Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Improved Wang-Landau algorithm for the joint density of states of continuous models CHENGGANG ZHOU, Computer Science and Mathematics Div., Oak Ridge Natl. Lab., T.C. SCHULTHESS, D.P. LANDAU, Center for Simulational Physics, Univ. of Georgia, Athens, GA 30602 — The joint density of states of a statistical physical system is the key to calculating thermodynamic observables at all temperatures and external fields. For example, $\rho(M,\ E)$ of a Heisenberg ferromagnet is a generalization of $\rho(E)$, from which magnetization and susceptibility at all temperatures can be obtained. A well-known method to calculate $\rho(E)$ is the Wang-Landau algorithm [1], which can be in principle extended to the joint density of states. Unfortunately, a straightforward application of the Wang-Landau algorithm to this type of problem turns out to be inefficient. We thus adopt a number of strategies to accelerate the simulation and to increase the performance of the algorithm in low-density regimes. In particular, we replace the conventional binning scheme with kernel density estimation, so that the algorithm is intrinsically suitable for continuous systems. This version of the Wang-Landau algorithm is also generally applicable to classical statistical physics models, including discrete models with large size. We also discuss other promising applications to magnetic nano-particles and in biophysics. [1] F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001). *This research is supported by the Department of Energy through the Laboratory Technology Research Program of OASCR and the Computational Materials Science Network of BES under Contract No. DE-AC05-00OR22725 with UT-Battelle LLC, and by NSF DMR-0341874.

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Date submitted: 06 Dec 2004 Electronic form version 1.4