Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Reaching extended length-scales with temperature-accelerated dynamics[1] JACQUES G. AMAR, YUNSIC SHIM, University of Toledo — In temperature-accelerated dynamics (TAD) a high-temperature molecular dynamics (MD) simulation is used to accelerate the search for the next low-temperature activated event. While TAD has been quite successful in extending the time-scales of simulations of non-equilibrium processes, due to the fact that the computational work scales approximately as the cube of the number of atoms, until recently only simulations of relatively small systems have been carried out. Recently, we have shown that by combining spatial decomposition with our synchronous sublattice algorithm, significantly improved scaling is possible. However, in this approach the size of activated events is limited by the processor size while the dynamics is not exact. Here we discuss progress in developing an alternate approach in which high-temperature parallel MD along with localized saddle-point (LSAD) calculations, are used to carry out TAD simulations without restricting the size of activated events while keeping the dynamics "exact" within the context of harmonic transition-state theory. In tests of our LSAD method applied to Ag/Ag(100) annealing and Cu/Cu(100) growth simulations we find significantly improved scaling of TAD, while maintaining a negligibly small error in the energy barriers.

[1]Supported by NSF DMR-0907399.

Jacques G. Amar
University of Toledo

Date submitted: 11 Dec 2012 Electronic form version 1.4