Harnessing GPU speed to accelerate LAMMPS particle simulations

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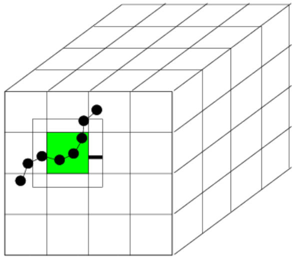
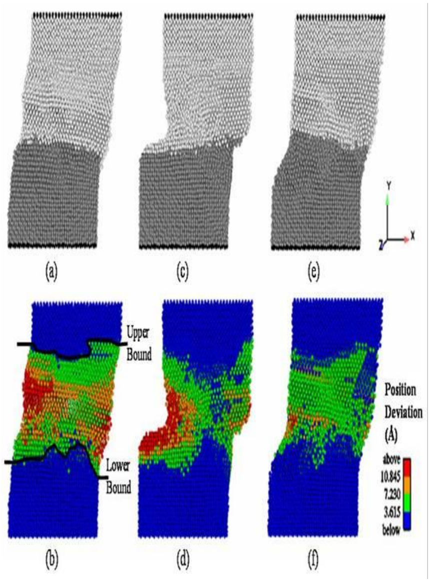
LAMMPS

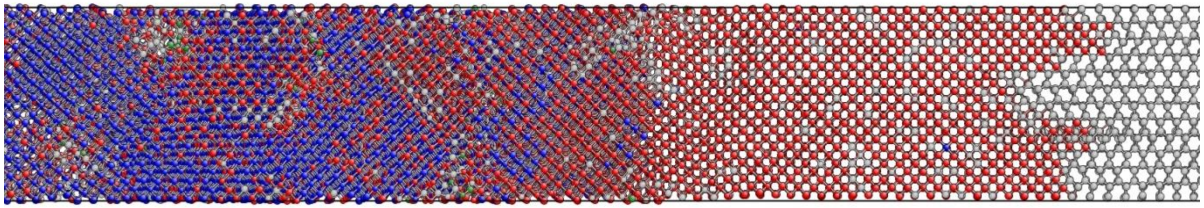
(Large-scale Atomic/Molecular Massively Parallel Simulator)

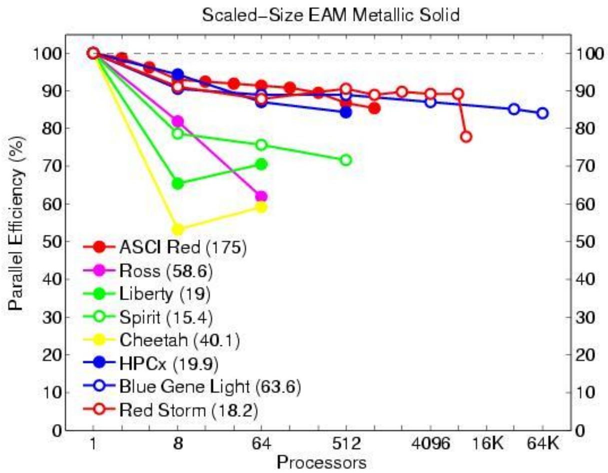
http://lammps.sandia.gov





- Classical MD code.
- Open source, highly portable C++.
- Freely available for download under GPL.
- Easy to download, install, and run.
- Well documented.
- Easy to modify or extend with new features and functionality.
- Active user’s e-mail list with over 300 subscribers.
- Since Sept. 2004: over 20k downloads, grown from 53 to 125 kloc.
- Spatial-decomposition of simulation domain for parallelism.
- Energy minimization via conjugate-gradient relaxation.
- Radiation damage and two temperature model (TTM) simulations.
- Atomistic, mesoscale, and coarse-grain simulations.
- Variety of potentials (including many-body and coarse-grain).
- Variety of boundary conditions, constraints, etc.





Why enable LAMMPS to run on GPUs?

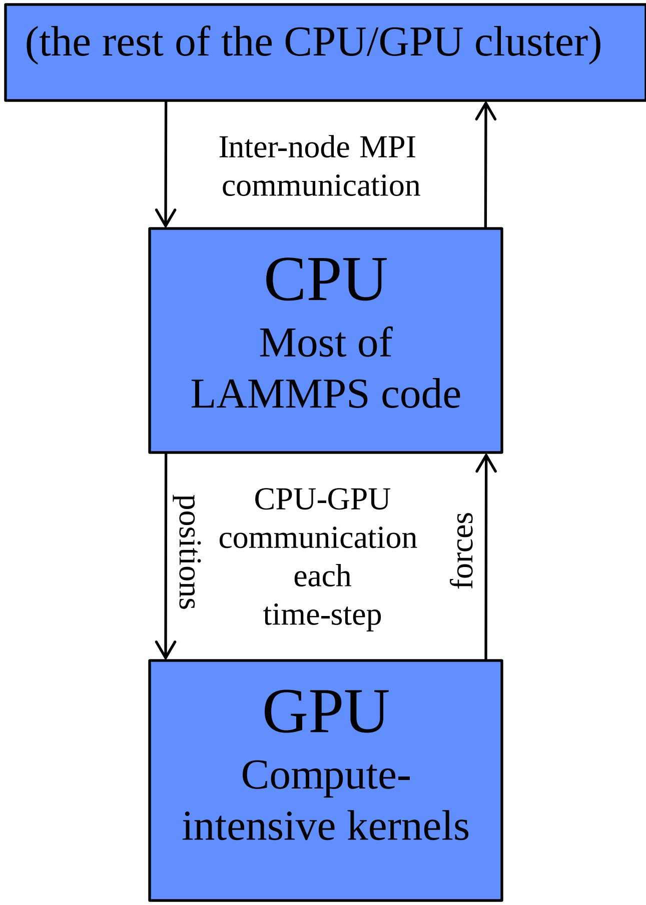
- **Other MD codes are running on GPUs and showing big speed-ups.**

- **The future is many-core, and GPU computing is leading the way.**

- **Next generation supercomputers will have accelerators, like LANL’s Road Runner, but the accelerators will be GPUs in many cases.**

GPU-LAMMPS strategy

- **Enable LAMMPS to run efficiently on future CPU-based clusters that have GPU accelerators.**
- **Not aiming for running on a single GPU.**
- **Not aiming to rewrite all of LAMMPS in CUDA.**
- **Rewrite the most compute-intensive LAMMPS kernels in CUDA.**
- **At each time-step, ship particle positions from CPU to GPU, compute forces on the GPU, and then ship forces back to the CPU.**



(the rest of the CPU/GPU cluster)
Inter-node MPI communication
CPU
Most of LAMMPS code
positions
CPU-GPU communication each time-step
forces
GPU
Compute-intensive kernels

Current status of the GPU-LAMMPS project

- GPU library and package available for download with LAMMPS: http://lammps.sandia.gov
- CUDA kernels written for two pairs styles: LJ and Gay-Berne
- Pre-release developer's version of GPU-LAMMPS available for subversion checkout at: http://code.google.com/p/gpulammps/
  - Faster CUDA kernel for LJ
  - Cell list built on the GPU to avoid reneighboring on the CPU
  - More LAMMPS pair styles coming soon
- To offer feedback, or join the GPU-LAMMPS team, send e-mail to: Paul Crozier (pscrozi@sandia.gov)

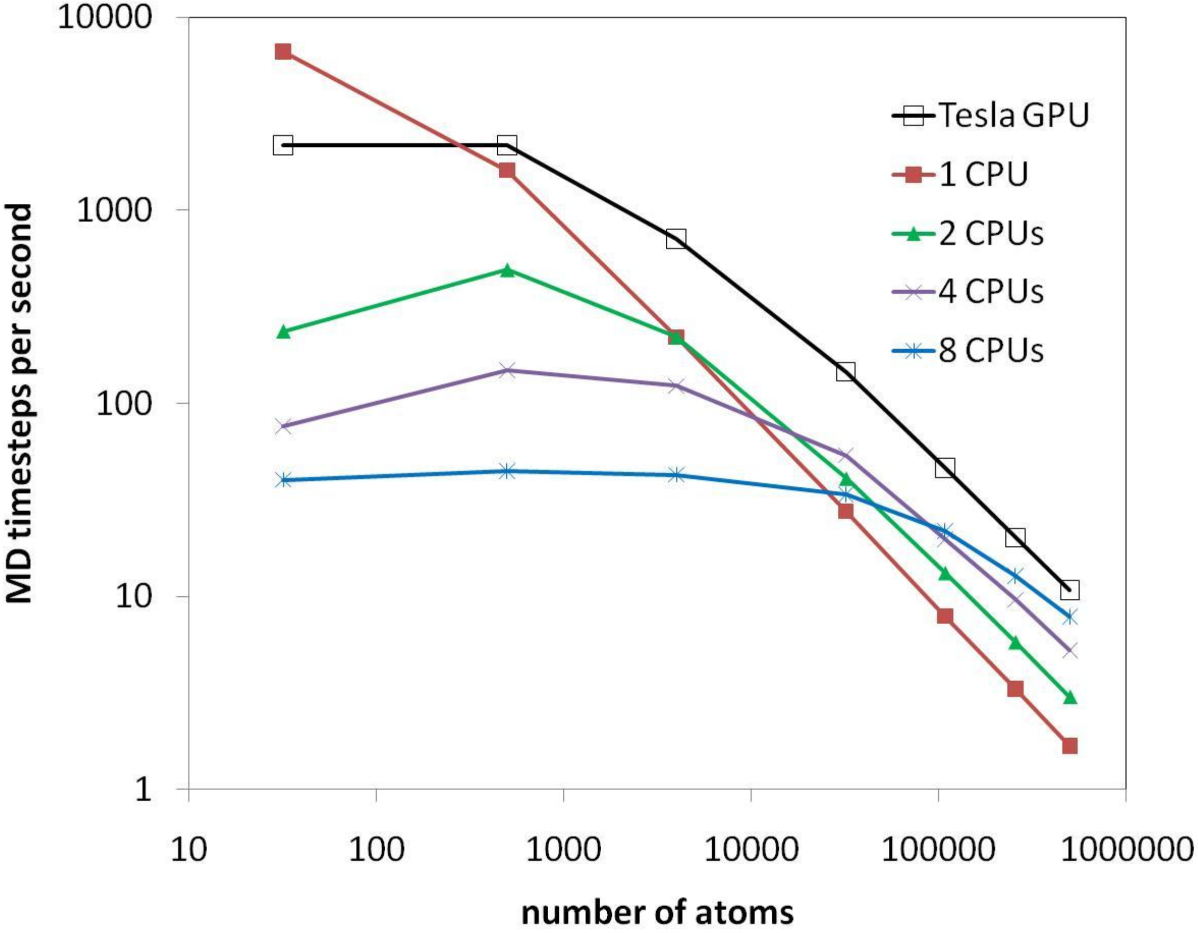
Results for LAMMPS LJ benchmark

- Dual Quad Core Intel® Xeon® Processors X5560 2.8GH

- 1 Tesla C1060 GPU

- Use of Tesla is almost always faster than not using it on this machine.

- Tesla 3.2x faster than Dual Quad Core for 4000 atom system.



Gay-Berne Potential for Liquid Crystal Simulation

- **Gay-Berne for dissimilar biaxial ellipsoids**
- **S is the shape matrix, A rotation, *h*$_{12}$ distance of closest approach**
- **The E matrix characterizes the relative well depths of side-to-side, face-to-face, and end-to end interactions**
- **~30 times the cost of an LJ interaction**

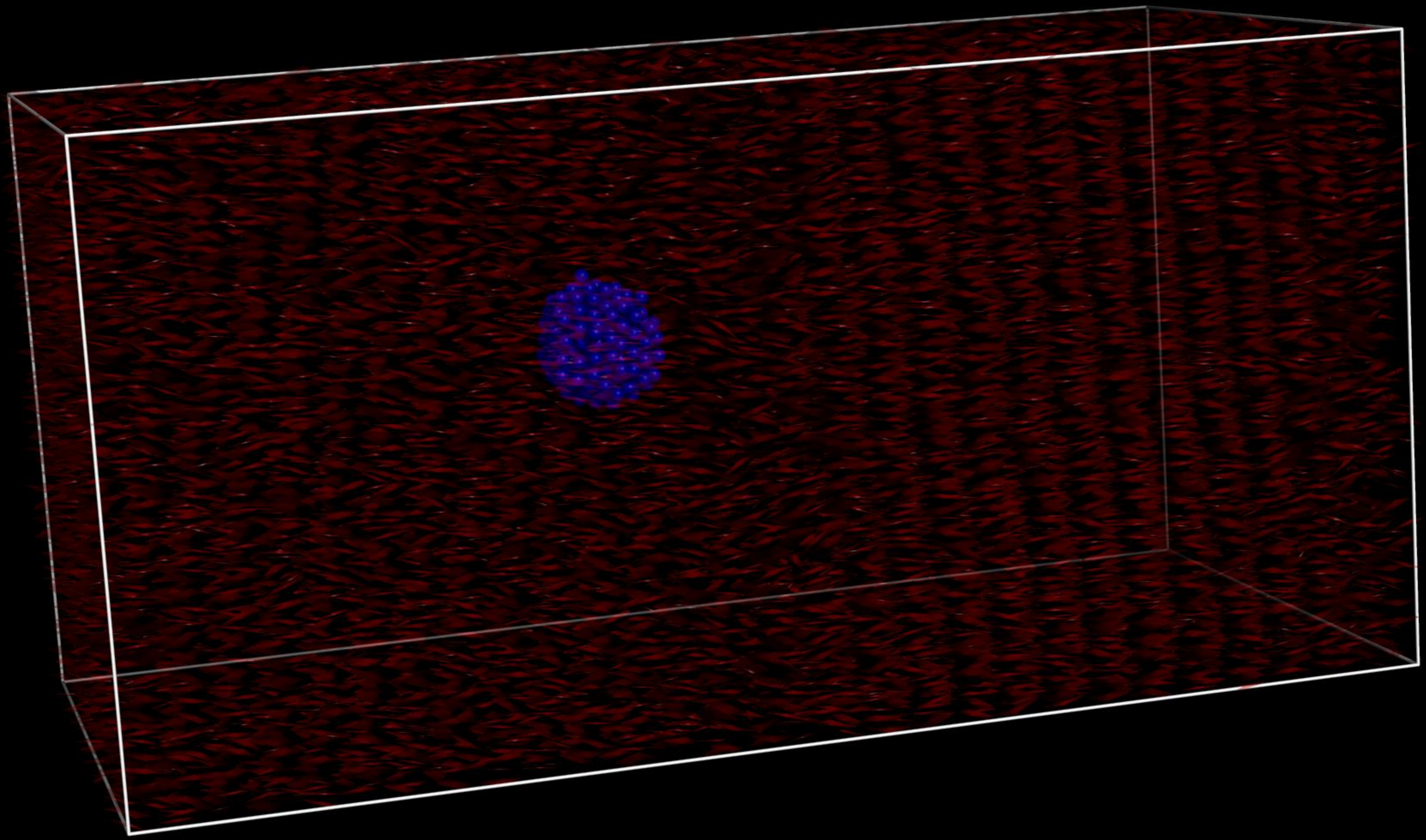
$$U = U_r\left(\mathbf{A}_1,\mathbf{A}_2,\mathbf{r}_{12}\right)\eta_{12}\left(\mathbf{A}_1,\mathbf{A}_2\right)\chi_{12}\left(\mathbf{A}_1,\mathbf{A}_2,\hat{r}_{12}\right)$$

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

$$\eta_{12} = \left[\frac{2s_1s_2}{\det\left[\mathbf{A}_1^T\mathbf{S}_1^2\mathbf{A}_1 + \mathbf{A}_2^T\mathbf{S}_2^2\mathbf{A}_2\right]}\right]^{\upsilon/2}$$

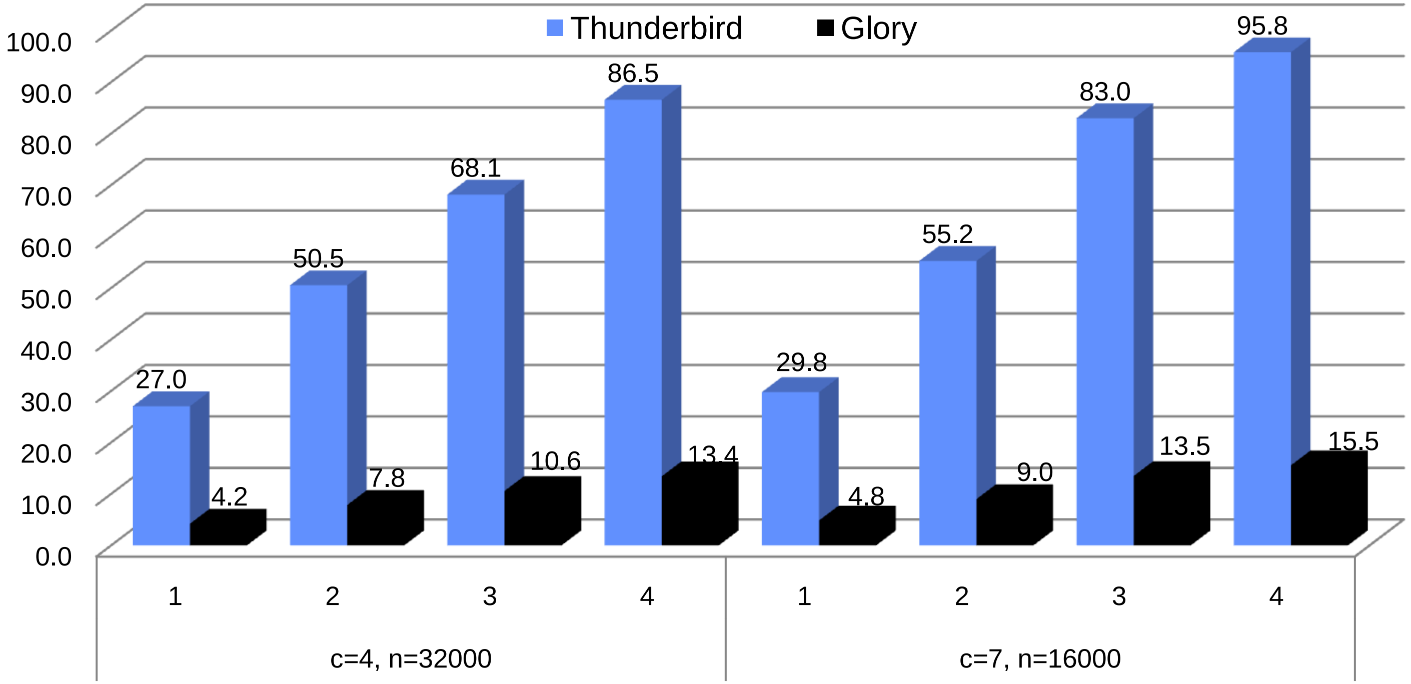
$$s = \left[a_ib_i + c_ic_i\right]\left[a_ib_i\right]^{1/2}$$

$$\chi_{12} = \left[2\hat{\mathbf{r}}_{12}^T\left(\mathbf{A}_1^T\mathbf{E}_1\mathbf{A}_1 + \mathbf{A}_2^T\mathbf{E}_2\mathbf{A}_2\right)^{-1}\hat{\mathbf{r}}_{12}\right]^{u}$$



GPU Times Speedup vs 1 Node

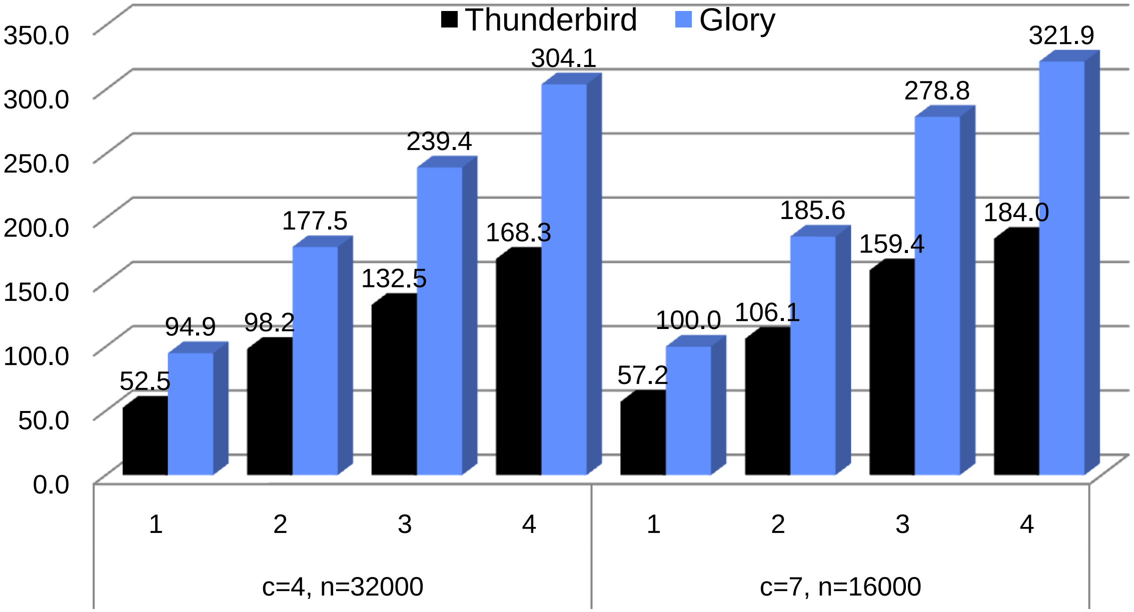
(*c*=cutoff, *n*=particles)



GPU: 1, 2, 3, or NVIDIA, 240 core, 1.3 GHz GPUs
Thunderbird: *2 procs, Dual 3.6 GHz Intel EM64T processors*
Glory: *16 procs, Quad Socket/Quad Core 2.2 GHz AMD*

GPU Times Speedup vs 1 Core

(*c*=cutoff, *n*=particles)



GPU: 1, 2, 3, or 4 NVIDIA, 240 core, 1.3 GHz GPUs
Thunderbird: *1 core of Dual 3.6 GHz Intel EM64T processors*
Glory: *1 core of Quad Socket/Quad Core 2.2 GHz AMD*

Plans for further GPU-LAMMPS work

Before SC10, we plan to:

- Focus on fast biomolecular simulations on CPU/GPU hybrid supercomputers.
- Do efficient 3D FFTs on CPU/GPU hybrid cluster for faster long-range electrostatics.
- Improve CUDA kernel efficiency of LJ and GB pair styles.
- Add more CUDA kernels for additional LAMMPS pair styles until most of LAMMPS's 40 or so pair styles are done.

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