Atomify app: LAMMPS on an iPhone or Android
Google for “app store atomify lammps” - Wed AM talk
Welcome and What’s New in LAMMPS

Steve Plimpton
Sandia National Labs
sjplimp@sandia.gov

5th LAMMPS Workshop and Symposium
August 2017 - Albuquerque, NM
Thanks

- **Logistics:** Phyllis Rutka and Christine Trujillo
- **Tutorials:** Matt Lane, Aidan Thompson, Richard Berger, Anders Hafreager
- **Breakouts:** Ray Shan, Mark Stevens, Dan Bolintineanu, Jeff Greathouse, Pieter in ’t Veld, Mitch Wood, Stan Moore
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- **JSOL and Materials Design** - providing lunches!
- **Scienomics** - providing snacks and drinks!
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- **Invited speakers**
  - George Karniadakis *(Brown)*, **keynote**
  - Nir Goldman *(LLNL)*
  - Amalie Frischknecht *(Sandia)*
  - Tim Mattox *(Engility)*
  - Ale Strachan *(Purdue)*
  - Danny Perez *(LANL)*
  - Mike Chandross *(Sandia)*
One invited speaker has an unusual skill

Walter White, chemist
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Mike Chandross, physicist
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Winner

2012 Walter White look-alike contest
Social activities
August is a hot or stormy month to visit ABQ and NM!
Thanks to our user community

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- Attendees from **other countries** (registration list)
  - Australia, Brazil, Canada, Chile, China, England, Germany, India, Israel, Japan, Netherlands, Norway, South Korea, Turkey
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- Please talk to LAMMPS developers whenever/wherever you can find us. Or just send us an email.
New interatomic potentials (pair styles)

- **MGPT** from first-principles quantum DFT
  - Tomas Oppelstrup & John Moriarty (LLNL)
  - simplified model for generalized pseudopotential theory
  - d-band transition metals

- **SMTBQ** tight-binding model
  - Nicolas Salles, Emile Maras, Olivier Politano, Robert Tetot (LAAS-CNRS, France)
  - second moment tight-binding with QEq
  - metal oxides

- **Vashishita** 3-body potential
  - Yongnan Xiong (Hunan U)
  - Coulombics and bond-angle energies
  - inorganic compounds

- **Gao-Weber** 3-body potential
  - German Samolyuk (ORNL)
  - Si and C, also ZBL option
New optimized versions of popular potentials

**MEAM**
- Sebastian Hutter (Otto-von-Guericke U, Germany)
- MEAM/C version of Fortran MEAM potential
- can now be used with pair hybrid

**ReaxFF**
- Kokkos version:
  - Ray Shan (Materials Design) & Stan Moore (Sandia)
- OpenMP version: Metin Aktulga (MSU)
- faster, more memory efficient, more robust

**CHARMM + CMAP**
- Robert Latour (Clemson U) and collaborators
- new fix cmap command for CHARMM 5-body interactions
- new versions of CHARMM pair styles (cut and long)
  - that exactly match current CHARMM ff
New USER-DPD package

- Jim Larentzos, Tim Mattox, John Brennan (ARL and Engility Corp)
- Dissipative particle dynamics for energetic materials
- DPD for solids and reactions (!)
- Energy-conserving integrators for NVE, NVT, NPT
- 10000× speed-up vs all-atom models due to length/time scales

- Shock wave thru 40×40×2500 nm³ polycrystalline sample
- Wed AM talk by Tim
New USER-MANIFOLD package

- Stefan Paquay & Remy Kusters
  (Eindhoven U of Tech, Netherlands)
- Constrained motion on arbitrary 2d surface (manifold)
- User can define new manifolds
New USER-CGDNA package

- Oliver Henrich (U Strathclyde and U Edinburgh, UK)
- Coarse-grained DNA model
- Simulate sequence-specific strands
- Setup tools for single- and double-helices

Automated installation of external libraries

- Some packages require pre-build of provided or external libraries
- See lammps/lib in distro: atc, colvars, kim, mscg, voronoi, etc
- All of them now have an **Install.py** script
- Can download, install, build external libs this way
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KIM example:

```
make lib-kim      # see help
make lib-kim args="-b . OpenKIM"  # all models
make yes-kim
make mpi
```
Weighting options for dynamic load balancing

- Axel Kohlmeyer (Temple U)
- Geometric balance of particle count per processor
- Can now weight particles based on CPU time, group, neighbor count, or per-atom variable
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2d SPH “water” flowing over a dam
Georg Ganzenmueller (Ernst Mach Institute, Germany)
Granular models: normal/tangential forces, friction, history
- Geometric regions become boundaries on granular particles
- Regions can move or rotate
- Enabled by new fix wall/gran/region command
LAMMPS app for your phone

- Anders Hafreager (U Oslo, Norway)
- Wed AM talk, right before lunch
- Atomify app, available from Apple app store
- iOS or Android (phone), Mac, or browser
- On-the-fly high-quality viz and plotting
- Edit script parameters

Why run molecular dynamics on a phone?

At least two uses:
1. Give a this-is-what-I-do elevator speech to your boss or funder
2. Stress-test your cell phone battery
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Development via GitHub

- https://github.com/lammps/lammps
- Axel Kohlmeyer & Richard Berger (Temple U)
- Preferred way to report bugs & submit new code
- Great way to stay current with LAMMPS distro
- Entire tutorial on it this AM, see PDFs

More ways to invoke Python code from your input script

- Richard Berger (Temple U), Wed AM talk
- variable python, pair python, fix python
- see doc/Section_python.html for details
New and enhanced features (2)

- **Fix controller** command
  - Aidan Thompson (Sandia)
  - control loop with feedback (PID)
  - adjust one parameter, monitor another
  - zoom in on melting temperature
  - adjust pressure via wall position

- **NEB** command for barrier heights
  - now allow multiple MPI tasks per replica
  - Emile Maras (CEA, France) added options for more efficient inter-replicas forces and first/last replicas
New and enhanced features (3)

- Coupling LAMMPS to quantum codes
  - Two density-function tight-binding codes
  - DFTB+, Nir Goldman (LLNL), Tues PM talk
  - LATTE, Christian Negre (LANL), Thurs AM talk
  - plans for NWChem and possibly VASP, already QE

- Fix mscg command
  - Lauren Abbott (Sandia) & Jacob Wagner (U Chicago)
  - enables use of Voth group MSCG library to fit CG potentials
  - Soft matter breakout

- Fix halt command
  - stop a simulation run based on evaluated variable criterion
Coming attractions (1)

- **Body-style** aspherical granular particles
  - Trung Nguyen (Northwestern U)
  - 2d and 3d rounded polygon Langston potentials
Stan Moore, *Performance breakout*

Supported hardware via 5 acceleration packages:
- CPUs: Vanilla, OPT, USER-OMP, Intel/CPU, Kokkos/OMP
- KNLs: Intel/KNL, Kokkos/KNL
- GPUs: GPU, Kokkos/Cuda

Goal of webpage: help users run as fast as possible

Give the details:
- several benchmark problems on several machines
- how LAMMPS was built (makefiles) with packages
- how each package was run (mpirun and LAMMPS options)
- tarballs with input/output files

Plots and Tables:
- best performance of any package on different hardware
- relative performance of packages on CPU or KNL or GPU

For each plot, each curve, each data point:
- launch command used
- link to logfile produced
Stan Moore, Performance breakout

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  - Christoph Junghans (LANL) & Richard Berger (Temple U)
  - short talk in Developers breakout

- **Fix react** command
  - Jake Gissinger (U Colorado), Tues PM talk
  - define before/after local bond topology for a reaction
  - define criteria for reaction to take place
  - optionally relax system after reaction occurs

- **Global and local hyperdynamics**
  - in collaboration with Art Voter & Danny Perez (LANL)
  - new hyper, fix hyper/global, fix hyper/local commands
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- Come to Developers breakout for more details