GPU Accelerated Molecular Dynamics Algorithms for Soft Matter Systems using HOOMD-Blue

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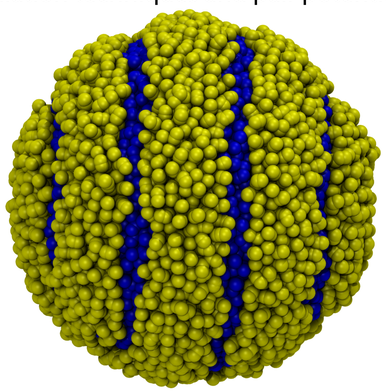
HOOMD-blue

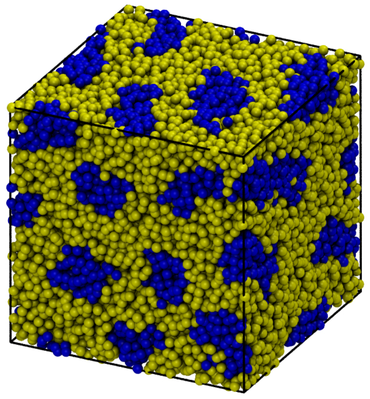
See Session 2062, 3pm Thursday

Soft Matter Simulations

The rheological, thermodynamic, and self-assembly behavior of liquids, colloids, polymers, foams, gels, granular materials and biological systems are often studied in simulation by using coarse-grained models based on molecular dynamics algorithms. The open source general purpose particle dynamics code HOOMD-Blue has been expanded to include the simulation techniques and pair potentials used to study this class of problems.



A DPD simulation immiscible polymer surfactants bonded to a nanoparticle surface forming stripes. Pons, Singh, Glotzer, 2010



A DPD simulation of 2,400 polymers of A7-B3 monomers self-assemble in the Hexagonal (H) Phase from Groot, Madden, Tildesley, 1999

Soft Matter Coarse-Grained Integration Methods

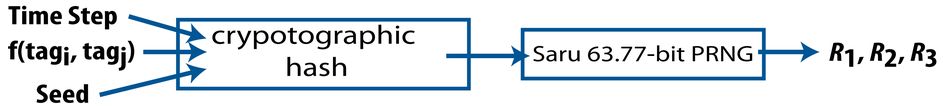
In Molecular Dynamics (MD), particles move in response to forces, usually defined between pairs of particles, by integrating Newton's equations of motions at each time step.

Brownian Dynamics (BD)- Solvent particles are modeled implicitly by subjecting each particle to a temperature-dependent stochastic force and drag force at each time step.

Dissipative Particle Dynamics (DPD) - Momentum is conserved by applying the stochastic and drag force between particle pairs.

GPU (SIMT) Challenge: BD and DPD require thousands of independent streams of random numbers used in small batches over many kernels calls.

Solution: Rather than store thousands of PRNG states or bank and distribute a single PRNG stream, at each kernel call, random numbers are generated by hashing three integers for each force calculation and then using this to seed a PRNG and produce a small batch of uniformly distributed random numbers.

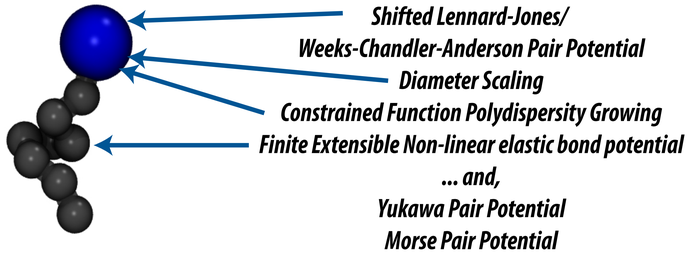


Advantages:

- Exchanges integer calculations (hidden by memory loads) for additional memory loads resulting in a net faster kernel execution time.
- For DPD, no need to exchange information between threads during force calculations.
- Trivial restart, rewind, and fast forward PRNG capability

Pair Potentials, Bonds, and Methods

Pair potentials, Bonds, and Computational Methods used to study Soft Matter Systems have been added to the library of available modules.

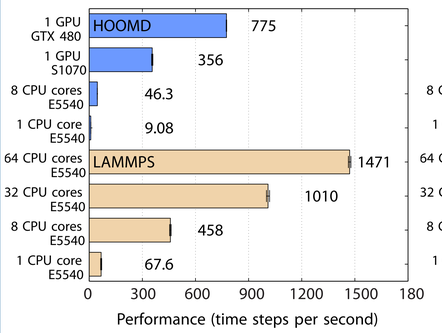


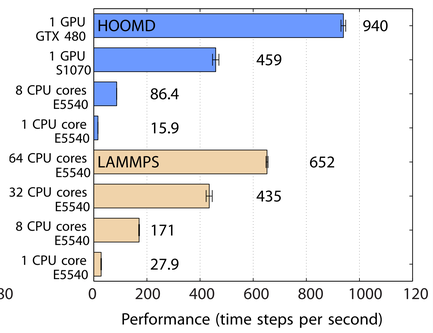
A Nanosphere tethered to a polymer modelled by 8 WCA beads bonded by FENE springs

Benchmarks

Polymer Tethered Nanospheres
The GPU version of the code is 35-70x faster than a (1) CPU version of the code. Compared to LAMMPS, which uses a better neighbor list building algorithm, HOOMD-Blue is equivalent to 6-26 CPU cores.

DPD Simulation of A7-B3 Polymers in the H Phase
The GPU version of the code is 30-45x faster than a (1) CPU version of the code. Compared to LAMMPS, HOOMD-Blue is equivalent to 32-100 CPU cores.



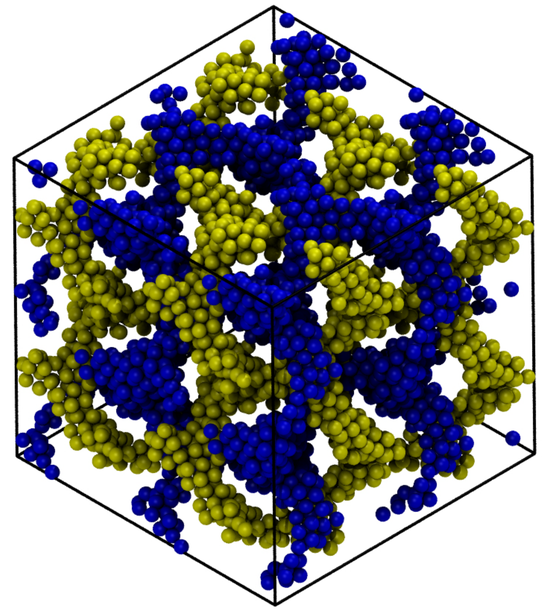


References

General purpose molecular dynamics simulations fully implemented on graphics processing units, Joshua A. Anderson, Chris D. Lorenz, and Alex Travesset Journal of Computational Physics 227 (2008) 5342-5359

Stability of the double gyroid phase to nanoparticle polydispersity in polymer-tethered nanosphere systems, Carolyn L. Phillips, Christopher R. Iacovella, Sharon C Glotzer, Soft Matter 6 (2010) 1693

The effect of polydispersity on the tethered nanosphere phase diagram, Carolyn L. Phillips, Sharon C. Glotzer, Preprint

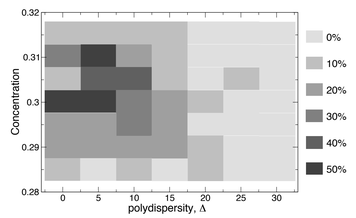


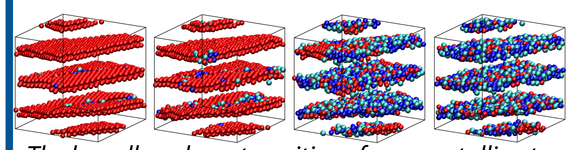
A BD simulation of 4040 Tethered Nanospheres (TNS) microphase separated into a Double Gyroid Phase colored blue and maize to distinguish the two halves . (polymers not shown)

Beyond Benchmarks

Using the HOOMD-Blue code package, the influence of polydispersity on the stability of TNS phase diagram was studied. This study required ~1500 simulation runs or ~50,000 GPU hours

A small amount of polydispersity was found to stabilize the Double Gyroid Phase.





The lamallae phase transitions from crystalline to liquid in response to increasing polydispersity.

Acknowledgements

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