Model Reduction for Chemical Reaction Networks: It's a Subtle Business!

Linda R. Petzold
Computer Science Department, University of California Santa Barbara, Santa Barbara, CA 93106, USA

REDUCED models, where a set of chemical reactions is replaced by a single reaction are often used in the simulation of deterministic chemical kinetics. Examples of such abridgements include Michaelis-Menten and Hill approximations. But how accurate are these approximations, in the context of discrete stochastic simulation? We examine the benefits and liabilities of replacing the simple three-reaction set $S_1 f S_2 \rightarrow S_3$ with a single S_3-producing reaction. We develop a novel criterion for deciding whether such an approximation can be accomplished in a way that accurately replicates the production of S_3 molecules, and we derive a formula for estimating the consequent speedup in stochastic simulation. We show that in all cases in which such an abridgment can be done accurately and with a significant gain in simulation speed, a procedure called the slow-scale stochastic simulation algorithm provides a robust and theoretically transparent way of implementing the abridgment.