DEPARTMENT OF MATHEMATICS AND COMPUTER SCIENCE
UNIVERSITY OF SOUTHERN DENMARK, ODENSE

COMPUTER SCIENCE COLLOQUIUM

PhD colloqium: Analysis of Generative Chemistries – Graph Grammars, Hyperflows and Composition of Rules

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IMADA's Seminar Room

Abstract:

We use labelled 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 direct derivations as directed hyperedges. On these hypergraphs (reaction networks) we define a hyperflow model in order to find interesting chemical pathways and specific pathway motifs, e.g., autocatalysis.

For exploring graph grammars directly we define a type of composition of transformation rules. This is used to infer higher level rules which represent chemical properties. We also present a general strategy framework for (chemical) graph transformation based on rule composition.

Host: