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:

(1) $p_i(n) = \frac{e^{-\beta u_i(j)}}{w_i(n)}$ (2) $w_i(n) = \sum_{j=0}^{n} e^{-\beta u_i(j)}$ (3) $\mathrm{W}(n) = \prod_{i=1}^{l} w_i(n)$

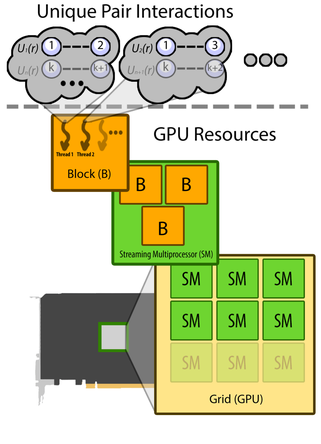
(4) $w_i(o) = e^{-\beta u_i(o)} + \sum_{j=0}^{n} e^{-\beta u_i(j)}$ (5) $\mathrm{W}(o) = \prod_{i=1}^{l} w_i(o)$

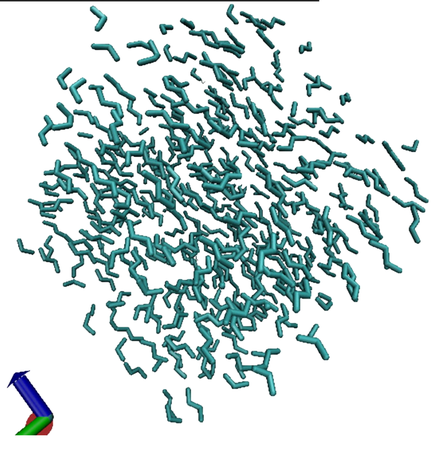
Initial trial locations are chosen randomly from the target box, second positions are constrained to a unit sphere of bond-length, and the remaining trial segments are selected in a fashion biased by the strong intramolecular forces.

Serial simulations were run on Intel(R) Core™ i5 (*Sandy Bridge*), Q6600 (*Penryn*), or Core-i7 (*Nehalem*, Ivy *Bridge*) systems with 8 GB of memory. For the GPU simulations, the system's NVIDIA(R) GeForce™ GTX 460, GTX 480, GTX 560 (*Fermi*), or GTX 660 (*Kepler*) by EVGA was also used.

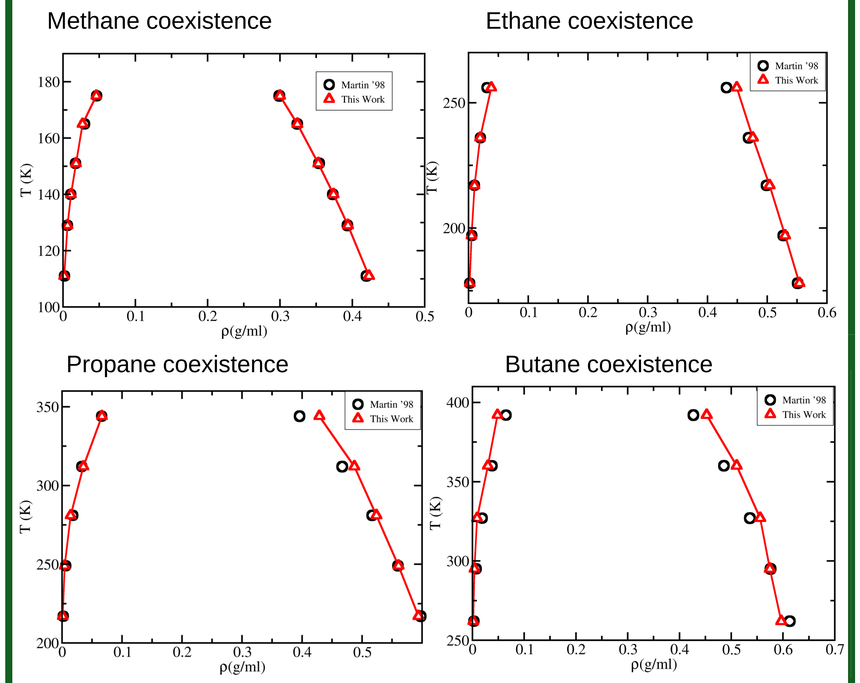
[Image Sources: *Ubergizmo*]

Applying the "Farm Algorithm" to Molecules on the GPU

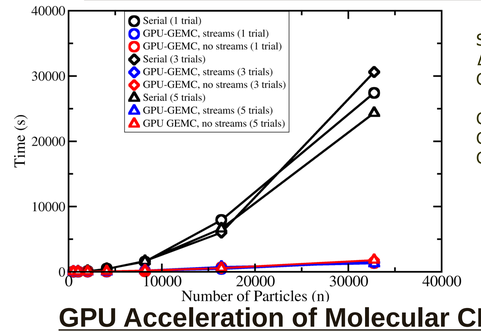




Validation of the GPU (CUDA) Code [9]



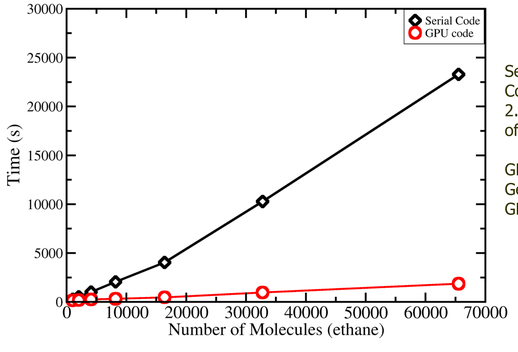
GPU Acceleration of Particle CB GEMC



Serial simulations run on *Ivy Bridge* Intel® Core™ i7-3770K CPU @ 3.5 GHz

GPU tests run on NVIDIA® GeForce™ GTX 660 with 2 GB of GDDR5 VRAM

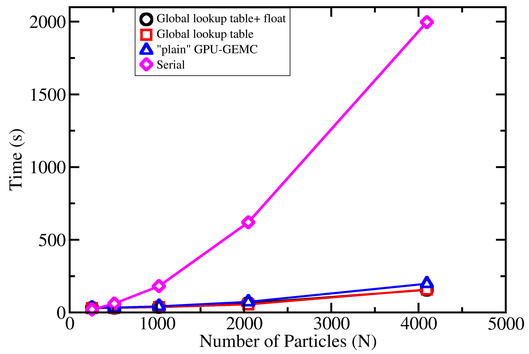
GPU Acceleration of Molecular CB GEMC



Serial simulations run on Intel® Core™ i7-870 CPU (*Nehalem*) @ 2.93 GHz. This system had 12 GB of DRAM.

GPU tests run on NVIDIA® GeForce™ GTX 460 with 1 GB of GDDR5 VRAM

Effects of Floating Point v. Double Performance on the GPU and Energetic Lookup Table



Run time was 1M MCS per trial.

Statistics were gathered from 3 trials.

Max. speedup for "plain" GPU CBMC was 10.09x for a system of 8192 particles.

With the lookup table in global memory, a max speedup of 12.64x was obtained.

Finally, by switching from double coordinates to float, a speedup of 12.85 was reached.

GPU tests were run on a GTX 480, serial tests were run on a Intel core i7 chip (*Sandy Bridge*)

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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