GPU Acceleration of Aspherical Particle Simulations

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Why Aspherical Particles?

- Particles in nature and manufacturing often have highly irregular shapes
- Liquid crystal simulations
- Coarse Graining
- Majority of computational particle mechanics (CPM) simulators treat only spherical particles
- Need a parallel and scalable implementation to attack realistic problems (LAMMPS)
Gay-Berne Potential

- Single-site potential for asphericals
- $S$ is the shape matrix
- The $E$ matrix characterizes the relative well depths of side-to-side, face-to-face, and end-to-end interactions
- $\sim 30$ times the cost of an LJ interaction

\[
U = U_r(A_1,A_2,r_{12})\eta_{12}(A_1,A_2)\chi_{12}(A_1,A_2,\hat{r}_{12})
\]

\[
U_r = 4\varepsilon\left[\left(\frac{\sigma}{h_{12} + \gamma\sigma}\right)^{12} - \left(\frac{\sigma}{h_{12} + \gamma\sigma}\right)^{6}\right]
\]

\[
\eta_{12} = \left[\frac{2s_1s_2}{\det[A_1^TS_1^2A_1 + A_2^TS_2^2A_2]}\right]^{v/2}
\]

\[
s = [a_ib_i + c_i c_i]^{1/2}a_ib_i
\]

\[
\chi_{12} = \left[2\hat{r}_{12}^T(A_1^TE_1A_1 + A_2^TE_2A_2)^{-1}\hat{r}_{12}\right]^\mu
\]
Liquid Crystal Simulations
Accelerated Gay-Berne in LAMMPS

- Good candidate for GPU acceleration
  - *Very* expensive force calculation

- Available in the GPU package (make yes-asphere yes-gpu)
  - Can run on multiple GPUs on a single node or in a cluster
  - Multiple precision options: Single/Single, Single/Double, and Double/Double
  - Can simulate millions of particles per GPU
GPGPU Times Speedup vs 1 Core
(c=cutoff, \(n\)=particles)

GPGPU: 1, 2, 3, or 4 NVIDIA, 240 core, 1.3 GHz GPGPUs
Thunderbird: 1 core of Dual 3.6 GHz Intel EM64T processors
Glory: 1 core of Quad Socket/Quad Core 2.2 GHz AMD
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GPGPU: 1, 2, 3, or NVIDIA, 240 core, 1.3 GHz GPGPUs
Thunderbird: 2 procs, Dual 3.6 GHz Intel EM64T processors
Glory: 16 procs, Quad Socket/Quad Core 2.2 GHz AMD
64K GB Particle Simulation on Stella

**Millions of Force Calculations/sec**

- 1 CPU
- 10 CPU
- 1 GPU
- 2 GPU
- 9 GPU (Stella)
Conclusions

- A single 4-GPU accelerated node can run a simulation faster than a 256-core simulation on Thunderbird or Glory.

- The power requirements for the GPU accelerated run were <1.2 kW versus 11.2 kW on Glory or 44.8 kW on Thunderbird