

309h An Equation-Free Probabilistic Steady State Approximation: Dynamic Application to the Stochastic Simulation of Chemically Reacting Systems

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'Small' systems of chemical or biochemical reactions typically require a mesoscopic mathematical representation, such as a jump Markov process. Kinetic Monte Carlo, also known as stochastic simulation, is a numerical method for generating trajectories of a jump Markov process. However, the computational cost of these simulations scale with the number of occurrences of reaction or diffusion events in the system. We present an equation-free probabilistic steady state approximation that speeds up the simulation of jump Markov processes which contain a separation in timescales. The method partitions the system into subsets of fast/discrete and slow/discrete reactions; detects the convergence of the unknown distribution to a stable quasi steady state; samples from the underlying distribution; and uses those samples to compute the waiting time of the next slow/discrete reaction and the state of the system at that time. The method is equation-free because the steady state distribution is not computed via the Master equation or any differential equation. Instead, by sampling directly from the unknown distribution, we only assume the quasi steady state distribution is ergodic. We present multiple examples and demonstrate the accuracy and efficiency of the proposed method. The presented ideas apply to both homogeneous and heterogeneous systems, but, for simplicity, we will focus on homogeneous ones.