Molecular Dynamics with LAMMPS on a Hybrid Cray Supercomputer

W. Michael Brown
National Center for Computational Sciences
Oak Ridge National Laboratory

NVIDIA Technology Theater, Supercomputing 2012
November 14, 2012
LAMMPS

- Large-scale Atomic/Molecular Massively Parallel Simulator

- General Purpose Classical Molecular Dynamics Software
  - Simulations for biology, materials science, granular, mesoscale, etc.

- Open source (GPL), with a user community
  - 1700 Citations
  - 100K downloads, 25K mail list messages
  - 100 contributors to code base

- Flexible and extensible:
  - 80% of code-base is add-ons by developers and users
  - styles: atom, pair, fix, compute, etc
Force Fields

• Biomolecules: CHARMM, AMBER, OPLS, COMPASS (class 2), Gromacs, long-range Coulombics via PPPM, point dipoles, ...

• Polymers: all-atom, united-atom, coarse-grain (bead-spring FENE), bond-breaking, bond-forming, ...

• Materials: EAM/MEAM for metals, Buckingham, Morse, Yukawa, Tersoff, COMB, AI-REBO, ReaxFF, GAP, ...

• Mesoscale: granular, DPD, SPH, PD, colloidal, aspherical, triangulated, ...
LAMMPS with Accelerators

• Acceleration for neighbor-list builds, short-range force calculation, and long-range electrostatics
• MPI Processes Share the Accelerator
  – Task-based parallelism to divide short-range and long-range calculations
  – Allows for parallelism of routines not ported to the accelerator that can run concurrently with accelerated routines
  – Allows for compatibility with all of LAMMPS features when using GPU acceleration
  – CPU/Accelerator/Data-transfer and Computation concurrency to achieve efficient simulation on hybrid nodes
• Deterministic Algorithms
  – Same result with same number of procs/random seed

## Host-Accelerator Concurrency

(- PPPM Acceleration) **Not to scale**

<table>
<thead>
<tr>
<th>GPU</th>
<th>CPU Core 1</th>
<th>CPU Core 2</th>
<th>CPU Core 3</th>
<th>CPU Core 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nbor Core 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nbor Core 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nbor Core 3</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nbor Core 4</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Data Transfer In</td>
<td>Pair Core 1</td>
<td>Pair Core 2</td>
<td>Pair Core 3</td>
<td>Pair Core 4</td>
</tr>
<tr>
<td>Data Transfer Out</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Neighboring is not performed every timestep. 1 in 10-20.
- Adjusts split of non-bonded force calculation automatically or by specifying a fixed split.
- Can run force models not ported to GPU concurrently with models ported to GPU (e.g. solvent on GPU).
Host-Accelerator Concurrency (+PPPM Acceleration)

Can run multiple kernels at the same time on some accelerators
X2090 Benchmark Results

• Jaguar upgrade to Titan consisted of:
  1. Upgrade XT5 to XK6 blades (AMD Interlagos Processors and Gemini Interconnect)
  2. Install *Titan Development Partition* with Fermi+ GPUs on 10 cabinets
  3. Upgrade to XK7 nodes (Installation of K20X Kepler II GPUs on all all nodes)

• XK6 Upgrade and Titan Development results are presented first
• *Early results with Kepler on Titan presented at end of talk*
• Benchmarks with acceleration used mixed-precision as compared to double precision
• Left: Strong Scaling for fixed-size simulations of approximately 256K particles
• Right: Weak Scaling with ~32K particles/node
• XK6 NP results use a new MPI process to grid mapping and a separate partition for long-range electrostatics (as do the GPU results)

Atomic Fluid

- Atomic fluid - microcanonical ensemble, Lennard-Jones potential, reduced density 0.8442, neighbor skin 0.3σ, cutoffs of 2.5σ and 5.0σ

XK6 Single Node: 1.17X
XK6 GPU Single Node: 3.03X, 5.68X

XK6 Single Node: 1.04X
XK6 GPU Single Node: 1.92X, 4.33X
XK6 GPU 512 Nodes: 2.92X, 5.11X
NP gives up to 20% improvement
Bulk Copper

- Copper metallic solid in the microcanonical ensemble. The force cutoff is 4.95Å with a neighbor skin of 1.0Å.
  - Requires additional ghost exchange during force calculation for electron densities

**Graphs:**

- **XT5**
- **XK6**
- **XK6 NP**
- **XK6 GPU**

---

**Performance:**

- **XK6 Single Node:** 1.07X
- **XK6 GPU Single Node:** 3.05X
- **XK6 GPU 512 Nodes:** 2.90X
- NP gives up to 12% improvement
Protein

- All-atom rhodopsin protein in a solvated lipid bilayer with the CHARMM force field. Isothermal-isobaric ensemble, SHAKE constraints, 2.0fs timestep. Counter-ions, water, 8Å/10Å cutoff
  - Long range electrostatics are calculated with P3M.

XK6 Single Node: 1.1X
XK6 GPU Single Node: 3.3X

XK6 Single Node: 1.1X
XK6 GPU Single Node: 2.6X
XK6 GPU 512 Nodes: 8X
NP gives up to 27% improvement
Liquid Crystal

- Liquid crystal mesogens are represented with biaxial ellipsoid particles, Gay-Berne potential, isotropic phase, isothermal-isobaric ensemble, 4σ cutoff with a 0.8σ neighbor skin
  - High arithmetic intensity

XK6 Single Node: .9X
XK6 GPU Single Node: 6.23X
XK6 Single Node: .9X
XK6 GPU Single Node: 5.82X
XK6 GPU 512 Nodes: 5.65X
XK6 vs XK6+GPU Benchmarks

### Speedup with Acceleration on XK6 Nodes

- 1 Node = 32K Particles
- 900 Nodes = 29M Particles

<table>
<thead>
<tr>
<th></th>
<th>Atomic Fluid (cutoff = 2.5σ)</th>
<th>Atomic Fluid (cutoff = 5.0σ)</th>
<th>Bulk Copper</th>
<th>Protein</th>
<th>Liquid Crystal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Speedup (1 Node)</td>
<td>1.92</td>
<td>4.33</td>
<td>2.12</td>
<td>2.6</td>
<td>5.82</td>
</tr>
<tr>
<td>Speedup (900 Nodes)</td>
<td>1.68</td>
<td>3.96</td>
<td>2.15</td>
<td>1.56</td>
<td>5.60</td>
</tr>
</tbody>
</table>
Example Science Problems 1.

- Controlling the movement of nanoscale objects is a significant goal of nanotechnology.

- Pulsed laser melting offers a unique opportunity to dictate materials assembly where rapid heating and cooling rates and ns melt lifetimes are achievable.

- Using both experiment and theory we have investigated ways of controlling how the breakage occurs so as to control the assembly of metallic nanoparticles.

- Here, we illustrate MD simulation to investigate the evolution of the Rayleigh-Plateau liquid instability for copper lines deposited on a graphite substrate.

- Simulations are performed with GPU acceleration on Jaguar at the same scales as experiment.
11.4M Cu Atom Simulations on Graphitic Substrate

2.7X Faster than 512 XK6 w/out Accelerators
Example Science Problems 2.

- Membrane fusion, which involves the merging of two biological membranes in a controlled manner, is an integral part of the normal life cycle of all living organisms.

- Viruses responsible for human disease employ membrane fusion as an essential part of their reproduction cycle.

- Membrane fusion is a critical step in the function of the nervous system
  - Correct fusion dynamics requires realistic system sizes

- Kohlmeyer / Klein INCITE Award

39M Particle Liposome System 2.7X Faster than 900 XK6 w/out Accelerators
The “Porting Wall”

- Although you can get performance improvements by porting existing models/algorithms and running simulations using traditional parameterizations...
  - There is a limit to the amount of parallelism that can be exposed to decrease the time-to-solution
  - Increasingly desirable to re-evaluate computational physics methods and models with an eye towards approaches that allow for increased concurrency and data locality
    - Parameterize simulations to shift work towards routines well-suited for the accelerator
    - Methods/models with increased computational requirements can perform better if they can increase concurrency, allow for larger time-steps, etc.

- Computational scientists will play a critical role in exploiting the performance of current and next-generation architectures

- Some very basic examples...
Electrostatics Example with Polyelectrolyte Brushes

- Electrostatics are typically solved by splitting the Coulomb potential into a short-range potential that decays to zero at the cutoff and a long-range potential that converges rapidly in k-space
  - Long-range component is typically solved with discretization on a mesh
    - Poisson solve with 3D FFTs
    - Communications bottleneck
  - The traditional parameterizations that work well on older high-performance computers are not necessarily optimal for many simulations
  - Shift the work towards the short-range component
    - Disproportionate performance improvements on accelerator with larger short-range cutoffs
    - Benefits from acceleration improve at larger node counts!

Electrostatics Example with Polyelectrolyte Brushes

- Eliminate the long-range component?
  - In condensed phase systems, charges can be effectively short-range due to screening from other charged particles in the system.
  - Use a large short range cutoff, correct for issues due to non-neutral spherical cutoff regions, and modify cell list calculation to be efficient for large cutoffs in parallel simulations.
  - Accurate results with faster time-to-solution for some simulations.

Alternative Potential Energy Models?

• Implementation of new models that can exploit high peak accelerator performance to improve accuracy and sampling
  – Computational cost of a single ellipsoid-ellipsoid interaction can be 15x that for Lennard-Jones on the CPU
  – With GPU acceleration, it is more competitive
    • Higher arithmetic intensity, so better speedup when compared to LJ acceleration
    • Better parallel efficiency relative to the CPU
      – Still get performance with fewer threads


Moore’s Law for Potentials

O(2^{T/2})

Cost [core-sec/atom-timestep]

Year Published

1980 1990 2000 2010
More Creative Examples...

• Advanced time integrators, time parallelism, etc...
Kepler II vs Fermi +

- More cores
  - Efficiently handle larger problems, better performance for complex models
- Improved thread performance
  - Faster time to solution for same problem
- Larger register file
  - Better performance for complex models such as the liquid crystal case
- Warp shuffle
  - Reduced shared memory usage for reductions across threads
- Hyper-Q
  - MPI processes sharing the GPU can share a context
    - Reduced memory overhead per process
    - Concurrent kernel execution from multiple processes
Early Kepler Benchmarks on Titan

**Atomic Fluid**

![Graph showing time vs. number of nodes for Atomic Fluid benchmarks.](image)

**Bulk Copper**

![Graph showing time vs. number of nodes for Bulk Copper benchmarks.](image)
Early Titan XK6/XK7 Benchmarks

Speedup with Acceleration on XK6/XK7 Nodes
1 Node = 32K Particles
900 Nodes = 29M Particles

<table>
<thead>
<tr>
<th></th>
<th>Atomic Fluid (cutoff = 2.5σ)</th>
<th>Atomic Fluid (cutoff = 5.0σ)</th>
<th>Bulk Copper</th>
<th>Protein</th>
<th>Liquid Crystal</th>
</tr>
</thead>
<tbody>
<tr>
<td>XK6 (1 Node)</td>
<td>1.92</td>
<td>4.33</td>
<td>2.12</td>
<td>2.6</td>
<td>5.82</td>
</tr>
<tr>
<td>XK7 (1 Node)</td>
<td>2.90</td>
<td>8.38</td>
<td>3.66</td>
<td>3.36</td>
<td>15.70</td>
</tr>
<tr>
<td>XK6 (900 Nodes)</td>
<td>1.68</td>
<td>3.96</td>
<td>2.15</td>
<td>1.56</td>
<td>5.60</td>
</tr>
<tr>
<td>XK7 (900 Nodes)</td>
<td>2.75</td>
<td>7.48</td>
<td>2.86</td>
<td>1.95</td>
<td>10.14</td>
</tr>
</tbody>
</table>
Ongoing Work

• Implementation and evaluation of alternative algorithms for long-range electrostatics.
  – Multigrid(-like) Methods for Poisson Solve, etc.
    • $O(N)$, no FFTs

• Implementation of complex models well suited for accelerators

• Improvements driven by specific science problems
Publications


Science Applications


Acknowledgements

• LAMMPS
  – Steve Plimpton (SNL) and many others

• LAMMPS Accelerator Library
  – W. Michael Brown (ORNL), Trung Dac Nguyen (ORNL), Peng Wang (NVIDIA), Axel Kohlmeyer (Temple), Steve Plimpton (SNL), Inderaj Bains (NVIDIA)

• Geryon Library
  – W. Michael Brown (ORNL), Manuel Rodriguez Rodriguez (ORNL), Axel Kohlmeyer (Temple)

• K-Space Partitions
  – Yuxing Peng and Chris Knight (University of Chicago)

• Metallic Nanoparticle Dewetting
  – Miguel Fuentes-Cabrera (ORNL), Trung Dac Nguyen (ORNL), W. Michael Brown (ORNL), Jason Fowlkes (ORNL), Philip Rack (UT, ORNL)

• Lipid Vesicle Science and Simulations
  – Vincenzo Carnevale (Temple), Axel Kohlmeyer (Temple), Michael Klein (Temple), et. al.

• Enhanced Truncation/Bottlebrush Simulations
  – Trung Dac Nguyen (ORNL), Jan-Michael Carrillo (UC), Andrew Dobrynin (UC), W. Michael Brown (ORNL)

• Multilevel Summation
  – Arnold Tharrington (ORNL)

• NVIDIA Support
  – Carl Ponder, Mark Berger