Accelerating Three-Body Molecular Dynamics Potentials Using NVIDIA Tesla K20X GPUs

GE Global Research
Masako Yamada
Overview of MD Simulations

- Non-Icing Surfaces for Wind Turbines
  - Large simulations ~ 1 million water molecules
  - Long simulations ~ 1 microsecond
  - Many simulations ~ 1000 independent droplets

- Awarded two DOE ALCC grants
  - 40M CPU-h on Jaguar Cray XK6 at ORNL
  - 40M CPU/GPU-h on Titan Cray XK7 at ORNL

*hybrid*
Overview of Titan

Total 18,600 nodes. Each node has

- 16 cores AMD Opteron CPUs
- 1 Tesla K20X GPU accelerator
  - 2688 compute cores
- Gemini interconnect (ASIC, MPI messages)
- PCI-Express 2.0 bus

LAMMPS was part of acceptance testing
Overview of MD

Atom-by-atom modeling of materials
  • N-body problem
  • Discrete, numerical integration

Biology, chemistry requires good water models
  • Dozens of potentials available
  • Most use pair-wise interactions
  • Most non-polarizable/rigid

MD always on the forefront of HPC
Overview of LAMMPS

Open-source molecular dynamics code developed by Sandia Nat’l Lab

Pre-populated with many popular pair-wise and many-body potentials

- TIP3P/TIP4P water potential
- Stillinger-Weber Three-Body potential
- User can also modify/define potential
Billion-fold growth in a (half) career

<table>
<thead>
<tr>
<th>Year</th>
<th>Software/Language</th>
<th># of Molecules</th>
<th>Hardware</th>
</tr>
</thead>
<tbody>
<tr>
<td>1995</td>
<td>Pascal</td>
<td>Few</td>
<td>Desktop Mac</td>
</tr>
<tr>
<td>2000</td>
<td>C, Fortran90</td>
<td>Hundreds</td>
<td>IBM SP, SGI O2K</td>
</tr>
<tr>
<td>2010</td>
<td>NAMD, LAMMPS</td>
<td>1000’s</td>
<td>Linux HPC</td>
</tr>
<tr>
<td>Present</td>
<td>GPU-enabled LAMMPS</td>
<td>Millions</td>
<td>Titan</td>
</tr>
</tbody>
</table>

1995  | 2000  | 2013  |
Why use a three-body potential?

Stillinger Weber 3-body particle = one water molecule

- mW water introduced in 2009, Nature paper in 2011
- Properties comparable or better than existing models
- Much faster than point-charge models
  - Exemplary test case by authors: 180x faster than SPC/E
  - Our production simulation: 40-50x faster than SPC/E

asymmetric million molecule droplet on engineered surface; loaded onto 64 nodes
Relevant GPU acceleration activity

Pair-wise potentials
- LAMMPS already GPU-enabled

Three-body potentials
- Impressive acceleration... but for crystal solids only

Present work
- >5x acceleration demonstrated using LAMMPS
- Works for liquids, glass, vapor
Parallelization scheme

Host
- Time integration
- Thermostat/barostat
- Bond/angle calculations
- Statistics

Accelerator
- 3-body potential
- Neighbor-lists
Generic 3-body potential

\[ U = \left\{ \sum_i \sum_{j \neq i} \sum_{k > j} \phi(p_i, p_j, p_k) \right\} \]

- \( r_{ij} < r_c, r_{ik} < r_c \)
- otherwise

Good candidate for GPU
1. Occupies majority of computational time
2. Can be decomposed into independent kernels/work-items

Stillinger-Weber
MEAM
Tersoff
REBO/AIREBO
Bond-order...

\( r_c = \text{cutoff} \)
\( r_\alpha = \text{neighbor} \)
Stillinger-Weber Parallelization

\[ U = \sum_{i} \sum_{j<i} \phi_2(r_{ij}) + \sum_{i} \sum_{j\neq i} \sum_{k>j} \phi_3(r_{ij}, r_{ik}, \theta_{jik}) \]

Atom \( i \)

3 kernels
no data dependencies

2-body operations

3-body operations
\((r_{ij} < r_\alpha) \ .AND. \ (r_{ik} < r_\alpha) == .TRUE.\)
update forces on i only

3-body operations
\((r_{ij} < r_\alpha) \ .AND. \ (r_{ik} < r_\alpha) == .FALSE.\)
neighbor-of-neighbor interactions
Redundant Computation Approach

Atom-decomposition
• 1 atom $\rightarrow$ 1 computational kernel only
• fewest operations (and effective parallelization) but
  – shared memory access a bottleneck

Force-decomposition
• 1 atom $\rightarrow$ 3 computational kernels required
• redundant computations but
  – reduced shared memory issues
  – many work-items = more effective use of cores
Neighbor List on GPU

- 3-body force-decomposition approach involves neighbor-of-neighbor operations
- Requires additional overhead
  - increase in border size shared by two processes
  - neighbor list for ghost atoms “straddling” across cores
- GPU implementation not necessarily faster than CPU but less time spent in host-accelerator data transfer (note: neighbor lists are huge)
>200x overall speedup since 2011

1. Switched to mW water potential
   3-body model is more expensive/complex than 2-body but
   • Particle reduction – at least 3x
   • Timestep increase – 10x
   • No long-range forces

2. LAMMPS dynamic load balance – 2-3x

3. GPU acceleration of 3-body model – 5x

2011: 6 femtosecond/1024 CPU-second (SPC/E)
2013: 2 picoseconds/1024 CPU-second (mW)
Post-processing and Viz

Big Data – Total 50TB
- 1 million molecules per snapshot
- Dozens of snapshots per file
- 10,000’s files

Big Compute – NOT a simple search/sort
- Execute three-body calculation again
- Subtle pattern-matching of intra-molecular position
- Post-processing a Titan job in itself!!!

Big Visualization – need dedicated viz resource
Visualizing crystalline regions

Steinhardt-Nelson order parameter  particle mobility
Credits

- Mike Brown (ORNL) – GPU acceleration
- Paul Crozier (Sandia) – dynamic load balancing
- Valeria Molinero (Utah) – mW potential
- Aaron Keyes (Umich, Berkeley) – Steinhardt-Nelson order parameters
- Art Voter/Danny Perez (LANL) – Parallel Replica method
- Mike Matheson (ORNL) -- Visualization
- Jack Wells, Suzy Tichenor (ORNL) – General
- Azar Alizadeh, Branden Moore, Rick Arthur, Margaret Blohm (GE Global Research)

This research was conducted in part under the auspices of the Office of Advanced Scientific Computing Research, Office of Science, U.S. Department of Energy under Contract No. DEAC05-00OR22725 with UT-Battelle, LLC. This research was also conducted in part under the auspices of the GE Global Research High Performance Computing program.
Backup
Load 1 million molecules on Host/CPU

1 million molecules
• 64 nodes
• Processor sub-domains correspond to “spatial” partitioning of droplet

• 8 MPI tasks/node
• 1 core/paired-unit
Per node ~ 15,000 molecules

Host
AMD Opteron 6274 CPU

Core0
Core1
Core2
Core3
Core4
Core5
Core6
Core7
Core8
Core9
Core10
Core11
Core12
Core13
Core14
Core15

Core0
Core1
Core2
Core3
Core4
Core5
Core6
Core7
Core8
Core9
Core10
Core11
Core12
Core13
Core14
Core15

"Kernel"

Accelerator
NVIDIA Tesla K20X GPU

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Private

Core 2
Private

Core 192
Private

Core 1
Dynamic load balancing

Introduced in LAMMPS in 2012

Adjusts size of processor sub-domains to equalize number of particles

2-3x speedup for 1 million molecule droplets on 64 nodes (with user-specified processor mapping)
Development of water-surface interaction potential

Interaction potential developed at GE Global Research
References

• C. Hou, J. Xu, P. Wang, W. Huang, X. Wang, Computer Physics Communications (2013)
• Shi, B. and Dhir, V. K. Molecular dynamics simulation of the contact angle of liquids on solid surfaces. The Journal of Chemical Physics, 130, 3 (01/21/ 2009), 034705-034705; Sergi, D., Scocchi, G. and Ortona, A. Molecular dynamics simulations of the contact angle between water droplets and graphite surfaces. Fluid Phase Equilibria, 332, 0 (10/25/ 2012), 173-177.