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Reaction Simulations: A Rapid Development Framework

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Reaction Simulations: A Rapid Development Framework

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Chemical Reaction Networks (CRNs) are a popular tool in the chemical sciences for providing a means of analyzing and modeling complex reaction systems. In recent years, CRNs have attracted attention in the field of molecular computing for their ability to simulate the components of a digital computer. The reactions within such networks may occur at several different scales relative to one another – at rates often too difficult to directly measure and analyze in a laboratory setting. To facilitate the construction and analysis of such networks, we propose a reduced order model for simulating such networks as a system of Differential Algebraic Equations (DAEs). Beginning from the continuous stirred-tank reactor ODE system model, we perform a change of basis on the system in which we may model the fast reactions as infinite, also accounting for their different scales of reaction relative to one another. The resulting DAE system consists of a set of implicit ODEs coupled with a set of algebraic constraints. We conclude by demonstrating our model on several sample networks.