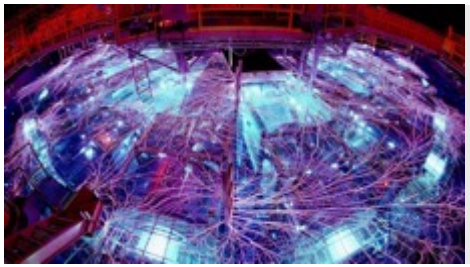
Exceptional service in the national interest

Sandia National Laboratories



CCR
Center for Computing Research

Introduction to LAMMPS

Stan Moore

SC22 Student Cluster Competition

U.S. DEPARTMENT OF ENERGY
NNSA

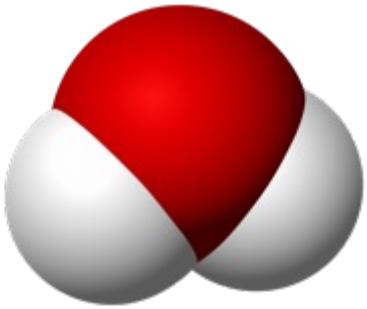
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. SAND2022-12475 PE

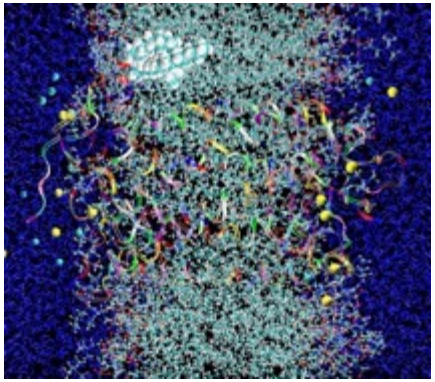
About Me

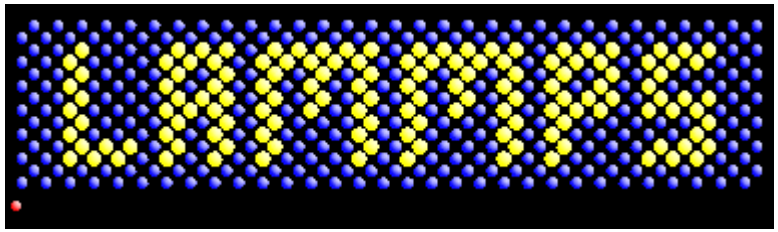
- Stan Moore
  - One of the LAMMPS code developers at Sandia National Laboratories in Albuquerque, New Mexico
  - Been at Sandia for 10 years
  - Main developer of the KOKKOS package in LAMMPS (runs on GPUs and multi-core CPUs)
  - Expertise in long-range electrostatics
  - PhD in Chemical Engineering, dissertation on molecular dynamics method development for predicting chemical potential

Molecular Dynamics

- Classical molecular dynamics (MD) models atom behavior using Newton's laws of motions
- Normally use an empirical expression for forces (**no explicit electrons**)
- Atom positions → forces → velocities → new positions
- Spherical cutoff gives *O*(N) linear scaling, can simulate billions of atoms on a supercomputer



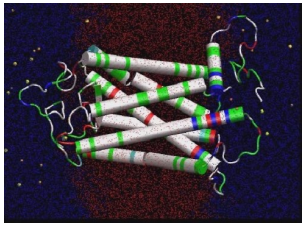
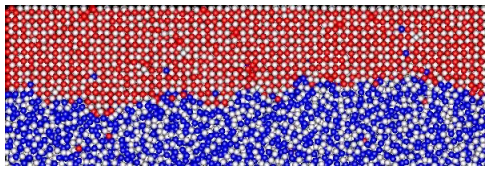
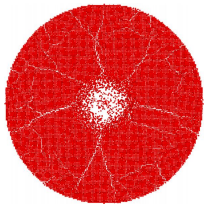




LAMMPS Overview

Sandia National Laboratories

- Large-scale Atomic/Molecular Massively Parallel Simulator
- https://lammps.org
  - Open source, C++ code
  - Bio, materials, mesoscale

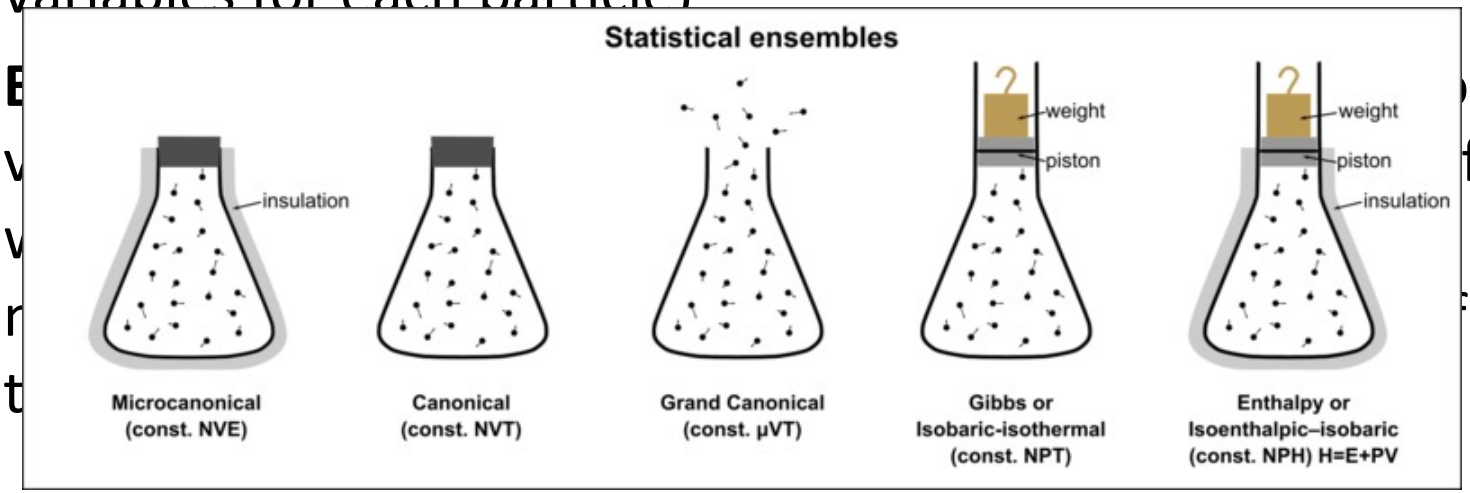
  - Particle simulator at varying length and time scales
    - Electrons → atomistic → coarse-grained → continuum
  - Spatial-decomposition of simulation domain for parallelism
  - Energy minimization, dynamics, non-equilibrium MD
  - GPU and OpenMP enhanced
  - Can be coupled to other scales: QM, kMC, FE, CFD, …

Statistical Mechanics Basics

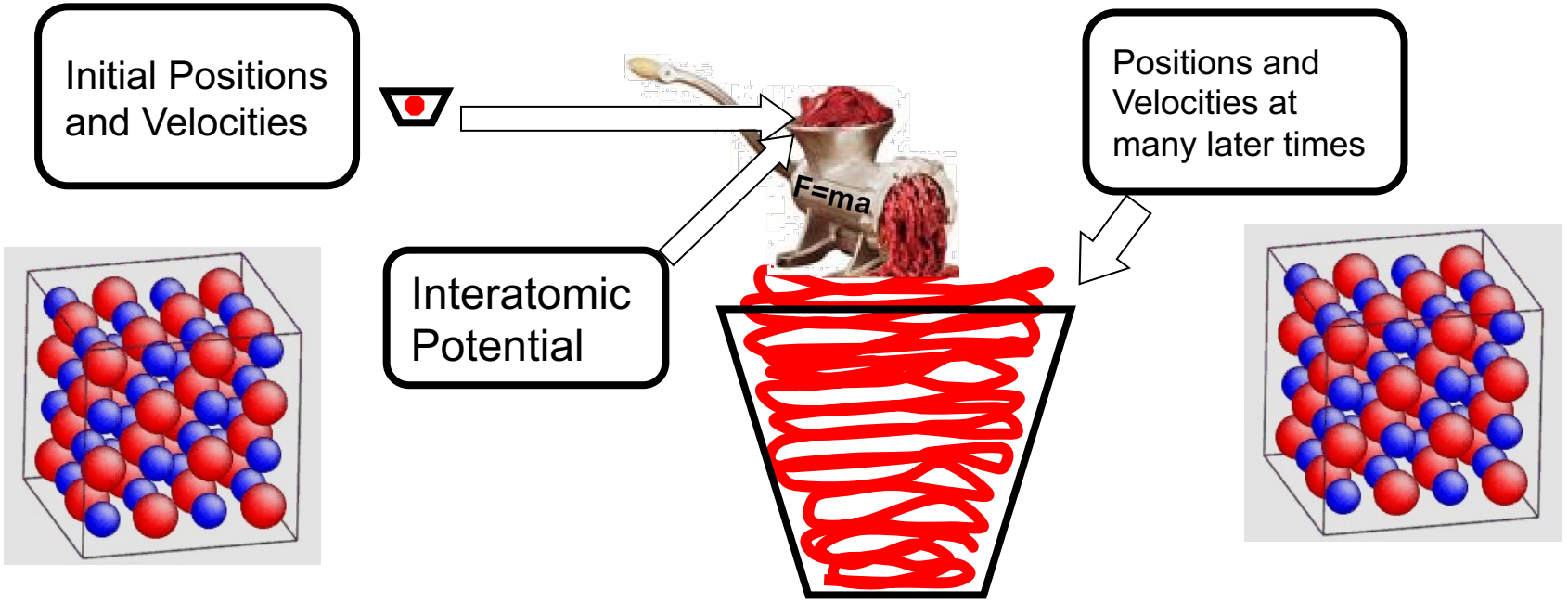
- **Statistical Mechanics:** relates macroscopic observations (such as temperature and pressure) to microscopic states (i.e. atoms)
- **Phase space:** a space in which all possible states of a system are represented. For *N* particles: 6*N*-dimensional phase space (3 position variables and 3 momentum variables for each particle)
- **Ensemble**: an idealization consisting of a large number of virtual copies of a system, considered all at once, each of which represents a possible state that the real system might be in, i.e. a probability distribution for the state of the system

Statistical Mechanics Basics

- **Statistical Mechanics:** relates macroscopic observations (such as temperature and pressure) to microscopic states (i.e. atoms)
- **Phase space:** a space in which all possible states of a system are represented. For *N* particles: 6*N*-dimensional phase space (3 position variables and 3 momentum variables for each particle)
- **B**



Molecular Dynamics: What is it?



Mathematical Formulation

- Classical Mechanics
- Atoms are Point Masses: r_1, r_2, ... r_N
- Positions, Velocities, Forces: r_i, v_i, F_i
- Potential Energy Function = $V(r^N)$
- $6N$ coupled ODEs

Newton's Equations:

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i$$

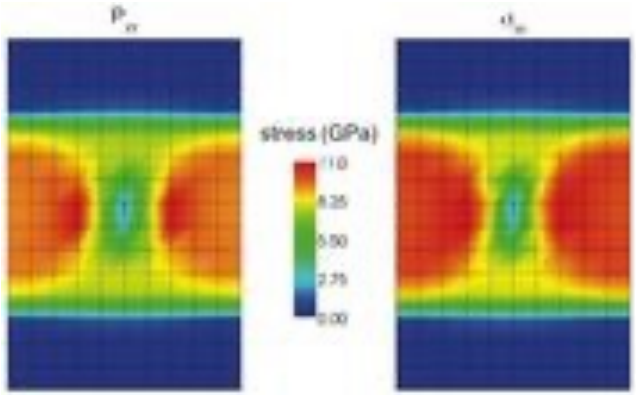
$$\frac{d\mathbf{v}_i}{dt} = \frac{\mathbf{F}_i}{m_i}$$

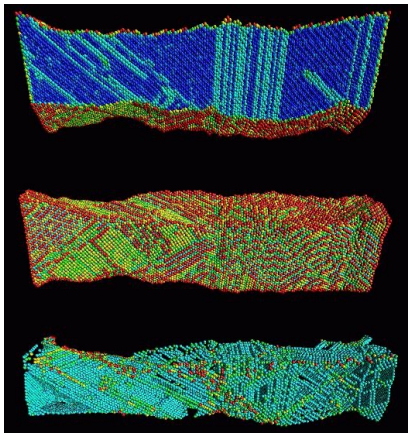
$$\mathbf{F}_i = -\frac{d}{d\mathbf{r}_i} V\left(\mathbf{r}^N\right)$$

MD Versatility

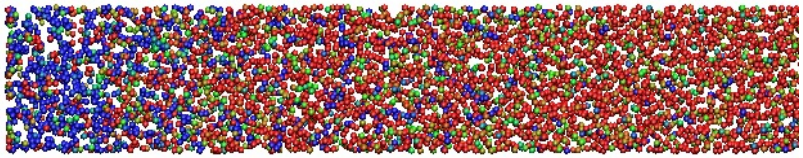
Sandia National Laboratories

Coupling to Solid Mechanics



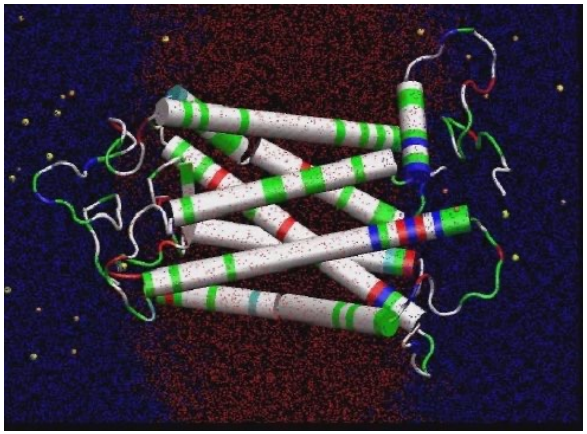


Materials Science

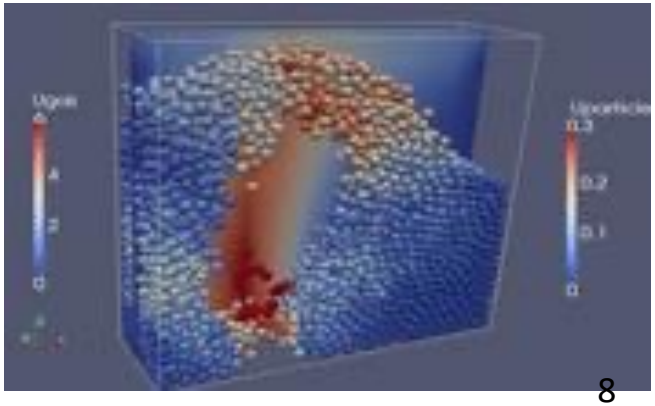


Chemistry

Biophysics

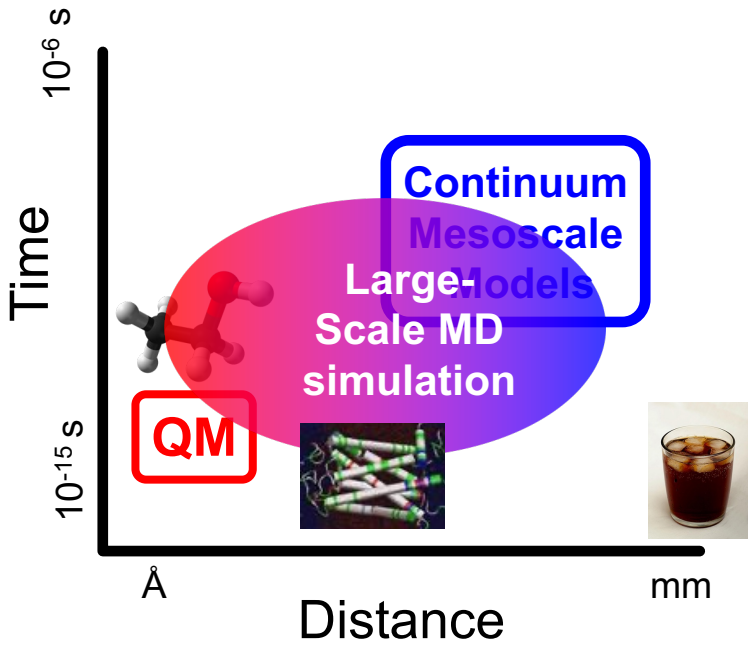


Granular Flow



MD Time & Length Scales

- Quantum mechanical electronic structure calculations (QM) provide accurate description of mechanical and chemical changes on the atom-scale, but limited to ~1000 atoms
- Atom-scale phenomena drive a lot of interesting physics, chemistry, materials science, mechanics, biology…but it usually plays out on a much larger scale
- Mesoscale: much bigger than an atom, much smaller than a glass of soda
- QM and continuum/mesoscale models (CM) can not be directly compared—large scale MD can bridge gap

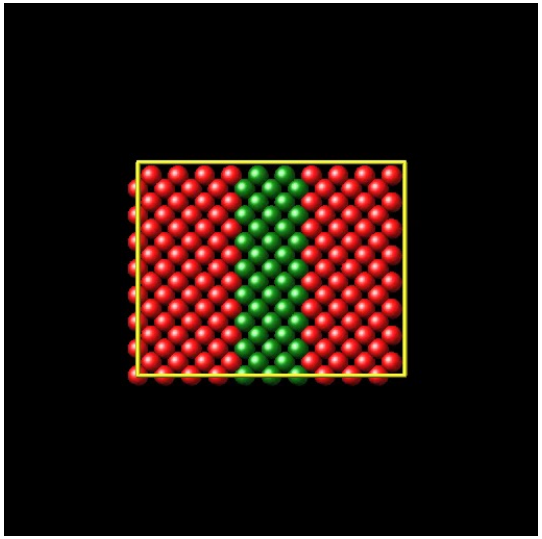


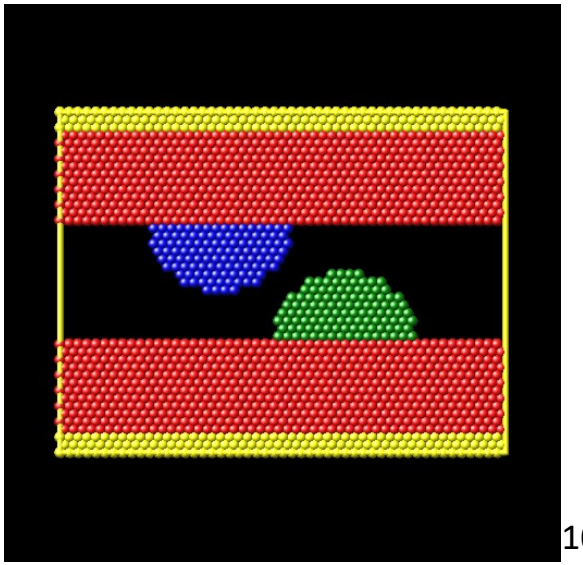
Picture of soda glass: by Simon Cousins from High Wycombe, England - Bubbles, CC BY 2.0, https://commons.wikimedia.org/w/index.php?curid=23020999

MD Basics

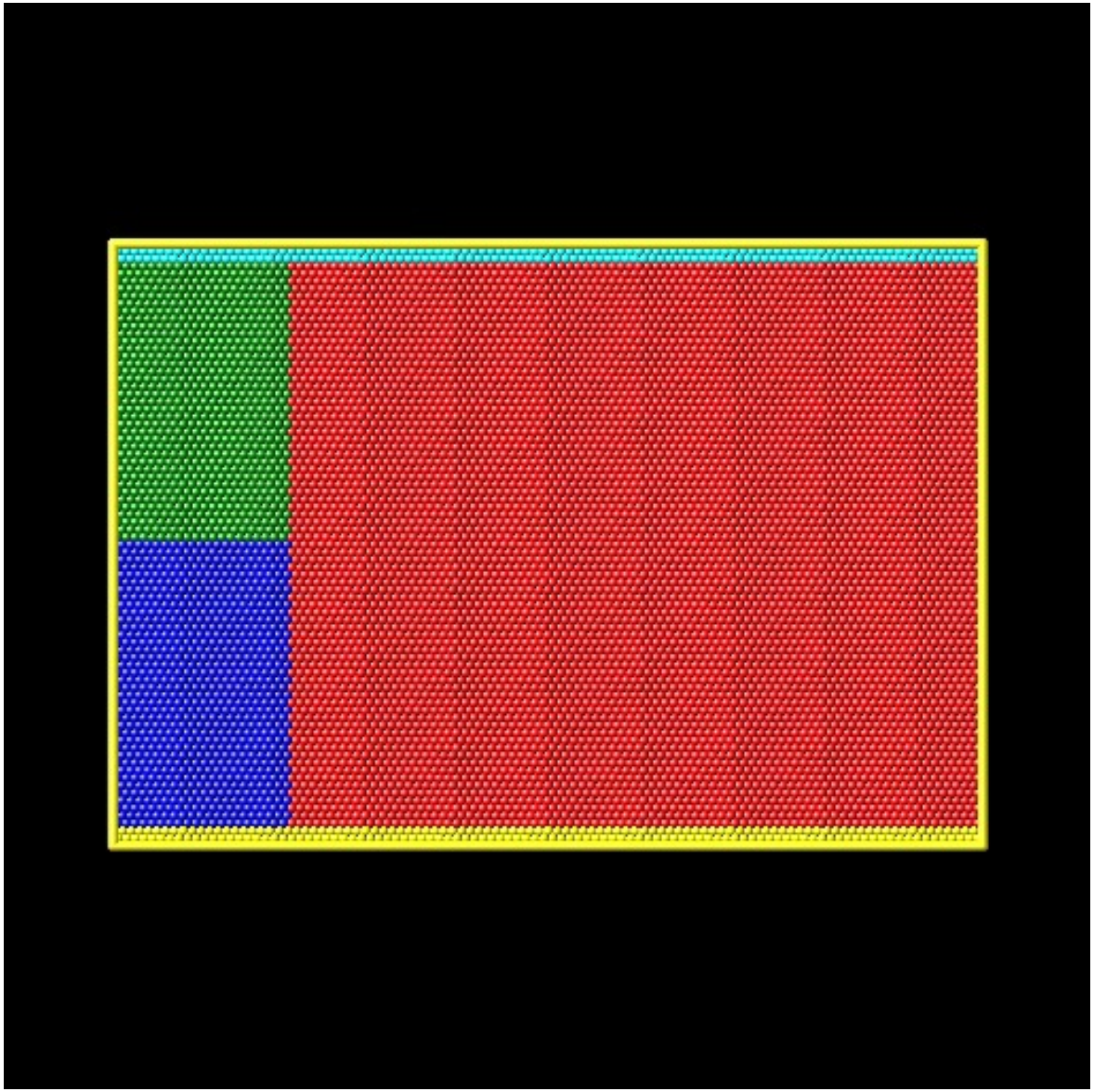
- Atoms can be modeled as points (most common), finite-size spheres, or other shapes (e.g. ellipsoids)
- Can model atomic-scale (all-atom model) or meso/continuum scale with MD-like models
- Typically use an orthogonal or triclinic (skewed) simulation cell
- Commonly use periodic boundary conditions: reduces finite size effects from boundaries and simulates bulk conditions

2D Triclinic



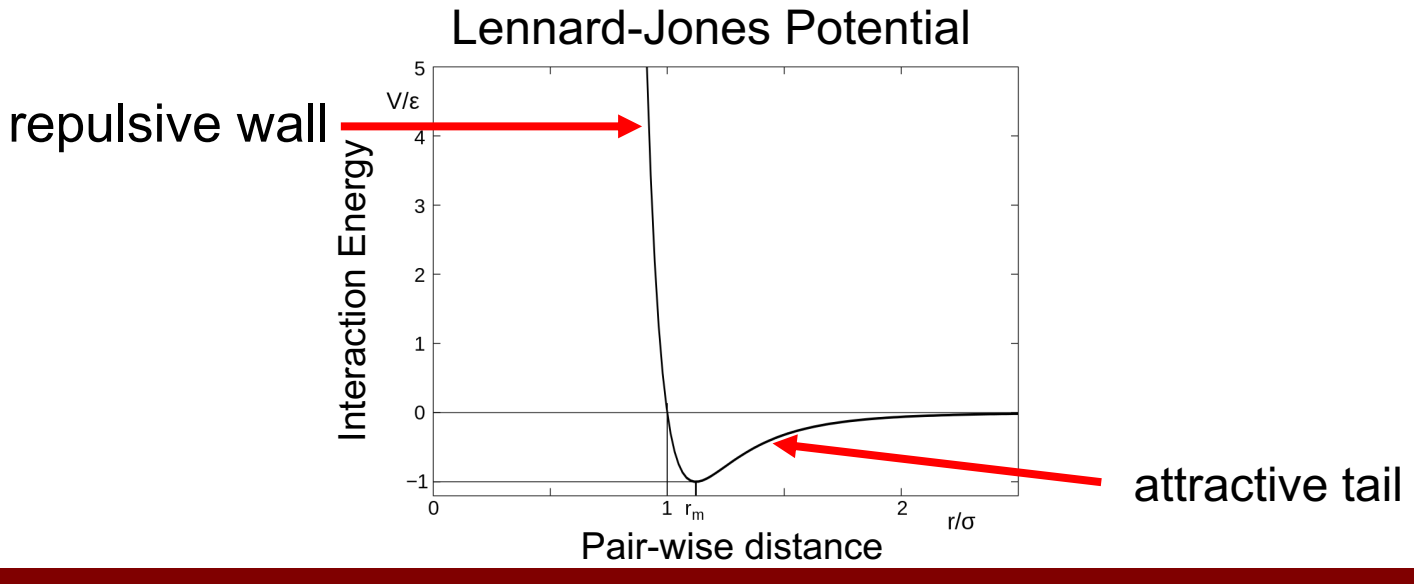


Simple Example: Crack

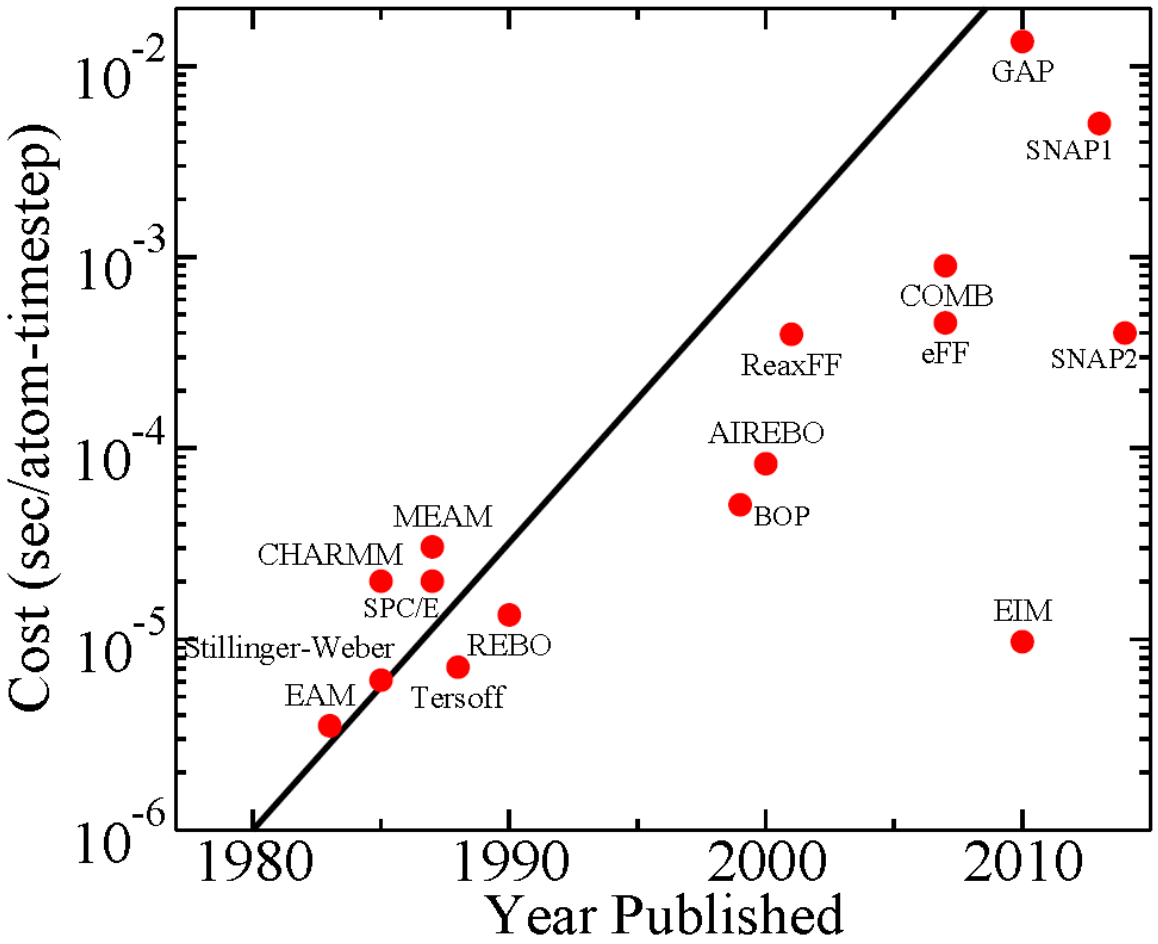


Interatomic Potentials

- Quantum chemistry: solves Schrödinger equation (electron interactions) to get forces on atoms. Accurate but very computationally expensive and only feasible for small systems: ~1000 atoms
- Molecular dynamics: uses empirical force fields, sometimes fit to quantum data. Not as accurate but **much** faster
- MD typically only considers pair-wise or three-body interactions, scales as *O*(N) (billion atom simulations are considered huge)



Accuracy = Higher Cost



Moore's Law for Interatomic Potentials

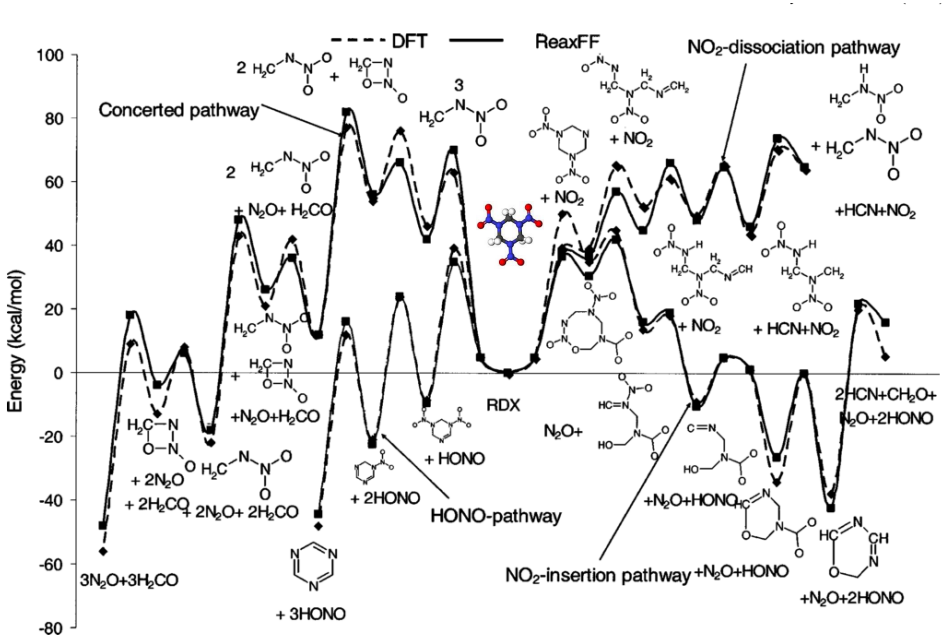
Plimpton and Thompson, MRS Bulletin (2012).

ReaxFF Potential

- Reactive model that captures bond breaking and formation via bond order parameter
- Many complex equations required to capture physics
- Includes charge equilibration model (QEq)

$$BO_{ij} = \exp\left[\rho_\sigma \left(\frac{r_{ij}}{r_0^\sigma}\right)^q_\sigma\right] + \exp\left[\rho_\pi \left(\frac{r_{ij}}{r_0^\pi}\right)^q_\pi\right] + \exp\left[\rho_{\pi\pi} \left(\frac{r_{ij}}{r_0^{\pi\pi}}\right)^q_{\pi\pi}\right]$$

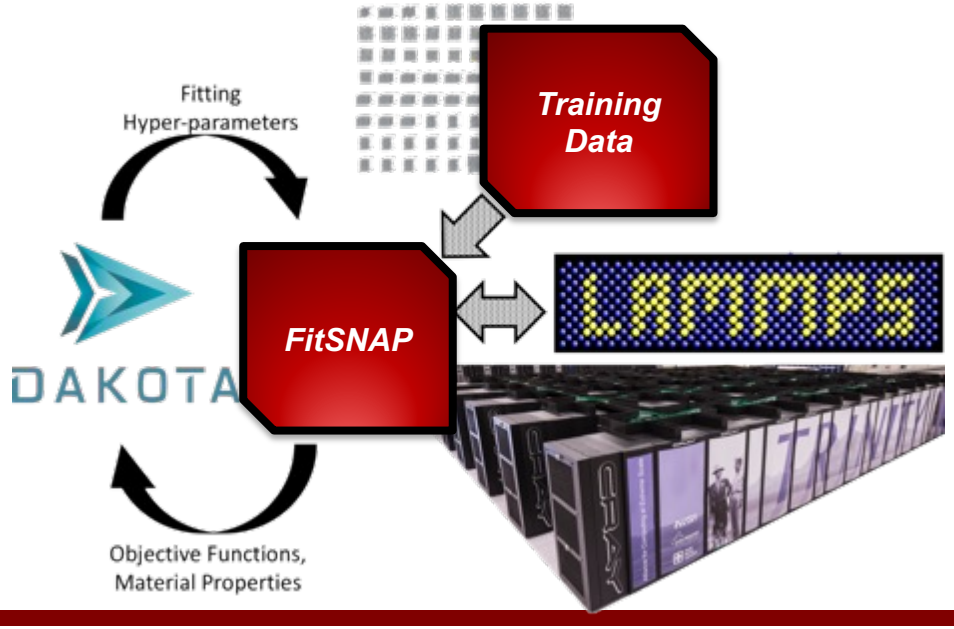
$$E_{system} = E_{bond} + E_{lone\ pair} + E_{over\ coord} + E_{under\ coord} + E_{valence\ angle} + E_{torsion} + E_{conjugation} + E_{H\ Bonds} + E_{vdW} + E_{coulomb}$$



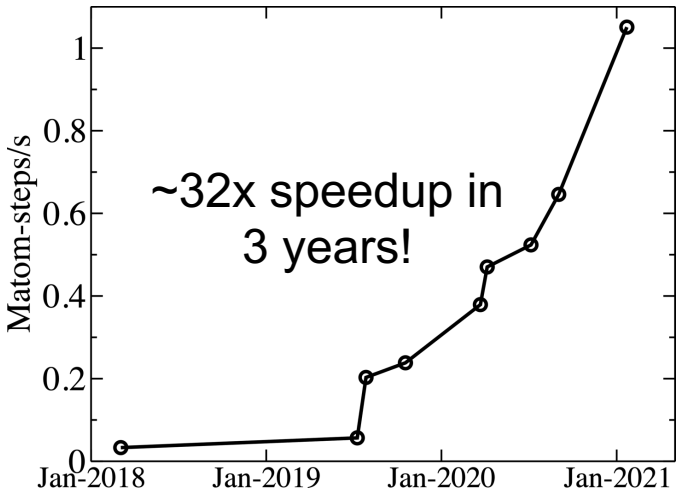
Chenoweth, van Duin and Goddard, J. Phys. Chem. A, 112, 1040-1053 (2008)
Strachan *et al.* J. Chem. Phys. 122, 054502 (2005)
Castro-Marcano *et al.* Combustion and Flame 159(3) 1272-1285 (2012)
Wood, van Duin, Strachan , J. Chem .Phys. A 118, 885 (2014)
Rappe and Goddard, J. Phys. Chem 1991, 95, 3358-3363

SNAP Machine Learning Potential

- ML interatomic potential (IAP) have three critical parts:
  - Descriptors of the local environment
  - Energy and force functions expressed in the descriptors
  - Training (regression method) on large amount of 'ground truth' energies and forces
- Demonstrated *ab initio* accuracy in classical MD!

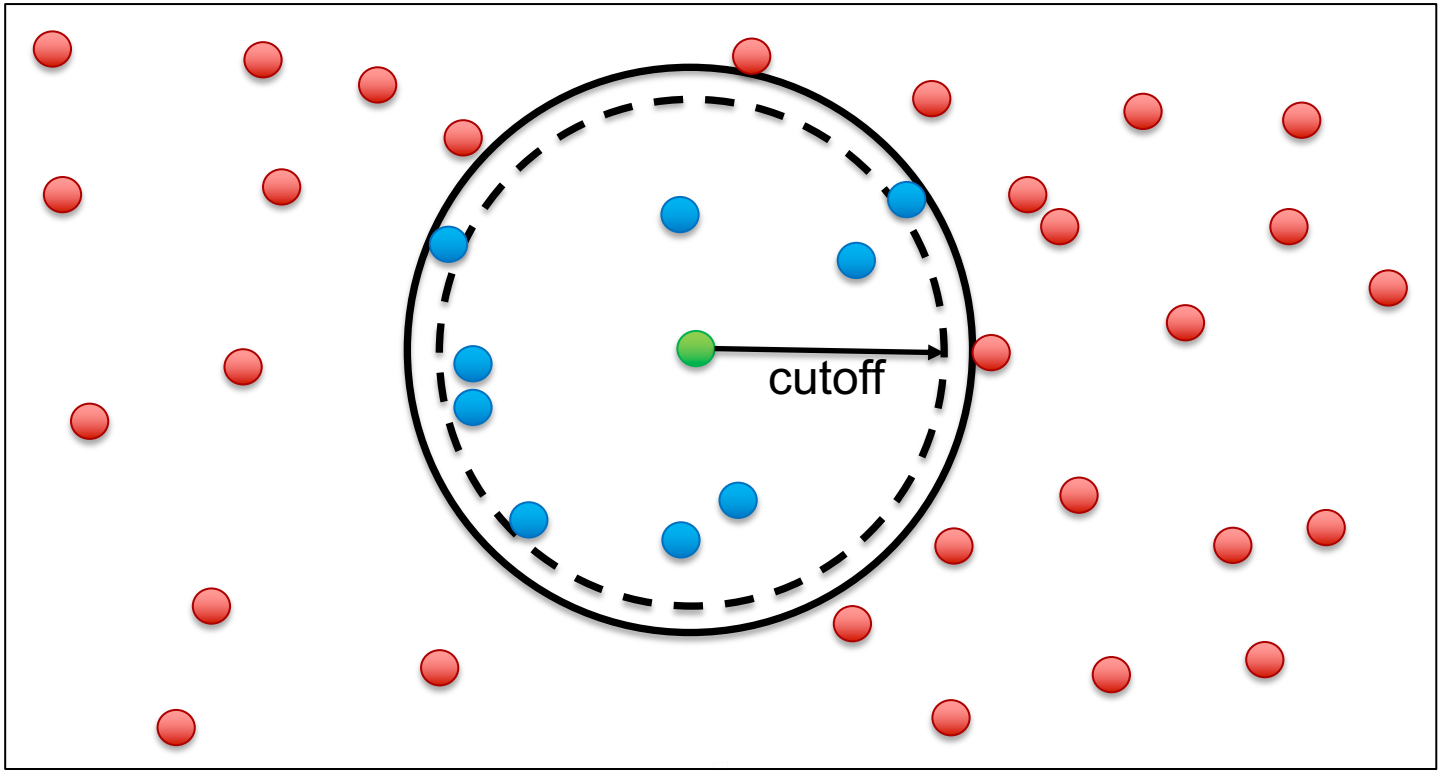


SNAP Performance on V100 GPU



Neighbor Lists

- Neighbor lists are a list of neighboring atoms within the interaction cutoff + skin for each central atom
- Extra skin allows lists to be built less often



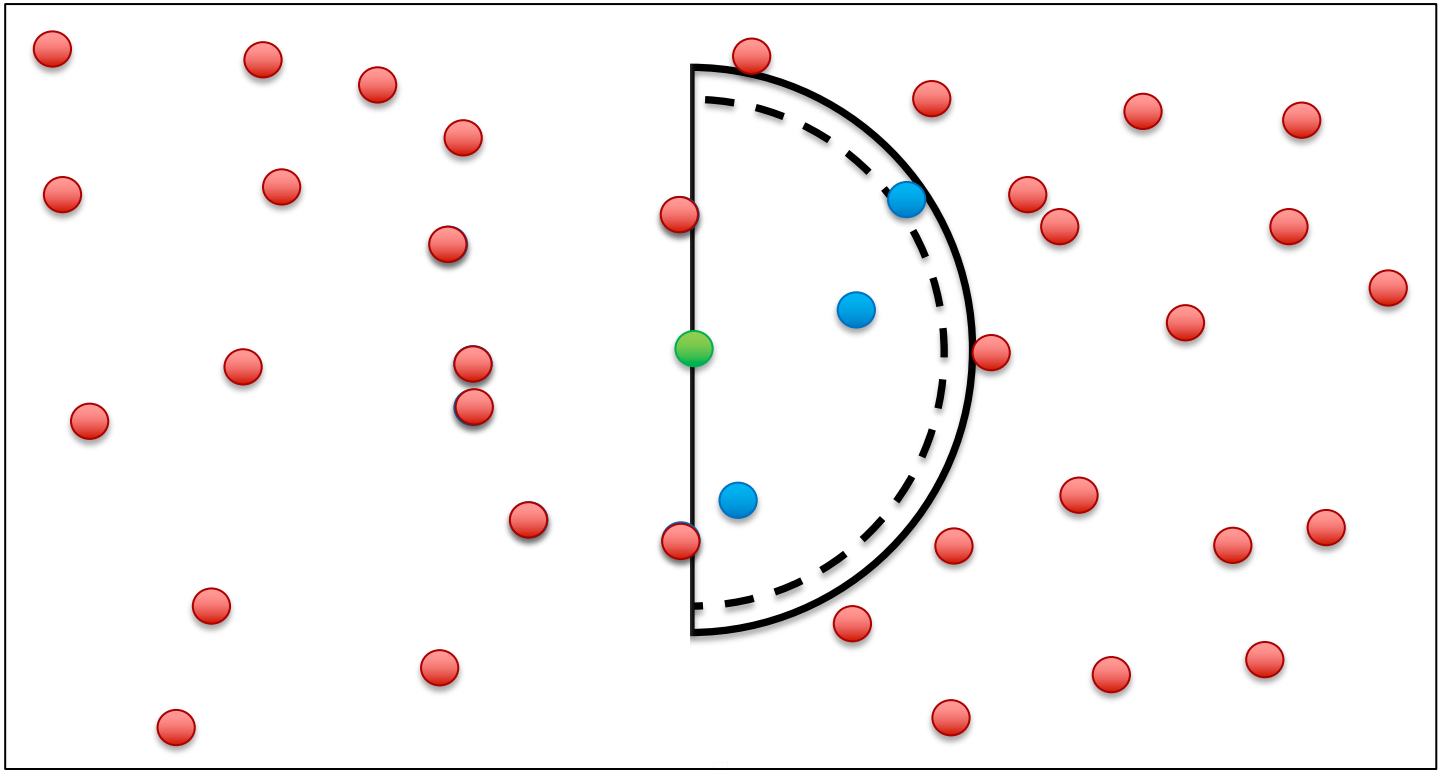
Newton Option

- Newton flag to *off* means that if two interacting atoms are on different processors, **both processors compute their interaction** and the resulting force information is not communicated
- Setting the newton flag to *on* saves computation but increases communication
- Performance depends on problem size, force cutoff lengths, a machine's compute/communication ratio, and how many processors are being used
- Newton off typically better for GPUs

```
newton on
newton off
```

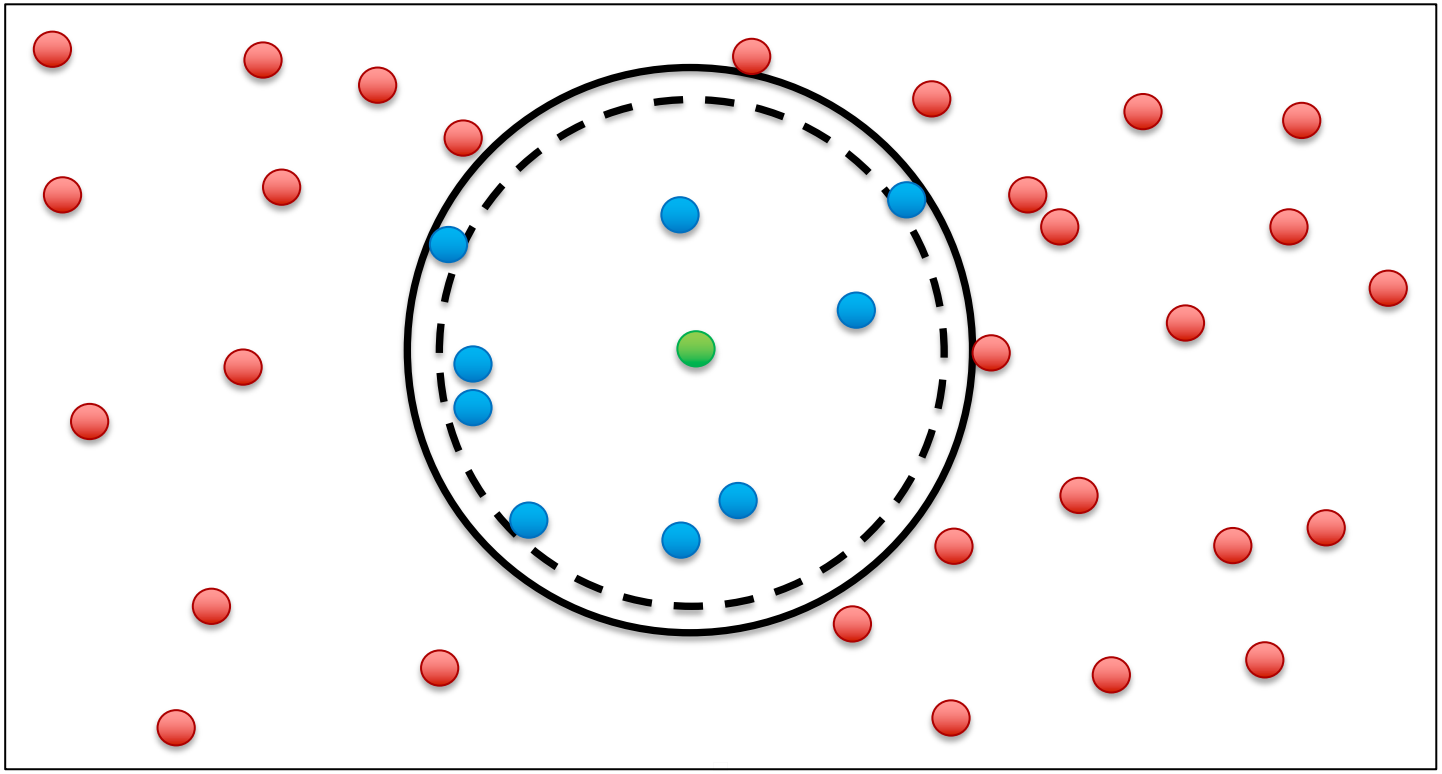
Half Neighbor List

- With newton flag on, each pair is stored only once (usually better for CPUs), requires atomic operations for thread-safety



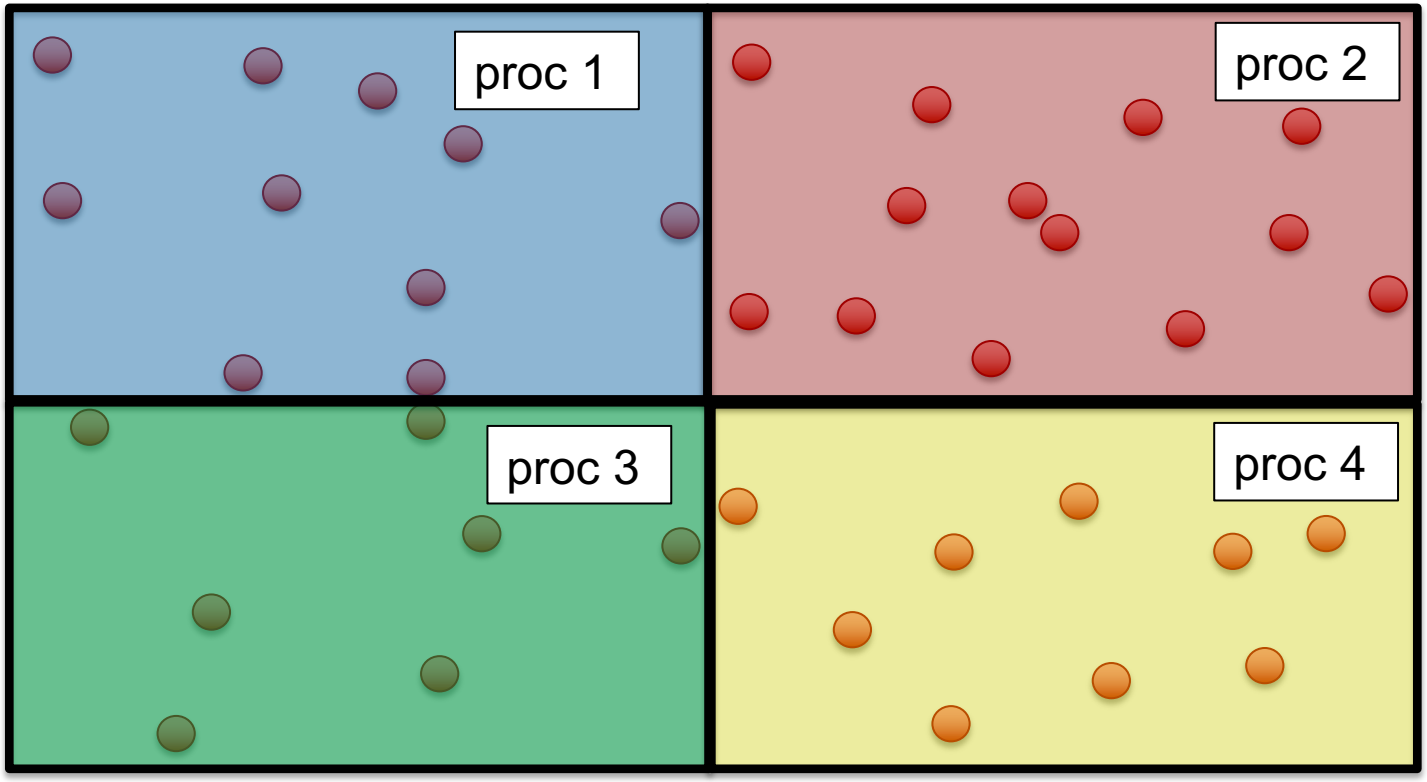
Full Neighbor List

- Each pair stored twice which doubles computation but reduces communication and doesn't require atomic operations for thread safety (can be faster on GPUs)



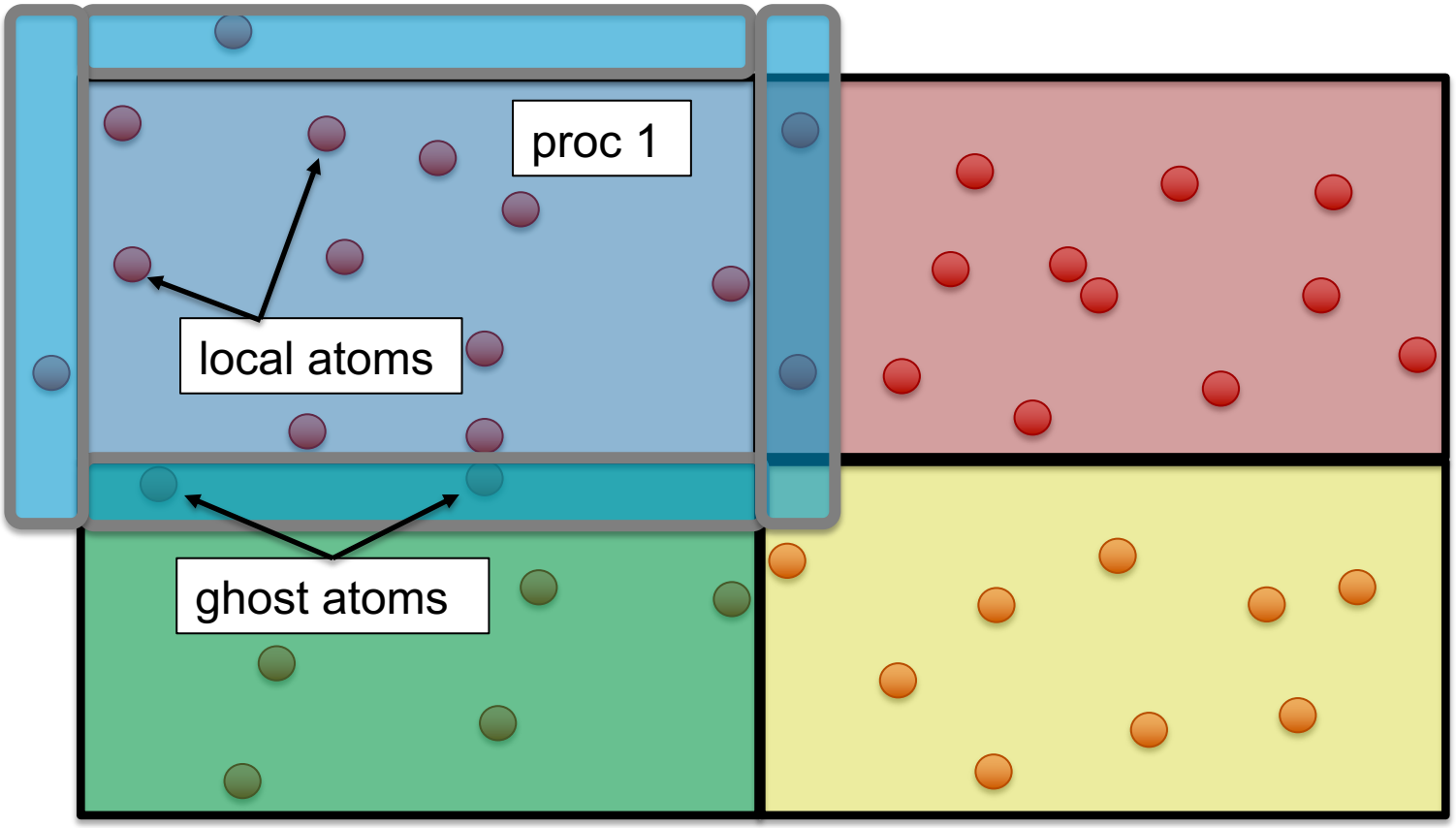
MPI Parallelization Approach

- Domain decomposition: each processor owns a portion of the simulation domain and atoms therein



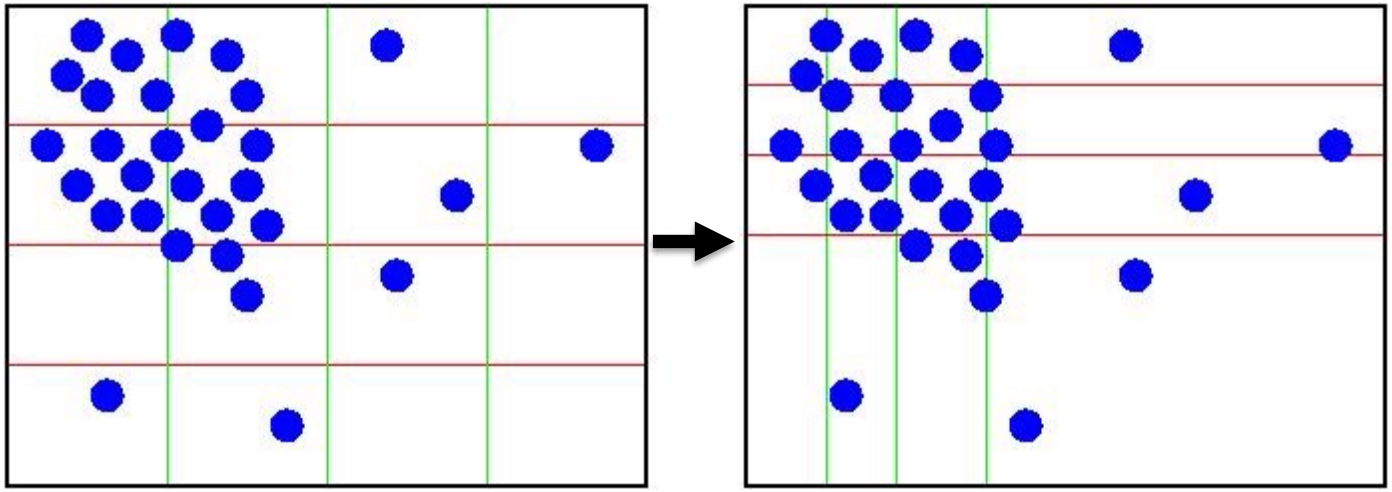
Ghost Atoms

- The processor domain is also extended include needed ghost atoms (copies of atoms located on other processors)
- Communicated via MPI (message passing interface)



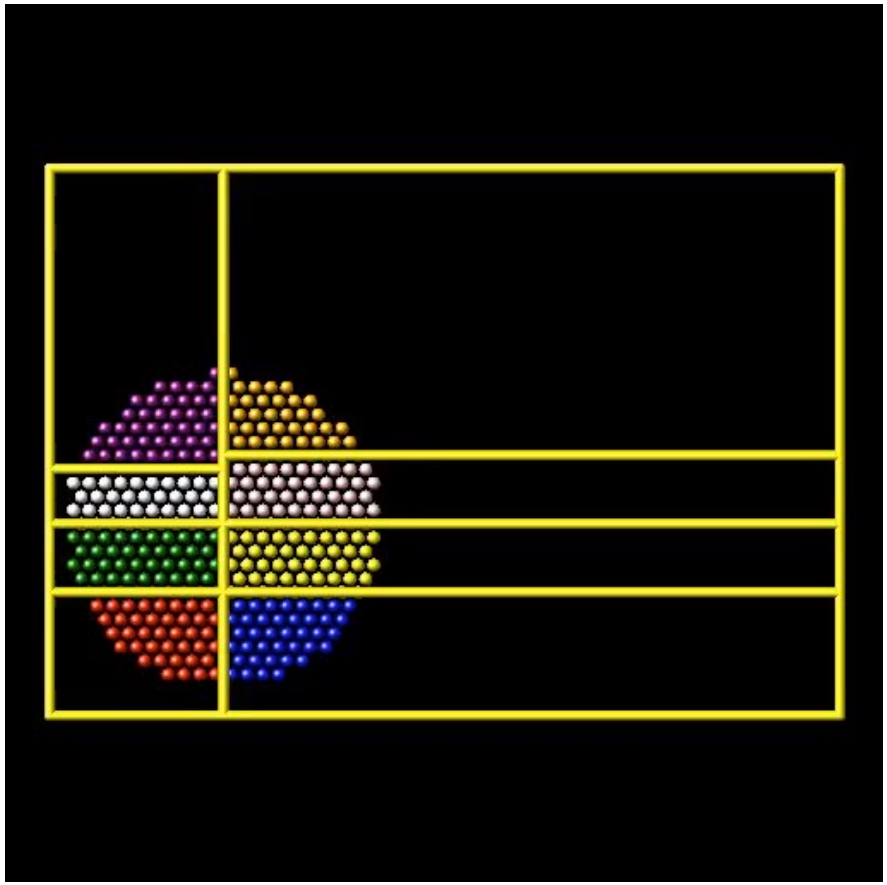
Load-balancing

- Balance (static) and fix balance (dynamic) commands
- "shift" style operates by adjusting planar cuts between processors
- Works well for 1D density variations
  - solid/gas or liquid/gas interfaces
- Less well for general 2D/3D variations



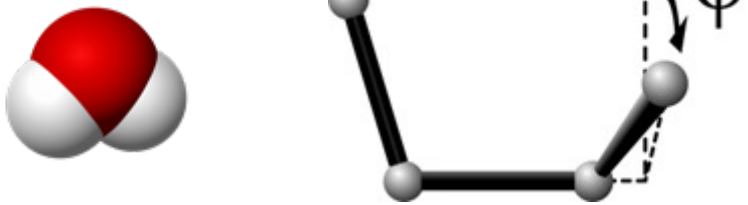
2D and 3D Load-balancing

- “rcb” style is a tiling method, works better for 2D and 3D variations



Molecular Topology

- Bonds: constrained length between two atoms
- Angles: constrained angle between three atoms
- Dihedrals: interactions between quadruplets of atoms
- Impropers: “improper” interactions between quadruplets of atoms




```
bond_style      harmonic
angle_style     charmm
dihedral_style  charmm
improper_style  harmonic
```

Long-Range Electrostatics

- Truncation doesn't work well for charged systems due to long-ranged nature of Coulombic interactions
- Use Kspace style to add long-range electrostatics. PPPM method usually fastest, uses FFTs
- Specify a relative accuracy (i.e. 1e-4)
- Use `pair_style *coul/long` such as `lj/cut/coul/long` instead of `*coul/cut`
- Can vary Coulomb cutoff length and get the same answer

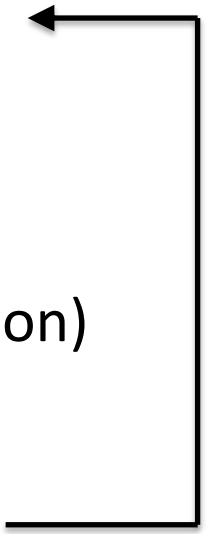
```
pair_style      lj/cut/coul/long 10.0
kspace_style    pppm 1e-4
```

Basic MD Timestep

Sandia National Laboratories

- During each timestep (without neighborlist build):

1. Initial integrate
2. MPI communication
3. Compute forces (pair, bonds, kspace, etc.)
4. Additional MPI communication (if newton flag on)
5. Final integrate
6. Output (if requested on this timestep)



*Computation of diagnostics (fixes or computes) can be scattered throughout the timestep

LAMMPS Files

Sandia National Laboratories

- Input file: text file with LAMMPS commands used to run a simulation
- Log file: text file with thermodynamic output from simulation
- Dump file: snapshot of atom properties, i.e. forces
- Restart file: binary checkpoint file with data needed to restart simulation
- Data file: text file that can be used to start or restart simulation

Downloading LAMMPS

Sandia National Laboratories

- Github (https://github.com/lammps/lammps)
  - https://github.com/lammps/lammps/releases
  - Clone or download button, then download zip file
  - git clone … (beyond this tutorial)
- LAMMPS Website (https://lammps.org)
  - Go to “download” link
  - Download gzipped tar file
- Stable version: rigorous testing
- Development version: still tested but not as rigorous, latest features, performance optimizations, and bug fixes (but could also have new bugs)

Compiling LAMMPS

Sandia National Laboratories

- https://docs.lammps.org/Build.html
- Need C++11 compiler (GNU, Intel, Clang)
- Need MPI library, or can use the “STUBS” library
- Many Makefiles in src/MAKE
- LAMMPS also has CMake interface

Running LAMMPS

- https://docs.lammps.org/Run_basics.html
- Basic syntax: `[executable] -in [input_script]`
- In serial:

```
./lmp_serial -in in.lj
```

- In parallel:

```
mpirun -np 2 lmp_mpi -in in.lj
```

- Many other command line options, see https://docs.lammps.org/Run_options.html

Optional Packages

- https://docs.lammps.org/Packages_list.html
- LAMMPS is very modular and has several optional packages
- For example, SNAP potential needs ML-SNAP package installed

Traditional Make:

```
make yes-ml-snap
make no-ml-snap
```

CMAKE:

```
-D PKG_ML-SNAP=yes
```

Accelerator Packages

Sandia National Laboratories

- https://docs.lammps.org/Speed_packages.html
- Some hardware components like GPUs, and multithreaded CPUs require special code (i.e. OpenMP, CUDA) to fully take advantage of the hardware
- LAMMPS has 5 accelerator packages:
  - OPENMP
  - INTEL
  - OPT
  - GPU
  - KOKKOS

Running OPT Package

- 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

Sandia National Laboratories

- 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 code

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 CPUs (with or without OpenMP threading)
- Can also be used in conjunction 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

Sandia National Laboratories

- 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
- Provides NVIDIA and more general OpenCL support
- Supports reduced precision: mixed FP64+FP32 or pure single FP32

Running GPU Package

- 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`
- Best to use CUDA MPS (Multi-Process Service) if using multiple MPI ranks per GPU
- Automatically overlaps pair-style on GPU with Kspace on CPU

Kokkos

Sandia National Laboratories

- 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

Sandia National Laboratories

- https://docs.lammps.org/Speed_kokkos.html
- **Need C++14 compiler**
- Supports OpenMP and GPUs
- Designed so that everything (pair, fixes, computes, etc.) runs on the GPU, minimal data transfer from GPU to CPU
- GPU 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

Sandia National Laboratories

- 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

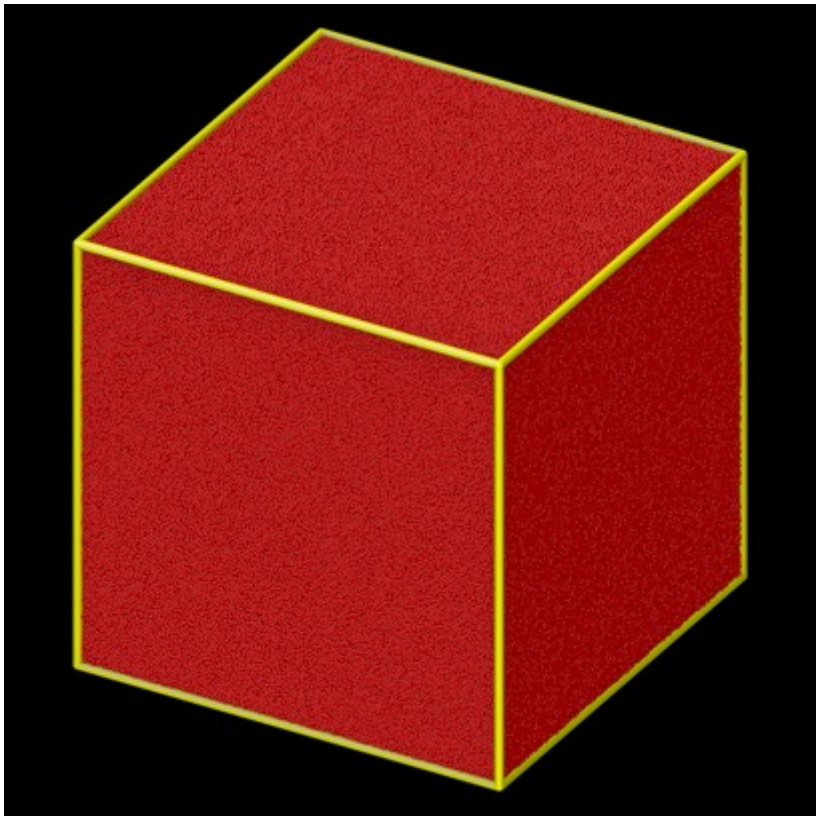
Sandia National Laboratories

- 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

Lennard-Jones Benchmark

Sandia National Laboratories

- lammps/bench/in.lj
- Simple pair-wise model
- Similar to argon liquid/gas

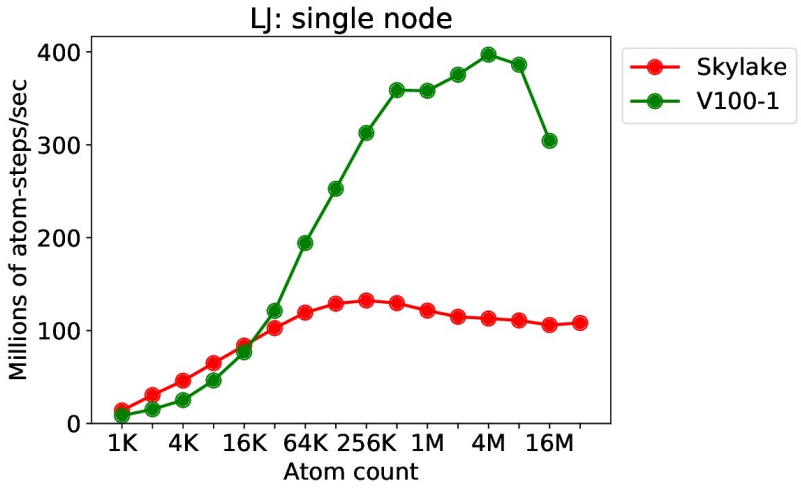


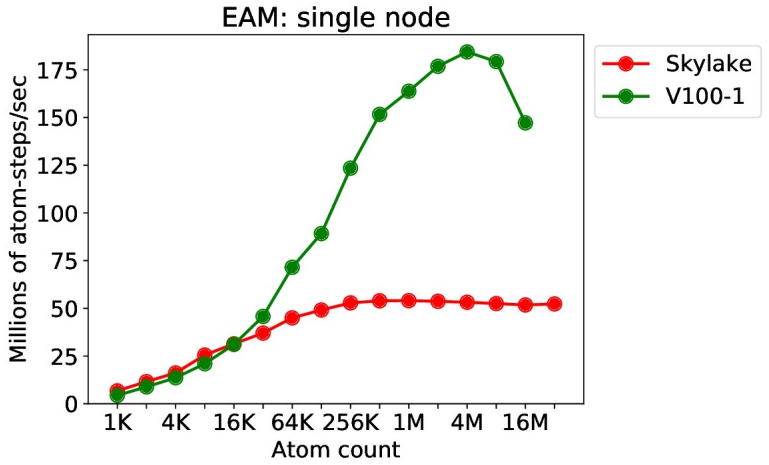
Measuring performance

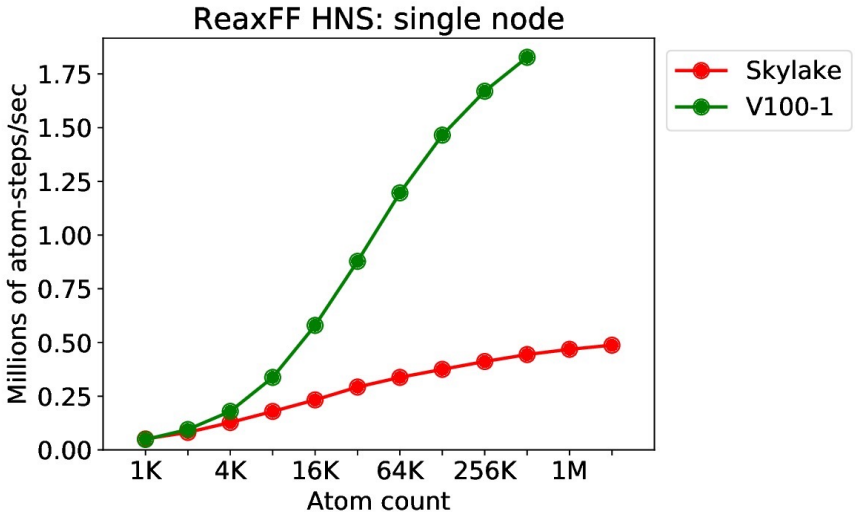
```
Loop time of 0.0174524 on 640 procs for 100 steps with 32000 atoms

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
```

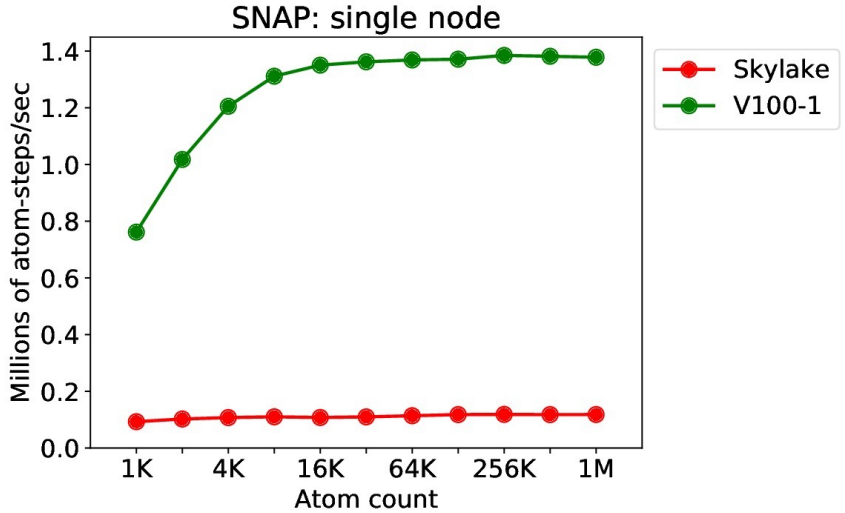
- For KOKKOS package on GPUs, timing breakdown won't be accurate without CUDA_LAUNCH_BLOCKING=1 (but will prevent kernel overlap and could slow down simulation)

Performance of Different Potentials









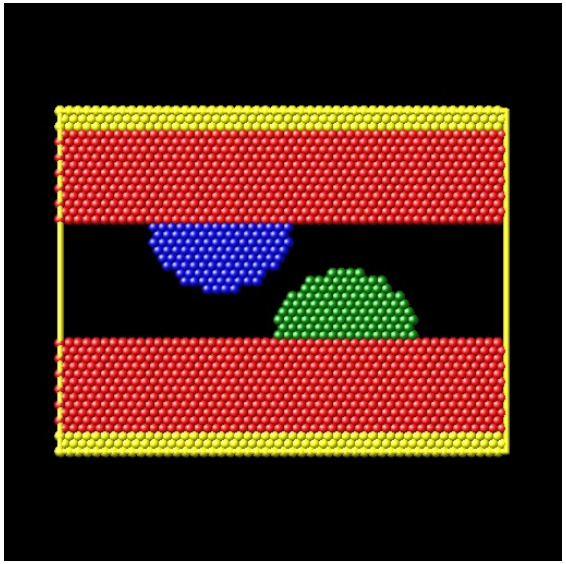
Parallel MD Performance

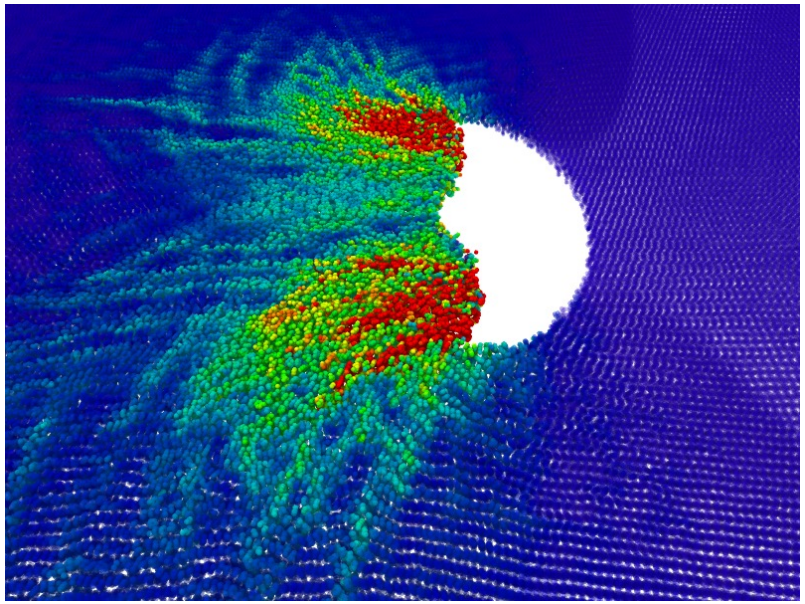
Sandia National Laboratories

- 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

Visualization Resources

- LAMMPS “dump image” command: https://docs.lammps.org/dump_image.html
- VMD: https://www.ks.uiuc.edu/Research/vmd/
- OVITO: https://www.ovito.org/about/ovito-pro/





Getting Help

- Look at LAMMPS documentation, latest version here: https://docs.lammps.org/Manual.html
- Search the MatSci LAMMPS forum archives https://matsci.org/lammps or join and post new questions
- LAMMPS reference paper: gives an overview of the code including its parallel algorithms, design features, performance, and brief highlights of many of its materials modeling capabilities https://doi.org/10.1016/j.cpc.2021.108171

Thank You

Sandia National Laboratories

Questions?