

Exercises with the LAMMPS examples

[examples/README](#) has one-line descriptions of 40 examples

Quick runs (2d) and visually appealing:

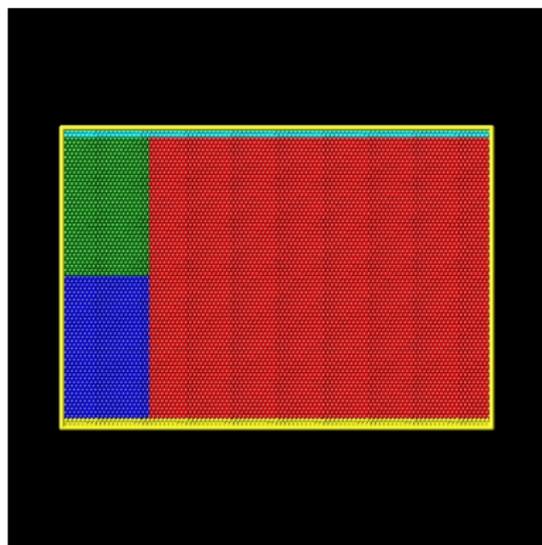
- **crack**: crack propagation
- **flow**: Couette and Poiseuille flow in a channel
- **friction**: frictional contact of spherical asperities
- **indent**: spherical indenter into solid
- **micelle**: self-assembly of small lipid-like molecules
- **obstacle**: flow around two voids in a channel
- **shear**: sideways shear of solid, with and without a void

Running and visualizing the examples

- Run in **serial**
 - `Imp_linux < in.friction`
- Run in **parallel**
 - `mpirun -np 4 Imp_linux < in.friction`
- Uncomment **dump image** and `dump_modify` lines
 - produce series of JPG (or PPM) files
- Uncomment **dump atom** line
 - produce snapshot file, can viz with VMD

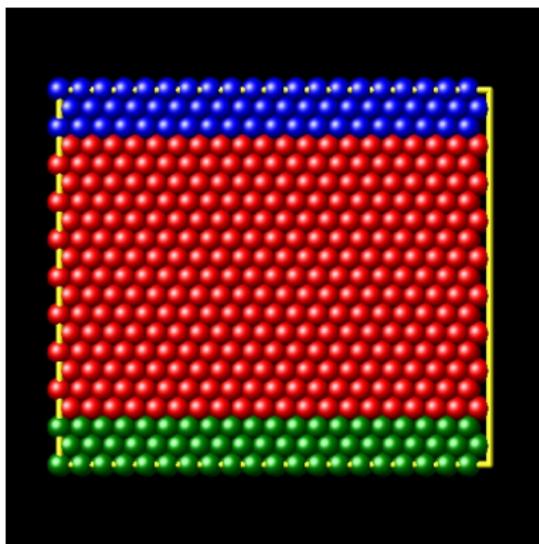
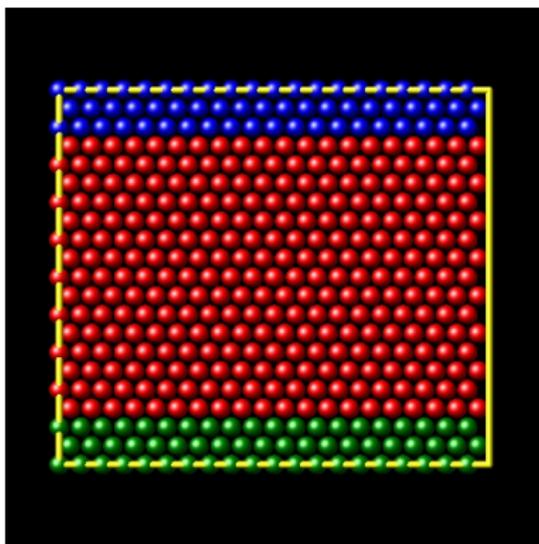
Crack problem

- 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



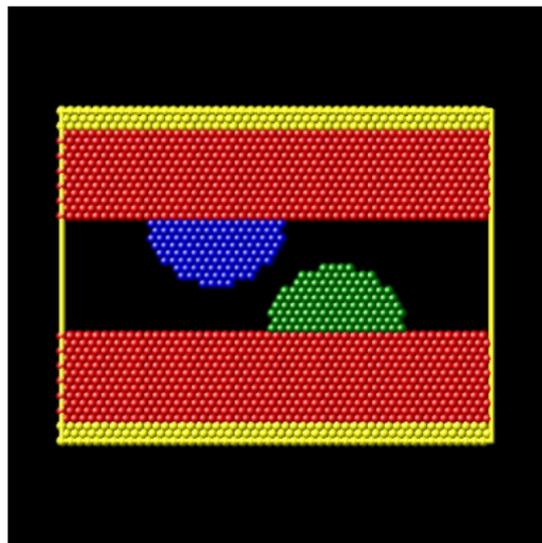
Flow problems

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



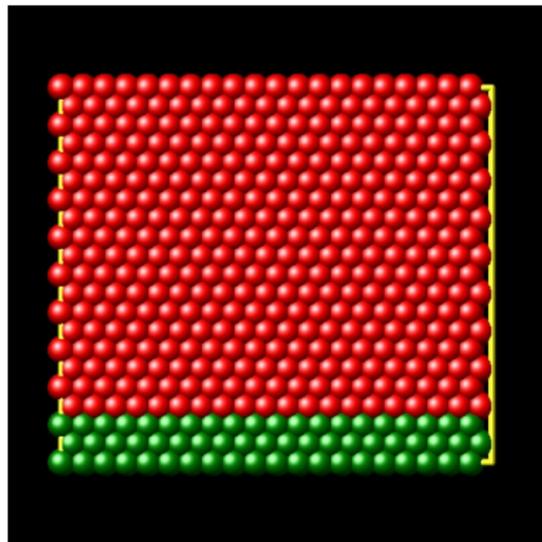
Friction problem

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



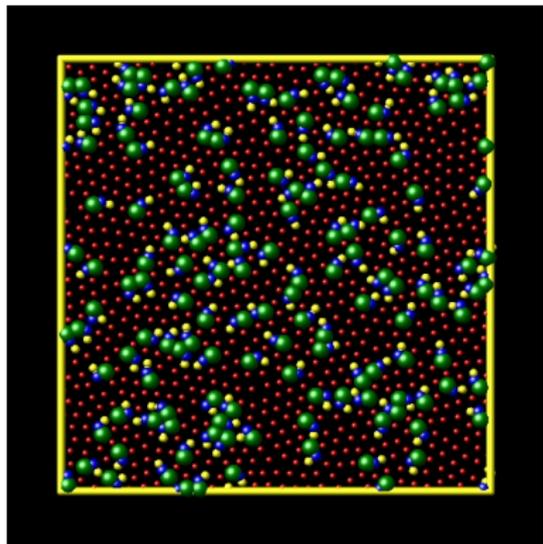
Indent problem

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



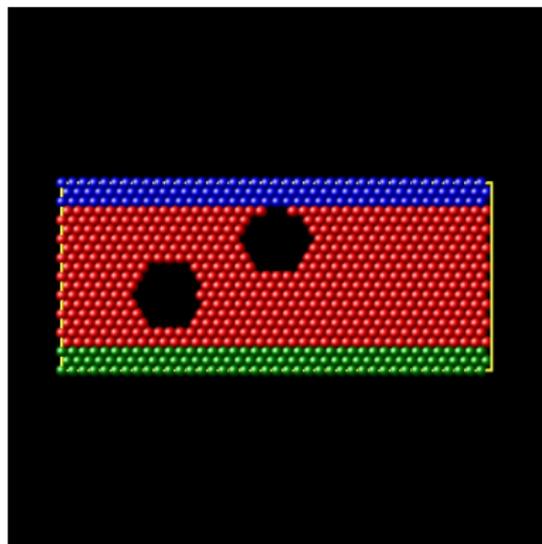
Micelle problem

- 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



Obstacle problem

- LJ flow around obstacle(s)
- 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



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

