



Future Plans for LAMMPS

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LAMMPS Workshop

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1. Soon to be released
2. Longer-term
3. Looking for help!
4. Additional ideas ?



But first ...

- Thanks to all for your participation in the workshop
- Please give us feedback on the workshop format
- Paul plans to post PDFs of all talks on the LAMMPS WWW site
- Please send us brief hi-lites of your work:
 - paragraph, pictures, movie, citation, link to you (email, WWW page)
 - lammeps.sandia.gov/pictures.html
 - lammeps.sandia.gov/movies.html
 - good advertising for you and for LAMMPS
 - many are doing things people don't know can be done with LAMMPS



Coming Soon

- New version of compute heat/flux for thermal conductivity (March)
directly from per-atom energy and stress
instead of via looping over neighbor list
will include all contributions (pair, many-body, etc) except long-range Coul
- NPT for triclinic boxes (Parinello/Rahman) (March)
kudos to Aidan
will include enhanced fix box/relax for minimizations
- NVT and NPT for for rigid composite particles (April)
Tony Sheh and Trung from U Michigan



Coming soon (2)

- Embedded ion method (EIM) potentials
Xiaowang's talk
- Free-energy alchemy methods for liquid/solid transitions
Sai's talk
- New C++-based ReaxFF implementation
Aidan and Ananth Grama group at Purdue
advertised as 10x faster
- EFF for modeling electrons and excited states
Anders talk



Coming Soon (3)

- Nudged elastic band for barrier finding (April)
similar to tempering or PRD with multiple replicas
uses LAMMPS partitions
- Triangle-shaped particles (May)
for granular and nanoparticle models
triangulated surfaces can be walls or aspherical particles
sphere-triangle interactions are easier
triangle-triangle interactions are harder



Longer Term

- Stochastic Rotation Dynamics (SRD)
 - work with Jeremy
 - coarse-grained solvent with point particles
 - no solvent/solvent interactions → much cheaper than LJ
 - allows for modeling of larger nanoparticles in solution
 - waiting for release approval from industrial partners
- Fast Lubrication Dynamics (FLD) version of Stokesian Dynamics (SD)
 - work with Jon Higidon group at U Illinois
 - implicit solvent model
 - allows for modeling of larger nanoparticles in solution
 - not full SD, so no long-range, so more parallel
 - waiting for release approval from Jon and partners



Longer Term (2)

- Temperature Accelerated Dynamics (TAD)
work by Aidan and Greg and Jon
Art Voter's method (LANL)
build on top of PRD and NEB kernels
- More GPU-enabled features
SNL/ORNL/Temple group effort, German group effort
merging the two efforts ?
looking for developers to add specific pairs, fixes, computes
within their framework(s)
- Granular model enhancements and granular/fluid coupling
talk by Christoph Kloss (JKU)
looking for users/collaborators/developers



Looking for Help!

- How to calculate per-atom energy and stress for long-range Coulombics?
Ewald and PPPM
- Version of PPPM that works for triclinic boxes
also Ewald
- Long-range PPPM solver for point-dipoles
short-range is there, see PairDipoleCut class
- AIREBO implementation is not fully tested, may have bugs?



Looking for Help! (2)

- New charge-equilibrated potentials
leverage stand-alone qEq capability in new ReaxFF implementation
e.g. Streitz and Mintmire potential
talk to Aidan
- Extend USER-ATC library to couple MD with FE for
mechanical deformation (stress/strain)
electro-mechanical properties (piezoelectrics)
talk to Reese, Jon, Jeremy
- Beef up the nascent DSMC capability, see PairDSMC class
talk to Paul
- Pair style for core/shell model, occasionally requested
- Metadynamics, been contacted by a couple groups
- Polarized force fields



Ideas from Workshop Discussions

- Post pre-built Linux RPMs on a WWW site
Axel has volunteered to work on this
- Create an external SVN repository (mirror)
Axel possibly has a server
SourceForge or Google Code?
- Create more user-created discussion content
education assistance, sample problems
share input scripts
share how-to knowledge and answer FAQs
on LAMMPS WWW site or elsewhere?



Additional Ideas ?

- Open to suggestions
- Feel free to contact us about efforts outlined on previous slides
- Feel free to form a working group interested in some new capability