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Dynamically equivalent reaction networks: a computational point of view

It has been known from the 'fundamental dogma of chemical kinetics' that different mass action type reaction networks can give rise to the same ordinary differential equations describing the time evolution of specie concentrations. Finding dynamically equivalent network structures with preferred properties can significantly enhance the application range of the known and continuously developing strong results on the relation between network structure and qualitative dynamical properties (deficiency theorems, structural conditions on the possibility of multiple steady states, Global Attractor and Persistency Conjectures etc.). It is also known primarily from systems and control theory that the numerical feasibility of many existence and design problems can often be checked via appropriately formulated optimization tasks even if the original problem is algebraically complex to treat. In this talk, an overview of linear programming (LP) and mixed integer linear programming (MILP) techniques will be given for the computation of reaction networks with prescribed properties. This includes the computation of structures with the minimal/maximal number of reactions/complexes, detailed/complex balanced, and fully/weakly reversible realizations.