Accelerated Algorithms for Discrete Stochastic Simulation of Reaction-Diffusion Systems

Wonryull Koh  
School of Computing  
University of Southern Mississippi

Abstract: Stochastic simulation of a reaction-diffusion system enables computational investigation of the system’s spatiotemporal activity and stochastic variations within, where experimental investigation can be difficult. Although an exact stochastic simulation that simulates every individual reaction and diffusion event gives the most accurate trajectory of the system’s state over time, it can be too slow for many practical applications. We present algorithms for accelerated stochastic simulation of biochemical reaction-diffusion systems. We present numerical results that illustrate the improvement in simulation speed achieved by our algorithms. We discuss strategies to facilitate adjusting the balance between the degree of exactness in simulation and the simulation speed.

Biography: Dr. Koh received her PhD in Computer Science from Texas A&M University under the direction of Dr. Bruce McCormick, where she worked on neuroinformatics tools for neuroanatomical structures. She then did a Postdoctoral Fellowship with Dr. Avrama Blackwell at George Mason University, where she developed algorithms and tools for stochastic simulations of neuroscience models. Currently Dr. Koh is an Assistant Professor of Computer Science at the University of Southern Mississippi.