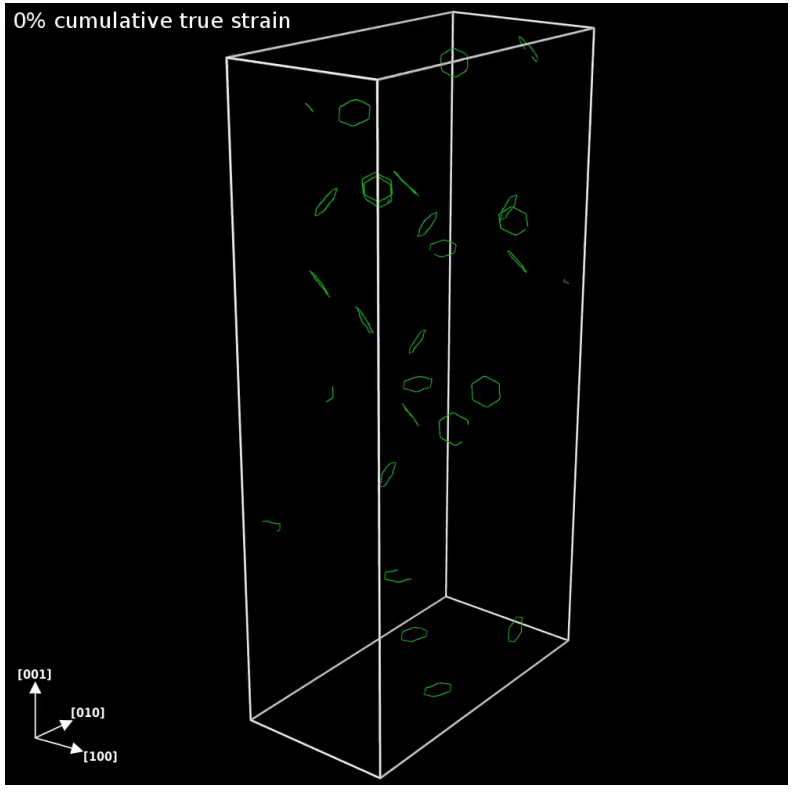
Next: keynote & invited talks by Vasily Bulatov and Alex Stukowski



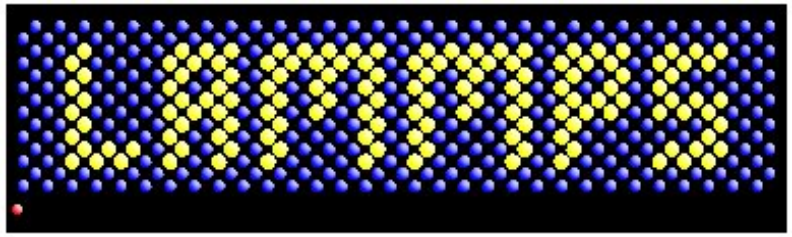
Anders Hafreager: atomify LAMMPS app on iPhone or Android

Google: app store atomify lammps

Welcome and What's New in LAMMPS

Steve Plimpton
Sandia National Labs
sjplimp@sandia.gov

6th LAMMPS Workshop and Symposium
August 2019 - Albuquerque, NM



Center for Computing Research

Sandia National Laboratories

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National Nuclear Security Administration

Thanks!

- Chair: Aidan Thompson Logistics: Christine Trujillo
- Tutorial: Axel Kohlmeyer Poster session: Julien Tranchida
- Breakouts: Mitch Wood, Richard Berger, Axel Kohlmeyer, Christoph Junghans, Pieter in 't Veld

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- DOE/NNSA ASC - funding for facility & equipment rentals
- JSOL Corp and Materials Design, Inc - lunches, snacks, coffee!
- LANL Center for Non-Linear Studies (CNLS) - travel $$

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- Invited speakers
  - Vasily Bulatov (LLNL), **keynote**
  - Niels Gronbech-Jensen (UC Davis)
  - Xiang-Guo Li (UC San Diego)
  - Susan Rempe (Sandia)
  - Ray Shan (Materials Design, Inc)
  - Alex Stukowski (Darmstadt U of Technology, Germany)

Social activities

Tonight: BBQ + tram ride

Plans for Thursday night dinner and Fri AM hike still TBD

Thanks to our user community

- August is a hot and stormy month to visit ABQ and NM

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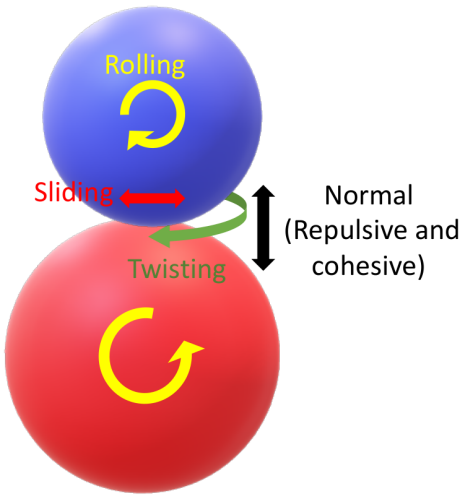
- Please talk to LAMMPS developers whenever/wherever you can find us. Or just send us an email.

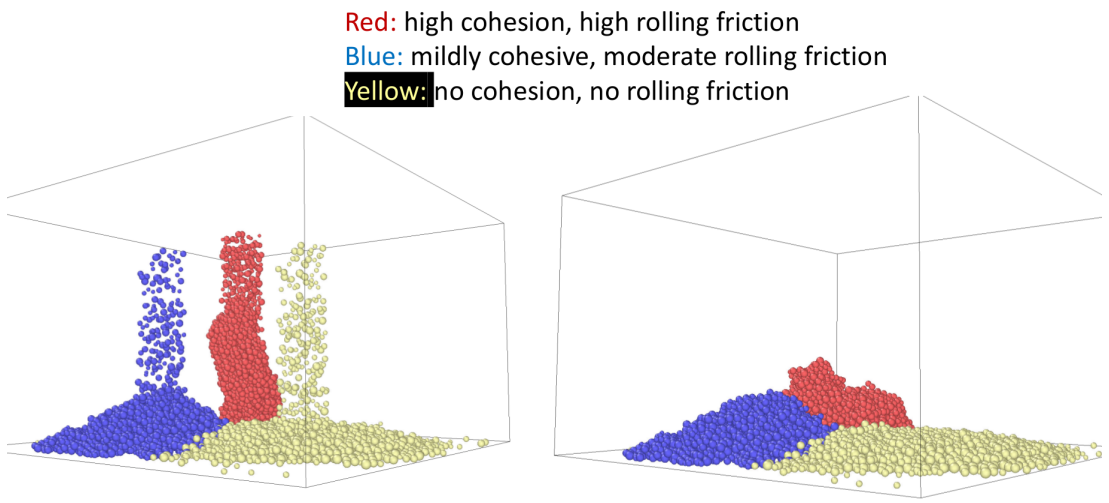
New commands

- Pair_style atm
  - Sergey Lishchuk (Sheffield Hallam U)
  - 3-body Axilrod-Teller-Muto potential (1943!)
- Fix bond/react
  - Jake Gissinger (U Colorado), talk: Today 4:45
  - heuristic model of chemical reactions
  - create/break bonds, form new molecules in flexible manner
- Enhancements to KIM package, interface to OpenKIM
  - Ryan Elliot & Ellad Tadmor (U Minnesota),
    Axel Kohlmeyer (Temple U)
  - large archive of interatomic potentials (and more!)
  - talks Today: 2:45 and 3:00

More general pair_style granular

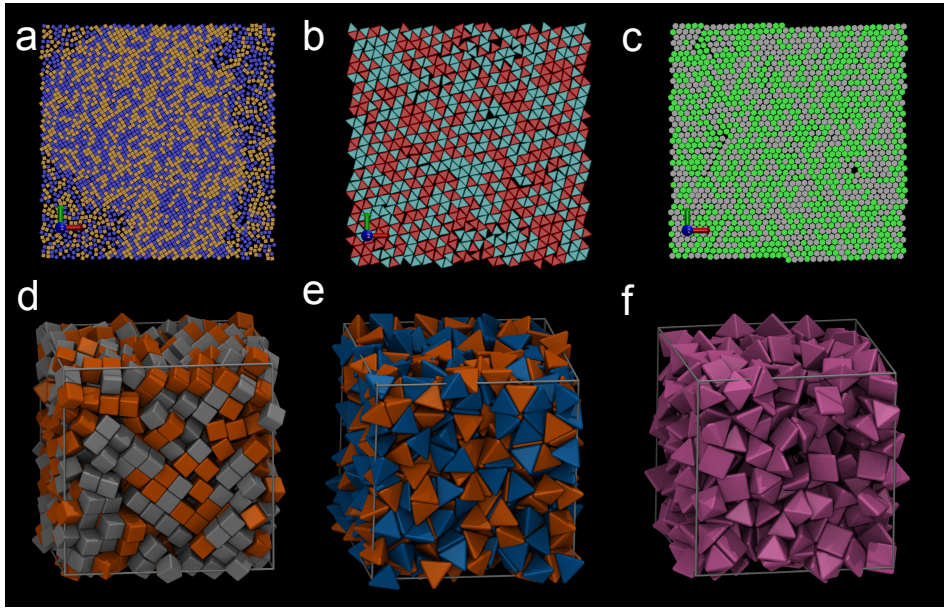
- Dan Bolintineanu, Ishan Srivastava, Jeremy Lechman (SNL), talks: Today 3:30 & Thurs 4:15
- new options for rolling, twisting, cohesion
- allows for per-type material properties

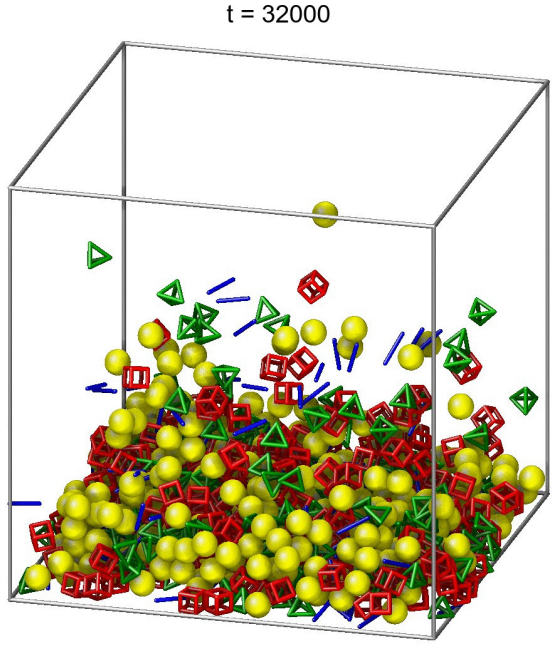




Atom_style body: rounded polygons and polyhedra

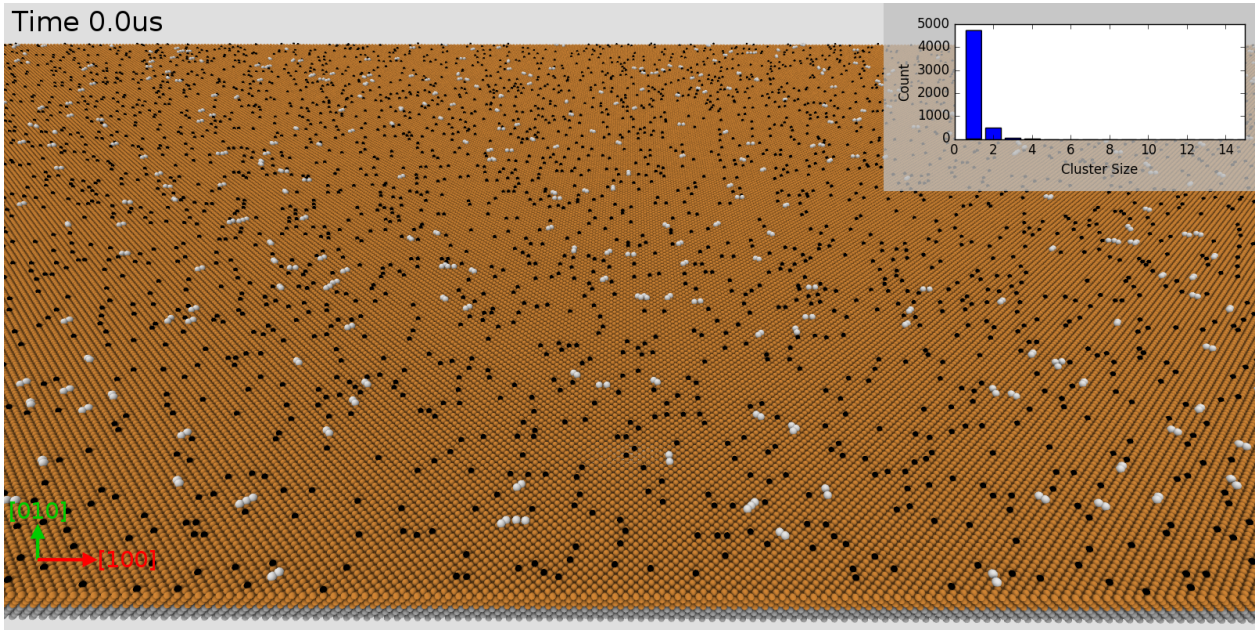
- Trung Nguyen (Northwestern U)
- 2d and 3d DEM models of aspherical particles
- Similar to granular spheres: pour, gravity, etc





Global and local hyperdynamics

- New commands = hyper, fix hyper/global, fix hyper/local
- Time-boost method of Art Voter (LANL) for rare-event MD
- Can apply orders-of-magnitude boost depending on T, ΔE



- 1.2M atoms, 1 ms (4000x boost), 400K events, 128 nodes
- OVITO viz: Thanks to Mitch Wood (Sandia)

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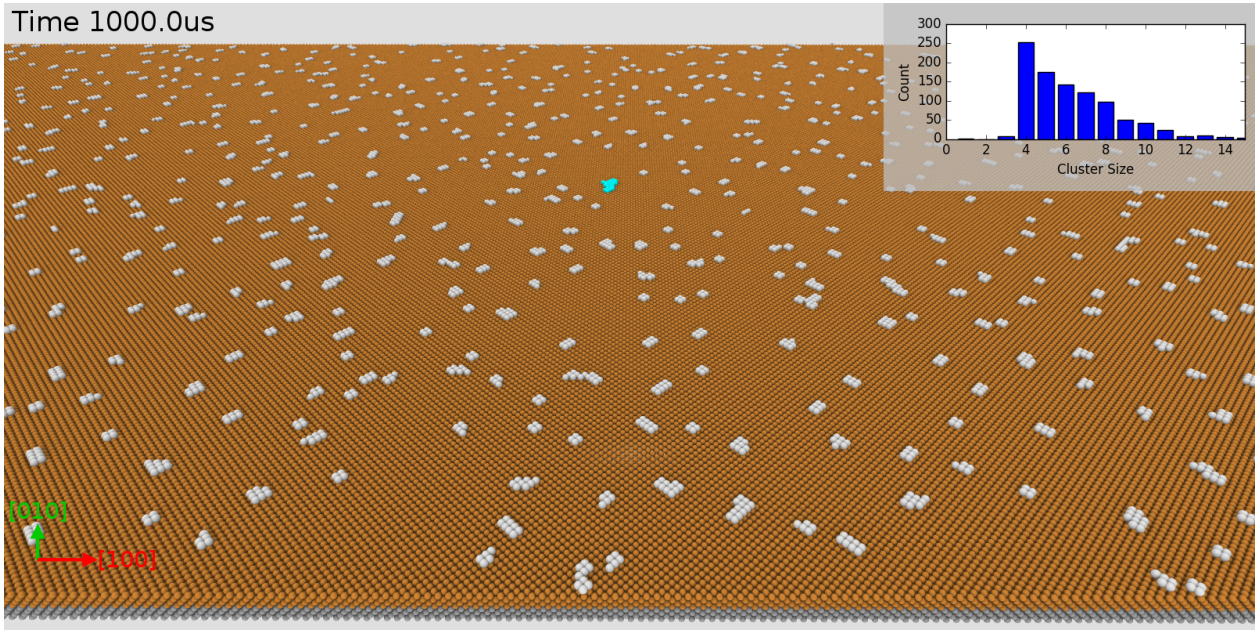

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Parallel rendezvous algorithm

- Collaboration with Chris Knight (ALCF)
- Improved performance for some large parallel setup operations
- Scales well to billions of atoms, millions of MPI tasks
- Setup: replicate, special bonds, SHAKE, rigid-body creation

		replicate		2/3/4 bonds		SHAKE setup	
Atoms	MPI	old	new	old	new	old	new
96M	2K	19	1.1	175	0.9	2	0.3
1.5B	32K	318	1.1	3060	1.8	29	0.6
37B	768K	7656*	2.7	73702*	13.2	693*	12.5

* = estimated time (too long to run!)

- Also a new, fast parallel read_dump

New CMake build system

- Christoph Junghans (LANL), Axel & Richard (Temple U)
- Alternative to traditional make, best option for desktop
- Auto-detects more than make system is capable of
- Released Aug 2018, continuously improved since
- Lots of work to enable all the LAMMPS build options!
- See http://lammps.sandia.gov/doc/Build_cmake.html
- Can be as simple as ...

```
% cd lammps
% mkdir build; cd build
% cmake [options ...]  ../cmake
% make
```

New packages

- LATTE
  - Christian Negre (LANL)
  - wrapper on open-source LATTE DFTB code
    density functional tight binding
  - *ab initio* MD with DFTB

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- MESSAGE
  - allows LAMMPS to act as client or server via CSlib
  - (1) MD (LAMMPS) as client, QM (VASP,NWChem) as server
  - (2) Monte Carlo as client, MD (LAMMPS) as server
  - *ab initio* MD or send select LAMMPS configs to DFT
  - client/server model:
    - messages via files, sockets, or MPI
    - 2 independent executables (LAMMPS, VASP)
    - LAMMPS can run on 1 proc, VASP on P procs
    - LAMMPS can talk to any QM code, w/out knowing details

More new packages

- SPIN
  - Julien Tranchida, talk: Today 11:00
  - coupling of magnetic spin dynamics with MD
  - ferromagnetics, magnetic alloys, amorphous magnetic materials
  - clever, high-accuracy, parallel time integration algorithm

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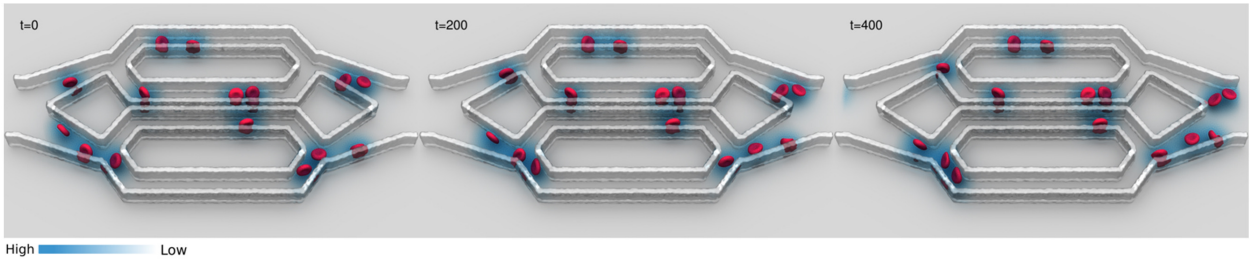
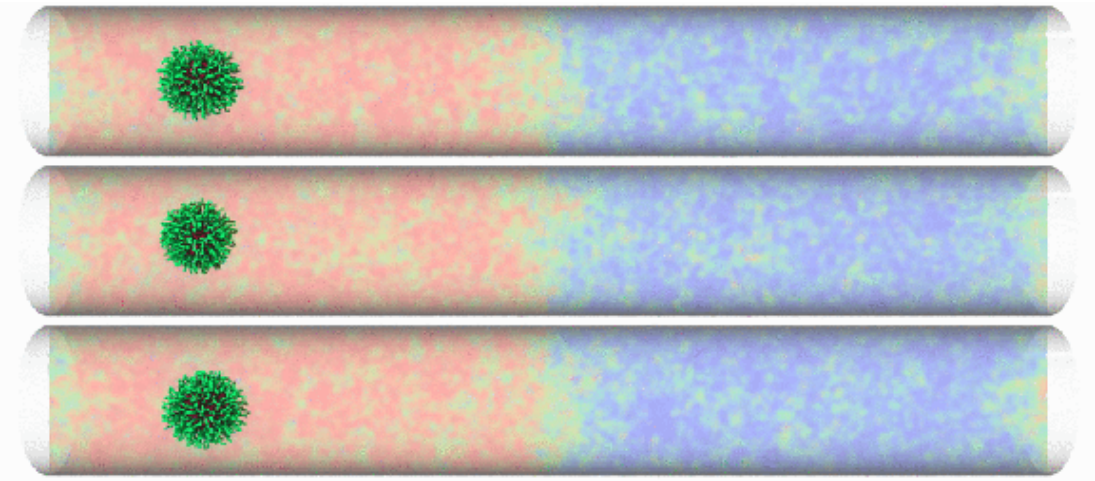
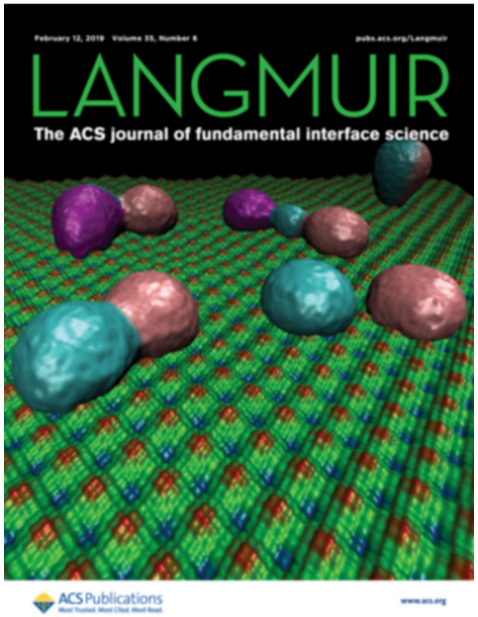
- USER-SCAFACOS
  - Rene Halver (Juelich Supercomputing Centre)
  - wrapper on ScaFaCoS parallel long-range solver
  - includes more KSpace solver options than LAMMPS has
  - Godehard Sutmann (JSC), talk: Thu 9:45

Another new package

- USER-MESO
  - Zhen Li (Brown U)
  - models for tDPD, eDPD, mDPD for soft mesoscale particles
  - t,e,m = transport, energy-conserving, many-body

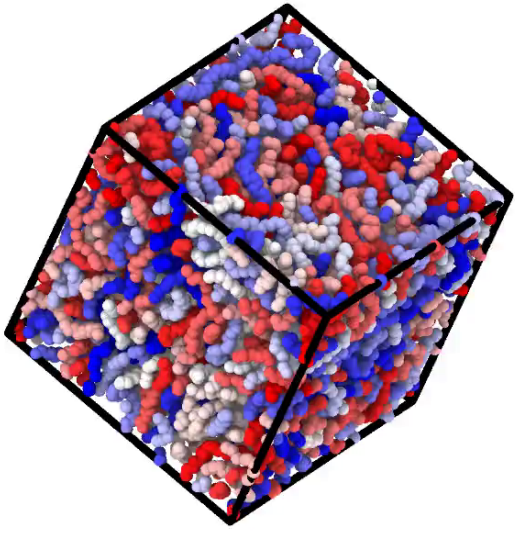






One more new package

- USER-UEF
  - David Nicholson (MIT)
  - NEMD method for continuous extensional flow with SLLOD
  - analogous to NEMD shear methods
  - continuous remapping of simulation box shapes



That's all!

Welcome to the workshop and let's start the technical program ...