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4 – Hands-on: Simple LAMMPS Examples

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Working with the LAMMPS examples

examples/README has one-line descriptions of 30 examples

Quick runs (2d) and visually appealing:

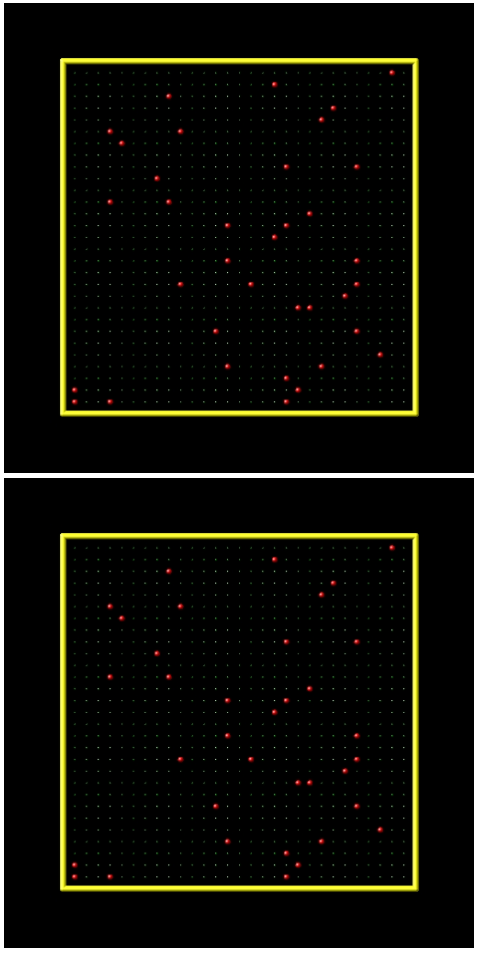
- colloid: colloidal particles in solution
- crack: crack propagation
- flow: Couette and Poiseuille flow in a channel
- friction: frictional contact of spherical asperities
- indent: spherical indenter into solid
- micelle: self-assembly of small lipid-like molecules
- nemd: continuous non-equilibrium shear of LJ liquid
- obstacle: flow around two voids in a channel
- pour: pouring of granular particles into a box
- shear: sideways shear of solid, with and without a void

Running and visualizing the examples

- Run in serial
  - % lmp_linux < in.friction
- Run in parallel
  - % mpirun -np 4 lmp_linux < in.friction
- Uncomment dump image and dump_modify lines
  - produce series of JPG (or PPM) files
  - convert image*jpg tmp.gif
  - open tmp.gif in your browser to animate
- Uncomment dump atom line
  - produce snapshot file, can viz with VMD

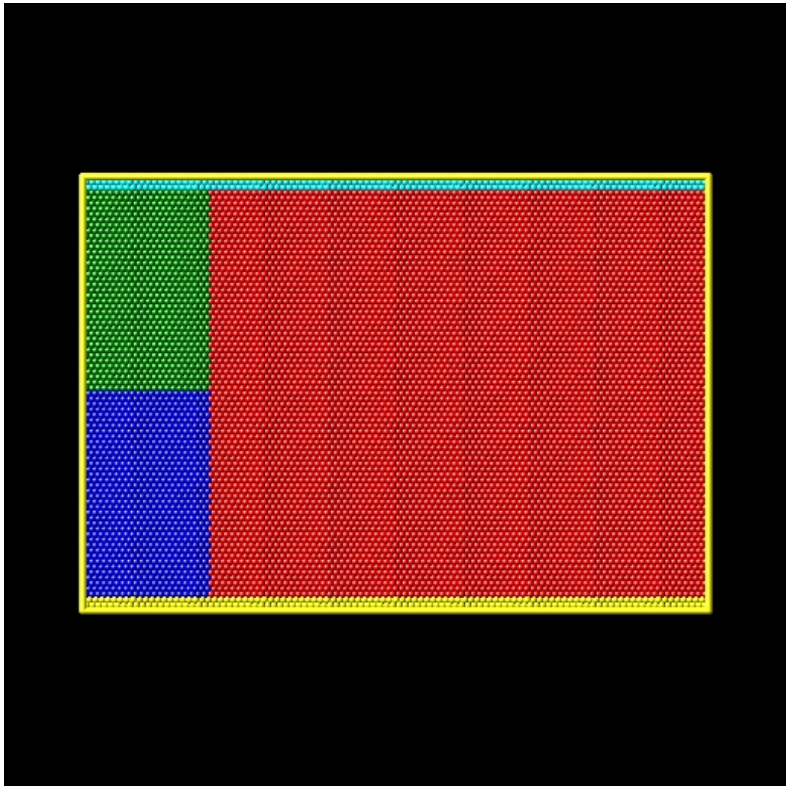
Colloid problem

- Colloids in background LJ fluid
- Set type/fraction 0.96
  4% colloid, 96% solvent
- Fix npt to avoid initial
  overlaps and shrink box
- Neighbor multi for efficient
  neighbor list building
- Options to play with:
  fix deform $\Rightarrow$ target density
  change colloid fraction
  CPU test of
    neighbor multi vs bin



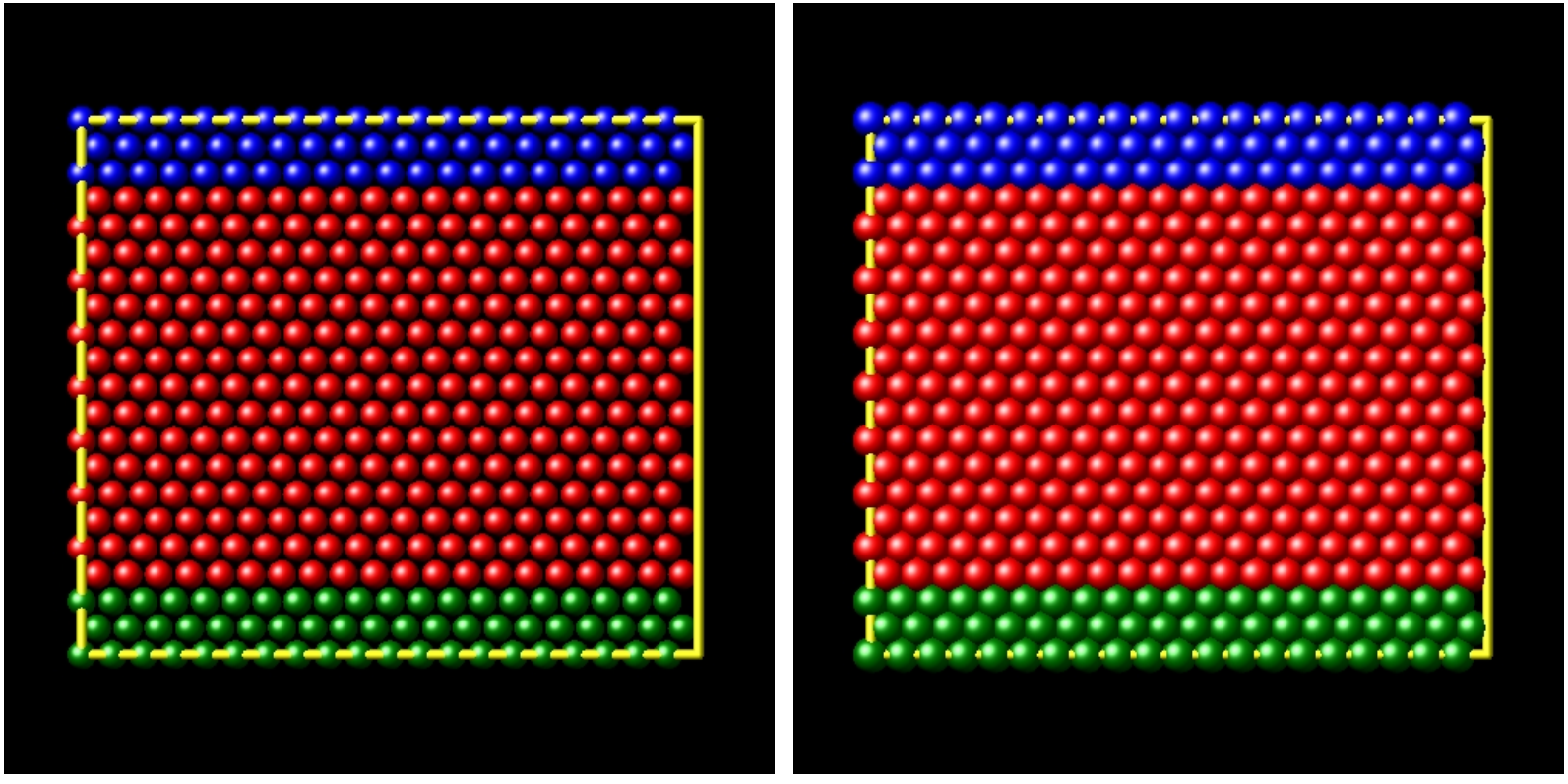
Crack problem

- Tensile pull on 2d LJ solid
- Slit crack between red/green
  neigh_modify exclude 2 3
- Uniform gradient pull
  velocity ramp command
  else shock waves or worse
- Need large system & slow pull
  else defects besides crack
- Options to play with:
  pull rate
  pair-wise cutoff
  turn off velocity ramp
  change NULL $\Rightarrow$ 0.0 in fix 2



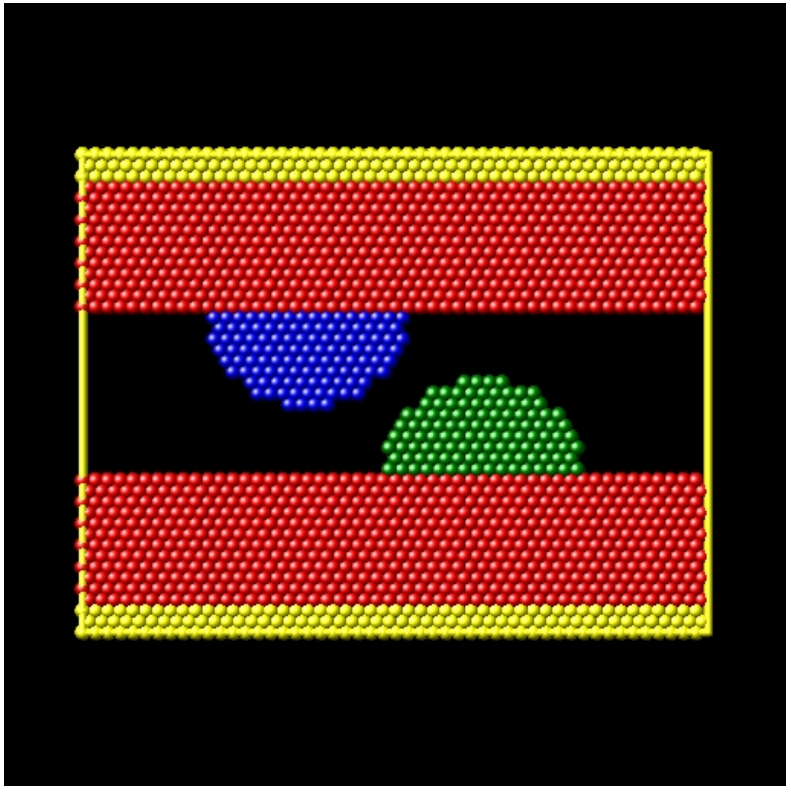
Flow problems

- Couette flow and Poiseuille flow
- Options to play with: wall velocity, force kick, temperature
- Monitor velocity profile via fix ave/spatial



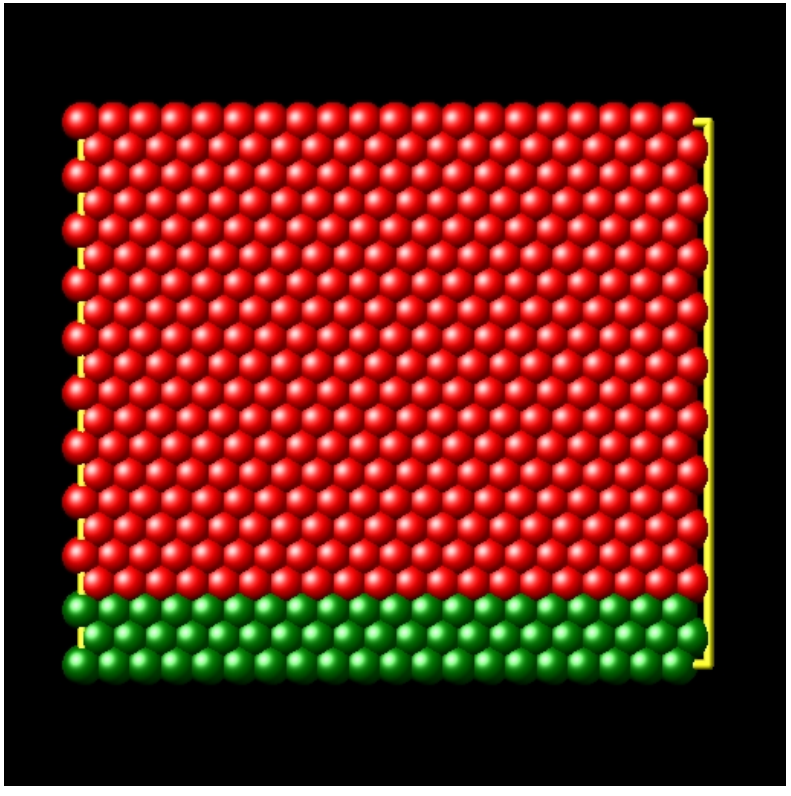
Friction problem

- Two non-planar surfaces
- Region commands
  to build geometry
- Options to play with:
  asperity size, shape
  asperity separation
  x-velocity
  multiple passes



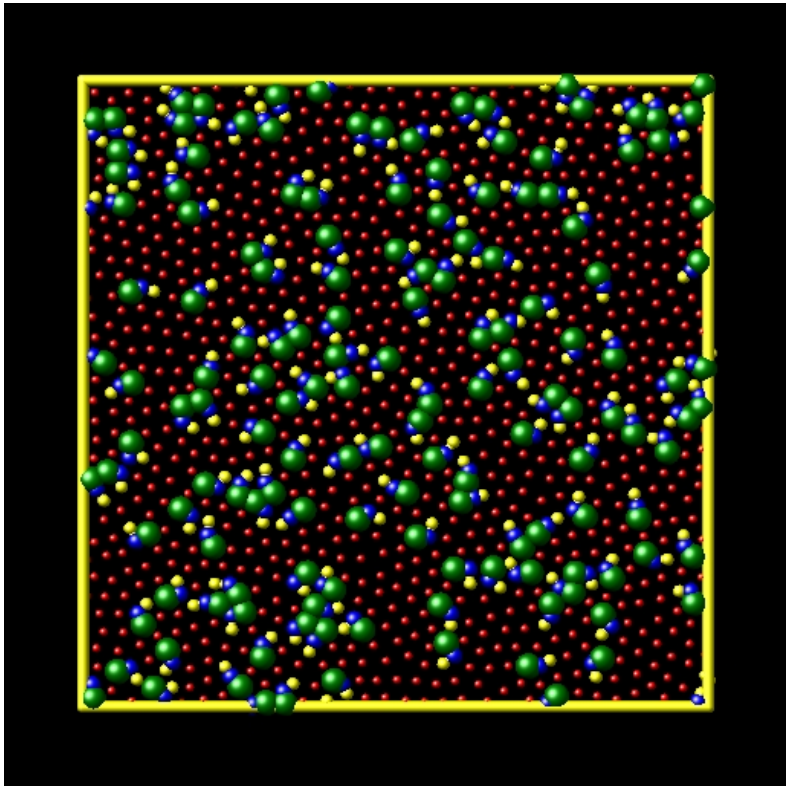
Indent problem

- 2d LJ solid
  - periodic in x
  - free upper y surface
- Spherical indenter
  - push downward, remove
- Defect creation & healing
- Options to play with:
  - speed & depth of indent
  - size of indenter
  - size of system



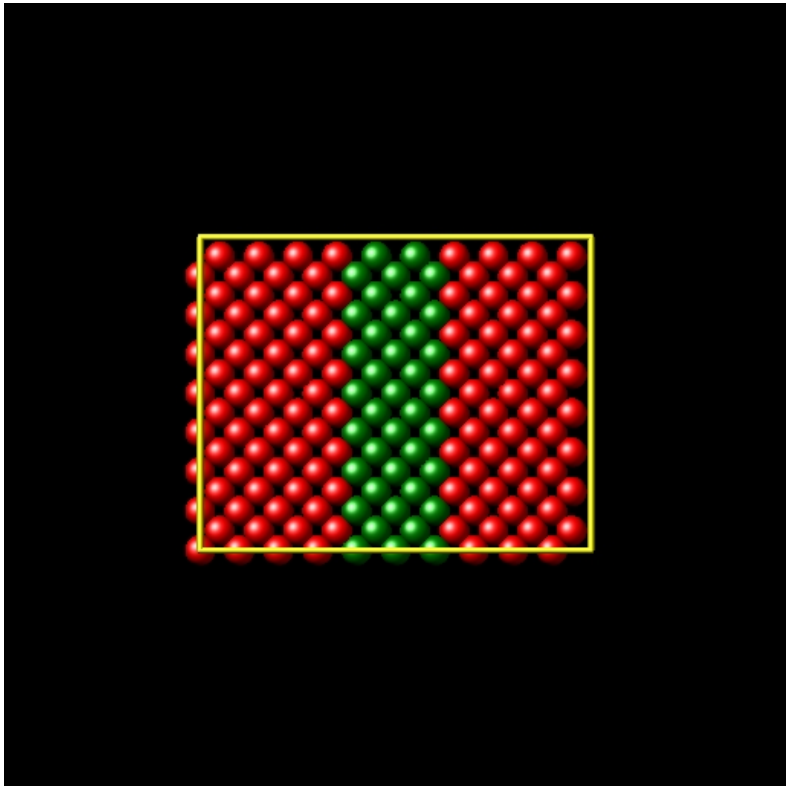
Micelle problem

- Simple lipid model
  - hydrophilic head
  - hydrophobic tail
  - monomer solvent
- 2d self-assembly
  - vesicles, bilayers
- Options to play with:
  - timestep size
  - # of timesteps
  - pair-wise coeffs



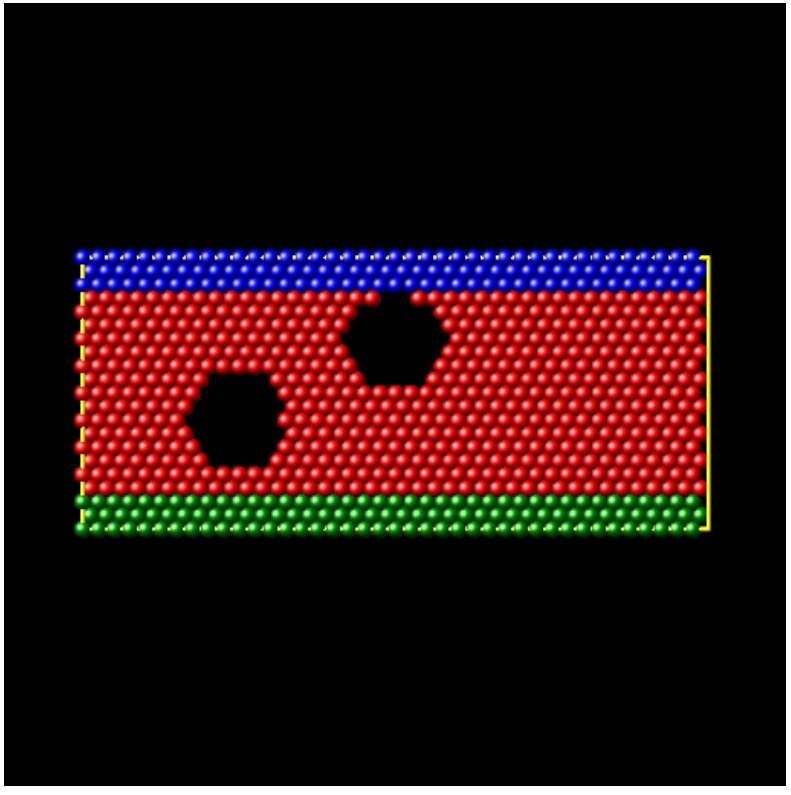
NEMD problem - non-equilibrium MD

- Continuous shear of LJ fluid
  - via fix deform xy
- Fix nvt/sllod for
  - thermostatting
- Red/green to illustrate mixing
  - via region and set type
- Options to play with:
  - system size
  - shear rate
  - velocity ramp for better
    - flow initialization



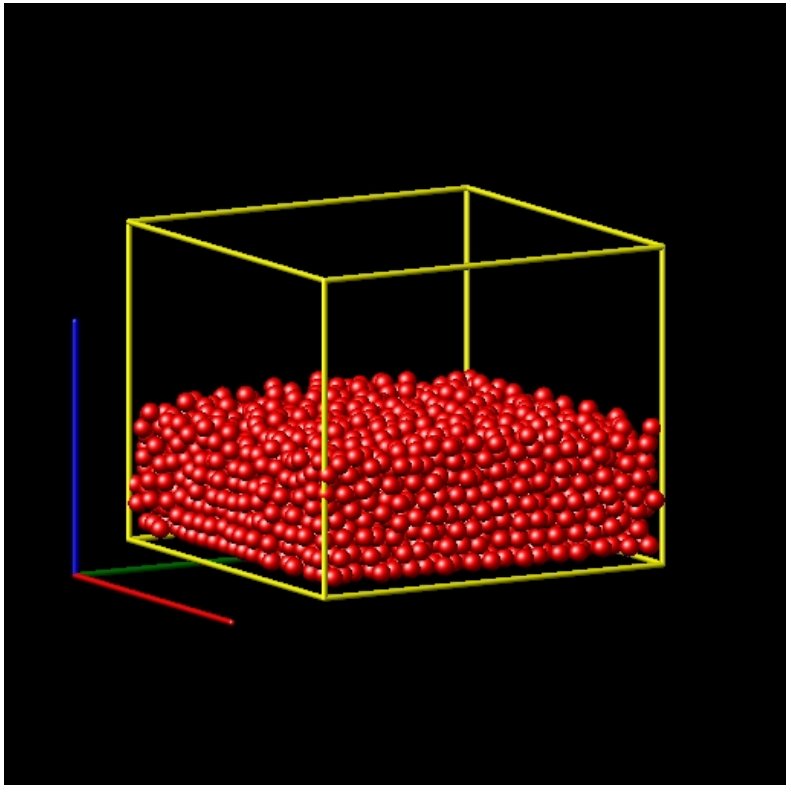
Obstacle problem

- LJ flow around obstacles
- Poiseuille kick added to atoms
  - pressure-gradient flow
- Top surface applies pressure
- Obstacle creation
  - delete_atoms command
  - fix indent command
- Options to play with:
  - size of force kick
  - size of system
  - size & position of obstacles
  - shape of obstacles
  - add a new obstacle



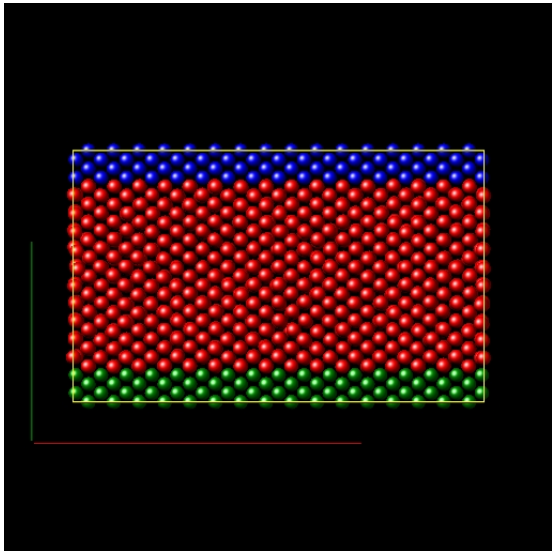
Pour problem

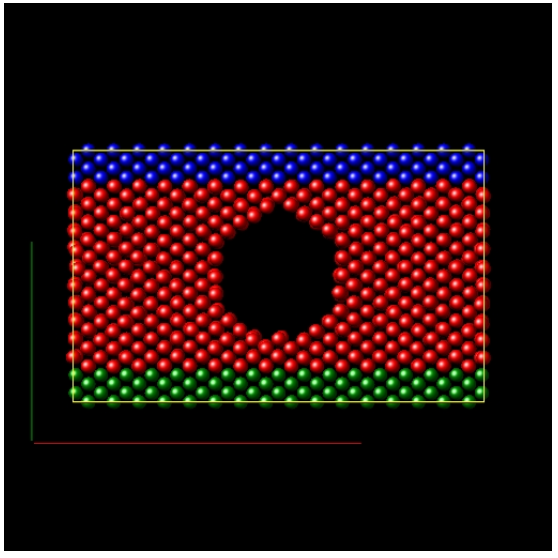
- Granular spheriods in box
- Normal & tangential friction
- Gravity for macroscopic system
  - angle induces chute flow
- 2d version also exists
- Upper/lower boundaries
  - fix pour command
  - fix wall/gran command
- Options to play with:
  - size of system
  - timescale of pour
  - direction of gravity
  - 2d input also exists



Shear problems

- Fixed-end shear in fcc Ni
- EAM potential
- Quasi-3d
  - non-periodic XY slab
  - thin in Z, periodic
- Defect formation without and with void
- Options to play with:
  - size of system
  - shear rate
  - turn off velocity ramp
  - change void shape, size
  - add another void





What does a hands-on session mean?

- Break into small teams
- Choose one or two example problems to work on
- Run simulations, play with the options
- Split up tasks among team members
- Ask questions as needed
- Last half hour:
  - present a couple of slides to group
  - 3 to 5 minutes max
  - include plots, images, movies
  - what did you learn?
  - what could be next steps?

- Let's see how this works!