Development of a GPU Accelerated Gibbs Ensemble Monte Carlo Simulation Engine

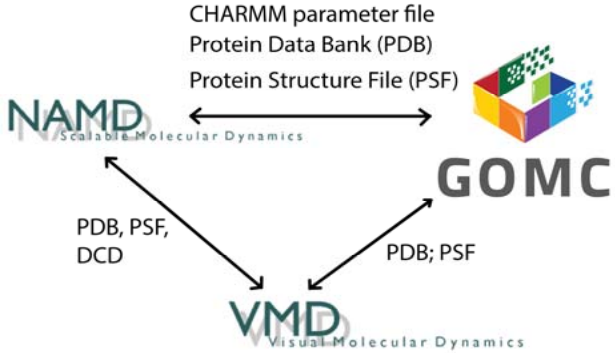
Jeffrey Potoff ‡ and Loren Schwiebert †

‡Department of Chemical Engineering & Materials Science, College of Engineering,

†Department of Computer Science, College of Engineering, Wayne State University, Detroit, MI, USA 48202

GPU **O**ptimized **M**onte **C**arlo (GOMC)
http://gomc.eng.wayne.edu

GOMC is a Gibbs Ensemble Monte Carlo simulation engine developed specifically for the simulation of phase equilibria for systems that contain 10,000-100,000+ interaction sites. It has been designed to use standardized input and output file formats, allowing users to work seamlessly between GOMC and other simulation engines (NAMD, CHARMM) and analysis tools (VMD).



Gibbs ensemble Monte Carlo

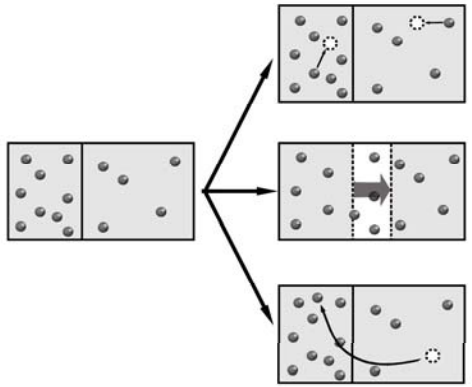


Figure 1: Schematic of the Gibbs ensemble Monte Carlo method. In the simulation, each box represents a region of the two phases in equilibrium. Equilibration occurs through a series of moves that include molecular displacements in each phase (top), the exchange of volume between phases (center), and the transfer of molecules between phases (bottom).

Pure Phase Equilibria

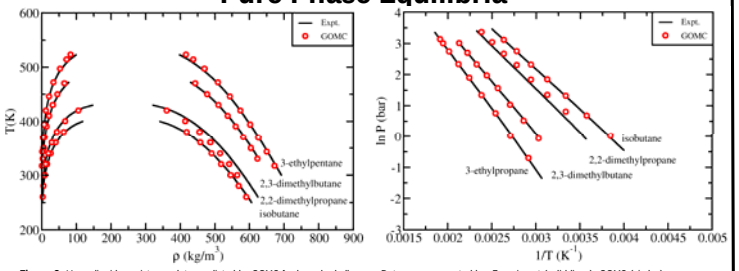


Figure 2: Vapor-liquid coexistence data predicted by GOMC for branched alkanes. Data are represented by: Experiment (solid lines); GOMC (circles).

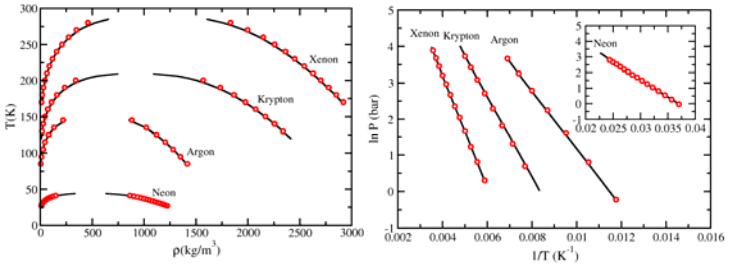


Figure 3: Vapor-liquid coexistence data predicted by GOMC for noble gases. Data are represented by: Experiment (solid lines); GOMC (circles).

Binary Phase Equilibria

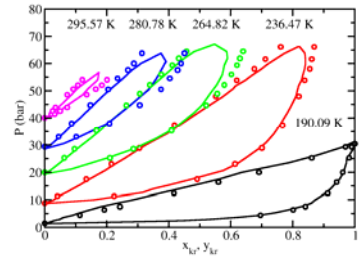


Figure 4: Pressure-composition data predicted by GOMC for the Krypton-Ethane binary mixture. Data are represented by: Experiment (solid lines); GOMC (circles).

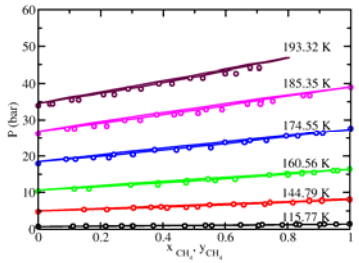


Figure 5: Pressure-composition data predicted by GOMC for Krypton-Methane binary mixture. Data are represented by: Experiment (solid lines); GOMC (circles).

Cell List

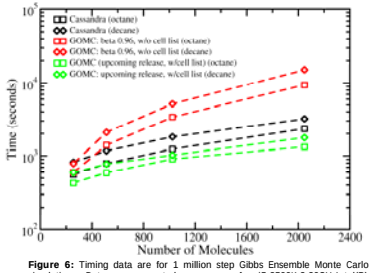
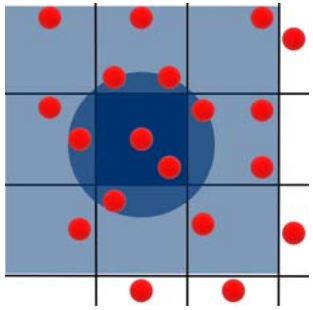


Figure 6: Timing data are for 1 million step Gibbs Ensemble Monte Carlo simulations. Data were generated on one core of an i5-2500K 3.30GH Intel(R) CPU. For a system of 2048 molecules, the CPU cell list implementation is 6 (octane) to 7.5 (decane) times faster than the baseline CPU-optimized code utilizing a simple pair-wise cutoff evaluation (without cell list).



Multi-Threading / Architecture Performance

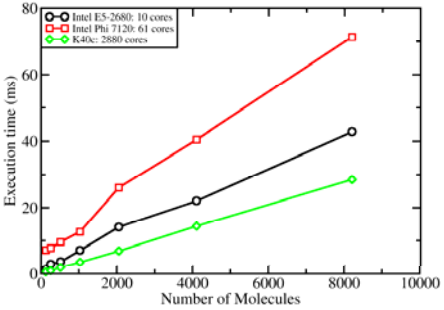


Figure 7: Comparison of code performance on various parallel architectures. Calculations correspond to a single evaluation of the total system energy. Calculations were performed on an Intel E5-2680 (red squares), Intel Phi 7120 (black circles) and NVIDIA K40c (green diamonds).

Products

Journal Publications

1. Loren Schwiebert, Eyad Hailat, Kamel Rushaidat, Jason Mick, Jeffrey Potoff, "An Efficient Cell List Implementation for Monte Carlo Simulation on GPUs," arXiv:1408.3764 [cs.DC]
2. Jeffrey J Potoff and Ganesh Kamath, "Mie potentials for phase equilibria: application to alkenes," J. Chem. Eng. Data 59, 3144-3150 (2014) [Invited Article]. DOI: 10.1021/je500202q
3. Eyad Hailat, Vincent Russo, Kamel Rushaidat, Jason Mick, Loren Schwiebert, and Jeffrey Potoff, "Parallel Monte Carlo simulation in the canonical ensemble on the graphics processing unit," Int. Journal of Parallel, Emergent and Distributed Systems (2013) DOI:10.1080/17445760.2013.833617
4. Jason R. Mick, Eyad Hailat, Vincent Russo, Kamel Rushaidat, Loren Schwiebert, and Jeffrey J. Potoff, "GPU-accelerated Gibbs ensemble Monte Carlo Simulations of Lennard-Jonesium," Computer Physics Comm. 184, 2662-2669 (2013)

Conference Presentations

1. Jason R. Mick, Brock Jackman, Kamel I. Rushaidat, Loren Schwiebert and Jeffrey J. Potoff, "Mie Potentials for Phase Equilibria: Application to Alkynes," AICHE Annual Meeting, 749h, Atlanta, GA 2014.
2. Jason R. Mick, Kamel I. Rushaidat, Brock Jackman, Yuanzhe Li, Loren Schwiebert and Jeffrey J. Potoff, "Development of a GPU Optimized Gibbs Ensemble Monte Carlo Simulation Engine," AICHE Annual Meeting, 406d, Atlanta, GA 2014.
3. Jason R. Mick, Kamel I. Rushaidat, Brock Jackman, Yuanzhe Li, Loren Schwiebert and Jeffrey J. Potoff, "Development of a GPU Optimized Gibbs Ensemble Monte Carlo Simulation Engine", 2014 Midwest Thermodynamics and Statistical Mechanics Conference, June 2014.
4. Jason R. Mick, Eyad Hailat, Vincent Russo, Kamel Ibrahem, Loren Schweibert, and Jeffrey Potoff, " GPU Accelerated Configurational-Bias Monte Carlo Simulations for Linear Alkanes," AICHE Annual Meeting, 405d, Pittsburgh, PA, 10/29/2012.
5. Jason R. Mick, Eyad Hailat, Vincent Russo, Kamel Ibrahem, Loren Schweibert, and Jeffrey Potoff, "Optimization of a Lennard-Jones Particle Monte Carlo GPU Code," AICHE Annual Meeting, 51e, Pittsburgh, PA, 10/31/2012.
6. Jason Mick, Eyad Hailat, Vincent Russo, Loren Schwiebert, and Jeffrey Potoff, "GPU Accelerated Monte Carlo Simulations in the Gibbs and Canonical Ensembles," AICHE Annual Meeting, Minneapolis, MN, 2011.

Development Team

Jason Mick (ChE); Brock Jackman (CS); Kamel Rushaidat (CS); Mohammad Bargahi; Eyad Hailat (CS); Yuanzhe Li (CS); Younes Nejahi (CS); Jeffrey Potoff (ChE); Loren Schwiebert (CS)

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