Katsoulakis, Markos A.; **Majda, Andrew J.**; **Vlachos, Dionisios G.**

Coarse-grained stochastic processes and Monte Carlo simulations in lattice systems. (English)

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J. Comput. Phys. 186, No. 1, 250-278 (2003).

Summary: In this paper we present a new class of coarse-grained stochastic processes and Monte Carlo simulations, derived directly from microscopic lattice systems and describing mesoscopic length scales. As our primary example, we mainly focus on a microscopic spin-flip model for the adsorption and desorption of molecules between a surface adjacent to a gas phase, although a similar analysis carries over to other processes. The new model can capture large scale structures, while retaining microscopic information on intermolecular forces and particle fluctuations. The requirement of detailed balance is utilized as a systematic design principle to guarantee correct noise fluctuations for the coarse-grained model. We carry out a rigorous asymptotic analysis of the new system using techniques from large deviations and present detailed numerical comparisons of coarse-grained and microscopic Monte Carlo simulations. The coarse-grained stochastic algorithms provide large computational savings without increasing programming complexity or the CPU time per executed event compared to microscopic Monte Carlo simulations.

MSC:

82C80 Numerical methods of time-dependent statistical mechanics (MSC2010)
65C05 Monte Carlo methods
65C35 Stochastic particle methods
60K35 Interacting random processes; statistical mechanics type models; percolation theory

Cited in **2** Reviews
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Keywords:

Hierarchy of Monte Carlo algorithms; Coarse-grained processes and; coarse-grained Monte Carlo simulations; Birth-death processes; Detailed balance; Large deviations

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