Pushing the timestep limit of molecular dynamics with hamiltonian monte carlo

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The quantitative accuracy of molecular dynamics simulations is limited by timestep discretization error. This error can be eliminated by the use of metropolization, e.g. hamiltonian monte carlo. This rigorous approach has been largely unused by the molecular simulation community for reasons of interpretation and computational efficiency. Herein we combine multi-timestep integration, GPU accelerated molecular dynamics, and hamiltonian monte carlo to provide substantial speed improvements. Furthermore, the guaranteed thermodynamic fidelity provided by hamiltonian monte carlo enables the treatment of sampling as a blackbox optimization problem with little human intervention.

Keywords: molecular dynamics

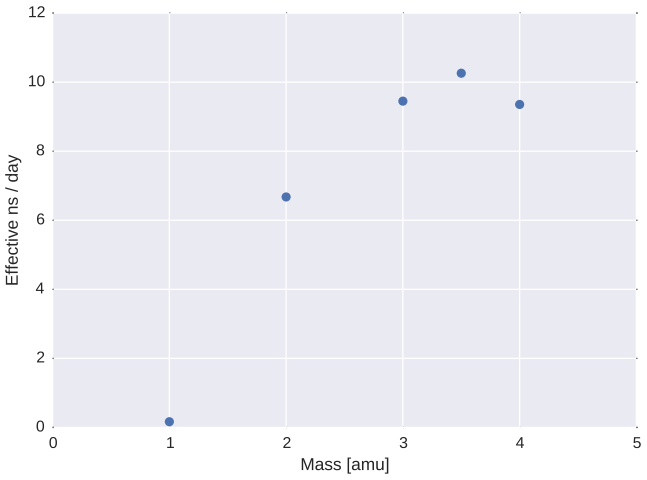

FIG. 1. HMR MASSES. HMR MASSES

I. INTRODUCTION

Molecular

II. THEORY

A. Quantifying Performance and Sampling

Quantifying sampling performance requires consideration of several distinct elements. The main objective is to draw uncorrelated samples from some target distribution $P(x)$.

1. Effective step size: $p_{accept} * \Delta t$ 2. Effective nanoseconds (simulation) per day (wall clock) 3. Effective sample size / ineffefiency

III. RESULTS

A. Hydrogen Mass Repartitioning

B. Choice of steps per HMC iteration

C. Multiple Timestep GHMC: MTSGHMC

D. Alanine Populations and escape times

E. XCGHMC and XCMTSGHMC

IV. CONCLUSIONS

Density

V. ACKNOWLEDGEMENTS

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