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Dynamics-preserving model reduction using bipartite-graph representations of biochemical systems

At a fundamental level, biochemical systems can be represented as sets of elementary reactions. These mechanistic descriptions can in turn be represented as bipartite graphs, with one vertex type representing chemical species, and the other chemical reactions. Specially constructed subsets of the bipartite graph known as fragments have a one-to-one correspondence with terms in the characteristic equation arising in stability analysis, whether for ODEs representing a well-mixed system, or for reaction-diffusion PDEs. Accordingly, there is a connection between the structure of the bipartite graph and stability. Specifically, critical fragments, those corresponding to terms in the characteristic equation with negative coefficients, are necessary to allow for Andronov-Hopf, saddle-node, or Turing bifurcations. Because biochemical networks are typically very large, it is often desirable to simplify the corresponding models. This talk will explore an idea for using the bipartite-graph representation of a biochemical network to reduce a biochemical model while preserving its dynamics, by carrying out graph transformations that preserve critical fragments.