Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Reaching extended length-scales with accelerated dynamics[1] BRADLEY HUBARTT, YUNSIC SHIM, JACQUES AMAR, University of Toledo — While temperature-accelerated dynamics (TAD) has been quite successful in extending the time-scales for non-equilibrium simulations of small systems, the computational time increases rapidly with system size. One possible solution to this problem, which we refer to as parTAD[1] is to use spatial decomposition combined with our previously developed semi-rigorous synchronous sublattice algorithm[2]. However, while such an approach leads to significantly better scaling as a function of system-size, it also artificially limits the size of activated events and is not completely rigorous. Here we discuss progress we have made in developing an alternative approach in which localized saddle-point searches are combined with parallel GPU-based molecular dynamics in order to improve the scaling behavior. By using this method, along with the use of an adaptive method to determine the optimal high-temperature[3], we have been able to significantly increase the range of time- and length-scales over which accelerated dynamics simulations may be carried out. [1] Y. Shim et al, Phys. Rev. B **76**, 205439 (2007); ibid, Phys. Rev. Lett. **101**, 116101 (2008). [2] Y. Shim and J.G. Amar, Phys. Rev. B **71**, 125432 (2005). [3] Y. Shim and J.G. Amar, J. Chem. Phys. 134, 054127 (2011).

[1]Supported by NSF-DMR 0907399

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Date submitted: 11 Nov 2011 Electronic form version 1.4