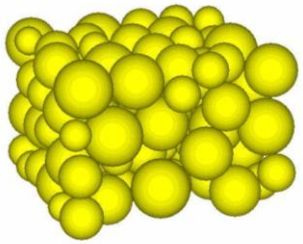
The challenge of simulating the stressing of dense samples of sand

George Marketos
Catherine O'Sullivan

Imperial College
London

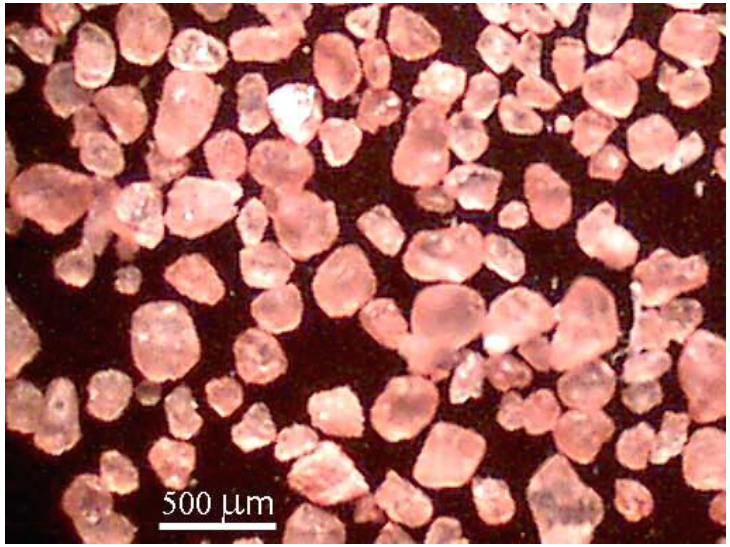
Talk overview

- Why LAMMPS is a Discrete Element code
- What materials the code can simulate
- What we need in order to simulate real sand samples
- How we check that the code does what it should
- A few ideas on desirable ‘new’ features

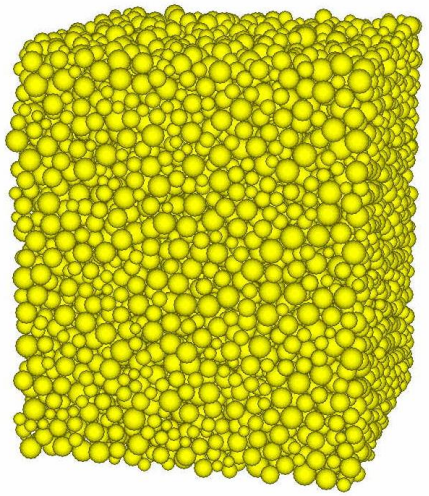


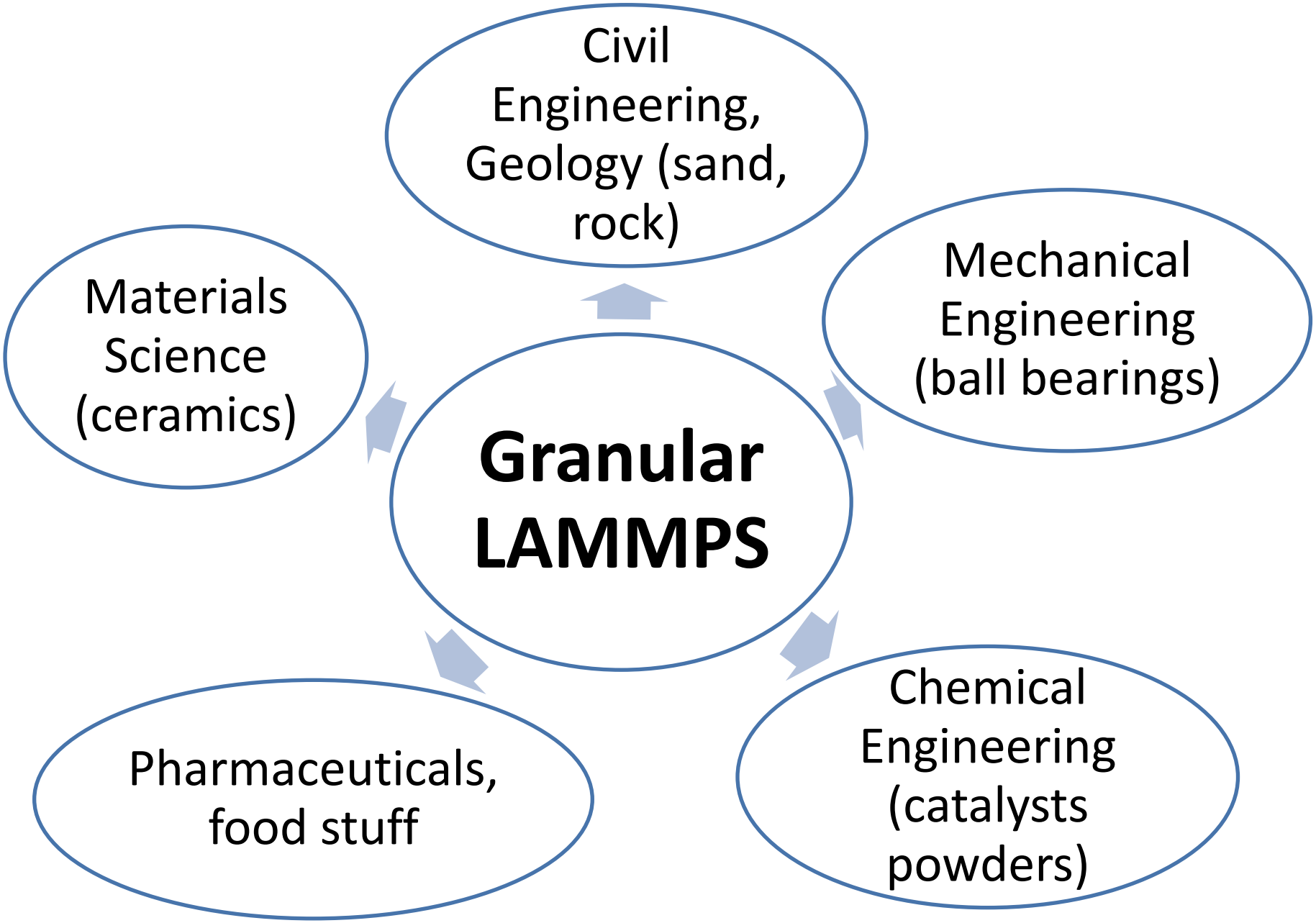
The case for using LAMMPS

- Each sand grain is a LAMMPS atom (sphere)
- Grains have radius and angular velocity
- Pairwise interactions with low cutoff
- Calculation steps within timestep the same
- Granular LAMMPS is a Discrete Element Method package!



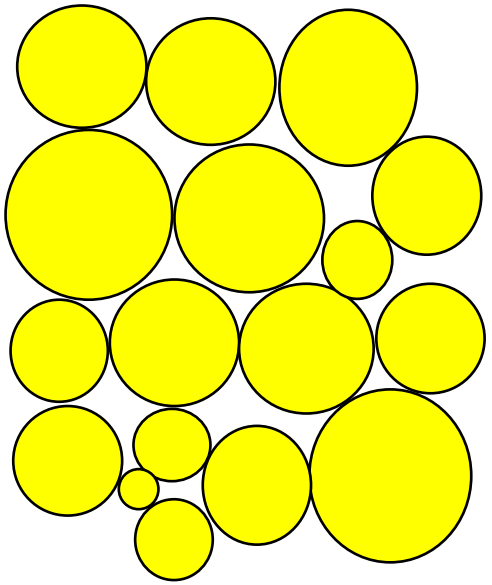
Picture reproduced from http://web.ncf.ca

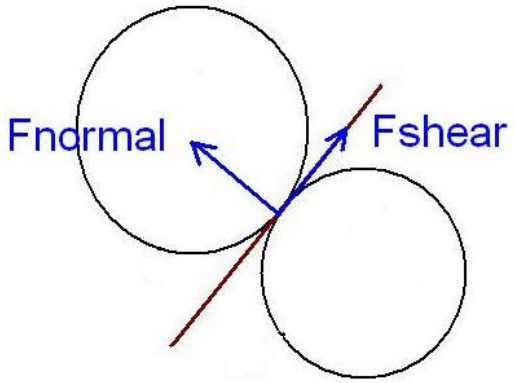



Civil Engineering, Geology (sand, rock)
Mechanical Engineering (ball bearings)
Chemical Engineering (catalysts powders)
Pharmaceuticals, food stuff
Materials Science (ceramics)
Granular LAMMPS

Simulating sand

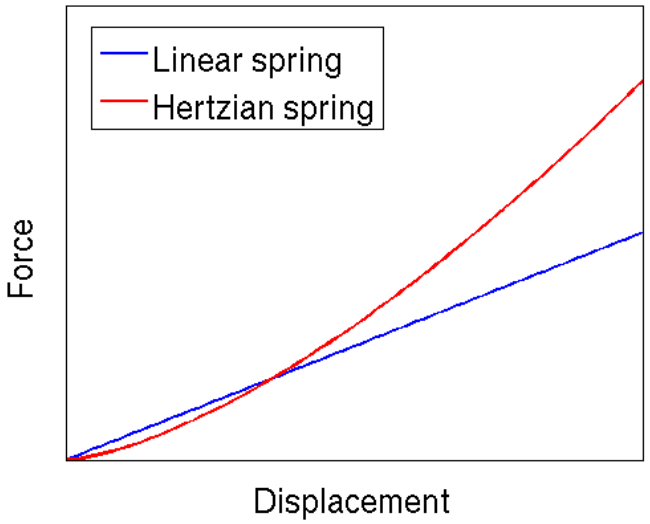
- Only touching grains interact
- Force split in normal and tangential directions
- Force now acting at the contact point
- Have large number of per-contact data
- Need ways of accessing them easily, extra per-contact memory slots

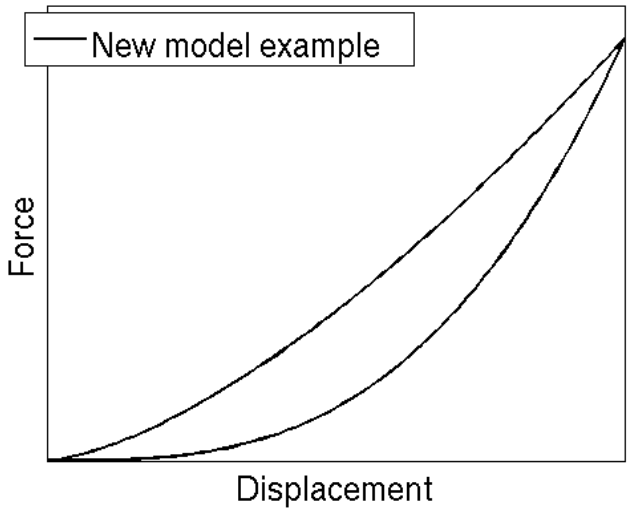




Real grains – the interaction model

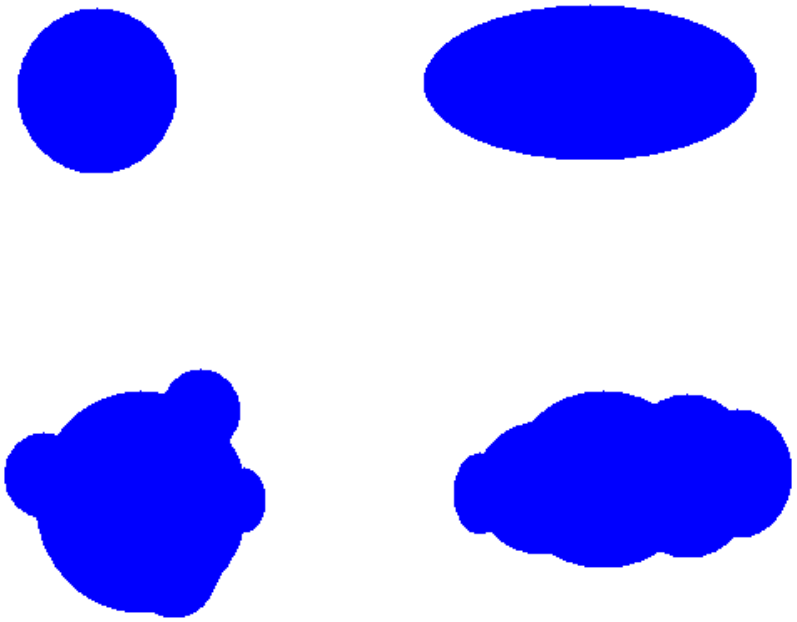
- LAMMPS has linear and Hertzian spring granular pair models
- Both based on elastic theory – OK for most work
- Real grains exhibit plasticity, hysteresis on load-unload
- Need to be able to implement these easily
- Granular models need storage of history parameters with neighbour list
- Also need model for bonding (sandstone cement)
- Working on new models





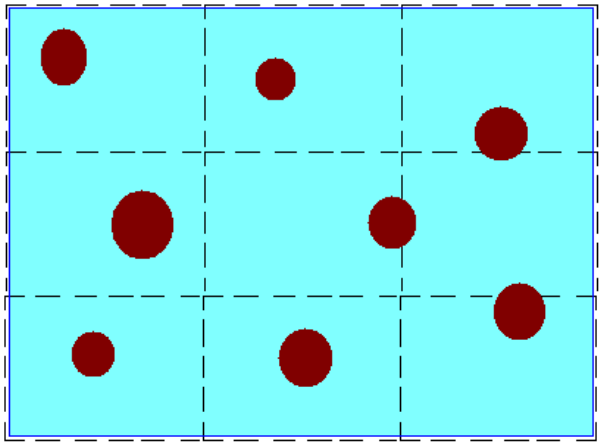
Real grains - shape

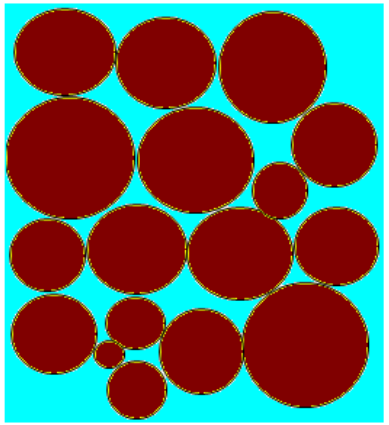
- Sand grains not spheres
- LAMMPS has ellipsoids but not integrated in granular yet
- Could cluster spheres
- Get more realistic packings, rolling resistance, response to cyclic loading



Real tests on sand- pore fluid

- Currently our simulations are dry
- Coarse fluid mesh on top of grains will work well for dilute suspensions of grains
- For dense packings we need more detail – model fluid inside pore
- Is this achievable?





Tests on sand - boundaries

- Apply force on samples by moving boundaries
- History parameters also stored for wall-atom interactions
- Specify velocity or force increase rate
- Latter needs control loop
- Could also have simulated ‘membrane’ boundaries
- Granular LAMMPS capabilities should be increased
- LIGGGHTS has triangle particles for boundaries

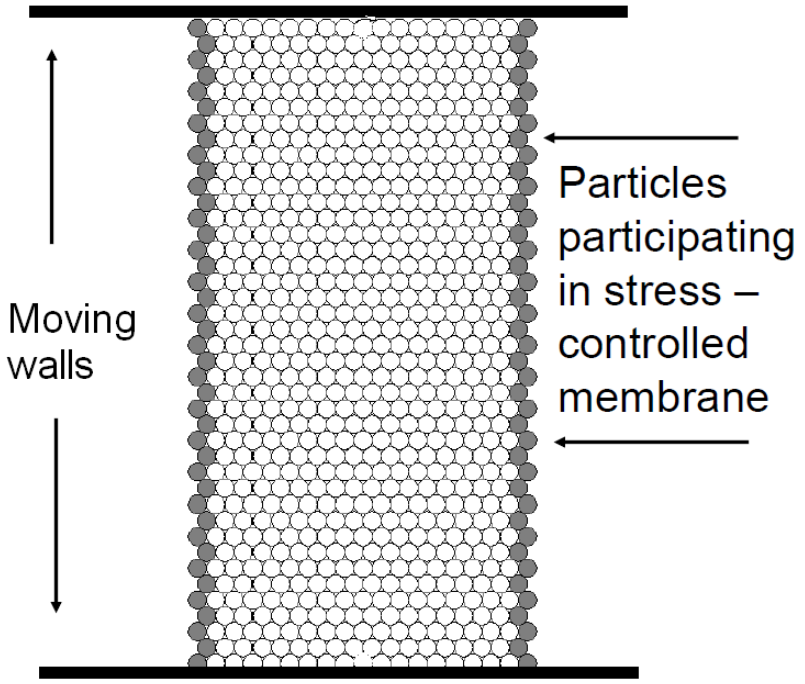
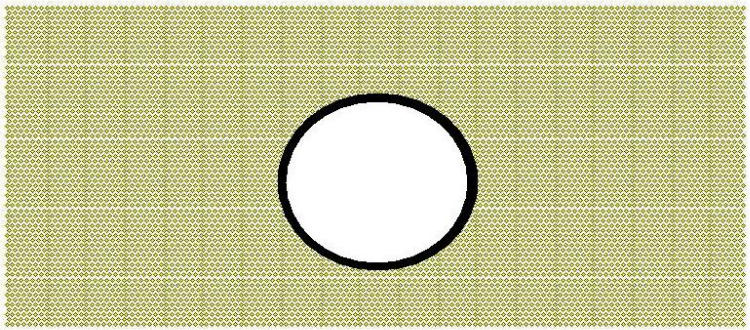


Figure courtesy of John O’Donovan

Large simulations

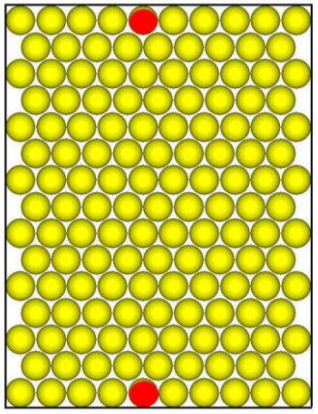
- Soil-structure interaction problems need huge numbers of grains
- Limited by sample generation step
- Need more efficient techniques
- Use maximum allowable timestep – more research needed to find it
- Inclusion of timestep calculation in LAMMPS

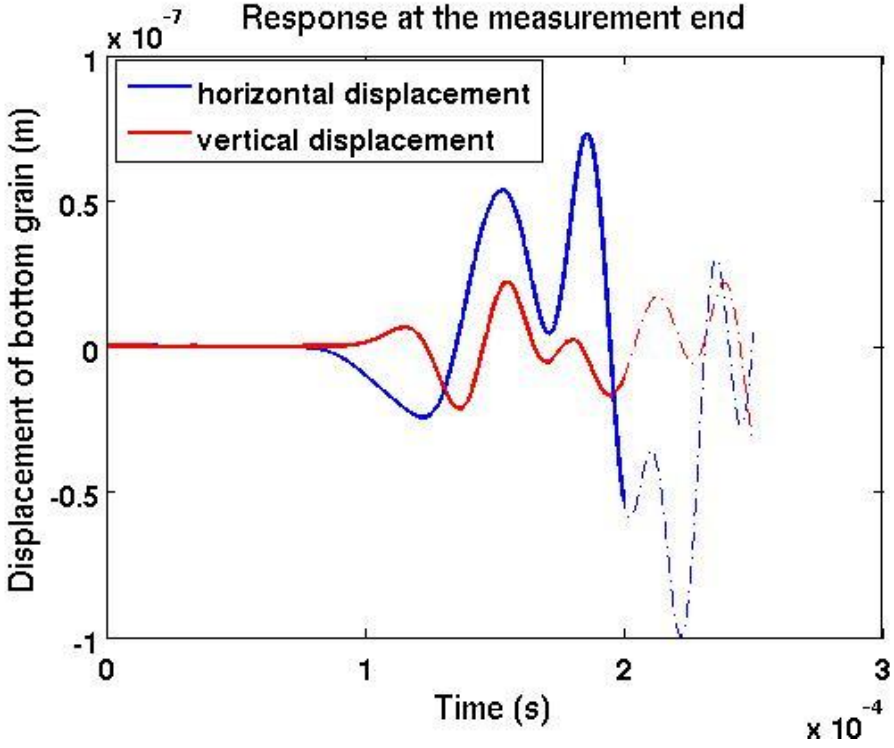


Tomas Bym's project

Need validation simulations

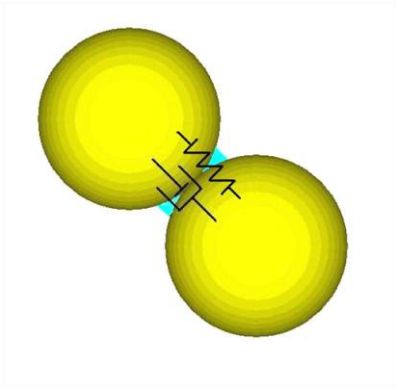
- Simple validation checks for which solutions are available
- Ball bouncing on a plane, rolling down a plane
- Wave propagation through a granular pack (see Marketos & O'Sullivan in prep.)
- Picked up a bug that was sorted out

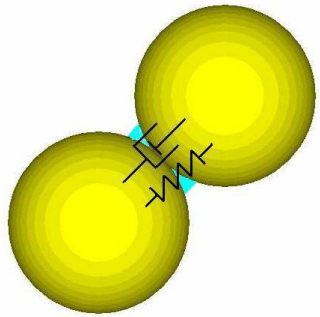




Also quality control needed

- LAMMPS is changing rapidly
- A set of simulations to be run regularly is needed to ensure no new bugs introduced
- Validation simulations cannot check everything – scripts that specifically check components of the code?





Granular LAMMPS – future efforts?

- Boundaries – movement, stress control
- New interaction models – Pairgen tool?
- Grain shapes
- Fluid modelling – is it achievable?
- Validation and quality control loops

Aim: Running parallel simulations of soil-structure interaction problems with large number of grains