Accelerating Simulations In the Gibbs and Canonical Ensembles with GPUs

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Introduction

Monte Carlo (MC) simulations [1] have been employed since the 1950s to determine thermodynamic data for simple model systems as well as complex force fields designed to reproduce the physical properties of specific compounds. Molecular Dynamics (MD has benefited greatly from the parallel computing revolution and many simulation engines [2-3] have added support for graphics processing units – powerful multi-core data processing devices. One MD engine – HOOMD – was even written from scratch for optimal GPU performance [4]. To date, MC codes have only been published for Ising lattice [5] and hard sphere simulations [6]. In this work, we introduce a fast, GPU-optimized code capable of simulations of a Lennard-Jones fluid in the canonical (NVT) and Gibbs ensembles [7].

Methodology

A series of simulations were run in canonical and Gibbs ensembles. All of these simulations utilized the ubiquitous Lennard-Jones potential [8]:

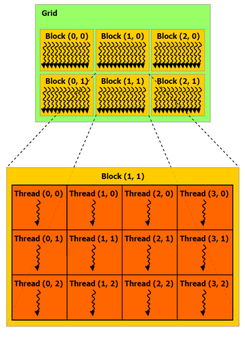
$$u(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

Simulations were performed for both truncated and long-range corrected potentials. These tail corrections utilize the assumption of a homogenous fluid and are defined as follows:

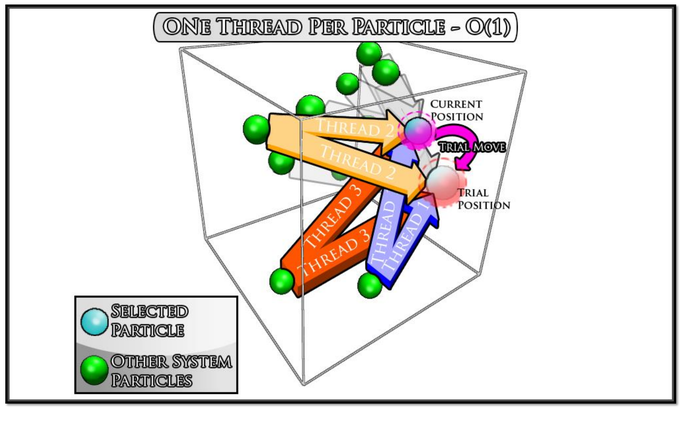
$$U^*(r_c) = \frac{8}{9}\pi\rho^*\epsilon\sigma^3\left[\left(\frac{\sigma}{r_c}\right)^9 - 3\left(\frac{\sigma}{r_c}\right)^3\right] \qquad P^*(r_c) = \frac{32}{9}\pi\rho^{*2}\epsilon\sigma^3\left[\left(\frac{\sigma}{r_c}\right)^9 - \frac{3}{2}\left(\frac{\sigma}{r_c}\right)^3\right]$$

All simulations were run on a machine with an Intel(R) Core™ i5-2500K CPU @ 3.30GHz, 8 GB of memory, and an NVIDIA(R) GeForce™ 560 GPU (336 processing cores, 850 MHz core clock, 1 GB memory) by EVGA.

[Image Sources: *Ubergizmo* (Above), NVIDIA (right)

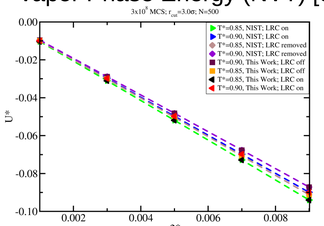


Schematic Representation of Multi-Threading Scheme

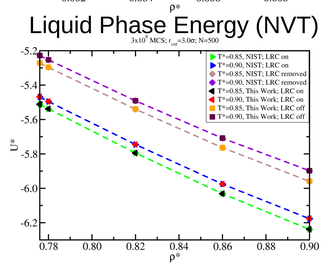


Validation of the GPU (CUDA) Code

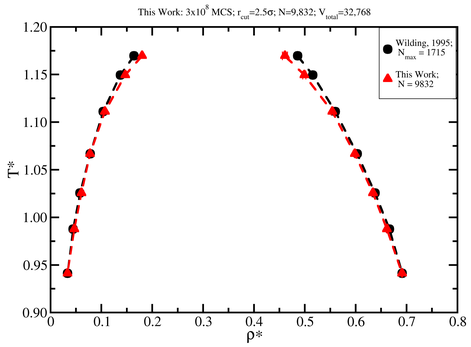
Vapor Phase Energy (NVT) [9]



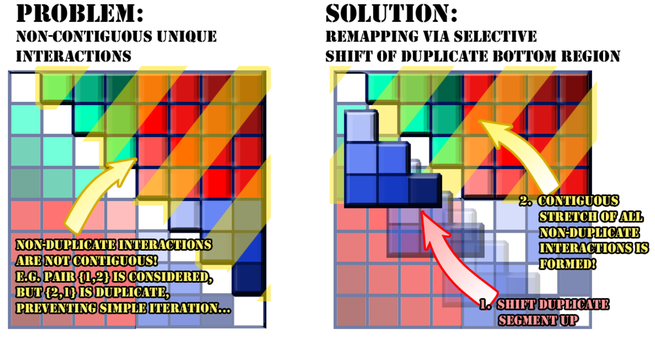
Liquid Phase Energy (NVT)



Density of coexisting phases (Gibbs) [10]

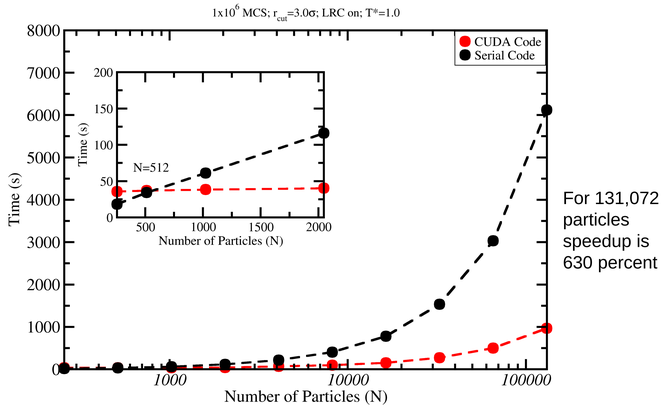


Creating a Contiguous Block of Unique Interactions



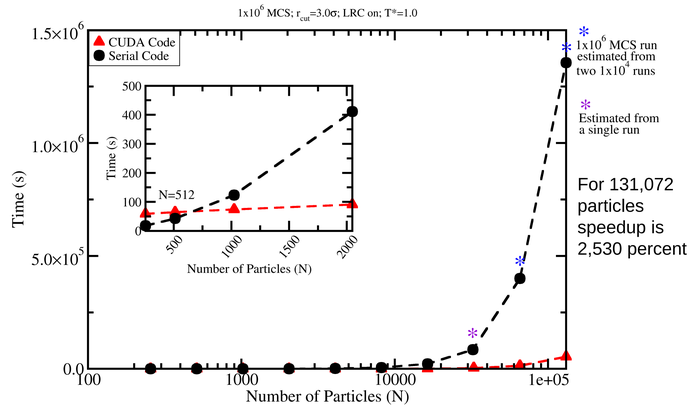
The volume move requires complete recalculation of all unique particle pair-wise interactions. When represented in two dimensions the problem of contiguous space becomes apparent -- a formula is necessary to map threads to series of interactions. We accomplish this by using a shift to create a contiguous region of unique interactions.

GPU Accelerates Simulations in the Canonical Ensemble



For 131,072 particles speedup is 630 percent

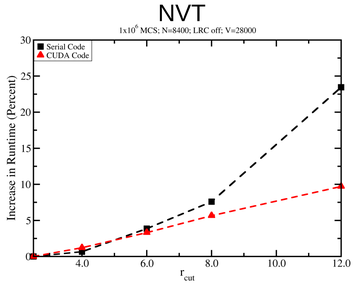
GPU Accelerates Simulations in the Gibbs Ensemble



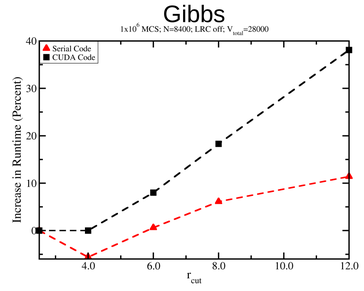
For 131,072 particles speedup is 2,530 percent

GPU Delivers Larger Cutoff at Less Time Cost

NVT



Gibbs



Conclusions

NVIDIA's Compute Unified Device Architecture (CUDA) is a powerful tool for scientific computing, providing a means to harness the power of GPUs to perform numerically intensive tasks. We have demonstrated the application of CUDA and GPUs to simulations in two ensembles, which show a "break even" point of around 500 particles. The effectiveness of the GPU was shown to improve with increasing potential cutoff radius and system size. Gibbs ensemble Monte Carlo appears to be particularly well suited to the GPU, as the GPU provides a means to flatten the volume move, which scales as $O(N^2)$.

References

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