The challenge of simulating the stressing of dense samples of sand

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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!
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