Abstract:

Stochastic simulation is widely used for chemical dynamics at the cellular level, where fluctuations in the small populations of key chemical species can have a large influence on system behavior. The Stochastic Simulation Algorithm (SSA) is widely used for simulation of spatially homogeneous systems. For spatially inhomogeneous systems, the spatial domain is discretized into small subvolumes. Reactions take place within each subvolume, and diffusion events between adjacent subvolumes are treated as first order reactions.

Generally speaking the reaction and diffusion processes are coupled. To accelerate the simulation it is convenient to split the two processes and simulate them separately. However, the splitting of the reaction and diffusion operators introduces a substantial error. We propose a new algorithm that uses the time dependent propensity function for the simulation, which takes into account the effect from the diffusion process. The new algorithm inherits the computational efficiency of operator splitting, while maintaining a high accuracy.