GPU-BASED MONTE CARLO SIMULATIONS FOR CANONICAL AND GIBBS ENSEMBLES

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Overview

Markov Chain Monte Carlo (MCMC) simulation of chemical systems allows examination of nonassociative thermodynamics and associated behavior at small time scales. These simulations tend to be computationally expensive, requiring days or more of CPU time to collect data. In order to remedy the inherent time complexity of these simulations and allow for easier exploration of physical phenomena, optimization work is essential. NVIDIA’s Compute Unified Device Architecture (CUDA) allows one to exploit the parallel nature of these scientific algorithms.

Motivation

In chemistry, computer simulations are considered a valid substitute to lab experiments to get information on the liquid state of a material. However, there is a class of problems that cannot be simulated using current methodologies. These problems require an open system, which employs an algorithm that allows for fluctuation in thermodynamics and associated behavior at small time scales. These problems require an open system, biological systems of interest.

Monte Carlo simulations require one to select a particular type of statistical thermodynamic ensemble to simulate the system. Molecular systems consist of several important correlated variables—volume, temperature, number of particles, system energy, and pressure. For each ensemble, specific variables are fixed, and others remain independent. The canonical ensemble is commonly employed to equilibrate and study the equilibrium structure and energy of small-molecular systems. Once equilibrated, the Widom insertion method allows for the direct calculation of chemical potential regions of system components. The Gibbs ensemble offers a way to directly simulate coexisting phases and calculate phase equilibria properties. This ensemble consists of two simulation boxes, where the canonical is limited to one.

Canonical and Gibbs Ensembles

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Computational Methods

Remapping Pairwise Interactions

Volume transfer requires a complete recalculation of all unique particle pairwise interactions. Representing particles as a matrix creates a problem of having a non-contiguous block of interactions. To overcome this problem, a remapping of the matrix is made by shifting, the lower triangle region up and remapping that part to create a contiguous block of unique particle interactions.

Performance Results

The results show performance gain in terms of execution time when using our CUDA implementation over the serial CPU implementation, especially on large sized systems with many particles. As the system size increases, the performance gap between the serial and parallel algorithm is increasing. However, there is no speed up noticed when the system size is less than 128 particles for the NVT and for a system size of 256 particles in each box for Gibbs ensemble, due to the parallel algorithm overhead and memory latency.

Gibbs ensemble on the GPU

The Gibbs ensemble parallel algorithm gains 14.4 times speed up and the parallel Canonical ensemble gains 8.3 times speed up over the serial algorithms. The two figures show rapid increase in the serial algorithms execution times, while the parallel algorithms are doing much better.

Canonical ensemble on the GPU

The algorithm shows a gain of energy vs. trial distance.

Code Validation

The engine code was compared with the literature [5-6].

- Canonical ensemble: evaluated liquid and gas phase reduced internal energies (U*) for various reduced densities (ρ*) and compared with data from NIST [5].
- Gibbs ensemble: evaluated vapor-liquid coexistence curve at different reduced temperatures (T*) and compared with histogram reweighted simulations of the grand canonical ensemble [6].
- The results showed good agreement with earlier work.

- Multi-Threading Scheme

Each thread is devoted to one particle, excluding the affected particle. The thread calculates the change in the particle interaction with the trial particle moving from its current position to the trial position. The sum of all particles is then compiled.

References


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Conclusion

- We have demonstrated the application of CUDA and GPUs to simulations in two ensembles, which show a “break even” point of around 100 particles.
- The effectiveness of the GPU was shown to improve with increasing 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(N²).