6d Multiscale Methods for Stochastic Simulation

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Kinetic Monte Carlo (KMC) simulations have emerged in the past few decades as one of the preeminent computational tools for science and engineering research, in diverse problems ranging from materials growth, to catalysis, to DNA/surface interactions, to image processing, and to modeling of metabolic pathways for biochemical engineering and bio-informatics. Despite their widespread use, KMC simulations are limited to short length and time scales, while device sizes and morphological features in experiments often involve much larger spatial and temporal scales.

In this talk various stochastic methods will be discussed. These methods will range from the exact stochastic simulation method for spatially homogeneous and distributed systems, to coarse-grained and approximate stochastic methods, to the chemical Langevin equation. The connections between the various methods will be highlighted. Finally, the need for stochastic simulation will be illustrated with examples from systems biology, nanoscopic systems, and interacting systems found in catalysis and crystal growth.