THE UNIVERSITY OF CHICAGO

Departments of Computer Science, Mathematics, and Statistics

SCIENTIFIC AND STATISTICAL COMPUTING SEMINAR

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Multilevel Approximations and Parametrization of Coarse-grained Dynamics in KMC Simulations

THURSDAY, January 31, 2013, at 4:30 PM

Eckhart 133, 5734 S. University Avenue

ABSTRACT

We discuss a hierarchy of approximation methods developed for accelerating sampling of microscopic dynamics in stochastic lattice systems. The approach is based on efficient coupling of different resolution levels, taking advantage of the low sampling cost in a coarse space and local reconstructions. We provide error estimates for (a) long-time stationary dynamics in terms of relative entropy, and (b) finite-time weak error estimates that control mesoscale observables. We present information-theoretic approach to parameterisation of coarse-grained dynamics defined as continuous time Markov chains. Rates of the coarse-grained process are parametrized and optimal parameters are selected by minimization of the relative entropy on the path space. This approach extends techniques also known as inverse Monte Carlo to models with *non-equilibrium stationary states*, for example systems driven by external parameters or reaction-diffusion systems in catalysis.

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