Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

A Local Superbasin Kinetic Monte Carlo Method[1] KRISTEN FICHTHORN, YANGZHENG LIN, Penn State University — A ubiquitous problem in atomic-scale simulation of materials is the small-barrier problem, in which the free-energy landscape presents "superbasins" with low intra-basin energy barriers relative to the inter-basin barriers. Rare-event simulation methods, such as kinetic Monte Carlo (KMC) and accelerated molecular dynamics, are inefficient for such systems because considerable effort is spent simulating short-time, intra-basin motion without evolving the system significantly. We developed an adaptive local-superbasin KMC algorithm (LSKMC) for treating fast, intra-basin motion using a Master-equation / Markov-chain approach and long-time evolution using KMC. Our algorithm is designed to identify local superbasins in an on-the-fly search during conventional KMC, construct the rate matrix, compute the mean exit time and its distribution, obtain the probability to exit to each of the superbasin border (absorbing) states, and integrate superbasin exits with non-superbasin moves. We demonstrate various aspects of the method in several examples, which also highlight the efficiency of the method.

[1]Supported by NSF DMR-1006452

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Date submitted: 11 Dec 2012 Electronic form version 1.4