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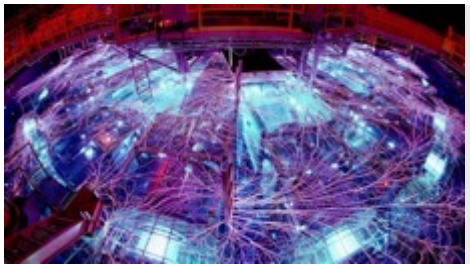
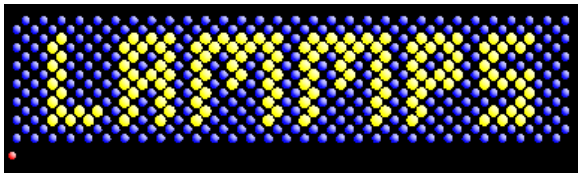


CCR
Center for Computing Research

Accelerator Packages and Performance



Stan Moore

2023 LAMMPS Beginners Tutorial

U.S. DEPARTMENT OF ENERGY NNSA

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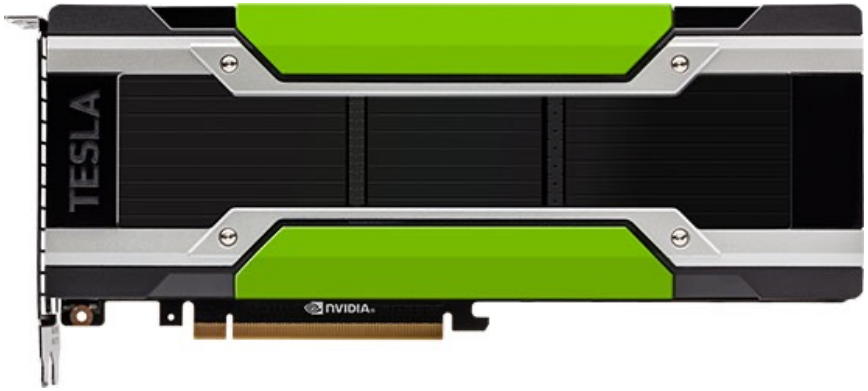
Supercomputer Hardware Trends

- Currently 7 out of the top ten supercomputers use GPUs (Graphics Processing Units), according to the June 2023 Top500 List (https://www.top500.org)
- All 3 US exascale machines will have GPUs: OLCF Frontier (AMD), ALCF Aurora (Intel), NNSA El Capitan (AMD)
- LAMMPS accelerator packages: special code (beyond regular C++ and MPI in LAMMPS) that is required to run well on GPUs and many-core CPUs (e.g. CUDA, OpenMP)



http://www.nvidia.com/object/tesla-p100.html

Accelerator Packages

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- LAMMPS has 5 accelerator packages:
  - OPENMP
  - INTEL
  - OPT
  - GPU
  - KOKKOS
- https://docs.lammps.org/Speed_packages.html

Running OPT Package

- OPT package includes optimized versions of some styles
- Compile LAMMPS with OPT package
- Run with 8 MPI: `mpiexec -np 8 ./lmp_exe -in in.lj -sf opt`
- `-sf opt` is the *suffix* command: automatically appends `/opt` onto anything it can
- For example, `pair_style lj/cut` automatically becomes `pair_style lj/cut/opt` (no changes to input file needed)
- https://docs.lammps.org/suffix.html

OPENMP Package

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- https://docs.lammps.org/Speed_omp.html
- Uses OpenMP to enable multithreading on CPUs
- **MPI parallelization in LAMMPS is almost always more effective than OpenMP on CPUs**
- When running with MPI across multi-core nodes, MPI often suffers from communication bottlenecks, so using MPI+OpenMP per node *could* be faster
- The more nodes per job and the more cores per node, the more pronounced the bottleneck and the larger the benefit from MPI+OpenMP
- OPENMP package may vectorize (SIMD) better than vanilla LAMMPS styles

Running OPENMP Package

- Compile LAMMPS with OPENMP package
- Run with 2 MPI and 2 OpenMP threads:

```
export OMP_NUM_THREADS=2
mpiexec -np 2 ./lmp_exe -in in.lj -sf omp
```

INTEL Package

- https://docs.lammps.org/Speed_intel.html
- Allows code to vectorize and run well on Intel (and other) CPUs, also supports OpenMP threading
- Can also be used with the OPENMP package
- Normally best performance out of all accelerator packages for CPUs
- Supports reduced precision: mixed FP64+FP32 or pure single FP32

Running INTEL Package

- Compile LAMMPS with INTEL package
- To run using 2 MPI and 2 threads on a Intel CPU:

```
mpiexec -np 2 ./lmp_exe -in in.lj -pk intel
0 omp 2 mode double -sf intel
```

- `-pk` is the package command that sets package options, see https://docs.lammps.org/package.html

GPU Package

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- https://docs.lammps.org/Speed_gpu.html
- Designed for one or more GPUs coupled to many CPU cores
- Only pair runs on GPU, fixes/bonds/computes run on CPU
- Atom-based data (e.g. coordinates, forces) move back and forth between the CPU(s) and GPU every timestep
- Asynchronous force computations can be performed simultaneously on the CPU(s) and GPU if using Kspace (e.g. PPPM)
- Provides NVIDIA and more general OpenCL support
- Supports reduced precision: mixed FP64+FP32 or pure single FP32

Running GPU Package

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- Compile GPU library found in lib/gpu
- Compile LAMMPS with GPU package
- Run with 16 MPI and 4 GPUs: `mpiexec -np 16 ./lmp_exe -in in.lj -sf gpu -pk gpu 4`
- **Important**: use CUDA MPS (Multi-Process Service) if using multiple MPI ranks per GPU
- Automatically overlaps pair-style on GPU with Kspace on CPU

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- Abstraction layer between programmer and next-generation platforms
- Allows the same C++ code to run on multiple hardware (GPU, CPU)
- Kokkos consists of two main parts:
  1. Parallel dispatch—threaded kernels are launched and mapped onto backend languages such as CUDA or OpenMP
  2. Kokkos views—polymorphic memory layouts that can be optimized for a specific hardware

- Used on top of existing MPI parallelization (MPI + X)
- See https://kokkos.github.io/kokkos-core-wiki for more info

LAMMPS KOKKOS Package

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- https://docs.lammps.org/Speed_kokkos.html
- **Need C++17 compiler**
- Supports OpenMP and GPUs
- Designed so that everything (pair, fixes, computes, etc.) runs on the GPU, minimal data transfer from GPU to CPU
- Relative performance penalty if kernel isn't ported to Kokkos
- Only double precision FP64 support
- Package options can toggle full and half neighbor list, newton on/off, etc.

```
-pk kokkos newton on neigh half
```

- https://docs.lammps.org/package.html

Running Kokkos Package

- Compile LAMMPS with the KOKKOS package
- Run with 4 MPI and 4 GPUs: `mpiexec -np 4 ./lmp_exe -in in.lj -k on g 4 -sf kk`
- Run with 4 OpenMP threads: `./lmp_exe -in in.lj -k on t 4 -sf kk`

Processor and Thread Affinity

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- Use mpirun command-line arguments (e.g. `--bind-to core`) to control how MPI tasks and threads are assigned to nodes and cores
- Also use OpenMP variables such as `OMP_PROC_BIND` and `OMP_PLACES`
- One must also pay attention to NUMA bindings between tasks, cores, and GPUs. For example, for a dual-socket system, MPI tasks driving GPUs should be on the same socket as the GPU

Measuring performance

```
Loop time of 0.0174524 on 640 procs for 100 steps with 32000 atoms

Performance: 2475308.243 tau/day, 5729.880 timesteps/s
94.1% CPU use with 640 MPI tasks x no OpenMP threads

MPI task timing breakdown:
Section |  min time  |  avg time  |  max time  |%varavg| %total
---------------------------------------------------------------
Pair    | 0.0010798  | 0.0013214  | 0.0016188  |   0.2 |  7.57
Neigh   | 0.00021591 | 0.00024434 | 0.0003079  |   0.0 |  1.40
Comm    | 0.015171   | 0.015479   | 0.01573    |   0.1 | 88.69
Output  | 9.0258e-05 | 0.00011218 | 0.00014501 |   0.0 |  0.64
Modify  | 0.00017915 | 0.00018453 | 0.00020567 |   0.0 |  1.06
Other   |            | 0.0001111  |            |       |  0.64
```

- For KOKKOS package on GPUs, timing breakdown won't be accurate without CUDA_LAUNCH_BLOCKING=1 (but will prevent kernel overlap and could slow down simulation)

Parallel MD Performance

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- MD parallelizes well: major parts of timestep (forces, neighbor list build, time integration) can be done in parallel through domain decomposition
- High communication overhead when strong scaling to a few 100 atoms/proc (depends on cost of the force-field)
- Strong scaling: hold system size fixed while increasing processor count (# of atoms/processor decreases)
- Weak scaling: increase system size in proportion to increasing processor count (# of atoms/processor remains constant)
- For perfect strong scaling, doubling the processor count cuts the simulation time in half
- For perfect weak scaling, the simulation time stays exactly the same when doubling the processor count
- Harder to maintain parallel efficiency with strong scaling because the compute time decreases relative to the communication time

Performance of Different Potentials

- See plots in LAMMPS reference paper
- https://doi.org/10.1016/j.cpc.2021.108171

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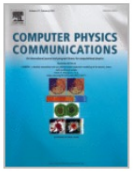

Feature article

LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales ☆, ☆☆

Aidan P. Thompson [a], H. Metin Aktulga [b], Richard Berger [c], Dan S. Bolintineanu [a], W. Michael Brown [d], Paul S. Crozier [a], Pieter J. in 't Veld [e], Axel Kohlmeyer [c], Stan G. Moore [a], Trung Dac Nguyen [f], Ray Shan [g], Mark J. Stevens [a], Julien Tranchida [a], Christian Trott [a], Steven J. Plimpton [a]

Thank You

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Questions?