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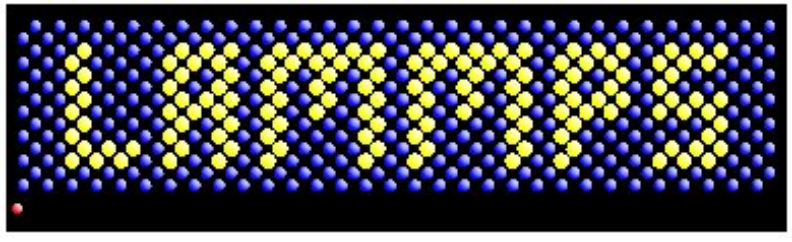
5th LAMMPS Workshop and Symposium
August 2017 - Albuquerque, NM



Center for Computing Research

Sandia National Laboratories

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National Nuclear Security Administration

Thanks

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- Tutorials: Matt Lane, Aidan Thompson,
  Richard Berger, Anders Hafreager
- Breakouts: Ray Shan, Mark Stevens, Dan Bolintineanu,
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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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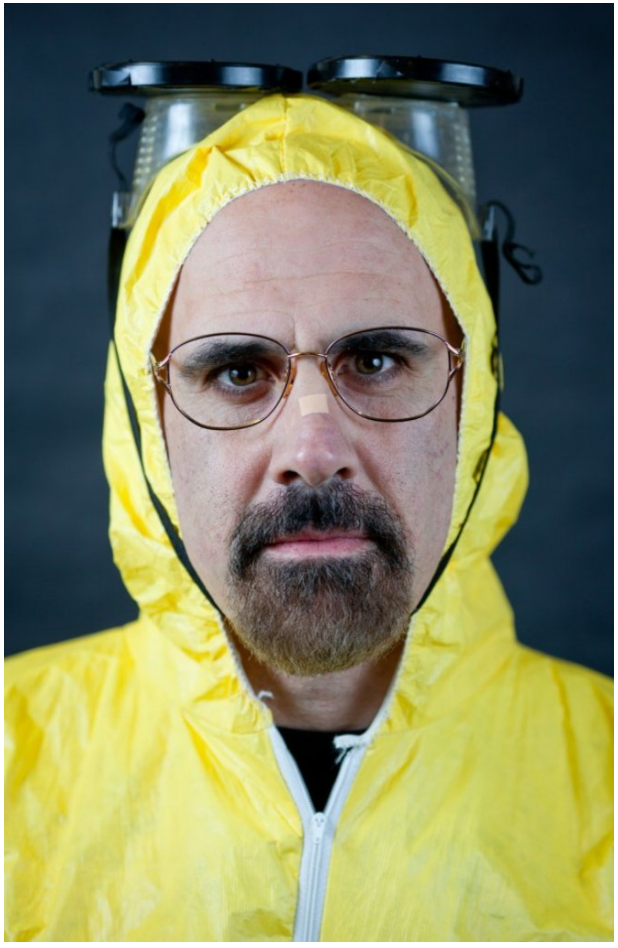
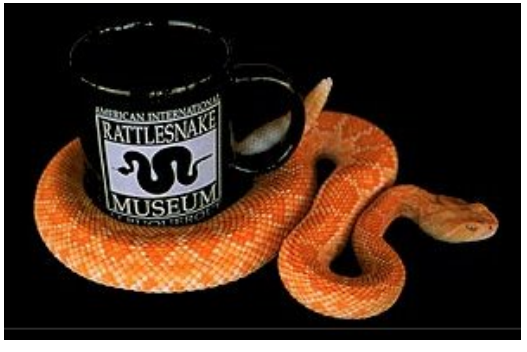


Winner
2012 Walter White look-alike contest

Social activities



Thanks to our user community

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  - 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)

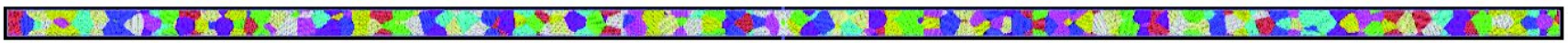
- MGPT from first-principles quantum DFT
  - Tomas Oppelstrup & John Moriarty (LLNL)
  - simplified model for generalized pseudopotential theory
  - d-band transition metals
- SMTBQ tight-binding model
  - Nicolas Salles, Emile Maras, Olivier Politano, Robert Tetot (LAAS-CNRS, France)
  - second moment 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

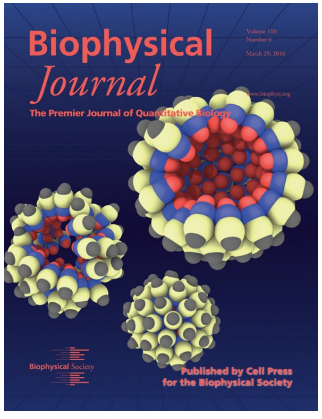
- Jim Larentzos, Tim Mattox, John Brennan
  (ARL and Engility Corp)
- Dissipative particle dynamics for energetic materials
- DPD for solids and reactions (!)
- Energy-conserving integrators for NVE, NVT, NPT
- 10000x speed-up vs all-atom models due to length/time scales

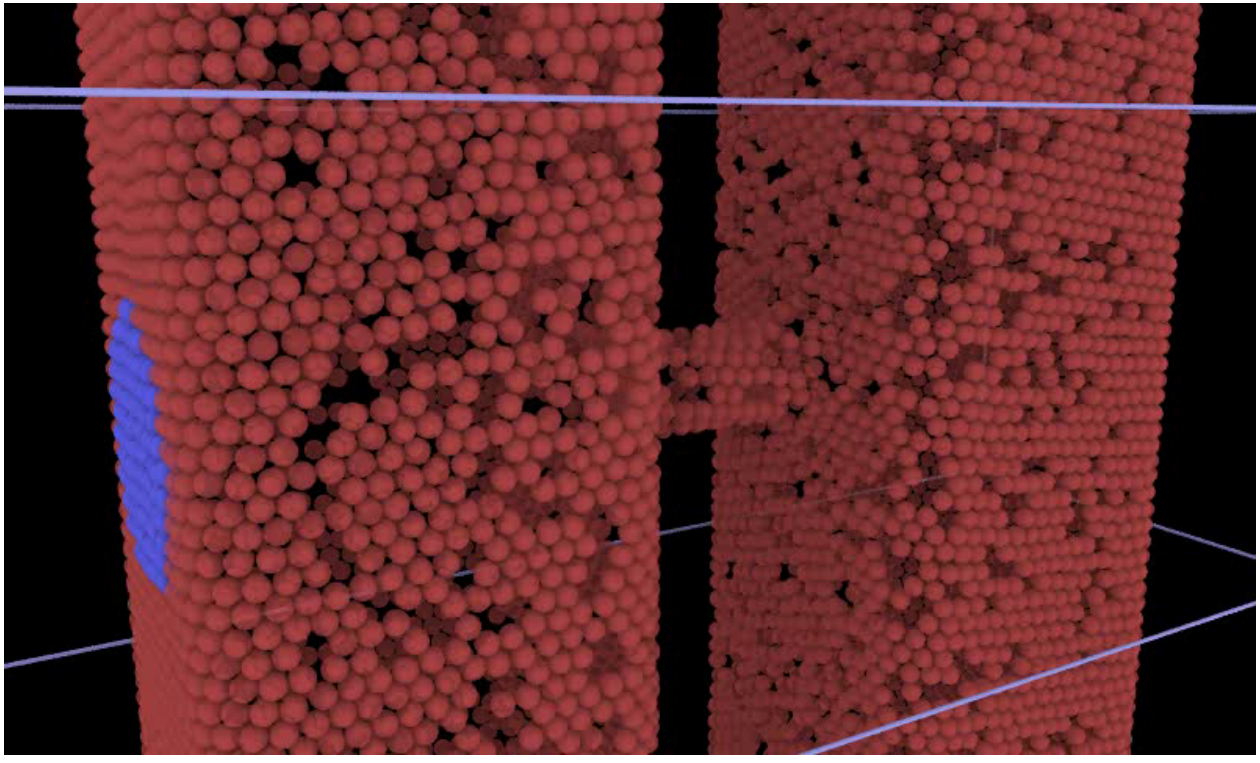


- Shock wave thru 40x40x2500 nm^3 polycrystalline sample
- Wed AM talk by Tim

New USER-MANIFOLD package

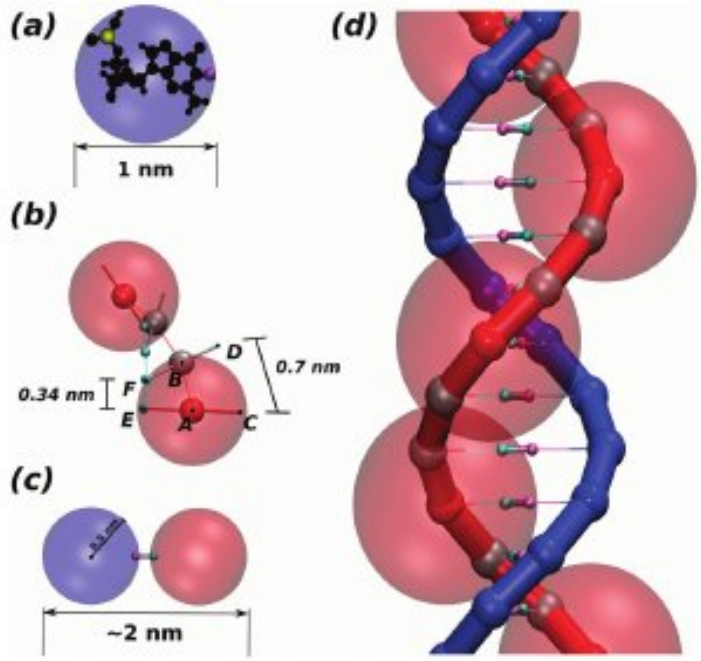
- Stefan Paquay & Remy Kusters
  (Eindhoven U of Tech, Netherlands)
- Constrained motion on arbitrary 2d surface (manifold)
- User can define new manifolds





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



- *Fosado & Henrich, et al, Soft Matter, 12, 9458 (2016).*

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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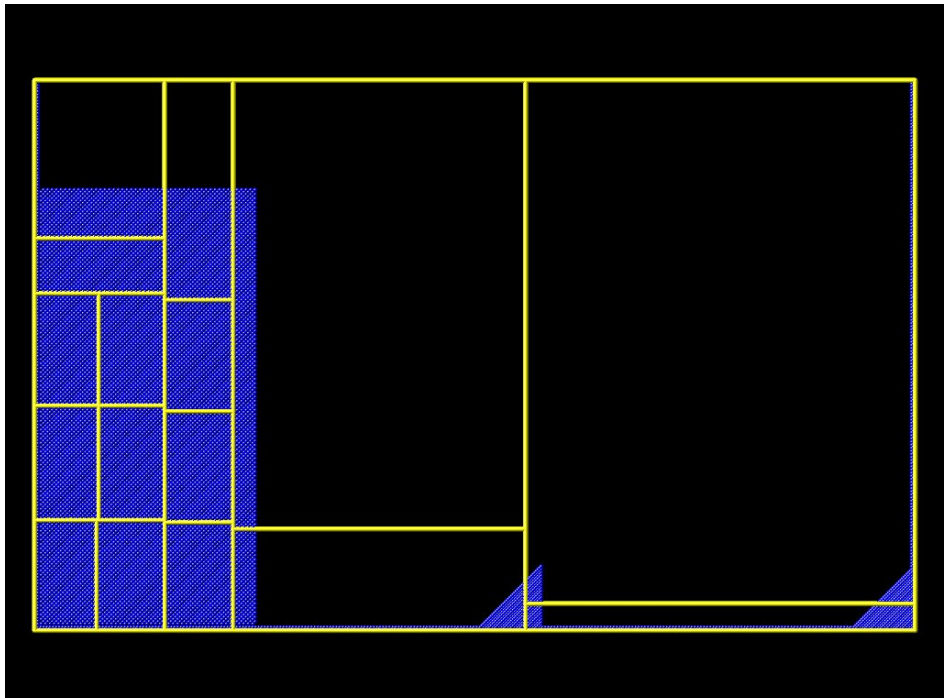
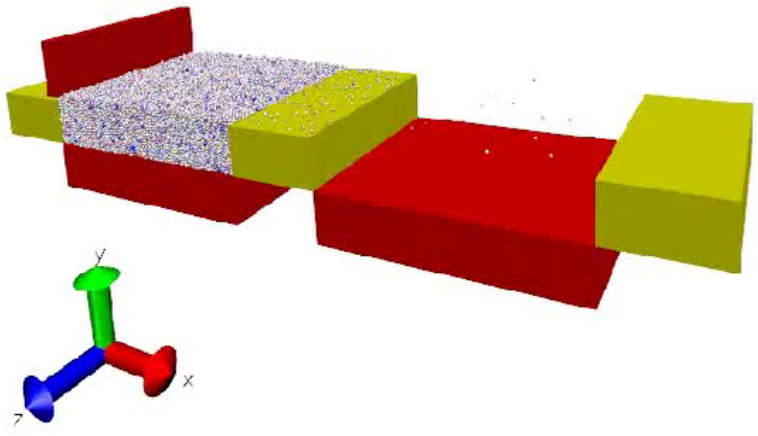
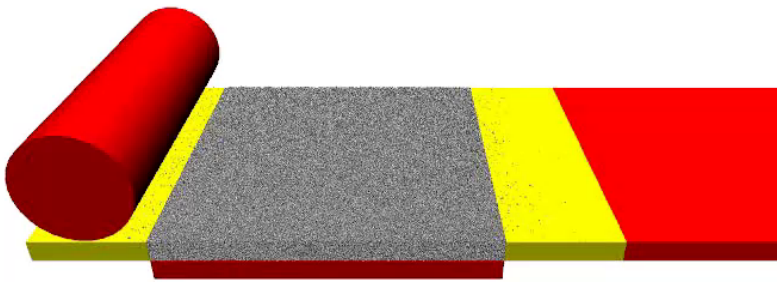
2d SPH "water" flowing over a dam
Georg Ganzenmueller (Ernst Mach Institute, Germany)



Additive manufacturing with granular materials

Dan Bolintineanu (Sandia), Tues PM talk
Powder processing:





- 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

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- At least two uses:

1. Give a this-is-what-I-do elevator speech to your boss or funder

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2. Stress-test your cell phone battery

New and enhanced featuresn (1)

- 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)

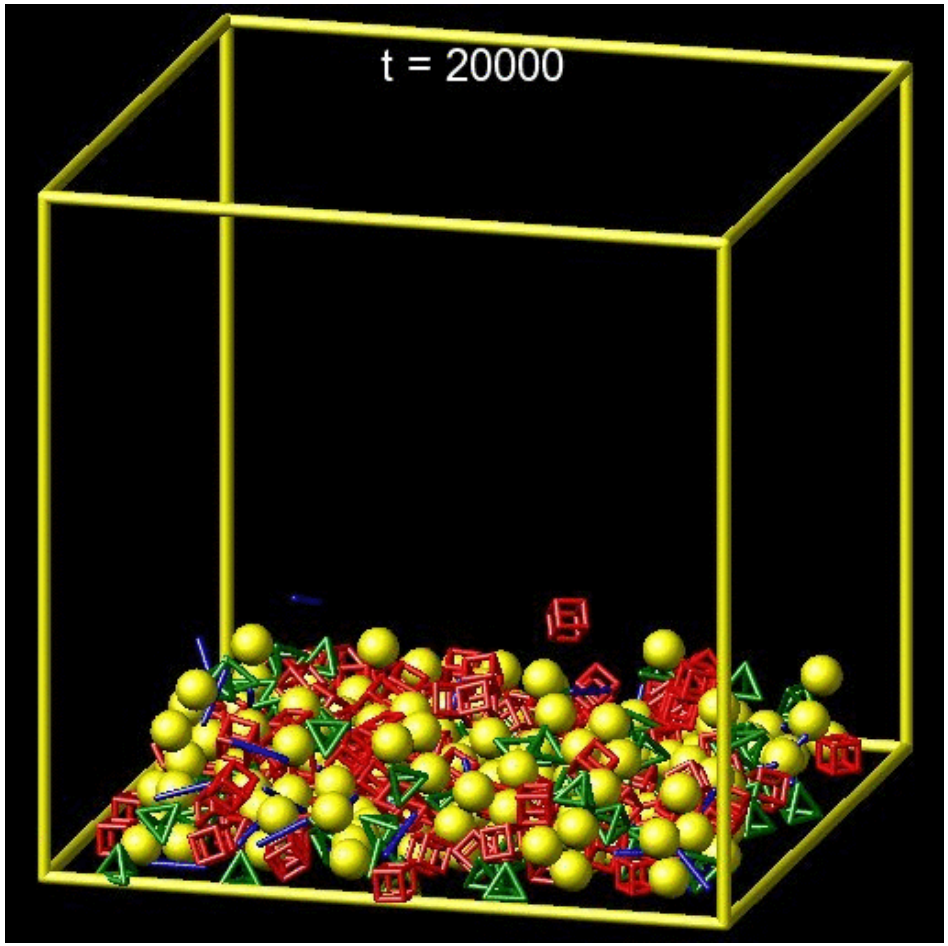
- Fix controller command
  - Aidan Thompson (Sandia)
  - control loop with feedback (PID)
  - adjust one parameter, monitor another
  - zoom in on melting temperature
  - adjust pressure via wall position
- NEB command for barrier heights
  - now allow multiple MPI tasks per replica
  - Emile Maras (CEA, 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



Coming attractions (2): New benchmarking web page

- 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

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- 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

Coming attractions (3)

- CMake build option for LAMMPS
  - 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)
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