Mesoscale models for fluids and solids in LAMMPS

Joel T. Clemmer, Thomas C. O'Connor,
Dan S. Bolintineanu, Jeremy B. Lechman

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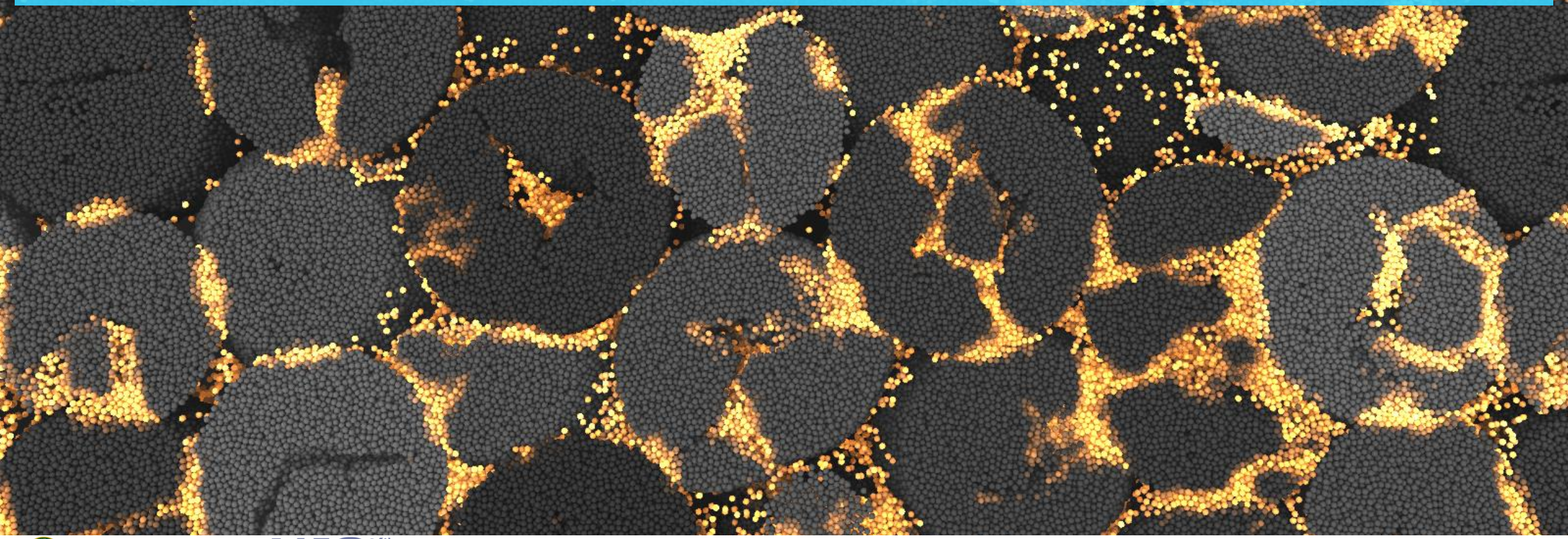

U.S. DEPARTMENT OF ENERGY
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Mesoscale Modeling in LAMMPS

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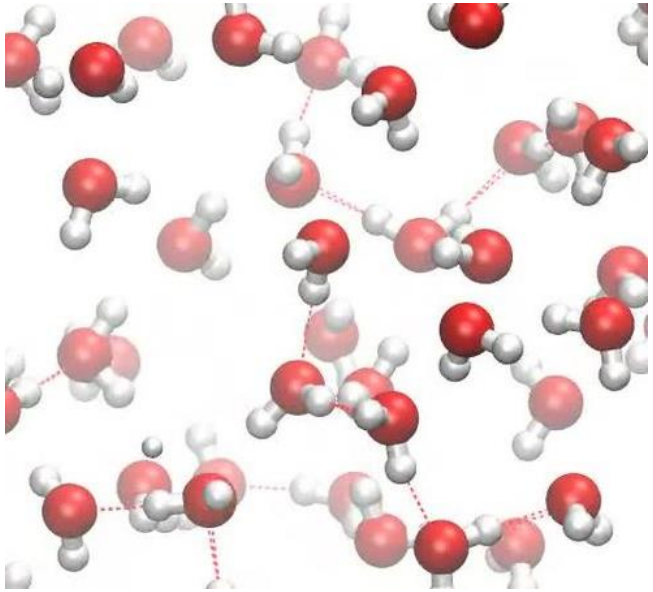
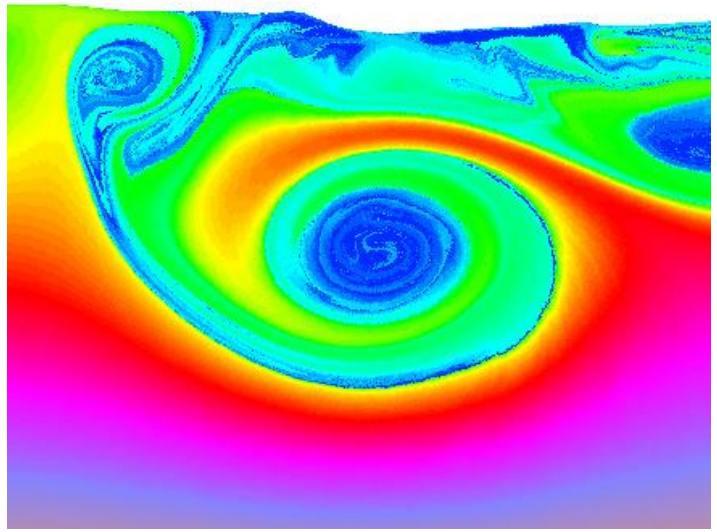


LAMMPS is a general particle simulation codebase, goes beyond MD

In mesoscale modeling, particles represent some coarse grained volume of fluid or solid, some models already implemented e.g.

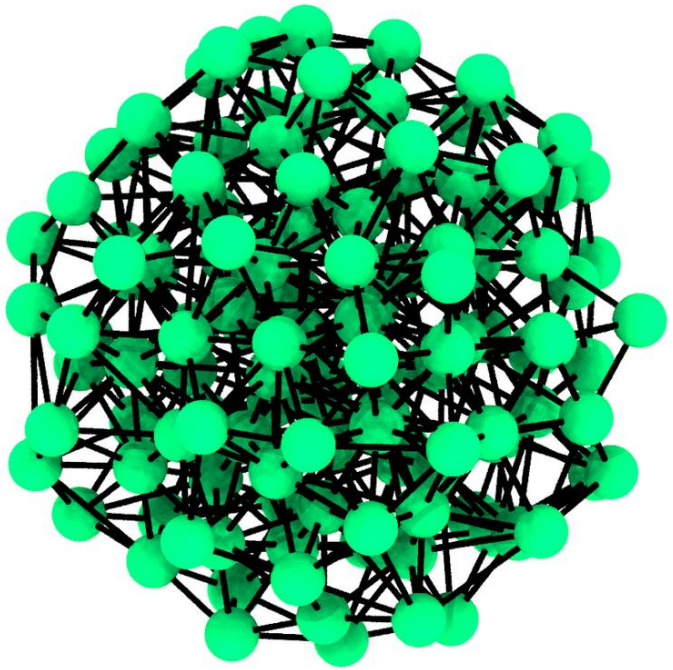
- Discrete element model (GRANULAR)
- Peridynamics (PERI)
- Dissipative particle dynamics (DPD-BASIC, DPD-MESO, …)
- Smoothed particle hydrodynamics (SPH)



New models to be released in LAMMPS:

- BPM package: bonded particle models for solids
- RHEO package: reproducing fluid models + hybridization with BPM

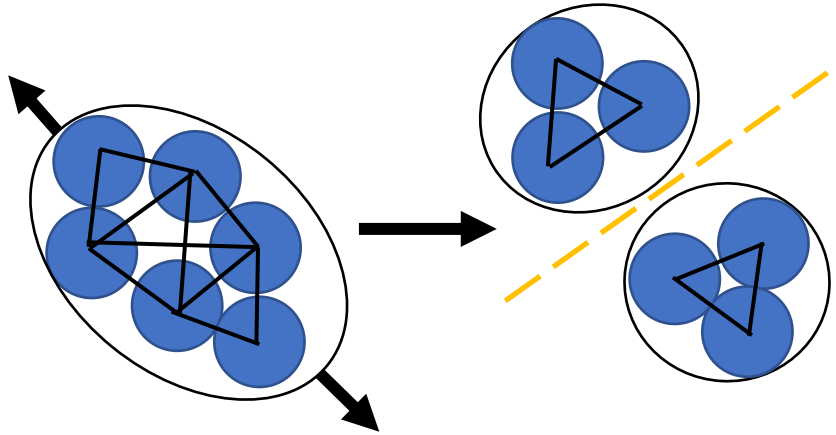
Bonded Particle Models (BPM)



Solids represented by particles connected by bonds

- Equilibrium length = initial length ⇒ stress-free ref. state
- Point particles: spring-like bonds
- Rotational particles: include shear forces and torques
- Can also include multibody terms

Bonds break when stretched beyond critical limit (like quartic)



Calibrate material properties by adjusting bond formulation:
Elastic moduli, Poisson's ratio (tricky), fracture toughness, etc

Implemented a general BPM package in LAMMPS which includes several specific models – adds new fix to store history of bonds

Utility of Approach

Advantages of particle-based methods:

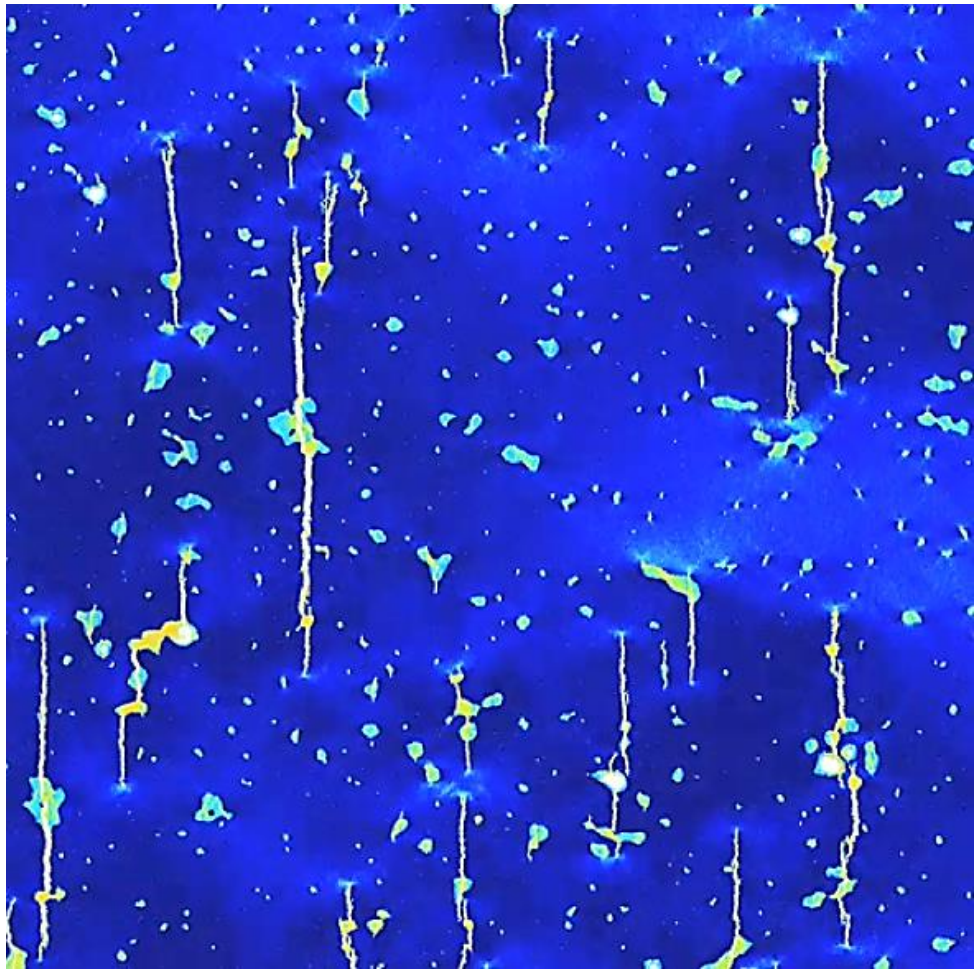
- Particles naturally treat discontinuities (meshfree)
- Full stress field – determines crack nucleation/growth

Disadvantages of BPM:

- Can’t easily implement arbitrary constitutive model
- No mechanic to rigorously enforce consistency
- Need to calibrate material properties

Advantages of BPM:

- Minimal model of fragmentation dynamics
- Efficient, can simulate large systems/resolutions



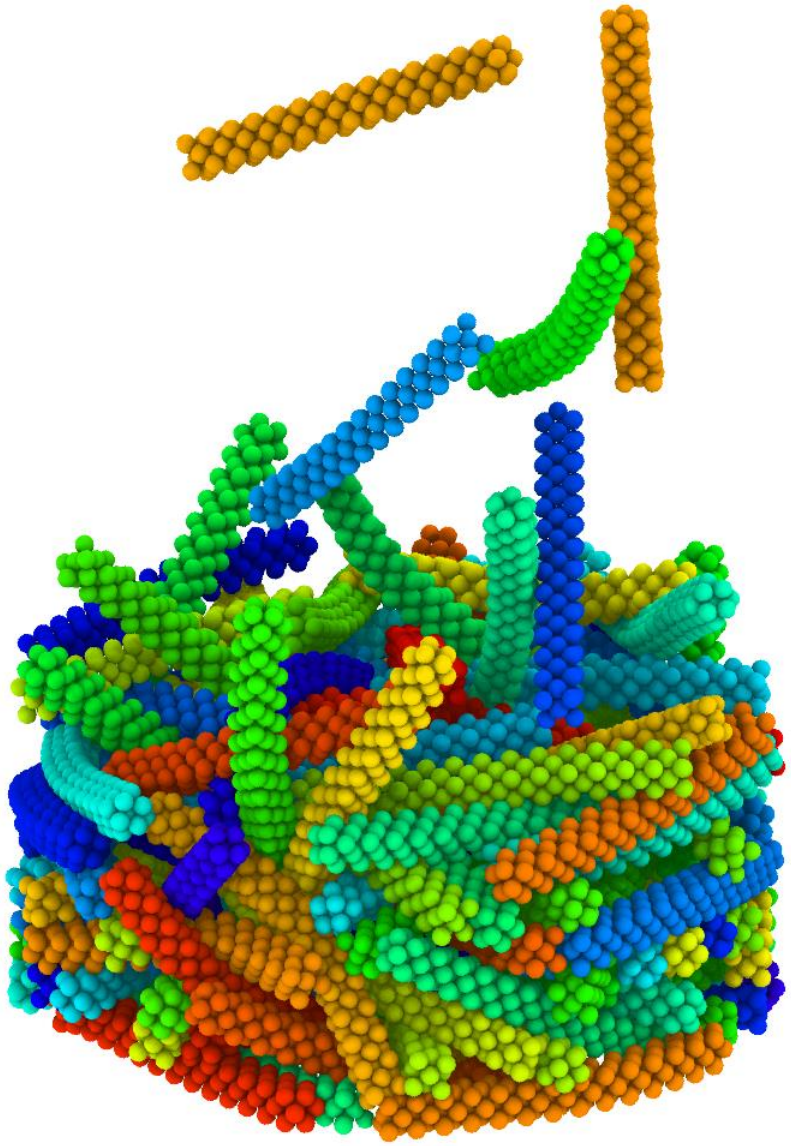
Cracks in uniaxially compressed solid w/ defects

Application 1: Extended Elastic Bodies

Like rigid package, can use BPM to model extended bodies (just turn off bond breakage)

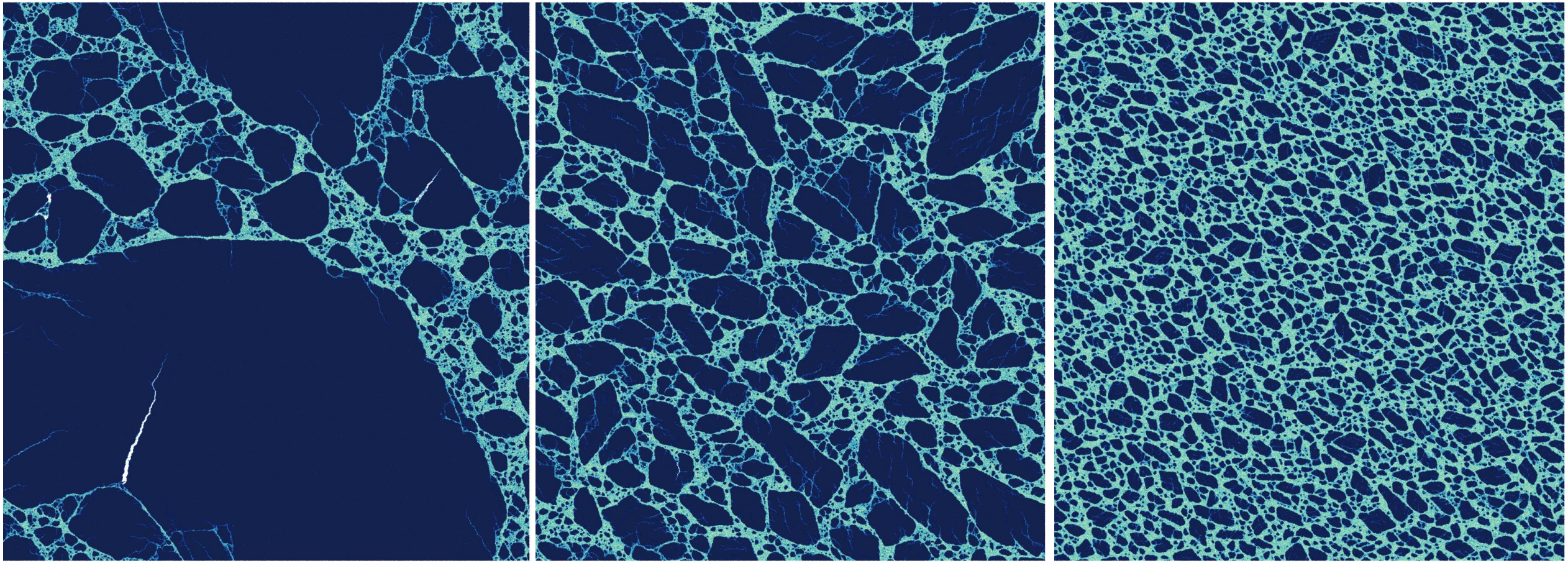
Unlike rigid package, can model soft particles and internal elastic deformation

As bonds remember initial lengths, only need one bond type regardless of internal atom structure



Application 2: Comminution of Solids

Under shear, brittle solids break up into fragments with power-law distributed sizes
Studied evolution of size distribution and effect of strain rate and material properties



Increasing strain rate

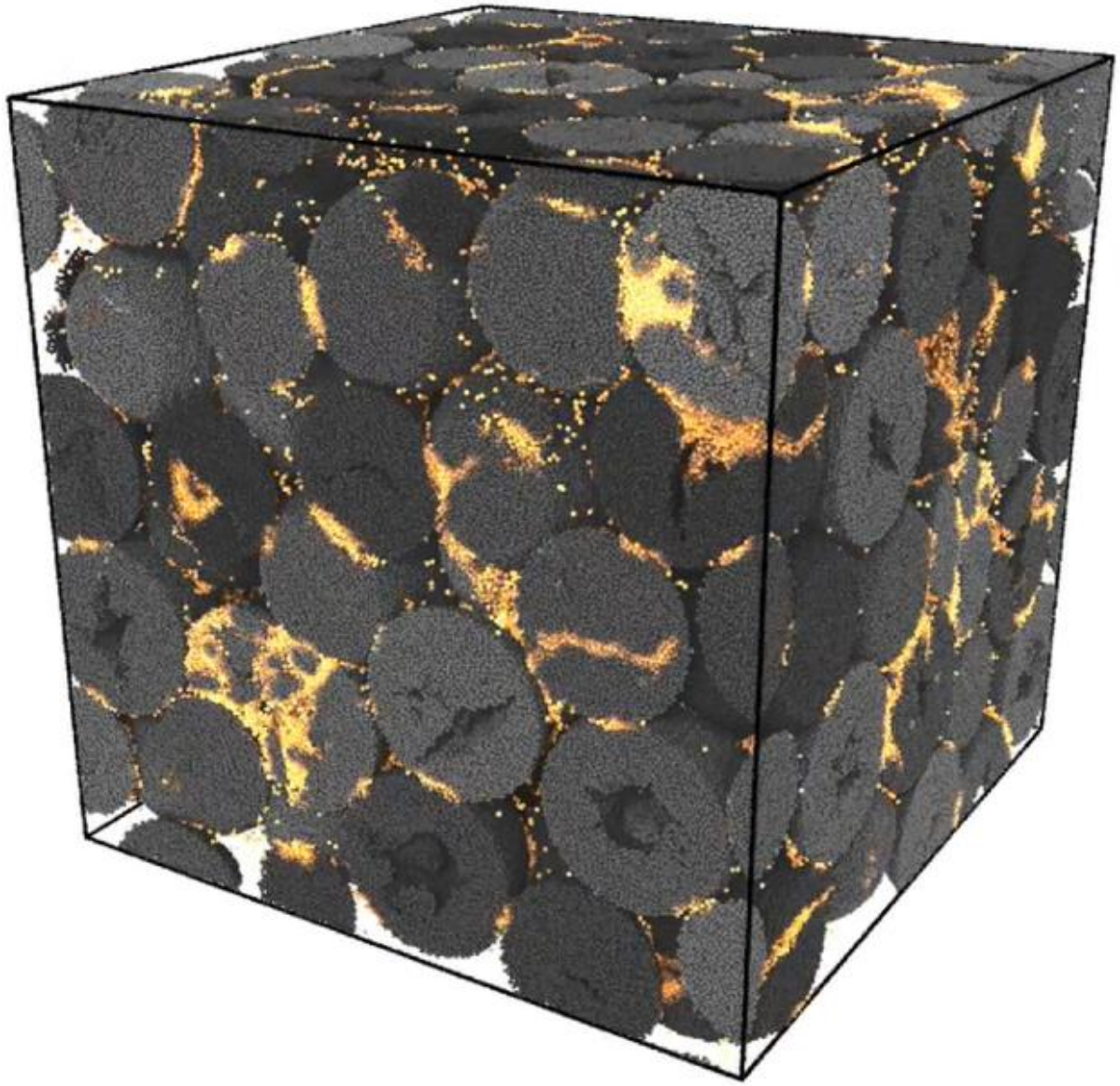
Clemmer, Robbins 2021

Application 3: Granular Compaction

Above the jamming transition, granular packings continue to densify with increased pressure

Grains will rearrange, deform, and eventually fracture

Model high pressure compaction using BPM, identify failure pressure for each grain to test densification theories



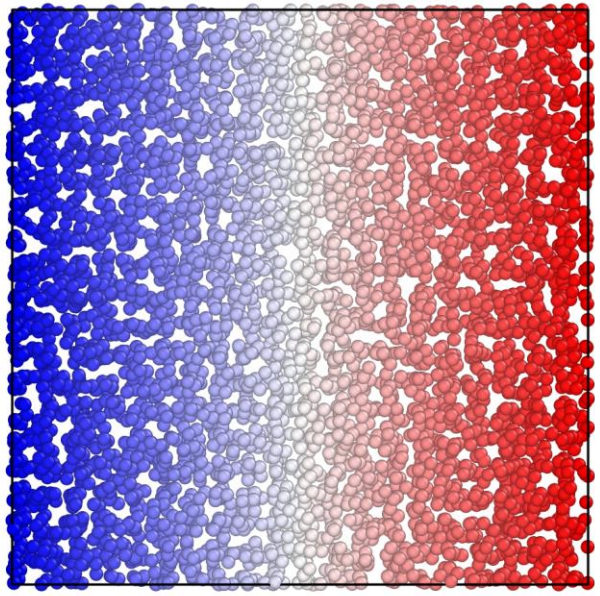
RHEO: Reproducing Hydrodynamics and Elastic Objects

Numerical solver of Navier-stokes equations, joint development with Thomas O'Connor (CMU)

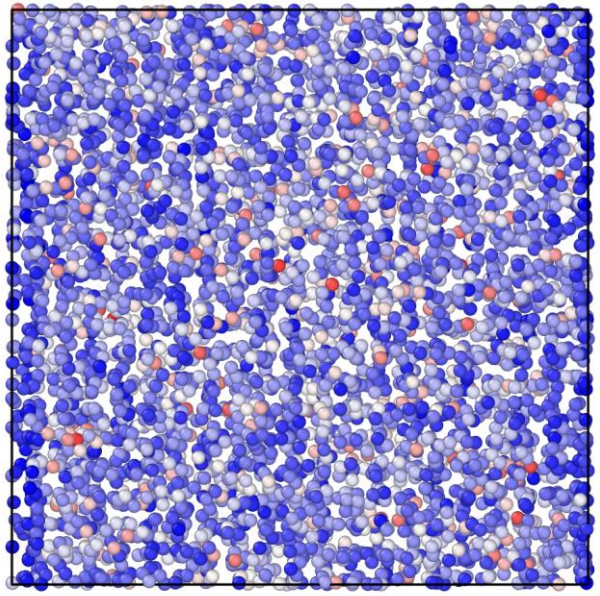
Like Smoothed Particle Hydrodynamics but each particle's kernel is locally built such that simulated continuum fields agree with the real solution up to a 2nd order polynomial (consistent)

Added advanced features:
Particle shifting, no-slip boundary conditions, spatially-varying viscosity models, and multiphase support

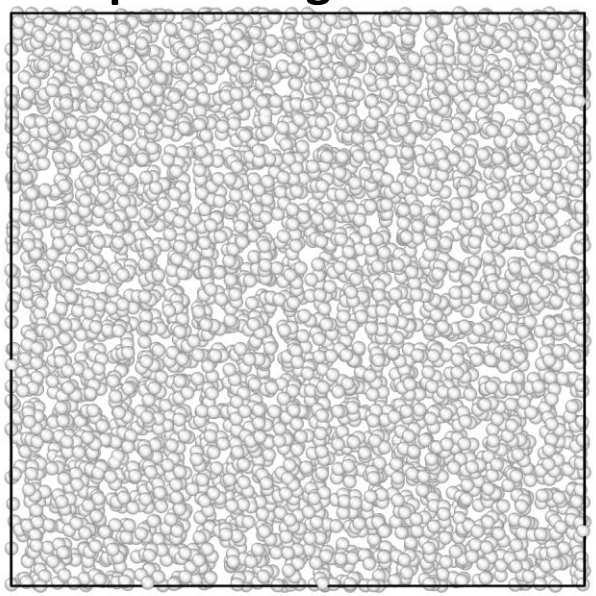
Linearly Increasing Field

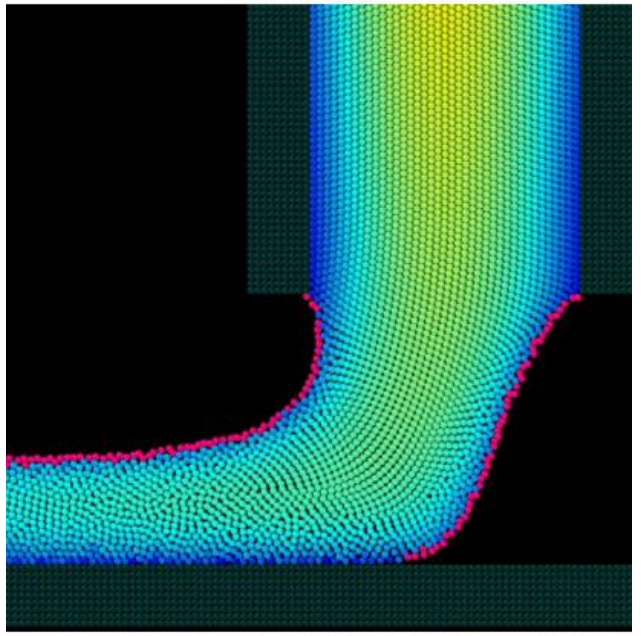


Standard SPH Gradient



Reproducing Gradient





Multiphase Modeling

Solids often represented using

- Frozen particles (no translation, no elasticity)
- A diverging viscosity (stiff equations, no elasticity)

Hybridize RHEO with BPMs to model multiphase problems by combining pair styles (hybrid/overlay) and fixes/computes

Interactions depend on state of each particle:

Temperature, oxidation, solid, fluid, etc…

Solids form/disappear by dynamically creating/breaking bonds

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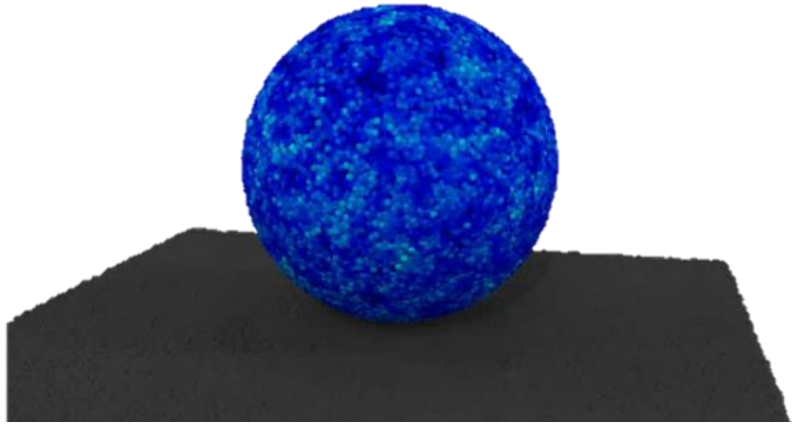
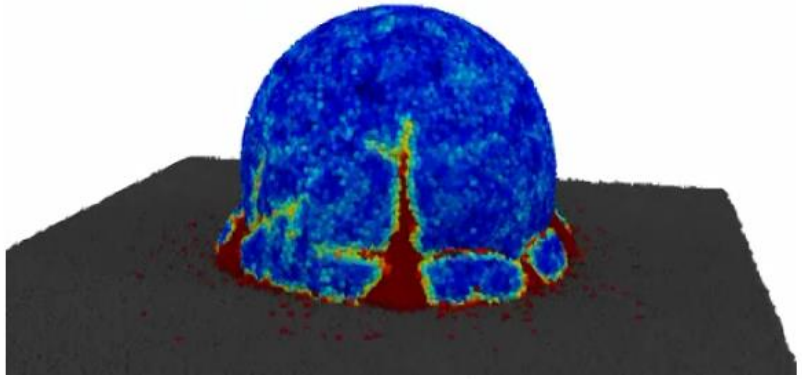
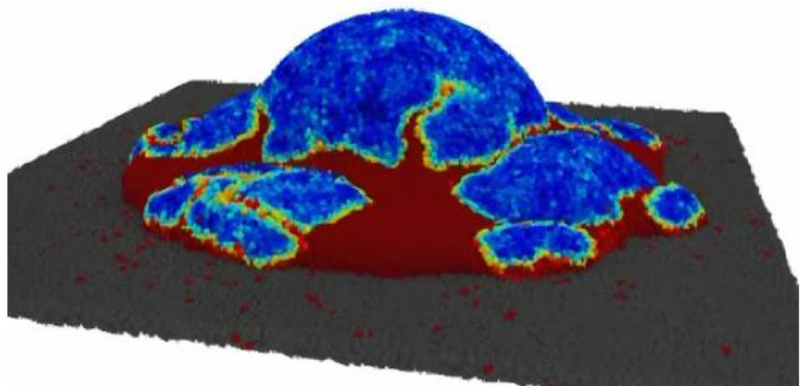
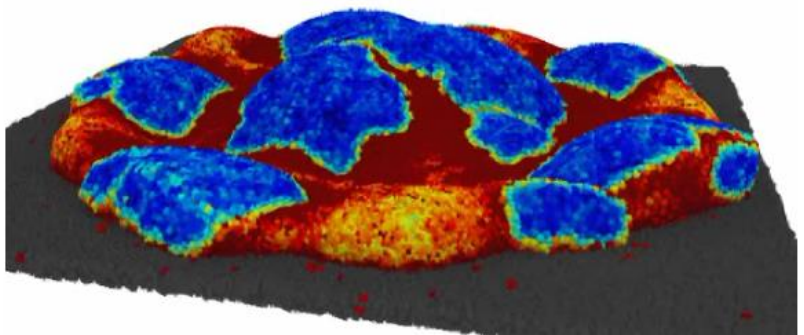
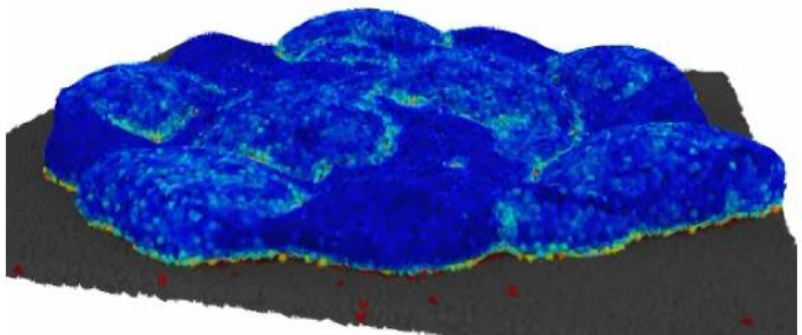
Oxidation/Surface Phase Changes











Certain metals (e.g. aluminum) readily oxidize, creating an elastic shell on surface

Model by tracking exposure of each particle to free surface, if exposed for sufficient time bond with nearby particles

Break bonds under large forces: shell can crack and heal

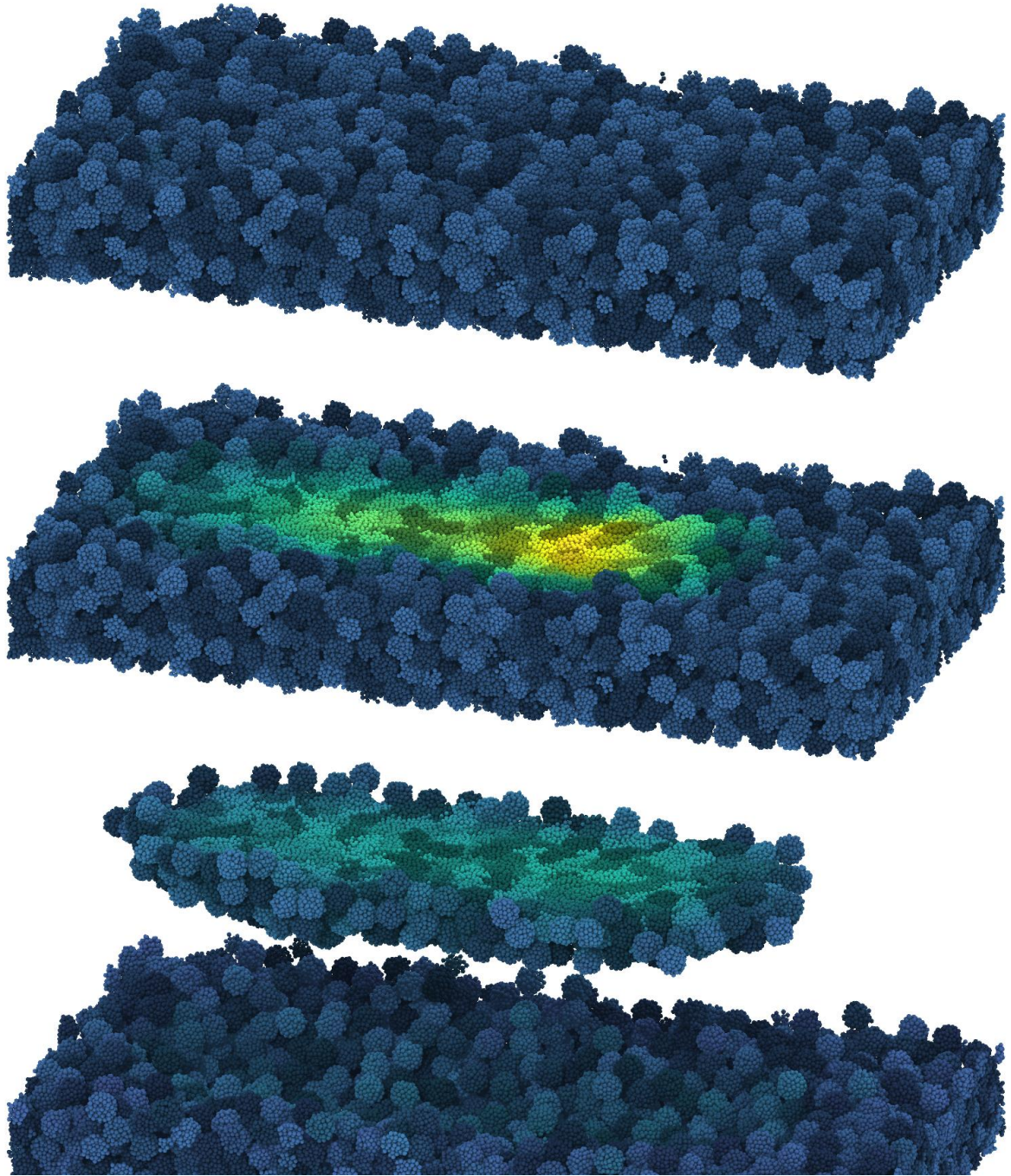
Solidification/Melting

Solve heat transfer between particles and to identify temperature/phase

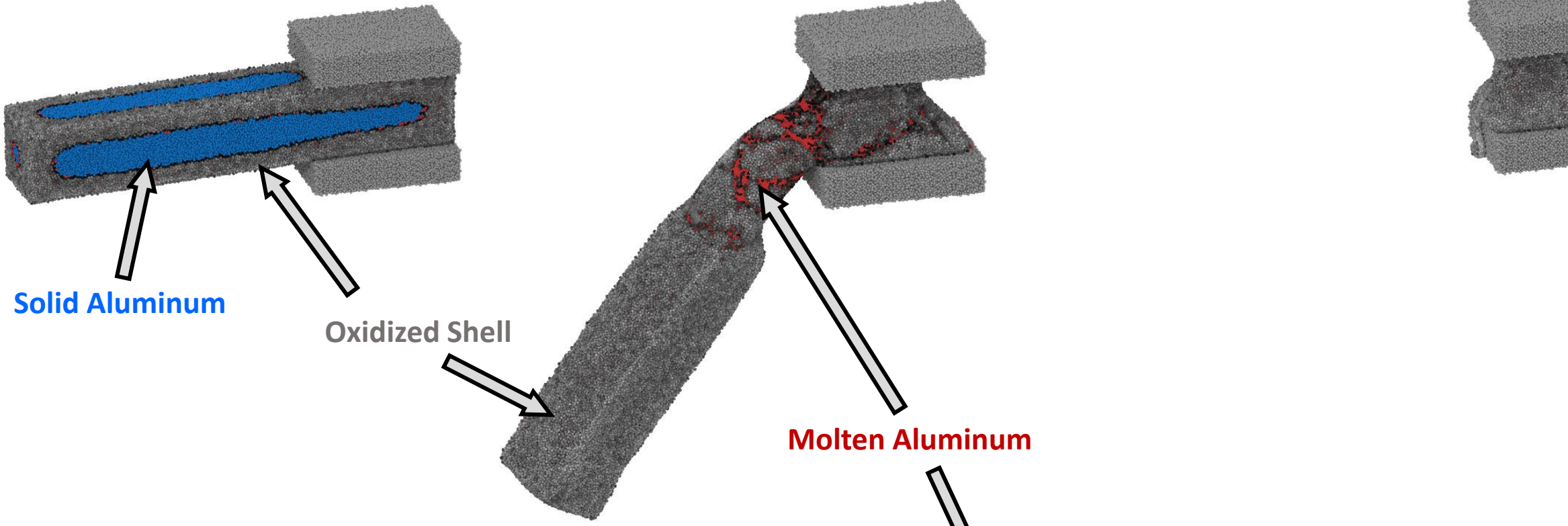
When solidifying, create bonds with all nearby solid particles, when melting break all bonds

Can seamlessly transfer between fluid/solid dynamics in a single simulation, e.g.

1. Pour solid grains
2. Locally melt with moving heat source
3. Cool and remove solidified product



Triple-Phase Problems



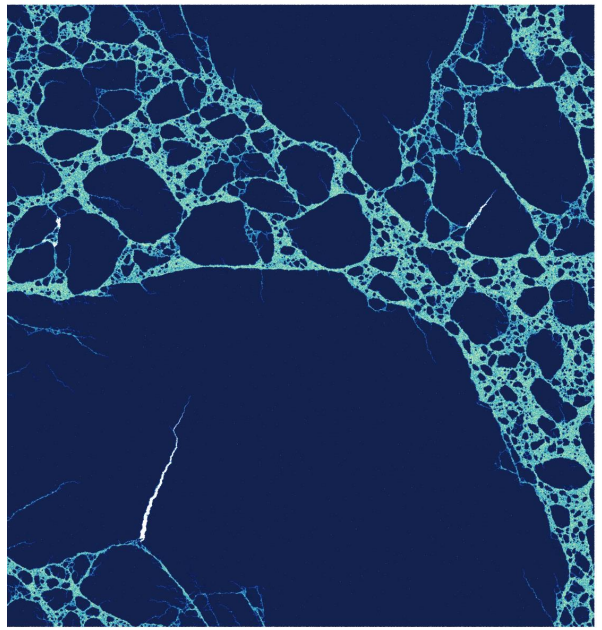
Can overlay multiple models of phase change for triple+ phase problems

Relocation of aluminum cantilever in a heated oven

Summary

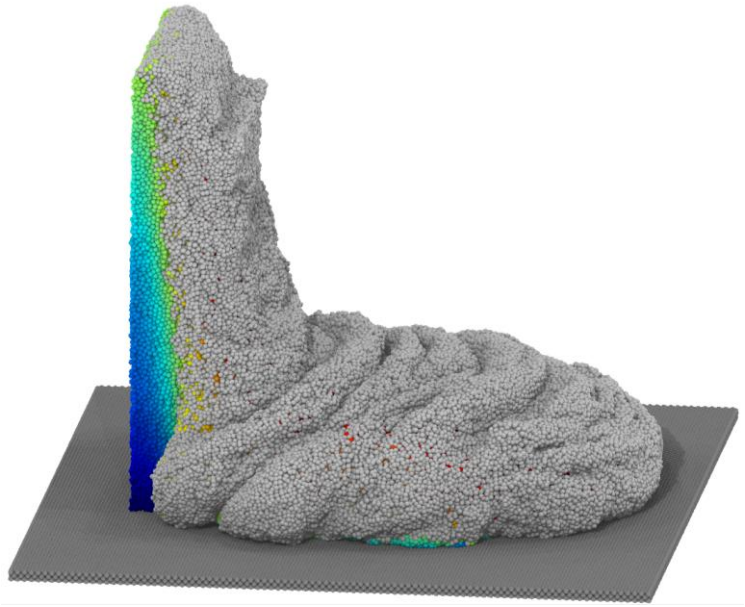
BPM package supports wide range of bonded particle models for solids and brittle fracture

Available now as a soft release, hopefully fully merged early fall



RHEO package provides a flexible platform for accurate solutions to NS equations and coupling to bonded models to support a multitude of multiphase applications

Hopefully submitted to LAMMPS in winter



All simulated images and videos rendered in Ovito