GPU Monte Carlo Developments: Biased Gibbs Ensemble Alkane Simulations and Architectural Optimizations

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Introduction

Invented in 1986, Gibbs ensemble [1] has provided a versatile tool for the study of equilibria properties, including adsorption and phase coexistence. Molecular dynamics studies have demonstrated graphics processing units (GPU) to be ideal computing devices for chemical systems [2-4]. Preliminary work to parallelize MC codes has been published for canonical [5], and grand canonical Monte Carlo systems [6]. Last year the authors demonstrated a fast GPU-driven simulation engine capable of performing Gibbs ensemble simulations on Lennard-Jonesium [7-8]. In this work configurational bias Monte Carlo simulations of Lennard-Jonesium and alkane molecules in the Gibbs ensemble is presented, along with a discussion of using energetic lookup tables and floating point precision coordinates to optimize device performance.

Methodology

A series of Gibbs ensemble simulations was performed. The TraPPE united atom forcefield [9] was used to describe methane molecules as single beads, while ethane, propane, and butane were described as multi-bead molecules. The particles are biased with a standard biasing [10] via calculation of \(k\) trial segments in the insertion box:

\[
p_i(t) = \frac{e^{-\Delta F_i(t)}}{w_i(t)}
\]

\[
w_i(t) = \sum_{j=0}^{\infty} e^{-\Delta F_i(j)}
\]

\[
W(t) = \prod_{i=1}^{n} w_i(t)
\]

Initial trial locations are chosen randomly from the target box, second positions are constrained to a unit sphere of bond-length, and the remaining trial segments are selected in a fashion biased by the strong intramolecular forces.

Serial simulations were run on Intel® Core™ i7 Sandy Bridge (Broadwell, Ivy Bridge) systems with 8 GB of memory. For the GPU simulations, the system's NVIDIA® GeForce® GTX 460, GTX 480, GTX 560 (Fermi), or GTX 660 (Kepler) by EVGA was also used.

Conclusions

Traditional CBMC techniques for systems of united atom alkanes have been ported to the graphics processing unit and show large preliminary speed gains. Optimization work is under way testing various device acceleration strategies, including the use of texture memory lookup tables, switching the coordinates to floating point values, and the use of neighbor lists. Further work will be done to improve selection of biasing algorithms and to combine the studied methods to produce a maximum acceleration of molecular CBMC simulations in the Gibbs ensemble.

References


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