BiRC Seminar – open to all

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Title: *Generative Chemistries - Graph Grammars, Chemical Motifs, and the Black Tar of Hydrogen Cyanide Polymers*

Time: Friday 8 March, 2013, 14:15 - 15:00

Place: Bioinformatics Research Centre (BiRC), Building 1110, Aud. 223, C. F. Møllers Allé 8, 8000 Aarhus C

Abstract:
We use labeled undirected graphs to model molecules and transformation rules in the Double Pushout formalism to model chemical reactions. A set of starting graphs and transformation rules, a graph grammar, implicitly defines a directed hypergraph with derivable graphs as vertices and the individual derivations as directed hyperedges. Within these iteratively generated hypergraphs (reaction networks) we find chemical reaction patterns with maximal outflow or specific pathway motifs like autocatalysis. We solve these NP-complete problems by Integer Linear Programming approaches.

Our Generative Chemistry framework is used in order to analyze a wide range of processes, including the Formose reaction, the Pentose Phosphate pathway, and the Citric Acid Cycle. Furthermore, we analyze the chemical system of polymerized hydrogen cyanide and its hydrolysis products, which constitute a plausible, but still poorly understood proposal for early prebiotic chemistry on Earth. Our goal is to demonstrate that a systematic exploration of complex chemical spaces is possible, despite the combinatorial explosions associated with such an endeavor. We demonstrate that experimental data, here obtained by mass spectroscopy, can be used to guide the exploration of the chemical space and makes it feasible to investigate likely pathways and chemical motifs even in potentially open-ended chemical systems.

After the seminar there will be beer/soda/coffee and chips in the coffee room on the 4th floor.

http://birc.au.dk/activities/seminar-series/

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