Large Scale Parallel Materials Simulations with LAMMPS

Dr. Axel Kohlmeyer

Senior Scientific Computing Expert
The Abdus Salam International Centre
for Theoretical Physics
&
Associate Dean for Scientific Computing
College of Science and Technology
Temple University

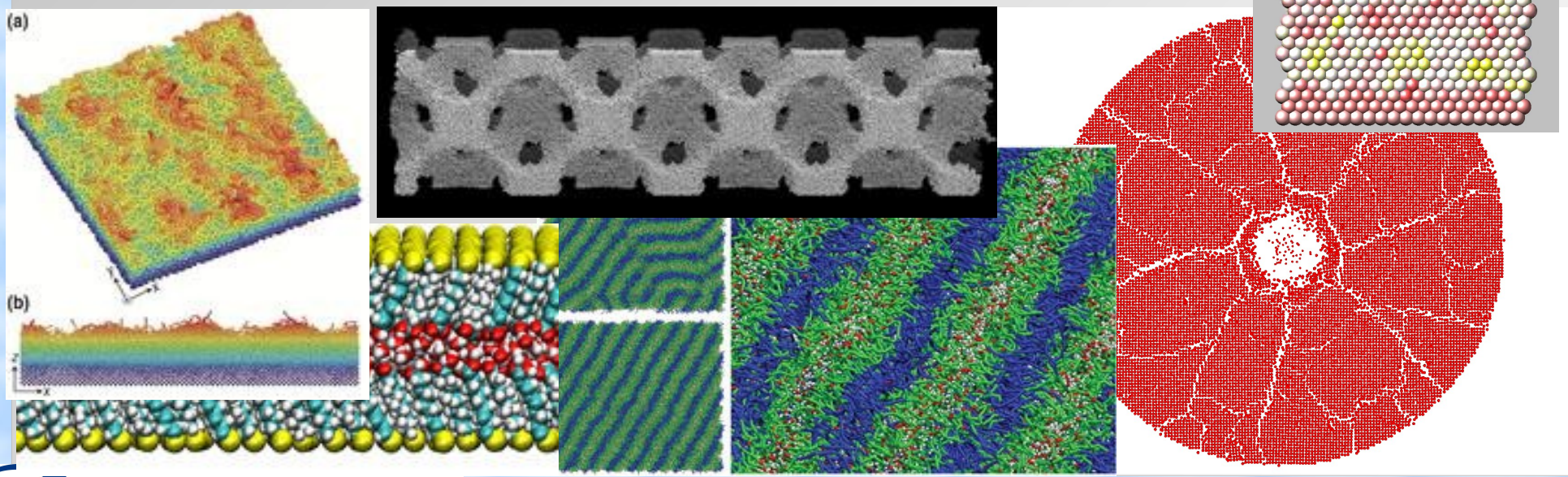
http://sites.google.com/site/akohlmey/

The Abdus Salam International Centre for Theoretical Physics

Industrial Forum for Multiscale Materials Modeling and Training, 11-13 Sept. 2013, Bologna, Italy

What LAMMPS Is

- **L**arge-scale **A**tomic/**M**olecular **M**assively **P**arallel **S**imulator
- Classical Molecular Dynamics (MD) framework for a variety of force fields and methods: biomolecules and polymers (soft matter), materials science (solids), mesoscale to continuum
- Open source, portable and extensible C++
- Home page: http://lammps.sandia.gov



LAMMPS General Properties

- Serial execution, MPI parallel, OpenMP parallel, CUDA and OpenCL acceleration
- Easy to compile and install, few dependencies
- Many pairwise, many-body and bonded models
- Analysis and post-processing during MD run, “rerun” option for additional post-processing
- Easy to extend with custom features (usually sufficient to just add C++ classes)
- Active developer and user community (Most of LAMMPS written by >100 contributors)

Not so Commonly Found Features

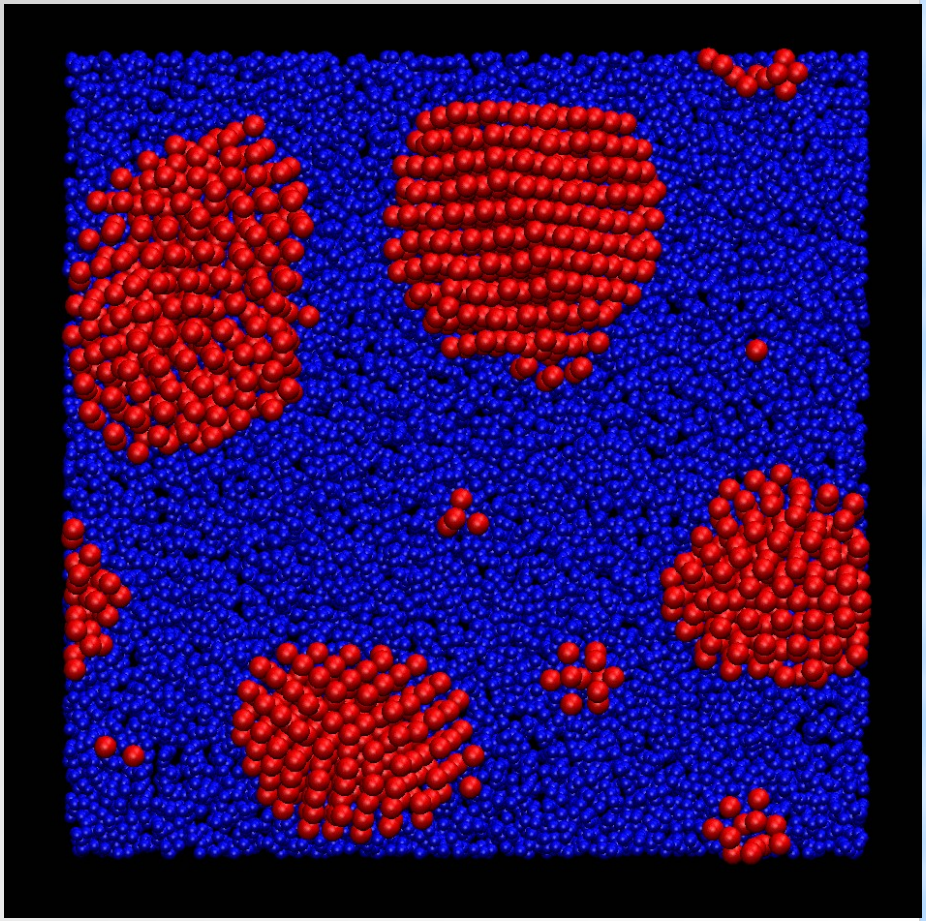
- Generalized Aspherical Particles (lines/meshes, “multi-bodies” with internal+external integrator)
- Stochastic Rotation Dynamics (SRD)
- Grand Canonical Monte Carlo (GCMC)
- Peridynamics mesoscale modeling
- Atom-to-Continuum coupling to FE solvers and back
- Discrete Element Modeling with CFD coupling (LIGGGHTS + OpenFOAM = CFDEM)
- Electron Force Field (eFF)
- Kinetic Monte Carlo Coupling (to SPPARKS)

Popular in Materials Modeling

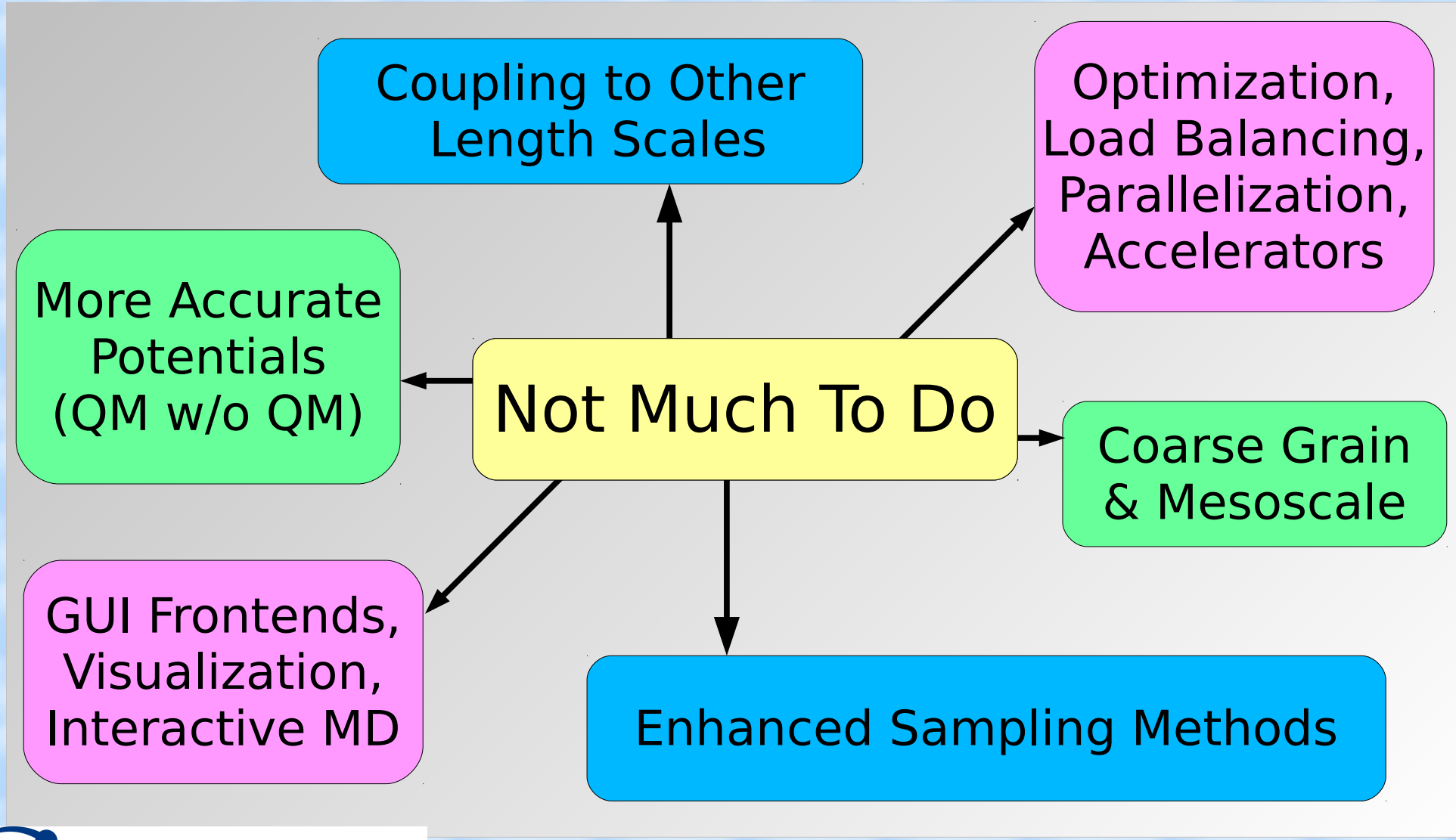
- Integrated scripting language
  - Loops, conditions, variables/functions etc. allow to build workflows for complex multi-step operations
  - Build complex systems from inside the MD code
  - Python interface for more complex scripting and integration into external frameworks
- Hybrid and multi-scale models
  - Combine multiple force field types via overlays or mechanical coupling
  - Coupling to external codes: FE, kMC, QM/MM

Hybrid Models

- Solid/liquid interfaces, solid/solid interfaces
  => mechanical coupling, simple model (LJ) for interface
- Metal islands on amorphous (LJ) substrate
- Specify 2 (or more) pair potentials:
  A-A, B-B, A-B, etc
- Overlay potentials:
  add explicit h-bonds
  add coulomb
- Hybrid in two ways:
  potentials (pair, bond, etc)
  atom style (bio, metal, etc)



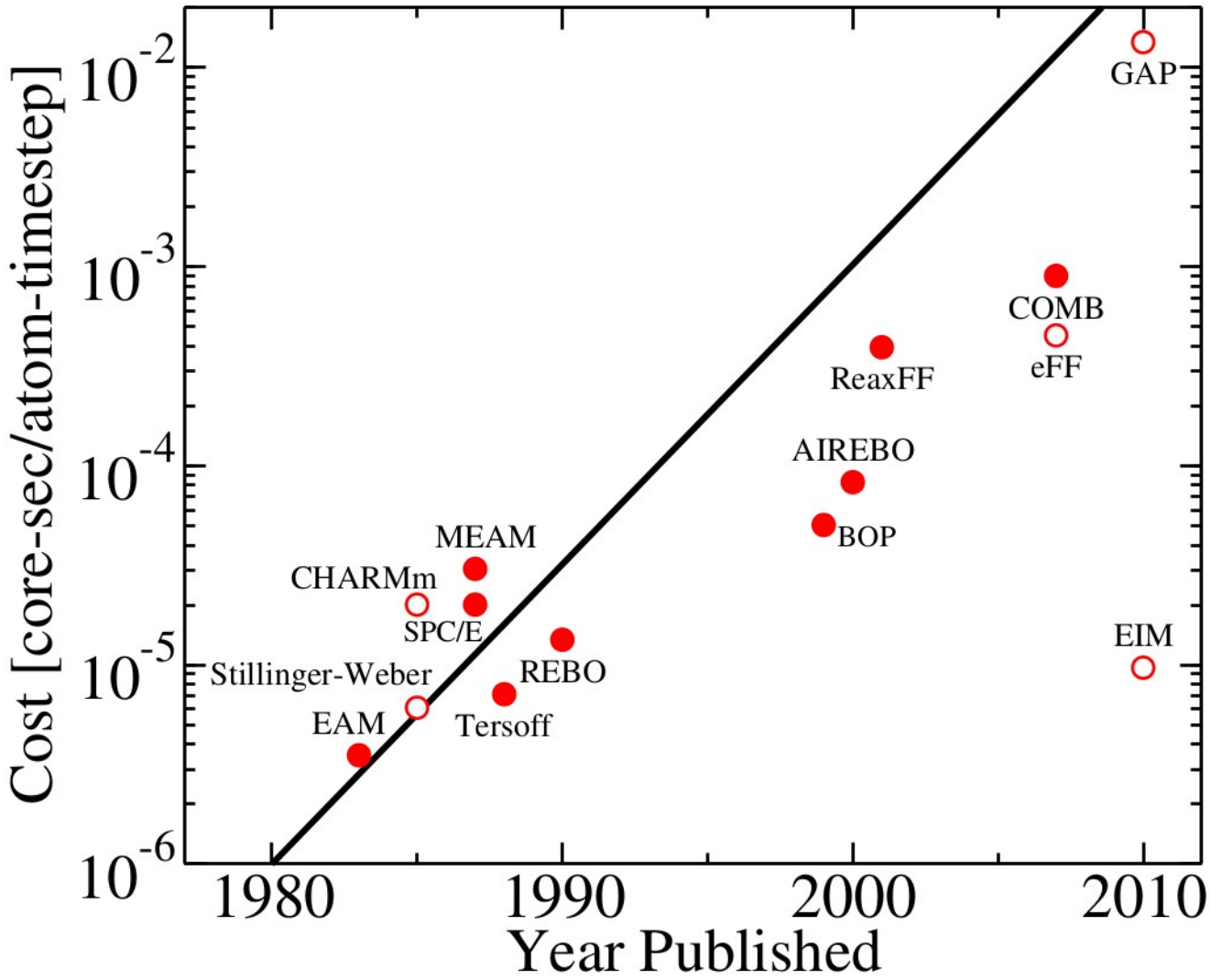
LAMMPS Development Trends



Methods to Bridge Time Scales

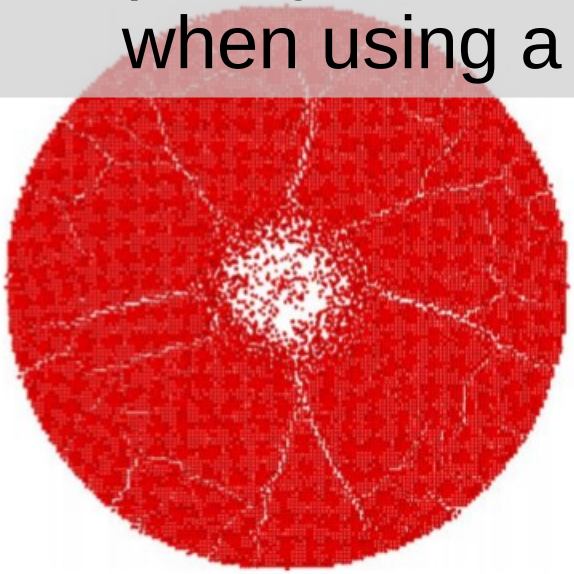
- Metadynamics, Adaptive Biasing Forces, Steered MD, Targeted MD and more
  => available via specialized fixes or commands
  => available via packages: USER-COLVARS (ported from NAMD) or PLUMED (external)
- Temperature Accelerated MD, Parallel Replica MD, Parallel Tempering Replica Exchange
  => available via internal commands
  => extensions under development externally (not always or not yet contributed back)

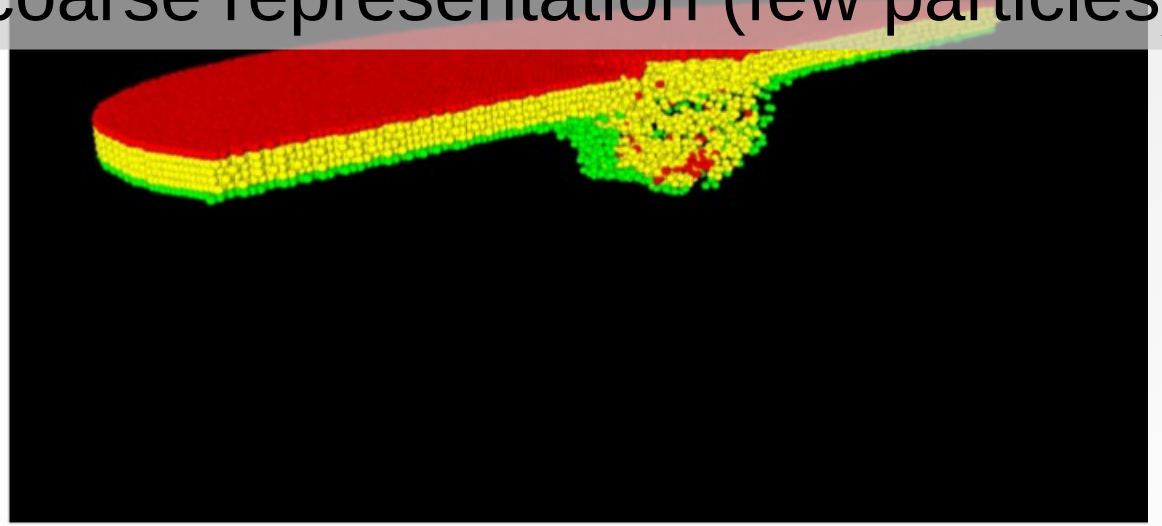
Moore's Law for Potentials



Mesoscale Modeling via Peridynamics

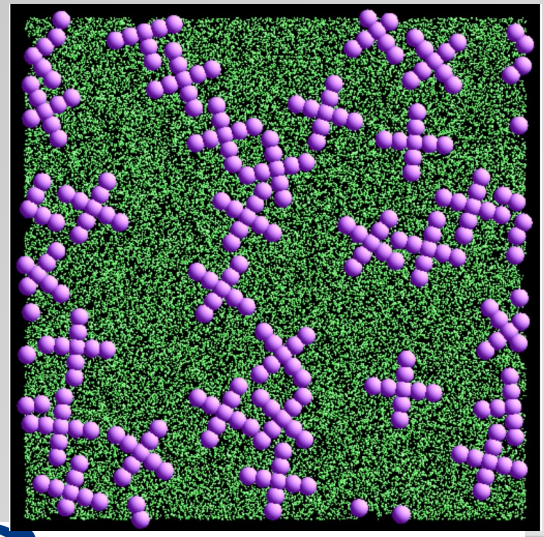
- Particle-based meshless non-local continuum model
- Constituent model implemented as pairwise force
- Particularly suited to model fracture of brittle materials
  => mesh-based models always exhibit bias in fracture
  => peridynamics leads to consistent results, even when using a coarse representation (few particles)

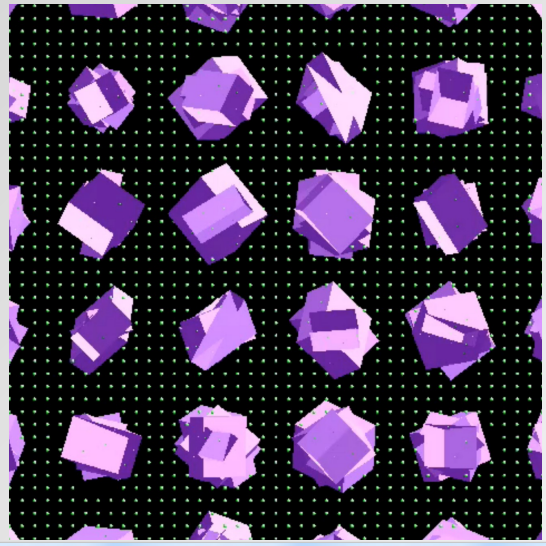


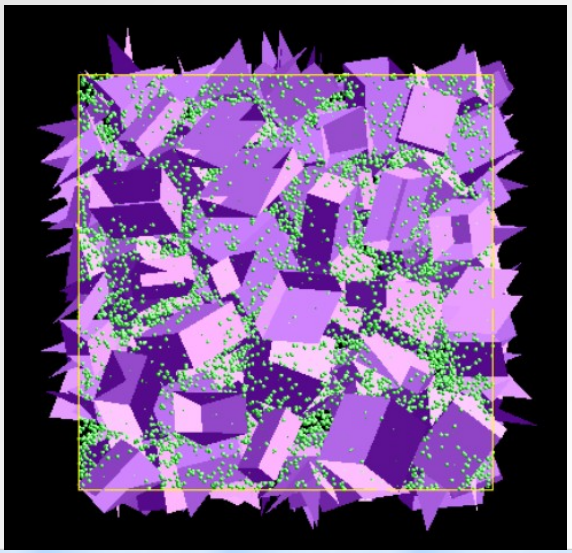


Stochastic Rotation Dynamics

- Effective model for solvated nanoparticles
- No solvent-solvent interactions to compute
- Simulation of micron-size partcles for seconds
- Study particle diffusivity, viscosity, aggregation





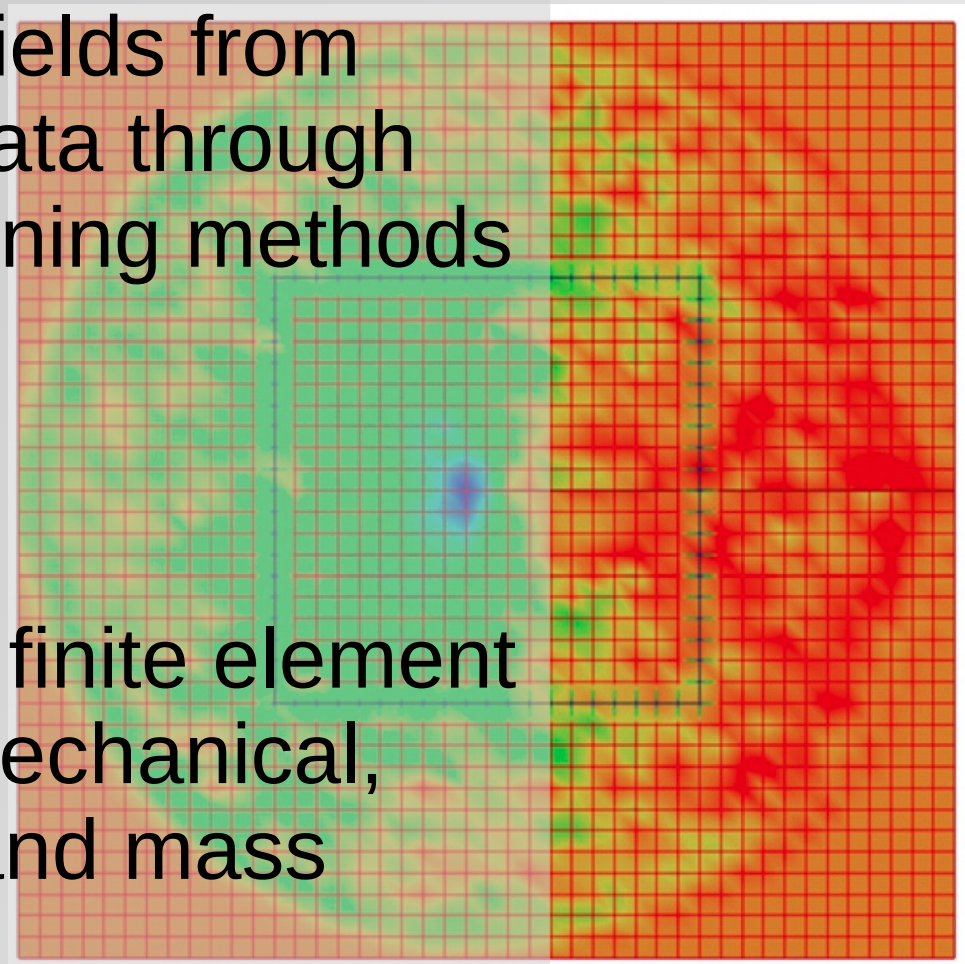


Atom-to-Continuum Package (AtC)

- **Estimate** continuum fields from atomistic simulation data through consistent coarse graining methods

Compressive stress field for an atomic simulation of shock loading

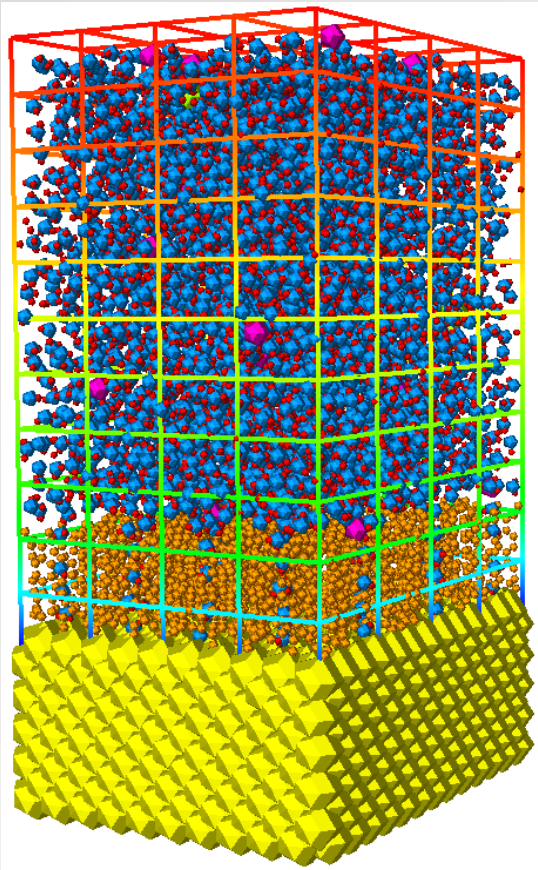
- **Couple** atomistic and finite element regions for thermal, mechanical, electrostatic, charge and mass transport simulations



Stress field around crack at finite temperature

AtC Library Components

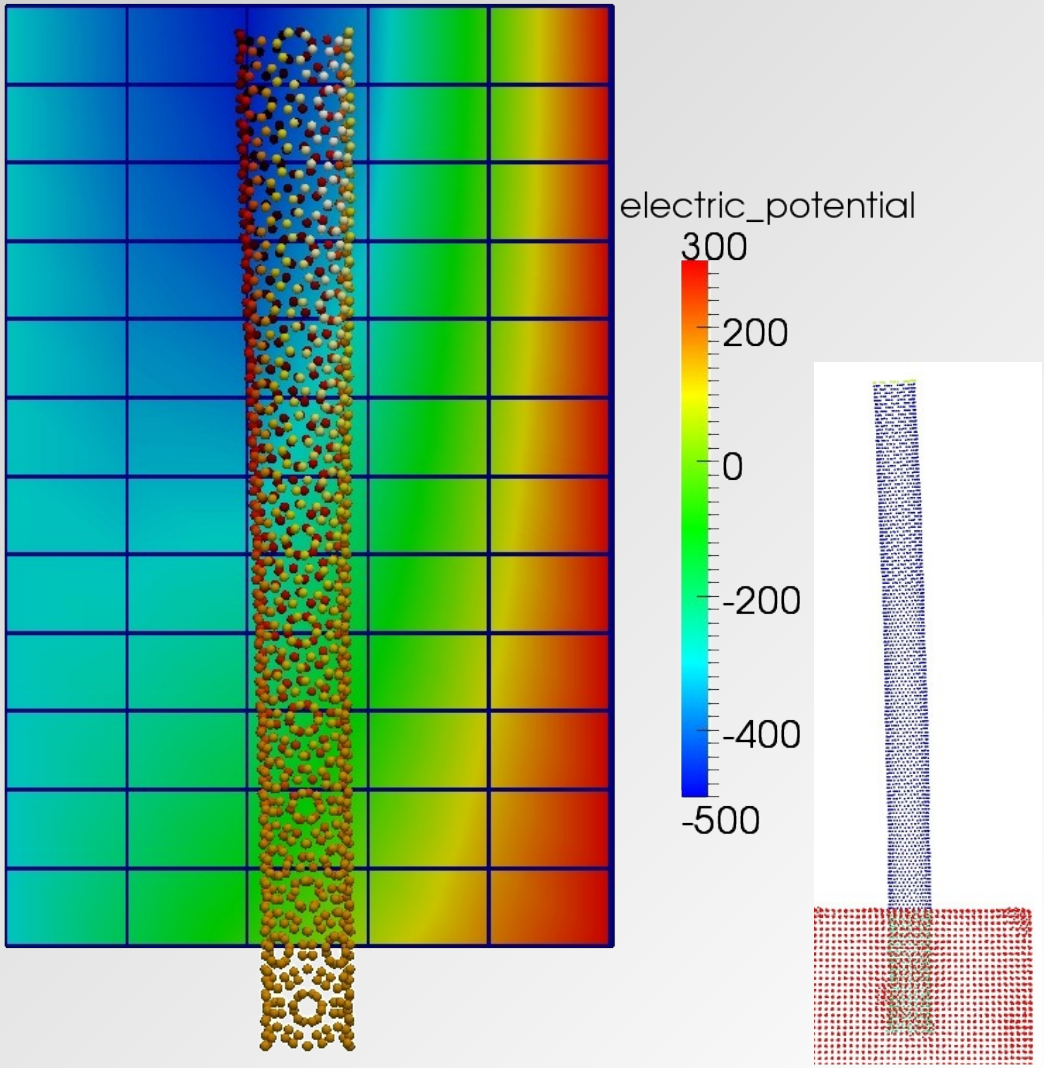
- Meshes (hexagonal, tetragonal)
- Filters (temporal and spatial)
- Coarse grain (transfer to mesh):
  - mass/charge density, dipole moment
  - dislocation, velocity, temperature
  - electric potential, stress and more
- Coupling:
  - charge diffusion, two-temperature
  - mechanical (momentum)
  - thermal (energy) and more



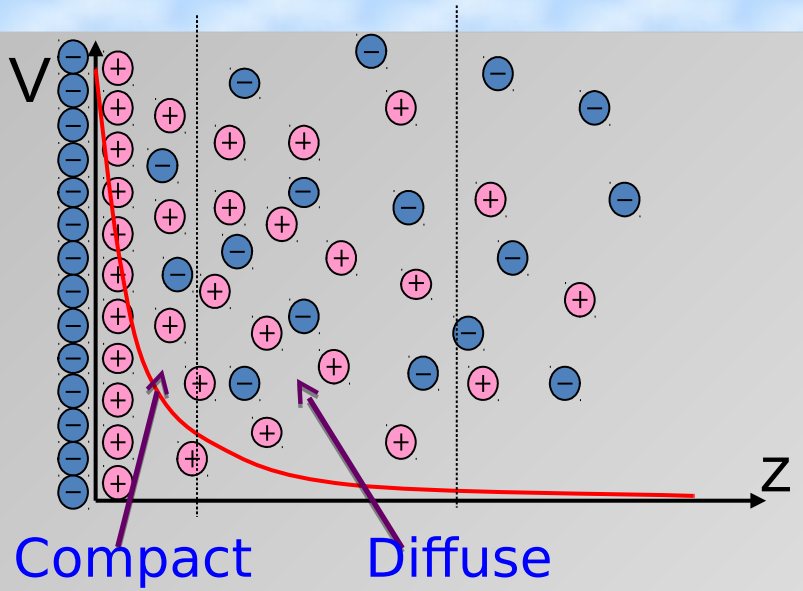
Saltwater-electrode-CNT system: mesh overlaps exactly with water-CNT atom region

AtC Example: Electrostatics

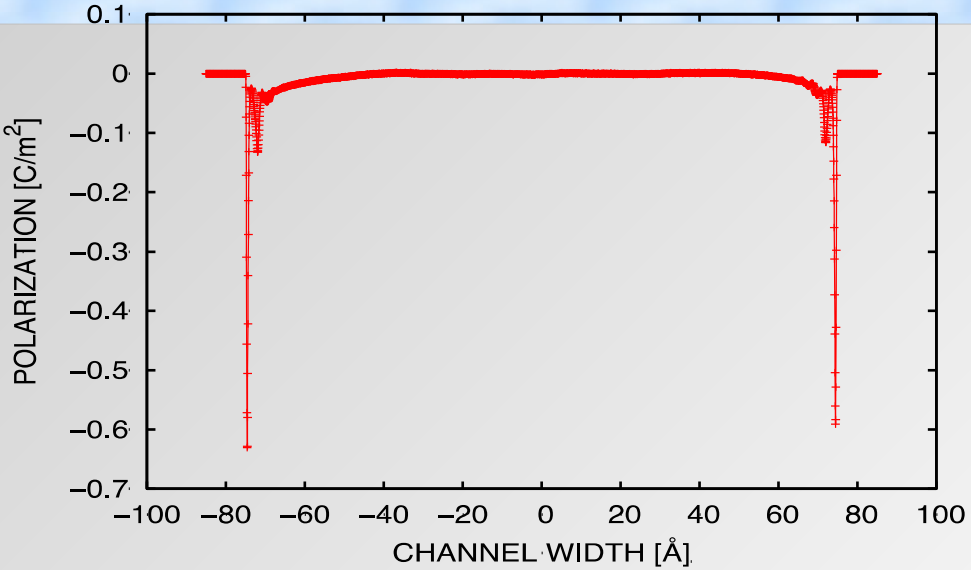
- Surrogate model for electron density
- Electrons segregate to tip
- Potential drop across short axis of CNT
- Mutual repulsion opens tip
- Net charge causes net tip displacement
- CNT anchored in a warm substrate



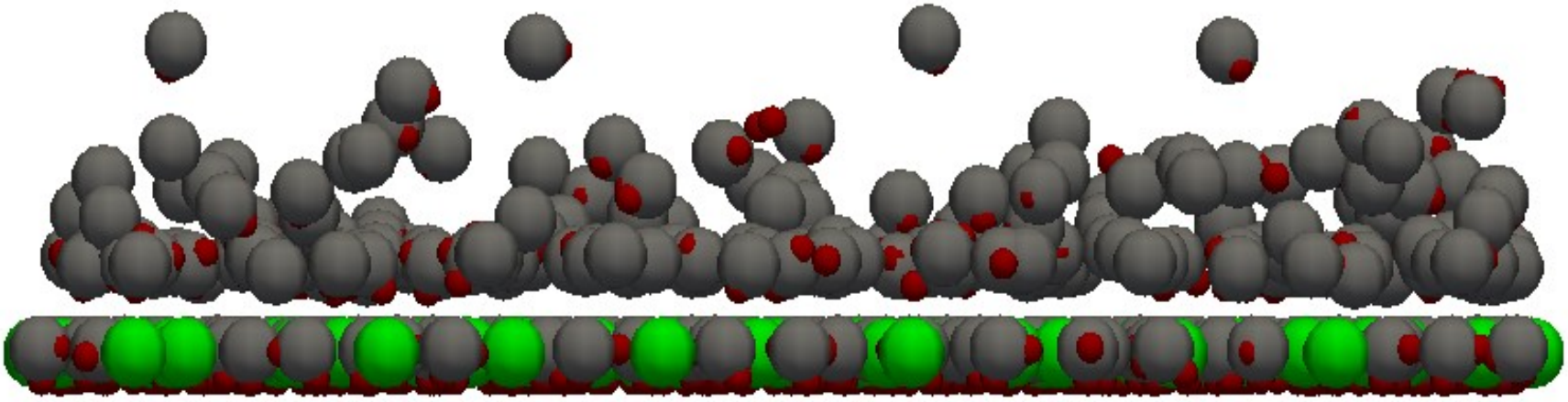
AtC: Electrical Double Layers



Computing the polarization field

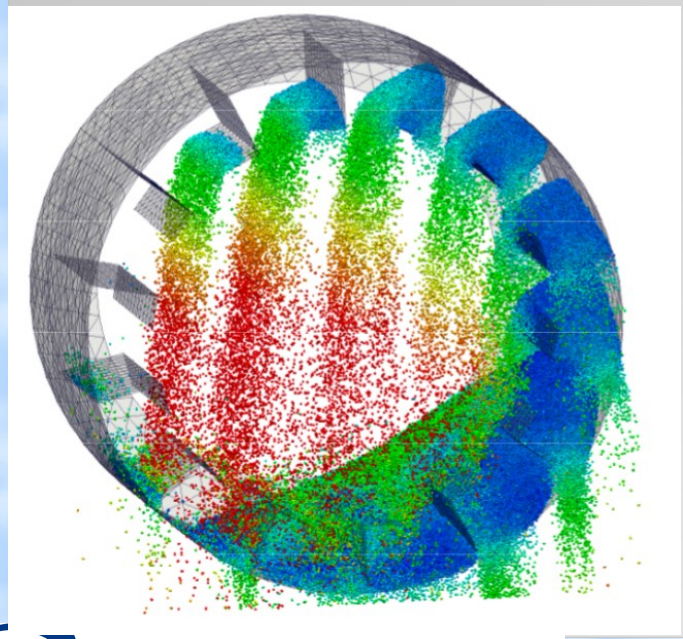


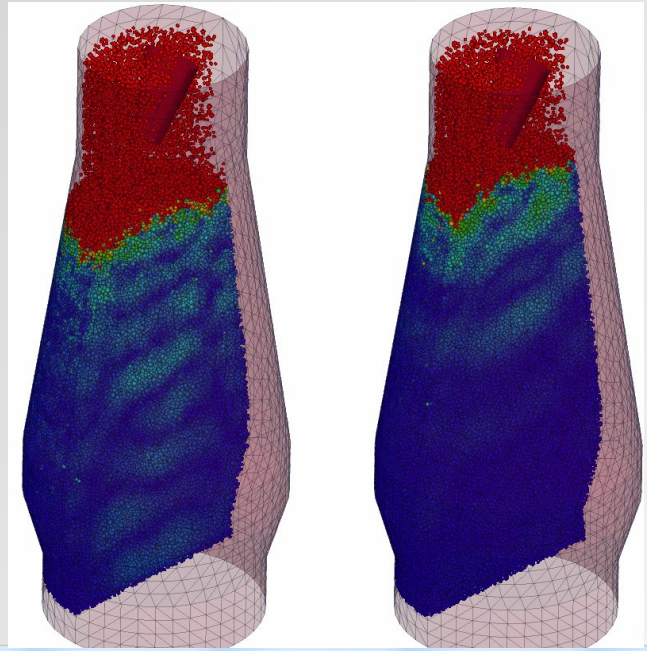
Polarization across the channel

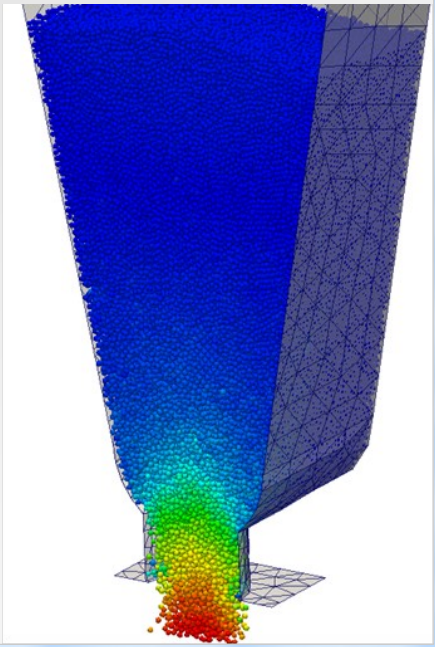


LIGGGHTS: Mesoscale Modeling for Granular Materials

- LIGGGHTS: fork of LAMMPS enhanced for discrete element modeling with CAD meshes
- Coupling to OpenFOAM (=> CFDEM) allows modeling of dry and wet granular materials







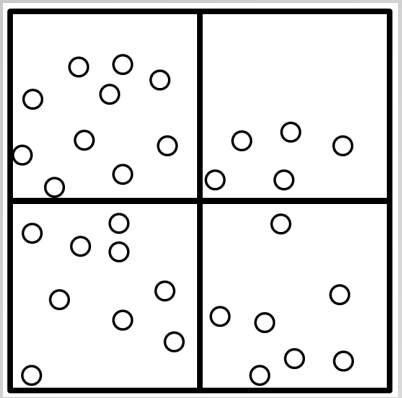
CFDEM Modeling Approaches

Fluid-particle interaction

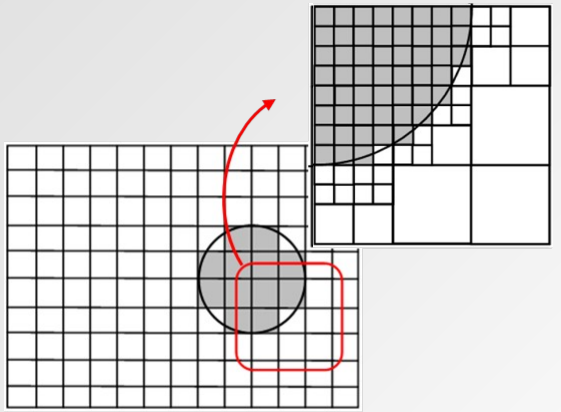
CFDEM coupling

Computational Fluid Dynamics (CFD) + **Discrete Element Method (DEM)**

LIGGGHTS



- **unresolved CFD-DEM**
- **resolved CFD-DEM**



- CFD-DEM*1*
- coarse grained CFD-DEM *2*
- MP-PIC*3*

- Immersed Boundary Method
- Fictitious Domain Method

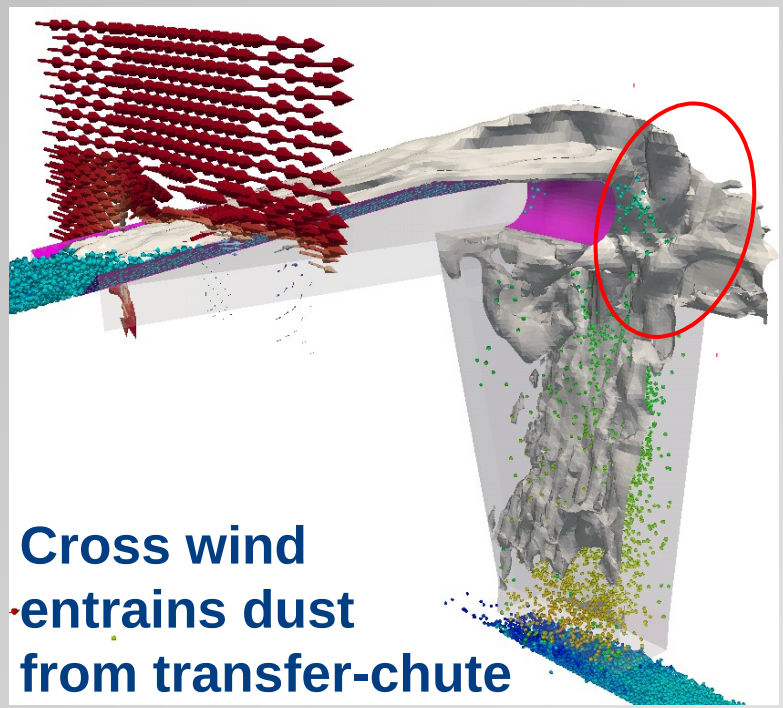
1) Goniva, C., Kloss, C., Deen, N.G., Kuipers, J.A.M. and Pirker, S. (2012): "Influence of Rolling Friction Modelling on Single Spout Fluidized Bed Simulations", Particuology, DOI 10.1016/j.partic.2012.05.002

2) Radl S., Radeke, Ch., Khinast, J., Sundaresan, S. (2011) : "Parcel-Based Approach for the Simulation of Gas-Particle Flows" , Proc. CFD 2011 Conference, Trondheim, Norway

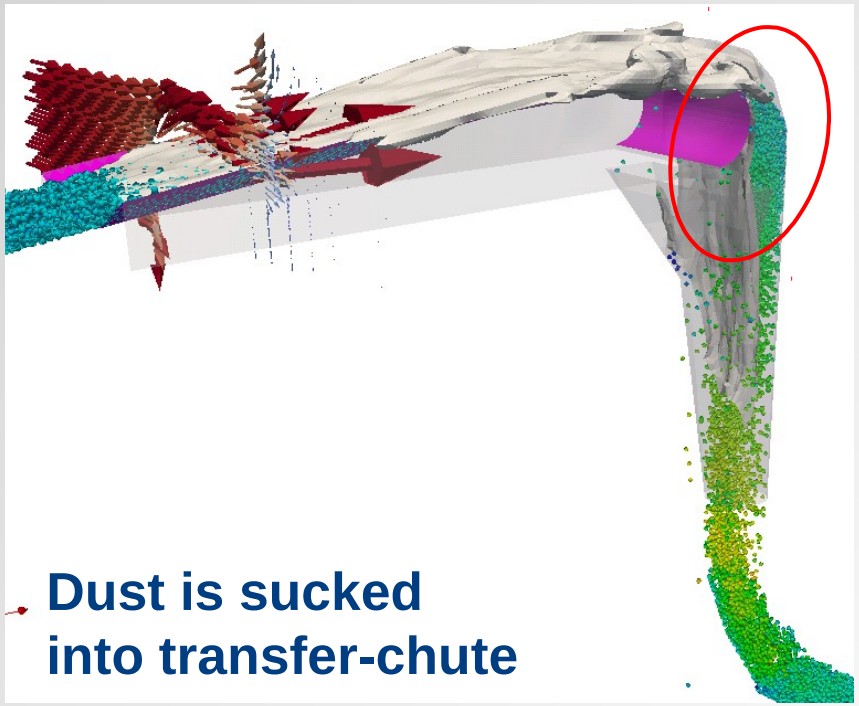
3) Andrews, M.J., O'Rourke, P.J. (1996): "The multi-phase particle-n-cell (MP-PIC) method for dense particle flow", Int. J. Multiphase Flow, 22, 379-402

Transfer Chute Dust Emission

Original Geometry



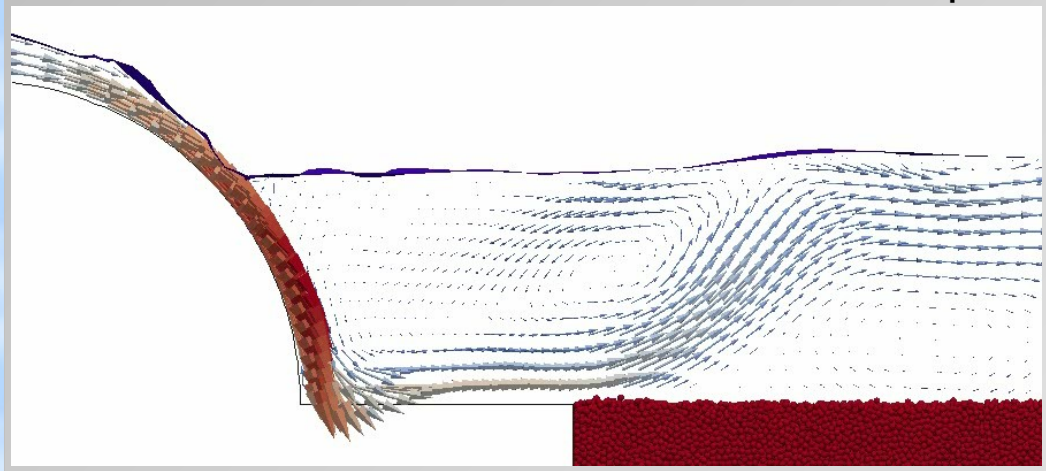
Optimized Geometry

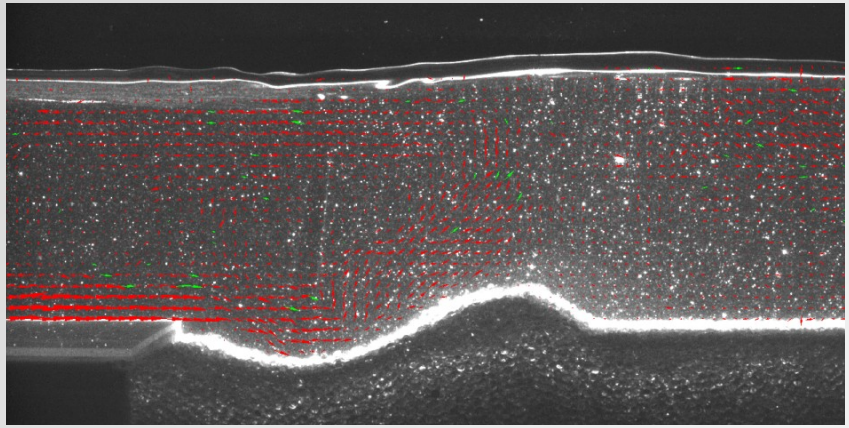


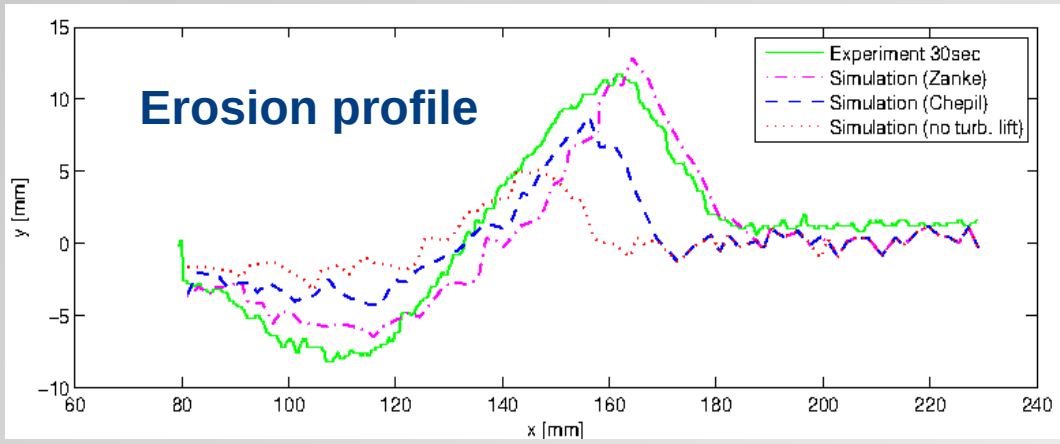
- Transported particles modeled via LIGGGHTS
- Conveyor and chute geometries from CAD meshes
- Dust modeled as continuum interacting with wind via OpenFOAM

Modeling of River Bed Erosion

- turbulent lift force is essential; best performance with Zanke (2003) model







Publications:

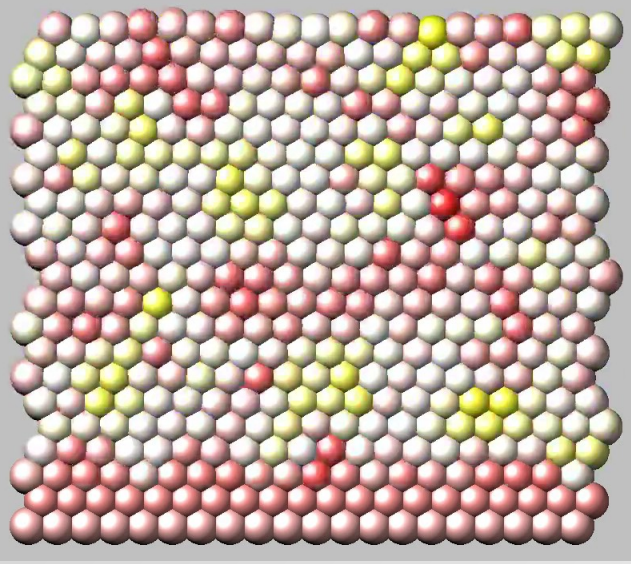
Gruber, K., Kloss, C., Goniva, C: NUMERICAL AND EXPERIMENTAL STUDY OF EROSION IN OPEN CHANNEL FLOW; Proc. IHAR 2012

Zanke, U. (2003). On the influence of turbulence on the initiation of sediment motion. *International Journal of Sediment Research*, pp. 17-31

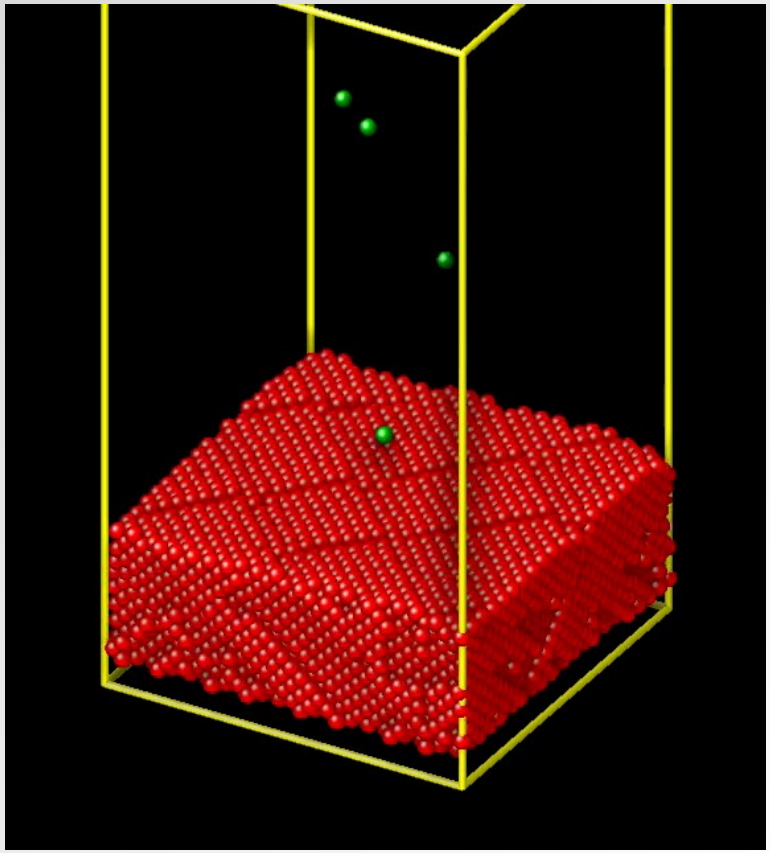
Chepil, W. (1961). The use of evenly spheres to measure lift and drag on wind-eroded soil grains. Soil Sci. Soc. Am, pp. 343-345

Movies From Internal Visualization

- Indent example using time averaged virial stress for colorization

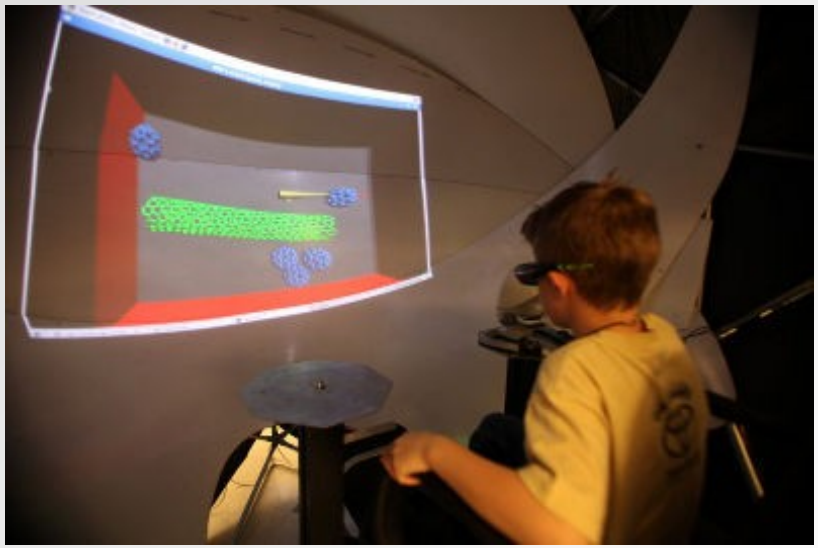


- Sputter example with ambient occlusion



LAMMPS for Outreach: The Nano Dome

- Single person immersive, stereo-3d, haptic, and interactive simulation/visualization environment
- Combines HPC, visualization, molecular simulation, virtual reality, and STEM outreach



LAMMPS MVPs

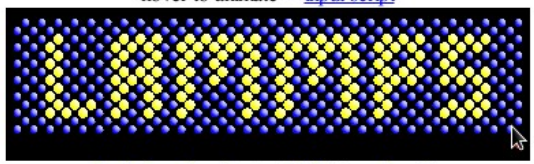
- Steve Plimpton (The Man)
- Aidan Thompson, Paul Croszier (His Deputies)
- Reese Jones, Jeremy Alan Templeton, Jonathan Zimmerman (Atom-to-Continuum)
- Christoph Kloss, Christoph Goniva (CFDEM)
- Greg Scantlen (Nanodome)
- ... and many more that don't all fit into this slide or the photo in the background

lammps.sandia.gov

LAMMPS Molecular Dynamics Simulator

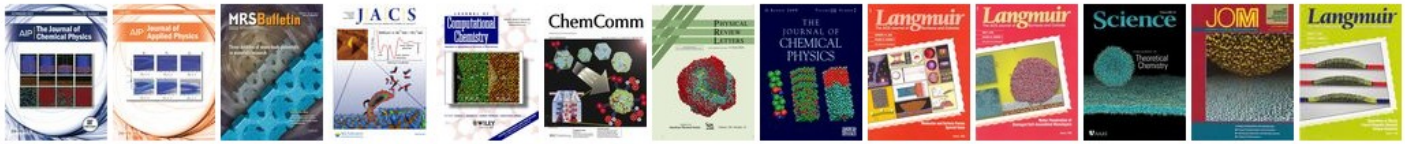
***lamp**: a device that generates light, heat, or therapeutic radiation; something that illumines the mind or soul* -- www.dictionary.com

hover to animate -- input script



physical analog (start at 3:25) & explanation

Big Picture	Code	Documentation	Results	Related Tools	Context	User Support
Features	Download	Manual	Publications	Pre/Post Processing	Authors	Mail list
Non-features	SourceForge	Developer Guide	Pictures	Pizza.py Toolkit	History	MD to LAMMPS glossary
FAQ	Latest Features & Bug Fixes	Tutorials	Movies	Offsite LAMMPS packages	Funding	User Scripts and HowTos
Wish list	Unfixed bugs	Commands	Benchmarks	Visualization	Open source	Workshops
.	.	.	Citing LAMMPS	Other MD codes	.	Contribute to LAMMPS



LAMMPS is a classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator.

LAMMPS has potentials for soft materials (biomolecules, polymers) and solid-state materials (metals, semiconductors) and coarse-grained or mesoscopic systems. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale.

LAMMPS runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain. The code is designed to be easy to modify or extend with new functionality.

LAMMPS is distributed as an open source code under the terms of the GPL. The current version can be downloaded here. Links are also included to older F90/F77 versions. Periodic releases are also available on SourceForge.

lammps.sandia.gov/#nogo ...andia National Laboratories, a US Department of Energy laboratory. The main authors of LAMMPS are listed on this page along with contact info and other contributors. Funding for

LAMMPS Workshop & Symposium @ ICTP, March 17 – 21st 2014

- First in such activity europe after three successful workshops in Albuquerque (Feb 2010, Aug 2011, Aug 2013)
- Bring together LAMMPS contributors and users
- Easier to reach from Europe and ICTP support for researcher from developing countries
- Two Tracks: a) In depth tutorial for beginners, b) developer training for experienced users
- General Symposium on March 21st 2014

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