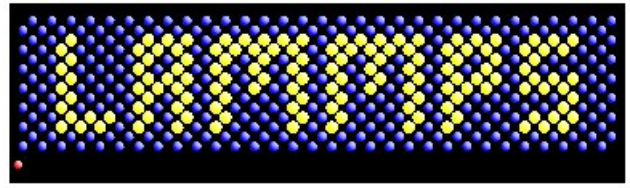

Welcome to the

2nd LAMMPS User Workshop

LAMMPS: Recent Features and Future Plans

Steve Plimpton
Sandia National Labs
sjplimp@sandia.gov

2nd LAMMPS User Workshop
August 2011 - Albuquerque, NM

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Thanks

- Paul Crozier - master of ceremonies
- Aidan Thompson - breakout (potentials)
- Axel Kohlmeyer (Temple U) - breakout (performance), mail list bad-cop (930 postings just in 2011!), repo manager, unofficial LAMMPS co-developer

- Rachel Lebya - administrative support
- John Aidun - $$ for venue

More thanks

- Todd Zeitler - breakout (solid-state materials)
- Stephanie Teich-McGoldrick - breakout (soft materials), poster session
- Mike Parks - breakout (coarse-graining)
- Greg Scantlen (Creative Consultants) - poster session refreshments
- Matt Lane - tutorial, tonight's dinner and tram ride
- Craig Tenney - tutorial, hike czar (Thursday PM)

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Thunderous applause

Paul Crozier, Aidan Thompson, Axel Kohlmeyer, Rachel Lebya. John Aidun, Todd Zeitler, Stephanie Teich-McGoldrick, Mike Parks, Greg Scantlen, Matt Lane, Craig Tenney

Thursday PM activities

- Hike:
  - peaceful mountain setting
  - fresh outdoor air
  - commune with nature

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- Hike:
  - peaceful mountain setting
  - fresh outdoor air
  - commune with nature
- Go-karting:
  - peaceful enclosed warehouse racetrack
  - fresh gasoline engine exhaust
  - commune with inner competitive ego and survival instincts

see http://www.abqkarting.com for details

Thanks to our user community

- August is not the best month to visit ABQ and NM

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- This is an informal workshop in all respects except for the aggressive schedule:
  - 12 minutes into talk: "gong" sounds, wrap-up
  - 15 minutes into talk: trapdoor opens

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

Significant LAMMPS enhancements since last workshop

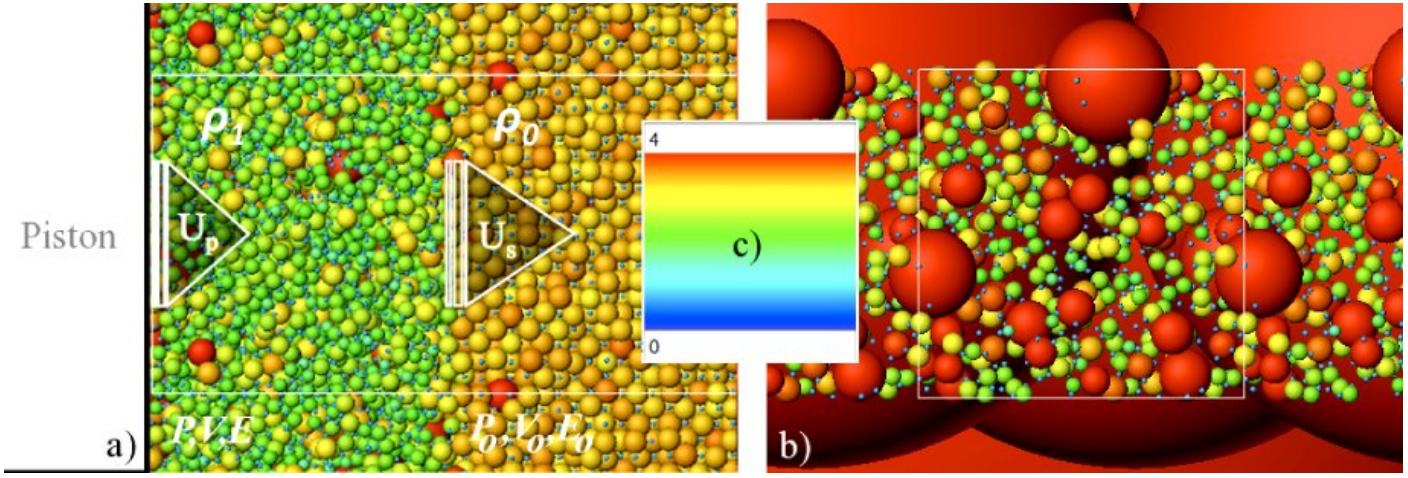
- SVN & Git repositories
  - Axel Kohlmeyer (Temple U), http://lammps.sandia.gov/download.html
  - 175 SVN users, 75 Git users
- NPT for triclinic (non-orthogonal) boxes
  - Aidan Thompson (Sandia)
  - dynamics and minimization (fix box/relax)
  - Nose/Hoover chains for NVT and NPT
- NVT for rigid bodies
  - Trung Dac Nguyen (U Michigan)
  - NPT coming soon
- Alchemy for free energy calculations
  - Sai Jayaraman (Sandia)
  - Yong Zhang (U Notre Dame), talk on Wed AM
  - see fix adapt and compute ti commands for details
  - associated pair styles and PPPM

New interatomic potentials

- COMB potential
  - Tzu-Ray Shan (U Florida), talk on Tues PM
  - metal and semiconductors and their oxides
- Embedded ion method potentials (EIM)
  - Xiaowang Zhou (Sandia)
  - ionic compounds
  - combo of Li, Na, K, Rb, Cs, F, Cl, Br, and I
- C++ version of ReaxFF
  - Metin Aktulga (LBNL), talk on Wed PM
  - can be faster than Fortran version by 2-3x

More interatomic potentials

- Electron force field (eFF)
  - Andres Jaramillo-Botero (Caltech), talk on Thurs AM
  - reigning go-kart champion
  - explicit electron dynamics in extreme conditions



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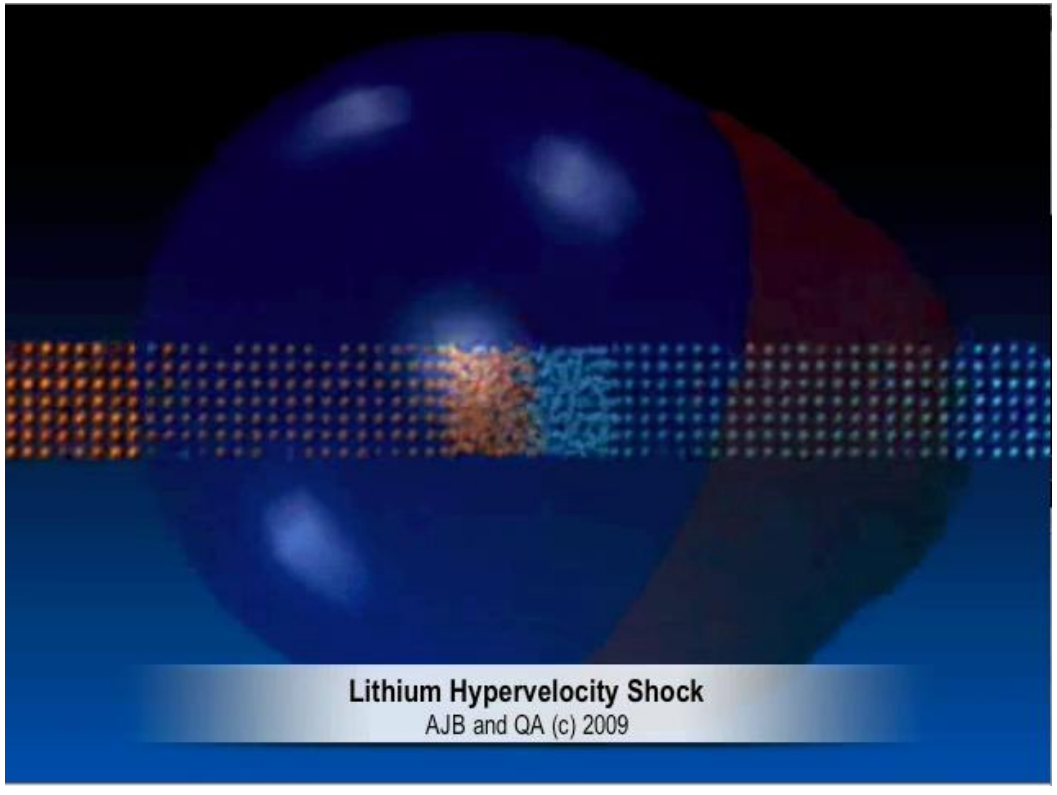
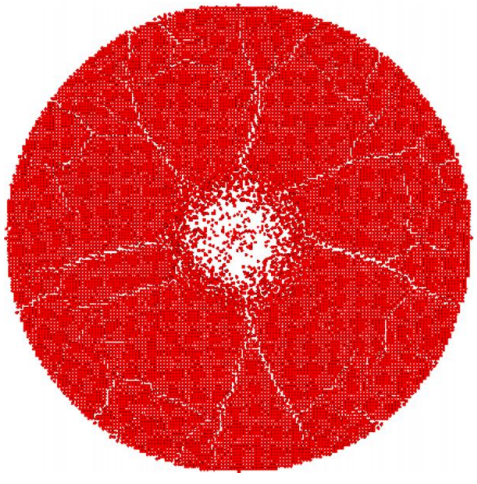


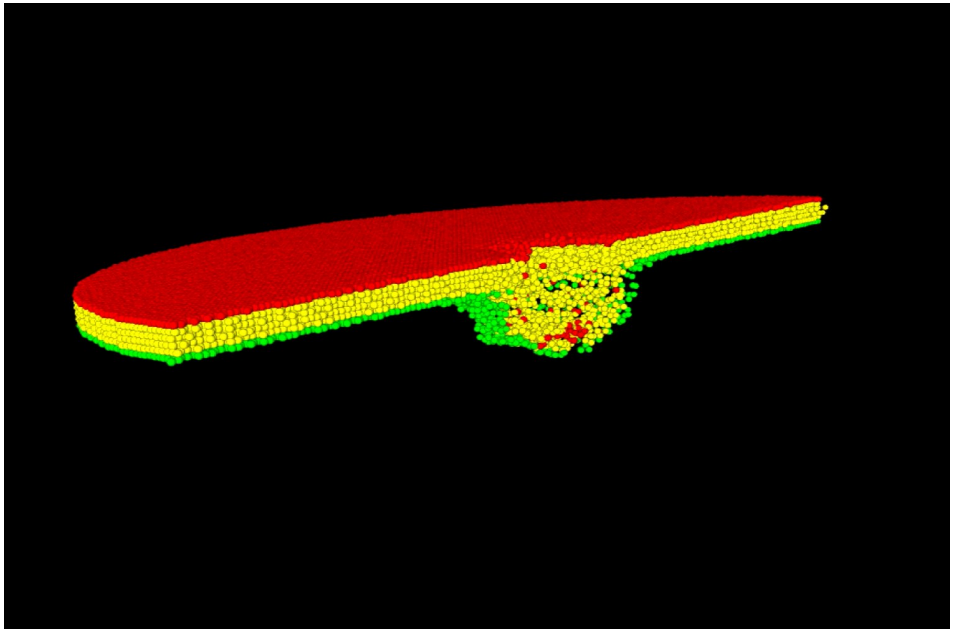
More interatomic potentials

- AIREBO potential bug fixes
  - Marcel Fallet & Steve Stuart (Clemson)
  - one more bug-fix upgrade is imminent
- Mishin ADP potential
  - Chris Weinberger (Sandia) & Chandra Veer Singh (Cornell)
  - angular-dependent EAM for metals and alloys
- Dreiding potential
  - Tod Pascal (Caltech)
  - hydrogen bonding for solvated bio-molecules

More interatomic potentials

- New Peridynamics potentials
  - Mike Parks & Stuart Silling (Sandia), talk on Wed PM
  - fracture at the meso and continuum scales





Interatomic potential bake-off

See http://lammps.sandia.gov/bench.html#potentials
Aidan Thompson (Sandia), talk on Wed AM

Potential	System	Atoms	Timestep	CPU	LJ Ratio
Granular	chute flow	32000	0.0001 tau	5.08e-7	0.34x
FENE bead/spring	polymer melt	32000	0.012 tau	5.32e-7	0.36x
Lennard-Jones	LJ liquid	32000	0.005 tau	1.48e-6	1.0x
DPD	pure solvent	32000	0.04 tau	2.16e-6	1.46x
EAM	bulk Cu	32000	5 fmsec	3.59e-6	2.4x
Tersoff	bulk Si	32000	1 fmsec	6.01e-6	4.1x
Stillinger-Weber	bulk Si	32000	1 fmsec	6.10e-6	4.1x
EIM	crystalline NaCl	32000	0.5 fmsec	9.69e-6	6.5x
SPC/E	liquid water	36000	2 fmsec	1.43e-5	9.7x
CHARMM + PPPM	solvated protein	32000	2 fmsec	2.01e-5	13.6x
MEAM	bulk Ni	32000	5 fmsec	2.31e-5	15.6x
Peridynamics	glass fracture	32000	22.2 nsec	2.42e-5	16.4x
Gay-Berne	ellipsoid mixture	32768	0.002 tau	4.09e-5	28.3x
AIREBO	polyethylene	32640	0.5 fmsec	8.09e-5	54.7x
COMB	crystalline SiO2	32400	0.2 fmsec	4.19e-4	284x
eFF	H plasma	32000	0.001 fmsec	4.52e-4	306x
ReaxFF	PETN crystal	16240	0.1 fmsec	4.99e-4	337x
ReaxFF/C	PETN crystal	32480	0.1 fmsec	2.73e-4	185x
VASP/small	water	192/512	0.3 fmsec	26.2	17.7e6
VASP/medium	CO2	192/1024	0.8 fmsec	252	170e6
VASP/large	Xe	432/3456	2.0 fmsec	1344	908e6

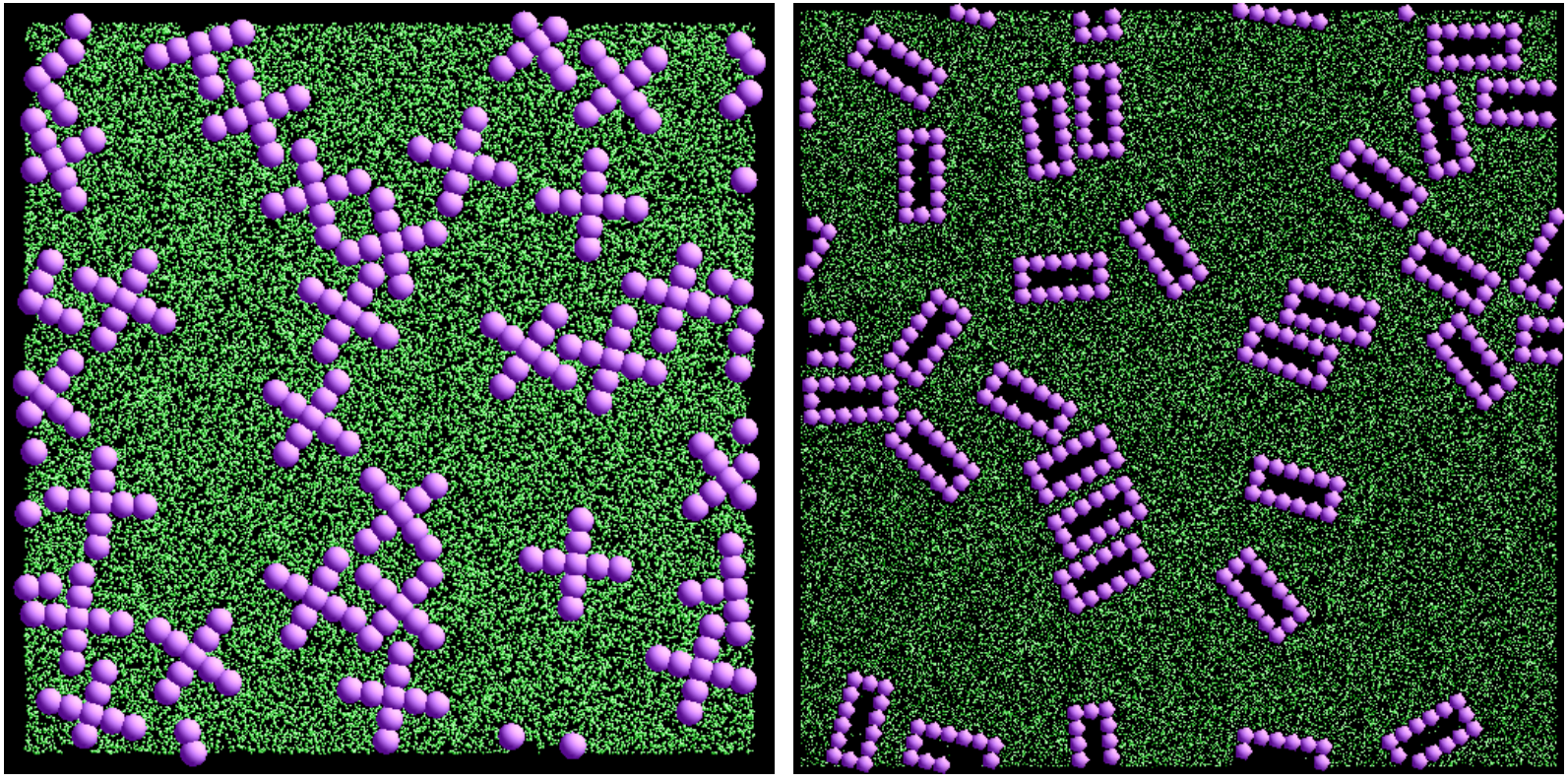
Multi-replica and accelerated time methods

- Nudged elastic band (NEB)
  - energy barrier height calculation for transition states
  - kernel in TAD
- Temperature accelerated dynamics (TAD)
  - method of Art Voter (LANL)
  - acceleration by lower barriers at high T
  - implemented by Aidan Thompson (Sandia)
- Parallel replica dynamics (PRD)
  - method of Art Voter (LANL)
  - acceleration by independent replicas sampling next event
  - implemented by Mike Brown (ORNL)

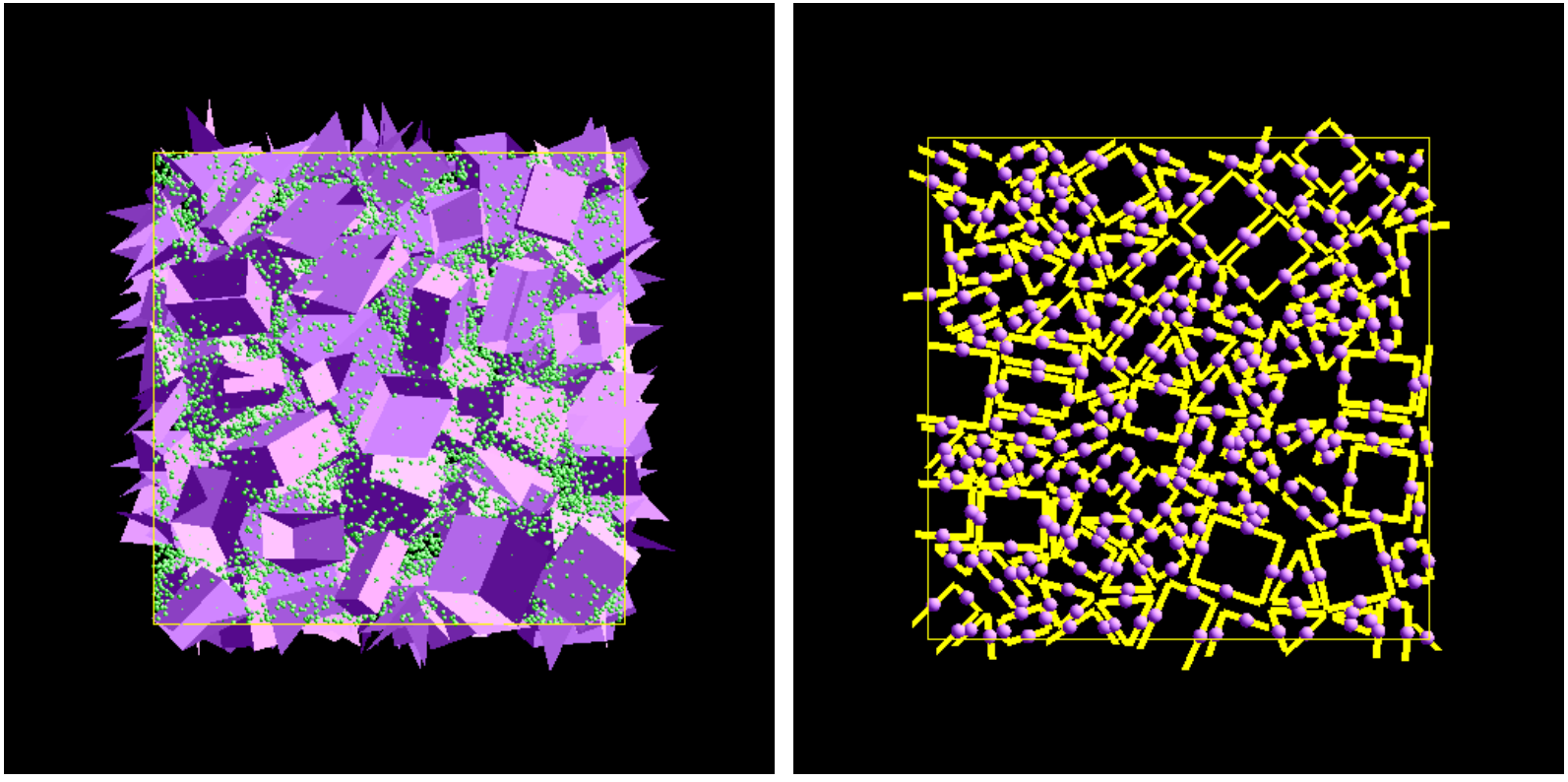
Coarse-graining methods

- Stochastic rotation dynamics
  - with Jeremy Lechman (Sandia) and Pieter in't Veld (BASF)
  - cheap solvent for nanoparticles
  - no solvent-solvent interactions
  - enables micron-size particles for seconds
- Fast lubrication dynamics (FLD)
  - Amit Kumar and Jon Higdon (U Illinois)
  - implicit solvent
  - fast variant of Stokesian Dynamics
  - enables micron-size particles for seconds
  - soon to be released
- Triangulated particles
  - generalized aspherical particles
  - soon to be released
  - merge ideas with granular LIGGGHTS package

Viscosity via stochastic rotation dynamics



Triangulated aspherical particles



GPU enhancements

- GPU package enhancements
  - Mike Brown (ORNL), talk on Wed AM
  - recent hybrid (CPU/GPU) and PPPM work
  - works well on multicore-CPU/GPU nodes
- USER-CUDA package
  - Christian Trott (U Tech Ilmenau)
  - just released (this morning!)
  - 28 pair styles, 14 fixes, 4 computes
  - impressive speed-up if simulation can stay on GPU
  - billion-particle LJ on 288 GPUs $\approx$ 10K Cray XT3 procs

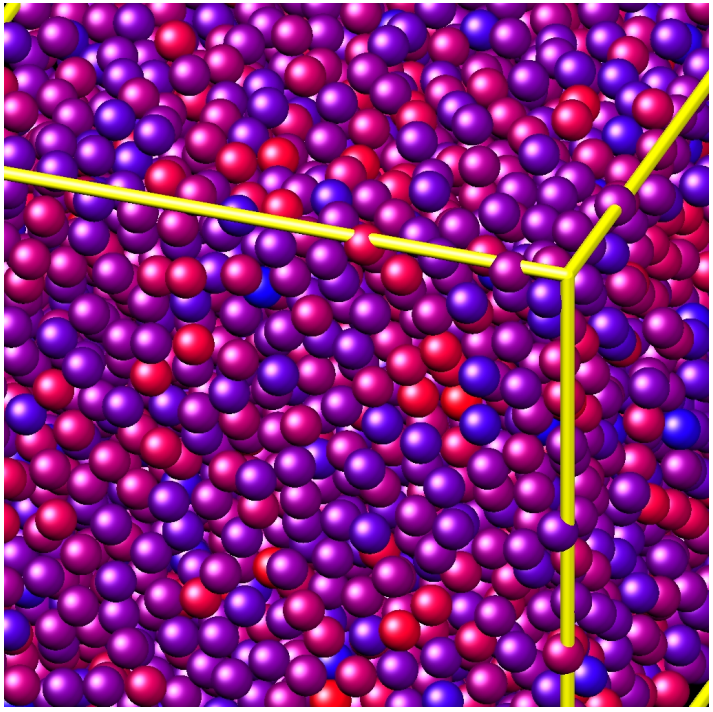
- See http://lammps.sandia.gov/doc/Section_accelerate.html

New cool and generally useful features

- 64-bit integers for atom count and timestep
  - 64 bits = $9x10^{18}$
  - 0.1 mm^3 of Cu atoms = Lincoln's nose (3d) on a penny
  - 2.5 hours (fmsec timestep)
  - hooks for 64-bit atom IDs are there, not coded yet
- Dump image command
  - Nathan Fabian (Sandia)
  - parallel output of ray-traced snapshots on-the-fly
  - JPEG or PPM (text format) files
  - non-interactive, but ...
  - good for instant viz, debugging, huge systems

Dump image example

```
variable      spin equal ramp(-110,110)
variable      zoom equal ramp(1.05,2.0)
dump          1 all image 10 image.*.jpg vx &
              type axes yes 0.8 0.02 &
              view 60.0 v_spin zoom v_zoom
```

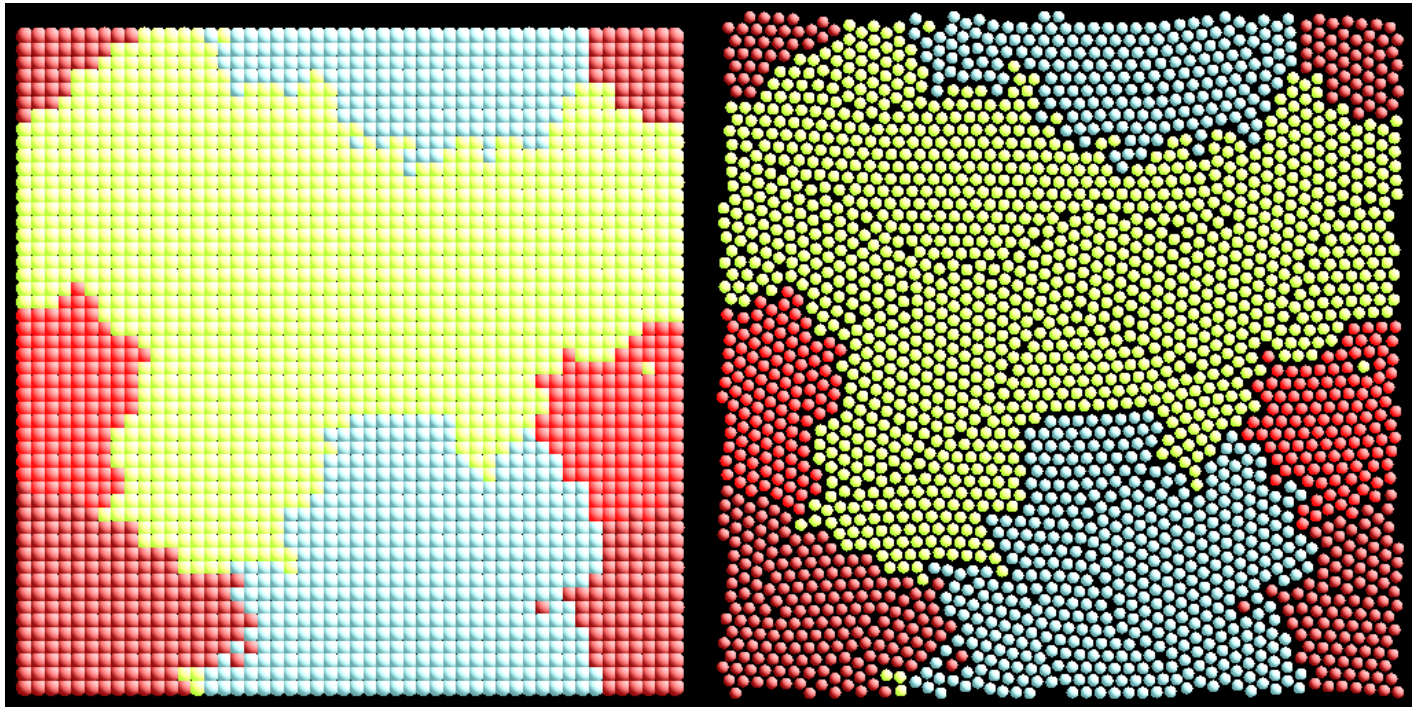


New cool and generally useful features

- Damped-dynamics minimizers
  - FIRE and QuickMin
  - used by NEB, can also be used stand-alone
- 3 methods for heat-flux and thermal conductivity
  - http://lammps.sandia.gov/doc/Section_howto.html#4_20
- Time-dependent variable options for many commands
  - time-dependent, spatially-dependent form of a setting
  - define formula via equal-style, atom-style variable
  - fix addforce, fix efield, fix indent, etc, etc
  - fix adapt can also change particle properties (diameter)
  - typically easy to implement, more on request
- Fix ave/spatial for 2d/3d binning

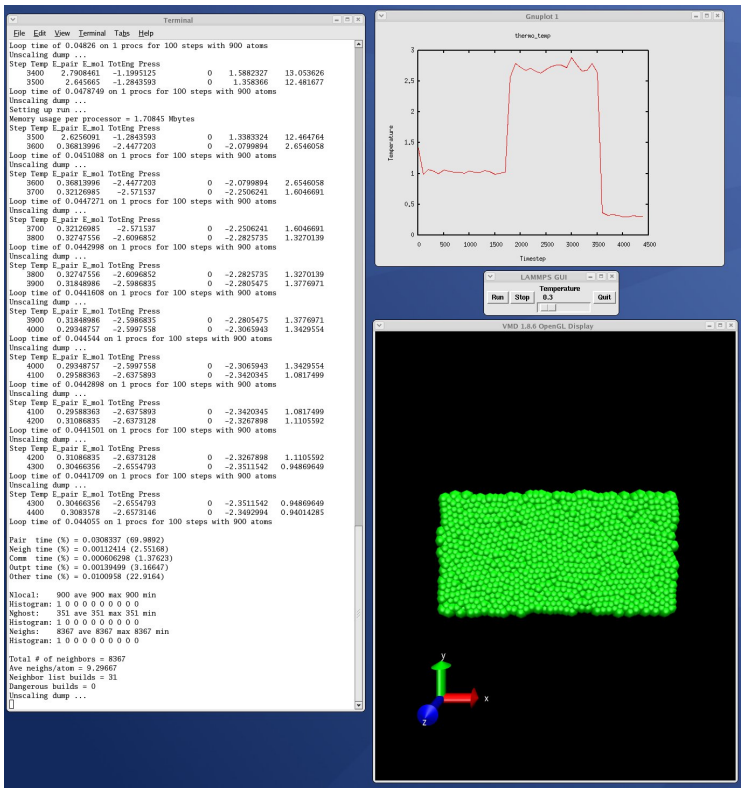
Coupling demos via LAMMPS library interface

- lammps/couple dir
- examples for loose coupling of MD to KMC or quantum DFT
- library to swap info in parallel between 2 apps every timestep



Python wrapping of LAMMPS library interface

- lammps/python dir
- write a Python script that calls LAMMPS or viz or plotting
- Viz options: VMD, AtomEye, PyMol
- Plotting options: GnuPlot, MatLab
- 170 lines of Python:



New potentials planned for LAMMPS

- Core/shell potential
  - Mike Chandross (Sandia)
  - zero-order model for polarization
- COMB potential (generation 3)
  - Tzu-Ray Shan (U Florida), next talk
  - more materials with polarization effects
- MGPT potential
  - from John Moriarty & Jaime Marian (LLNL)
  - transition metals

New potentials planned for LAMMPS

- BOP potential
  - Xiaowang Zhou (Sandia), talk on Tues PM
  - Don Ward (Sandia), poster on Wed PM
  - GaAs, CdTe, other III-V and II-VI semiconductors
- Gaussian approximation potentials (GAP)
  - Aidan Thompson (Sandia), talk on Wed AM
  - expensive, but quantum-level accurate in some cases
  - semiconductors & metals like InP, Ta, Be
- Interface to KIM potentials (https://openkim.org)
  - Ryan Elliott (U Minn), talk on Tues PM
  - Valeriu Smiricinschi (U Minn), talk on Wed PM
  - archive/database of potentials and material properties

New features planned for LAMMPS

- LIGGGHTS granular extensions $\Longrightarrow$ LAMMPS
  - Christoph Kloss, ckloss@jku.edu, talk on Tues PM
  - www.liggghts.com/www.cfdem.com
  - new potentials, cohesion, rigid bodies, coupling to fluids
  - amazing add-on package to LAMMPS

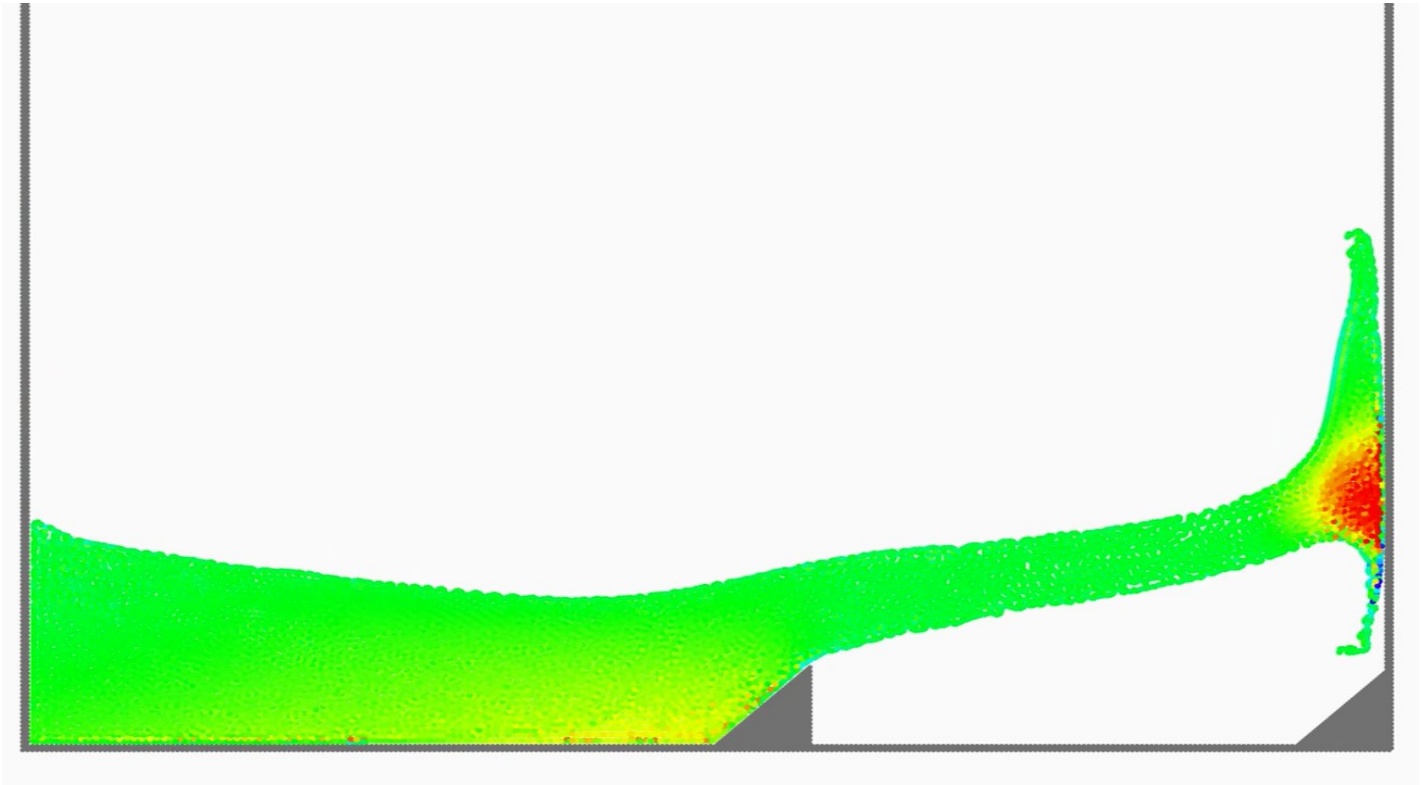
- Atom-to-continuum (ATC) package upgrades
  - Reese Jones & Jeremy Templeton & Jon Zimmerman (Sandia), talk on Wed PM
  - different flavors of coupling to continuum FE
  - another amazing add-on package to LAMMPS
  - who wants to work on parallel FEM?

New features planned for LAMMPS

- More GPU support
  - Mike Brown (ORNL)
  - Christian Trott (U Tech Ilmenau)
  - others can contribute as well via these frameworks
  - GPU-ized manybody potentials would be cool
- New long-range solvers
  - Paul Crozier & Stephen Bond (Sandia)
  - real-space and k-space
  - multi-level summation (MSM) method

New features planned for LAMMPS

- SPH capability
  - Georg Ganzenmüller (Franhofer-Institute, EMI, Germany)
  - soon to be released



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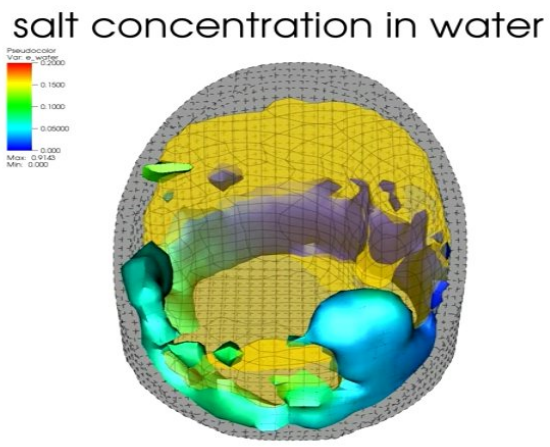
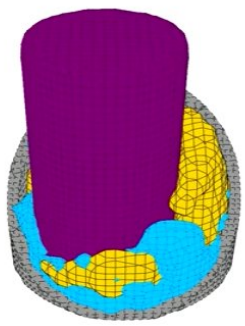
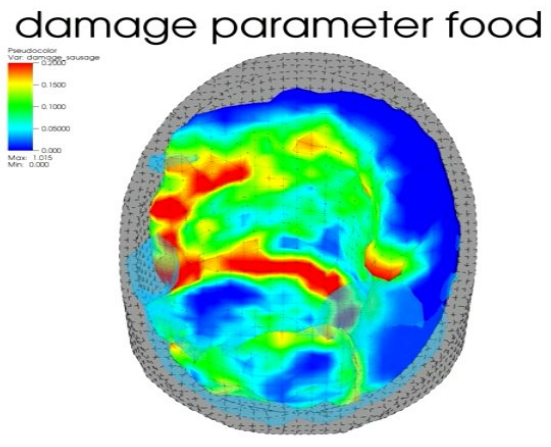






Wed PM breakout on LAMMPS development plans

- More details on items just mentioned
- Other ideas, posted to LAMMPS mail list
- Ideas for useful pre- and post-processing tools
- Add your ideas to the mix
- Make general suggestions on LAMMPS usability
- Volunteer your expertise & coding effort

New content for LAMMPS WWW site is always welcome

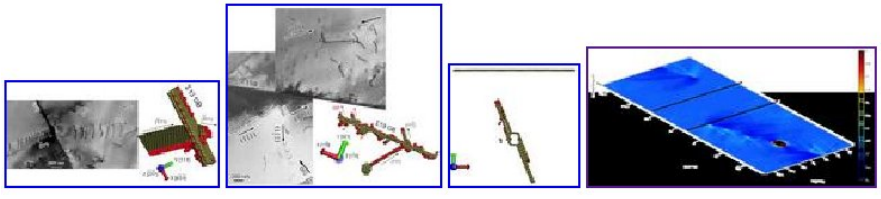
- Pictures http://lammps.sandia.gov/pictures.html
- Movies http://lammps.sandia.gov/movies.html

Dislocations moving thru grain boundaries

This is work by Mike Sangid (sangidm at gmail.com) at Purdue University (formerly at University of Illinois) to study the energy barriers for dislocations to transmit through and nucleate from specific types of grain boundaries (GBs).

The pictures display comparisons of in-situ TEM (transmission electron microscopy) images with snapshots of simulations indicating the same dislocation reactions are observed in experiments and simulations, in cases of slip transmission though a sigma 13 GB (left) and sigma 19 GB (right).

The first movie displays the dislocation reaction for slip transmission with a sigma 3 GB (coherent twin). For clarity, only the atoms representing defects are shown. The second movie displays a cross-sectional view of a contour plot of the energy for the same slip-sigma 3 GB reaction.



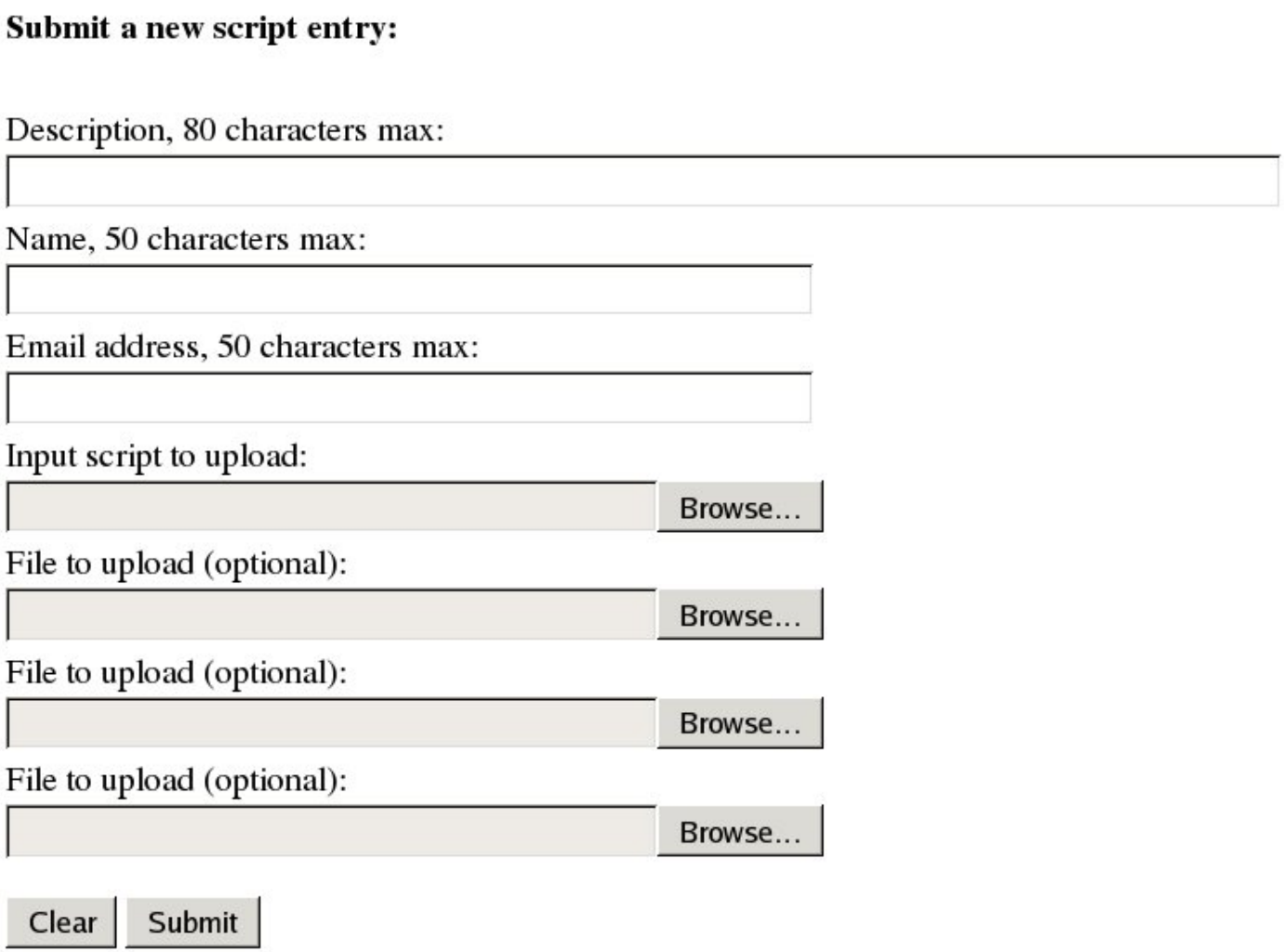
2 images and 2 AVI movies

This paper has further details:

Energy of slip transmission and nucleation at grain boundaries, M. D. Sangid, T. Ezaz, H. Sehitoglu, and I. M. Robertson, Acta Mater 59, 283-296 (2011). (abstract)

New content for LAMMPS WWW site is always welcome

- User Scripts: http://lammps.sandia.gov/scripts.html
- User HowTo: http://lammps.sandia.gov/howto.html



Submit a new script entry:

Description, 80 characters max:

Name, 50 characters max:

Email address, 50 characters max:

Input script to upload: Browse...

File to upload (optional): Browse...

File to upload (optional): Browse...

File to upload (optional): Browse...

Clear Submit