Towards the Multiscale Simulation of Biochemical Networks

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In microscopic systems formed by living cells, small numbers of reactant molecules can result in dynamical behavior that is discrete and stochastic rather than continuous and deterministic. In simulating and analyzing such behavior it is essential to employ methods that directly take into account the underlying discrete stochastic nature of the molecular events. This leads to an accurate description of the system that in many important cases is impossible to obtain through deterministic continuous modeling (e.g. ODE's). Gillespie's Stochastic Simulation Algorithm (SSA) has been widely used to treat these problems. However as a procedure that simulates every reaction event, it is prohibitively inefficient for most realistic problems.

We report on our progress in developing a multiscale computational framework for the numerical simulation of chemically reacting systems, where each reaction will be treated at the appropriate scale. The framework is based on a sequence of approximations ranging from SSA at the smallest scale, through a "birth-death" Markov process approximation, Gillespie's recently-developed tau-leaping approximation, a continuous stochastic differential equation (SDE) approximation, and finally to the familiar reaction rate equations (ODE's) at the coarsest scales.