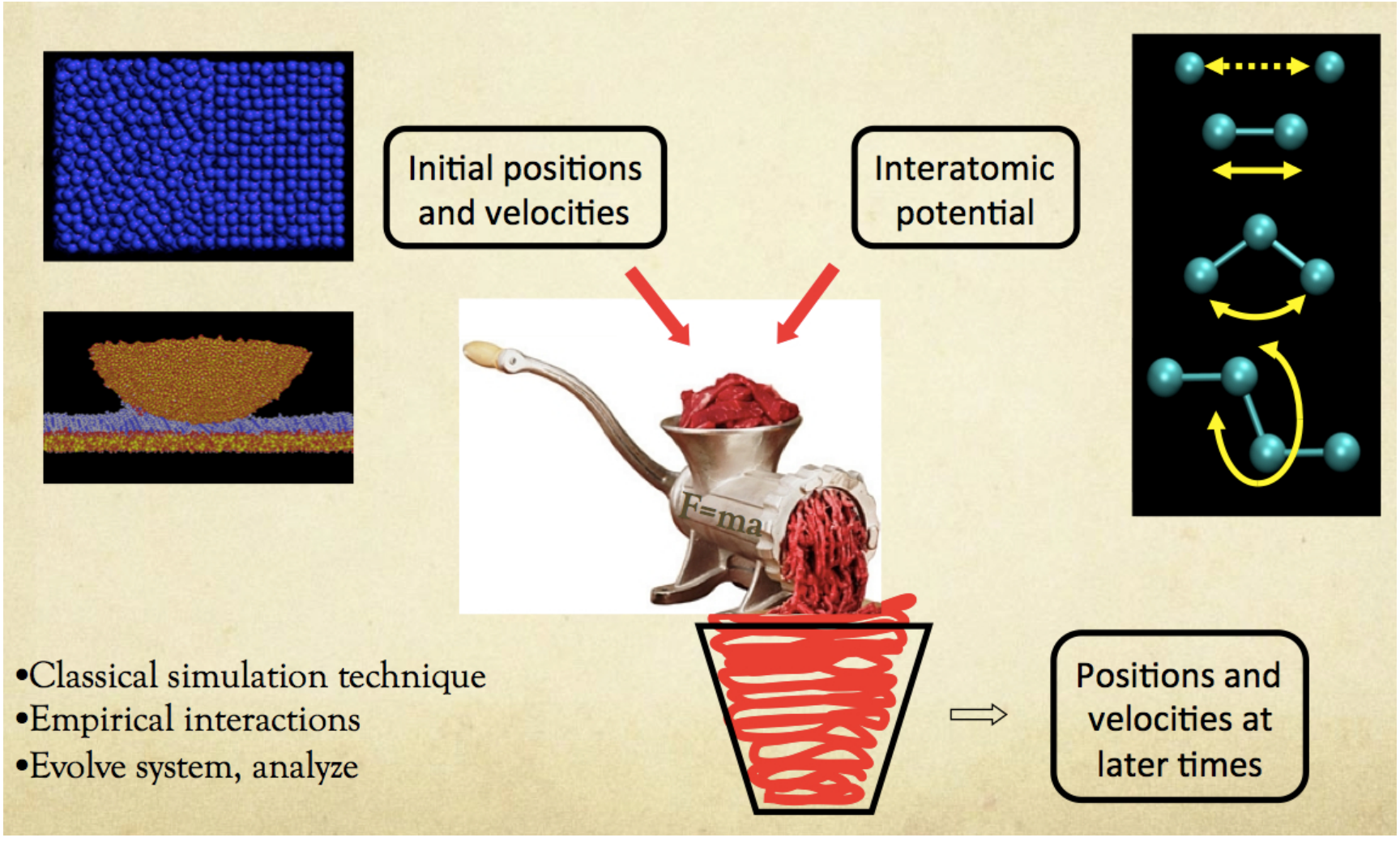
Molecular Dynamics



Welcome to the 3rd LAMMPS User Workshop

LAMMPS: Recent Features and Future Plans

Steve Plimpton
Sandia National Labs
sjplimp@sandia.gov

3rd LAMMPS User Workshop
August 2013 - 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
- Phyllis Rutka - administrative support
- Aidan Thompson - $$ for venue from his project
- Invited speakers (coming a long way!)
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- Organizers:
  Axel Kohlmeyer, Matt Lane, Stan Moore, Ray Shan, Stephanie Teich-McGoldrick Aidan Thompson, Christian Trott, Jon Zimmerman

Thursday evening extra-curricular activities

The good, the bad, the ugly ... but which is which?

Thanks to our user community

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

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  2012 stats:
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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

More GPU and threading support

- GPU package
  - Mike Brown and Trung Nguyen (ORNL)
  - 33 pair styles, PPPM
- USER-CUDA package
  - Christian Trott (Sandia)
  - 30 pair styles, 15 fixes, 4 computes, 4 atom styles, PPPM
- USER-OMP package
  - Axel Kohlmeyer (ICTP, Italy)
  - 88 pair styles, 29 fixes, PPPM, Verlet & rRESPA
  - 10 bond, 15 angle, 11 dihedral, 7 improper, 5 PPPM
- Come to developers breakout A2 on Wed PM
- See Christian Trott talk on Thurs AM

LAMMPS enhancements

Making life easier ...

- Pre-built executables
  - Ubuntu linux package - Anton Gladky
  - Fedora/RedHat/CentOS/openSUSE RPMs - Axel Kohlmeyer
  - Gentoo linux - Nicolas Bock and Christoph Junghans
  - OS X via Homebrew - Derek Thomas
  - new Windows installer - Axel Kohlmeyer

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- More efficient large-scale parallel I/O
  - with Christopher Knight
  - use subset of processors to write dump files
  - dump_modify nfile and fileper options

LAMMPS enhancements

Making simulations more flexible ...

- Added variable options to many commands
  - equal- and atom-style variables
  - use v_myVar in place of a numeric value
  - allows for more time- and spatial-dependence

LAMMPS enhancements

Making simulations more flexible ...

- Added variable options to many commands
  - equal- and atom-style variables
  - use v_myVar in place of a numeric value
  - allows for more time- and spatial-dependence
- Rerun and read_dump commands
  - read one or series of dump snapshots back into LAMMPS
  - compute on only those snapshots
    - compute energy/force with different potential
    - calculate diagnostics missed in initial run
    - example: RDF with longer cutoff

LAMMPS enhancements

New packages

- USER-PHONON package
  - Ling-Ti Kong (Shanghai Jiao Tong University)
  - calculates dynamical matrices
  - leads to phonon frequencies & dispersion relations

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  - Ling-Ti Kong (Shanghai Jiao Tong University)
  - calculates dynamical matrices
  - leads to phonon frequencies & dispersion relations
- USER-COLVARS package
  - Axel Kohlmeyer (ICTP, Italy)
  - built on top of collective variable lib
    - Giacomo Fiorin (Temple University)
    - Jerome Henin (IBPC, CNRS, Paris)
  - collective variables enable
    - adaptive biasing forces
    - metadynamics
    - steered MD
    - umbrella sampling & restraints

LAMMPS enhancements

Easy-peasy Python wrapping

- % make makeshlib
- % make -f Makefile.shlib g++
- % make install-python

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- >>> lmp = lammps()
- >>> lmp.file("in.polymer")
- see python/README for details & examples

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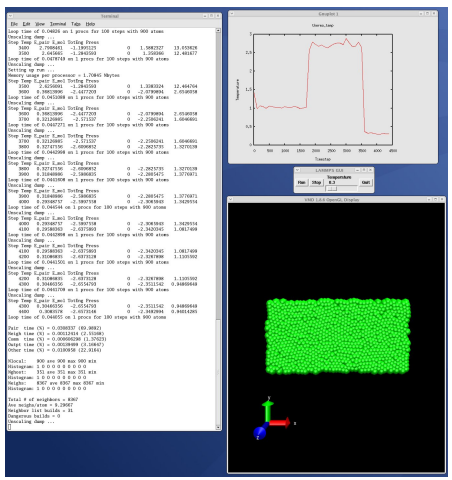
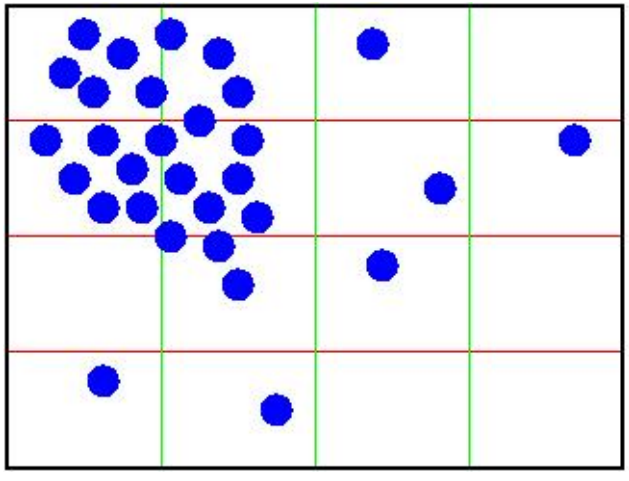
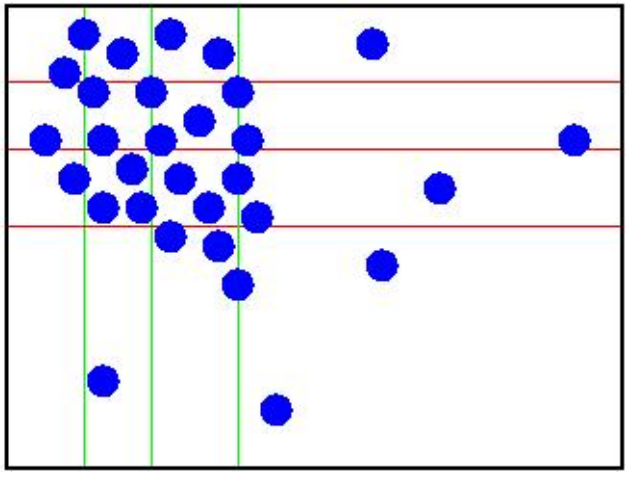


LAMMPS enhancements

Load-balancing

- With Christoph Kloss (JKU)
- Balance (static) and fix balance (dynamic) commands
- Operates by adjusting planar cuts between procs
- Works well for 1d density variations
  - solid/gas or liquid/gas interfaces
- Less well for general 2d/3d variations (stay tuned)

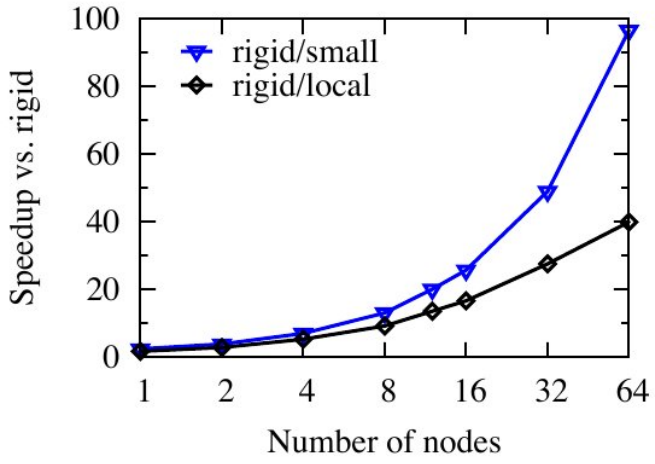




LAMMPS enhancements

Fix rigid/small command

- With Trung Nguyen (ORNL)
- Same functionality as fix rigid
- Except optimized for many small bodies
- Local communication instead of global
- Up to 100x performance improvement for some models
- See talk by Trung in breakout session B3 today



LAMMPS enhancements

- Builders for molecular systems
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  - VMD TopoTools (Axel Kohlmeyer, ICTP)
  - MC builder (Pieter in 't Veld, BASF)
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- Compute voronoi/atom command
  - Daniel Schwen (LANL)
  - uses Voro++ library of Chris Rycroft (LBNL)
  - calculate Voronoi volume & neighbors of each atom
  - useful for per-atom volume & defect analyses in solids

LAMMPS enhancements

- New and enhanced long-range Coulombic solvers
  - Stan Moore & Paul Crozier & Stephen Bond (Sandia)
  - MSM = multilevel summation method, $O(N)$
  - PPPM stagger, smooth, and run_style verlet/split
  - all KSpace styles now allow for:
    - triclinic geometries
    - per-atom energy and stress
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- Fast lubrication dynamics (FLD)
  - Amit Kumar and Jon Higdon (U Illinois)
  - implicit solvent
  - fast variant of Stokesian Dynamics
  - enables micron-size particles for seconds

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  - MC insertions and deletions of atoms/molecules
  - specify T and μ
  - also MC translations and rotations along with MD

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- Fix reax/c/species command
  - Ray Shan (Sandia)
  - identify ReaxFF molecules on-the-fly, in parallel
  - walk the active bonds, ID the molecules, output stats
  - useful for analyzing reactive simulations
  - see talk by Ray in breakout session A1 today

LAMMPS enhancements

Aspherical particles

- 2 formulations already exist
  - point ellipsoids and Gayberne-like potentials
  - rigid-body collections of point-particles and spheroids

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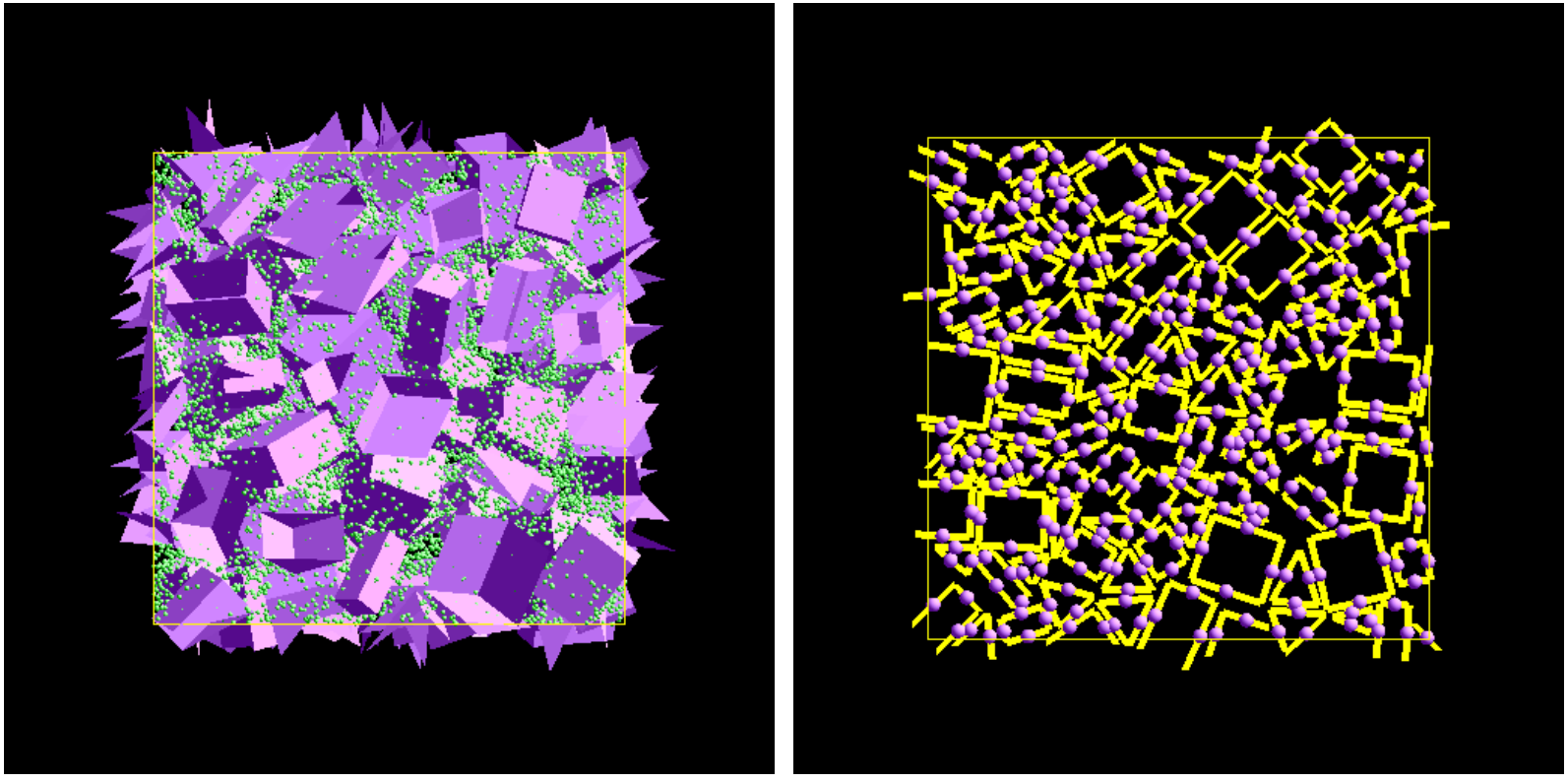
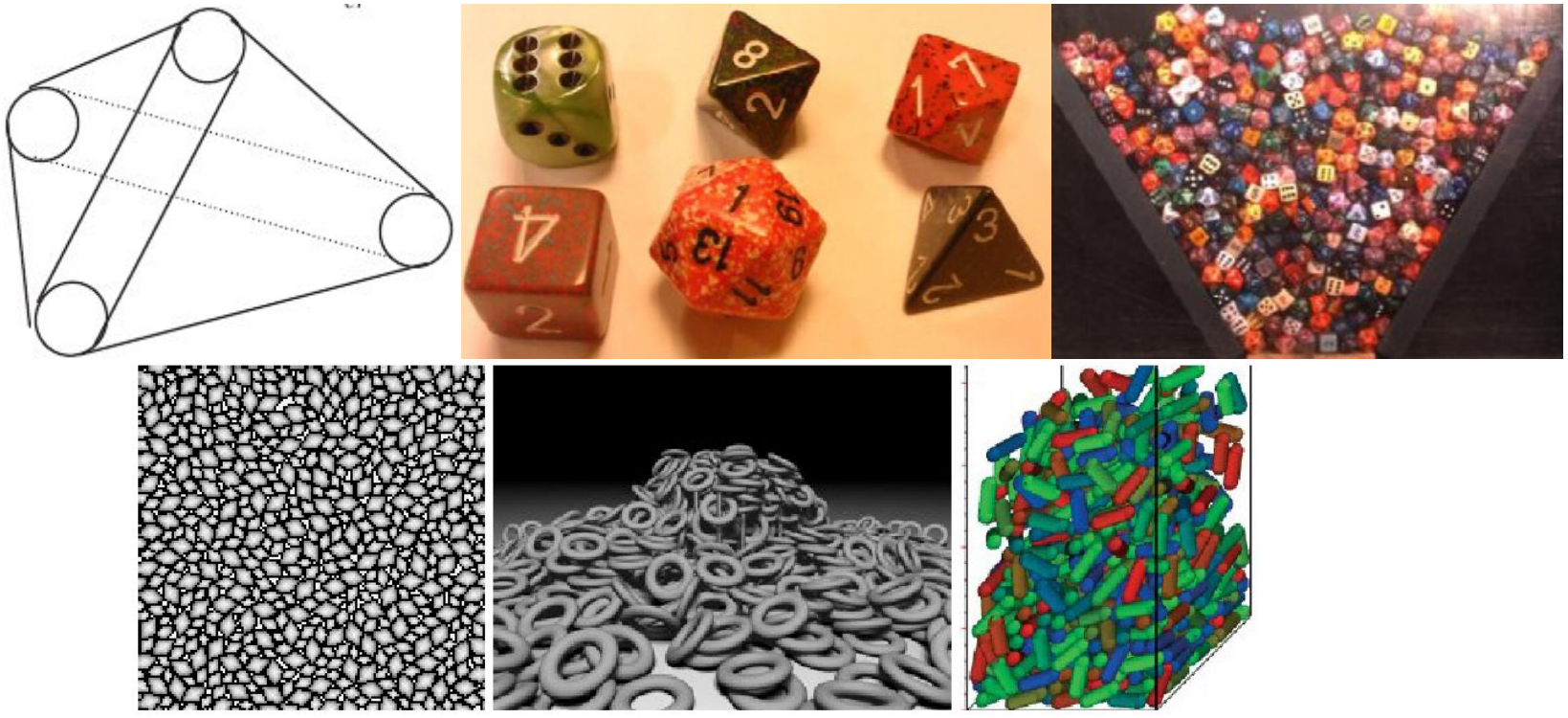
- New atom styles: line (2d), triangle (3d)
  - can build rigid bodies out of them
  - potentials for line/line and tri/tri interactions
- New atom style body for generalized asphericals
- Body particles store internal state
  - sub-particles, facets, etc
  - customizable Body class
  - see doc/body.html for details

Line and triangle particle examples



What we hope body-style particles enable



Pics from:
Mack, Langston, Webb, York, Powder Tech, 214, 431 (2011)
Bell, Yu, Mucha, Eurographics/ACM SIGGRAPH (2005)
Munjiza & Latham, Phil Trans Royal Soc Lond A, 362, 1817 (2004)
Williams & O'Connor, Engr Comp, 12, 185 (1995)

Near-term plans

- Generalized 3d load-balancing
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- Quantum-accurate potentials
  - fit to pre-computed DFT data
  - forces derived from atom's local conformation
  - expensive, but can approach quantum-level accuracy
  - automated development of new potentials for exotic materials
  - see talk by Aidan Thompson on Thurs AM

Give us your input on LAMMPS development plans

- Come to breakout A2 this afternoon
- Variety of topics will be discussed
- Input from attendees will be solicited
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