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NEW HYBRID MONTE CARLO METHODS FOR EFFICIENT SAMPLING: FROM PHYSICS TO BIOLOGY AND STATISTICS

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ABSTRACT

We will introduce a new class of hybrid methods designed to make feasible efficient and detailed simulation of large and complex systems and which can be used in a wide range of applications in physics, biology, materials science and statistics.

The methods, that we have called Generalized Shadow Hybrid Monte Carlo (GSHMC) methods, combine the best features of stochastic and deterministic simulation techniques. The GSHMC methods make use of multi-scale nature of complex systems and employ modified Hamiltonians [1 -3] in order to overcome exponential performance degradation with the system size.

The GSHMCs have been adapted to three simulation methodologies: atomistic simulation, particle simulation and Bayesian computation. This led to the development of three different types of GSHMC methods: (1) GSHMC (a thermodynamically consistent implementation of constant-temperature molecular dynamics); (2) meso-GSHMC (a Metropolis corrected dissipative particle dynamics method) and (3) Generalized shadow Hamiltonian Monte Carlo, GSHmMC (a Hamiltonian Monte Carlo approach which relies on modified Hamiltonians in the Metropolis test).

All above methods provide efficient sampling, remove drawbacks of their predecessors [3, 4] and are, due to their flexibility, easily combined with other enhanced sampling techniques. In addition, the methods are suitable for massively parallel computing and allow for a range of multi-level parallel strategies.

We shall highlight the ideas behind the GSHMC methods and discuss their implementation for different physical and biological applications on high performance computers. The effectiveness of GSHMC methods will be demonstrated through their comparison with multiple time stepping Langevin Dynamics (MTS LD), dissipative particle dynamics (DPD) and Hamiltonian Monte Carlo (HMC). More specifically, it will be shown that the GSHMC methods not only overcome well-known deficits of commonly used sampling techniques, e.g., resonance instabilities in MTS techniques or a non-preservation of thermodynamic equilibrium properties in DPD (**Fig. 1**), but also outperform such methods in sampling efficiency by an order of magnitude.

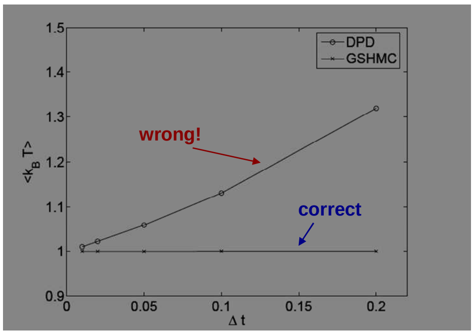

Figure 1. GSHMC exactly reproduce the target temperature while the DPD method leads to a nearly linear increase in the numerically observed temperature with respect to the step-size.