Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

GPU accelerated replica-exchange simulations of polymers
JONATHAN GROSS, MICHAEL BACHMANN, Center for Simulational Physics, University of Georgia, Athens, Georgia 30602, USA — Precise estimation of physical quantities using Monte Carlo computer simulations strongly depends on the amount of statistical data gathered during the simulation. Being able to increase the performance of the sampling process will allow more accurate results in a shorter time period. To employ the parallel tempering replica-exchange algorithm on parallel hardware such as multicore CPUs and GPUs turns out to be very suitable for the task. We achieve rapid speedups in our investigation of an exemplified bead-spring polymer model. Identification and classification of phase-like transitions were done by analyzing the microcanonical entropy.

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Date submitted: 26 Nov 2011 Electronic form version 1.4