dynamics can be contained in the controlled system. As an extension, feedback loop can be formed from the controlled system to the controller. However, it should not be necessary for the moment. The development of translator is demanded. Strategies for building a macro-to-micro translator: manual "intelligent" design, evolution, theory, mimicking, compiling, experiment and numerical inversion, etc.



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Primary Results

— Phase II —

1. N. Matsumaru, T. Hinze, P. Dittrich: **Organization-oriented Chemical Programming of Distributed Artifacts**, ***International Journal of Nanotechnology and Molecular Computation*** (submitted)
2. P. Dittrich, L. Winter: **Chemical Organizations in a Toy Model of the Political System**, *Advances in Complex Systems*, 11(04), 609-627, 2008
3. N. Matsumaru, T. Lenser, F. Centler, P. Speroni di Fenizio, T. Hinze, P. Dittrich: **Common Organizational Structures within Two Chemical Flip-Flops**, In *Natural Computing - 3rd International Workshop on Natural Computing*, 2008
4. N. Matsumaru, **Chemical Programming to Exploit Chemical Reaction Systems for Computation**, PhD Dissertation, Friedrich-Schiller-University Jena, Department of Mathematics and Computer Science, 2008
5. C. Kaleta, S. Richter, P. Dittrich: **Using Chemical Organization Theory for Model-Checking**, *Bioinformatics*, 2008 (submitted, under revision)
6. T. Lenser, N. Matsumaru, T. Hinze, P. Dittrich: **Tracking the Evolution of Chemical Computing Networks**, In *Proc. of Alife XI*, 2008

— Phase I —

7. N. Matsumaru, F. Centler, P. Speroni di Fenizio, P. Dittrich: **Chemical Organization Theory as a Theoretical Base for Chemical Computing**, *International Journal of Unconventional Computing*, 3(4), 285-309, 2007
8. P. Dittrich, N. Matsumaru: **Organization-Oriented Chemical Programming**, In *Proc. of 7th International Conference on Hybrid Intelligent Systems*, 2007
9. N. Matsumaru, T. Lenser, T. Hinze, P. Dittrich: **Designing a chemical program using chemical organization theory**, *BMC Systems Biology*, 1(Suppl 1):P26, 2007
10. N. Matsumaru, T. Lenser, T. Hinze, P. Dittrich: **Toward Organization-Oriented Chemical Programming: A Case Study with the Maximal Independent Set Problem**. *Advances in Biologically Inspired Information Systems: Models, Methods, and Tools. Series Studies in Computational Intelligence*, Vol. 69, pp. 147-163, Springer Verlag, 2007
11. N. Matsumaru, P. Dittrich: **Organization-oriented chemical programming for the organic design of distributed computing systems**, In *Proc. of BIONETICS* 2006
12. N. Matsumaru, P. Speroni di Fenizio, F. Centler, P. Dittrich: **On the Evolution of Chemical Organizations**, In: *Proc. 7th German Workshop on Artificial Life*, 2006
13. N. Matsumaru, F. Centler, P. Dittrich: **Chemical Organization Theory as a Theoretical Base for Chemical Computing** In: *Workshop on Unconventional Computing*, p. 71-82, Luniver Press, Beckington.

Secondary Results

— Phase II —

14. B. Ibrahim, S. Diekmann, E. Schmidt, P. Dittrich: **In-Silico Modeling of the Mitotic Spindle Assembly Checkpoint**, *PLoS ONE* 3(2):e1555, 2008
15. F. Centler, C. Kaleta, P. Speroni di Fenizio, P. Dittrich: **Computing Chemical Organizations in Biological Networks**, *Bioinformatics*, 24(14):1611-1618, 2008
16. C. Kaleta, F. Centler, P. Speroni di Fenizio, P. Dittrich: **Phenotype Preiction in Regulated Metabolic Networks**, *BMC Systems Biology*, 2:37, 2008
17. T. Hinze, R. Faßler, T. Lenser, N. Matsumaru, P. Dittrich: **Event-driven Metamorphoses of P Systems**, In *Proc. of 9th Workshop on Membrane Computing*, volume 5391 of LNCS, 209-225, 2008
18. T. Hinze, S. Hayat, T. Lenser, N. Matsumaru, P. Dittrich: **Biosignal-Based Computing by AHL 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

— Phase I —

19. C. Kaleta, F. Centler, P. Dittrich: **Analyzing Molecular Reaction Networks: From Pathways to Chemical Organizations**, *Mol. Biotechnol.*, 34(2):117-123, 2006
20. T. Hinze, S. Hayat, T. Lenser, N. Matsumaru, P. Dittrich: **Hill Kinetics Meets P Systems. In Membrane Computing**, *LNCS* 4860, pp. 320-335, Springer Verlag, 2007
21. T. Hinze, S. Hayat, T. Lenser, N. Matsumaru, P. Dittrich: **Hill Kinetics Meets P Systems: A Case Study on Gene Regulatory Networks as Computing Agents in silico and in vivo**. In *Proc. of the Eight Workshop on Membrane Computing (WMC8)*, pp. 363-381, SEERC Publishers, 2007
22. T. Hinze, R. Fassler, T. Lenser, N. Matsumaru, P. Dittrich: **Effizient chemisch rechnen durch deterministische Reaktionssysteme mit Regelpriorisierung**. In *Proc. 17. Theorietag Automaten und Formale Sprachen*, pp. 68-73, Universität Leipzig, 2007
23. N. Matsumaru, F. Centler, P. Speroni di Fenizio, P. Dittrich: **Chemical organization theory applied to virus dynamics**, *it - Information Technology*, 48(3), 154-160, 2006
24. F. Centler, P. Speroni di Fenizio, N. Matsumaru, P. Dittrich: **Chemical organizations in the central sugar metabolism of Escherichia Coli In *Mathematical Modeling of Biological Systems***, Volume I. A Birkhäuser book, 2007
25. N. Matsumaru, P. Speroni di Fenizio, F. Centler, P. Dittrich: **A Case Study of Chemical Organization Theory Applied to Virus Dynamics**, in *Systems Biology Workshop at ECAL 2005, Workshop Proceedings* CD-ROM, 2005