Title:
Parallel kinetic Monte Carlo simulations: algorithms and numerical analysis

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Abstract:
We present a class of algorithms that approximate underlying Markov jump process in lattice simulations of reaction-diffusion processes. The approximation is based on fractional-time step scheme for the Markov semi-group yielding different approximation schemes and processor communication schedules, including randomized schedules. We discuss error analysis and efficiency of the schemes and present examples of implementation on multi-core architectures and GPUs. Applications include models of reaction kinetics and diffusion processes in catalysis.