Recent developments and applications of LAMMPS for granular media

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2017 LAMMPS Workshop and Symposium

8/2/2017
What is ‘granular’?

**Molecular dynamics** vs. **Granular**

**Atoms (or small groups of atoms)**
- Particle length scale ~ atomic
- System length scale >> particle length scale

**Point particles → position, velocity**
- `atom_style atomic, full,...`
- `fix nve/nvt/npt,...`

**Long-range, conservative interactions**
- `pair_style lj/cut`

**Thermal, often equilibrium**
- `fix nvt`

**Representative sample, boundaries often periodic**
- `boundary ppp`

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**Macroscopic grains**
- Particle length scale >> atomic
- System length scale >> particle length scale

**Finite particles → position, velocity, orientation, angular velocity**
- `atom_style sphere,`
- `fix nve/sphere`

**Short-range, complex, dissipative interactions**
- `pair_style gran/hooke/history`

**Athermal, non-equilibrium**
- `fix nve/sphere, fix gravity`

**Often ‘full system’, boundaries complex, particles added/removed**
- `boundary fff, fix pour,`
- `fix wall/gran, ...`
Granular models: more details

Pair gran/hertz:

Analytical Hertz solution (1882 for normal contact force):

\[
\delta = R_i + R_j - \|r_i - r_j\| > 0
\]

\[
F_n = k_n \sqrt{R\delta^{3/2}} n - \sqrt{R\delta} m_\gamma n \nu_n
\]

What about oblique contact/tangential force?
\rightarrow friction, with option of accumulated shear

Pair gran/hertz/history

Dissipative term; Many damping models

Needs to account for rotating frame of reference
Larger world of granular simulations: discrete element method (DEM)

Traditional uses in geomechanics, mining industry, particle technologies

Many DEM codes: EDEM, Yade, PFC 2D/3D, Esys-Particle, LIGGGHTS

From EDEM youtube channel
Granular simulations in LAMMPS

- LAMMPS: used for seminal work in granular physics simulations (Grest, Silbert, Landry, others, ca. 2000)

- Historically: granular physics
  - spheres (often monodisperse)
  - simple contact potentials, w/ friction
  - simple geometries (periodic packings, flow down inclined plane,...)
    → glass beads

- More recent: engineering applications
  - Non-spherical particles
  - More realistic, complex contact potentials (e.g. cohesion, rolling/twisting friction)
  - Complex geometries
Recent capability: arbitrary particle shapes via overlapping spheres

- Algorithms to pack a shape represented on a voxel grid (3D image) optimally with overlapping spheres (pre-processing, external to LAMMPS):
  - Aggregates move as rigid bodies
  - Interactions are pairwise sums of sphere-sphere granular interactions

Credits: Leo Silbert, K Michael Salerno, Steve Plimpton
Arbitrary shape particles

molecule mymol shape1.data shape2.data
fix 1 all rigid/small molecule mol mymol infile moi
fix 2 all pour 1000 1 1234 mol mymol rigid 1

Study effect of shape on granular packing and rheology (Salerno et al, in prep)
Study effects of particle shape/size on battery electrode microstructure

Credits: Leo Silbert, K Michael Salerno, Steve Plimpton
Recent capability: complex boundaries for granular

region conereg cone z 0 0 5 20 10 30 open 1 open 2
...
fix 2 all wall/gran/region hertz/history &
   ${kn}$ ${kt}$ ${gamma_n}$ ${gamma_t}$ ${coeffFric}$ 1 region conereg
Application: additive manufacturing

Layer-by-layer powder bed fusion processes (e.g. SLM/SLS):

- Powder delivery
- Selective laser melting
- Powder delivery
- Selective laser melting

Very high cohesion
Moderate friction

No cohesion
Moderate rolling and sliding friction

No cohesion
Moderate sliding friction
No rolling/twisting friction
1.) Granular pair styles with **cohesion**, **rolling** friction, **twisting** friction:

pair gran/dmt/rolling, pair gran/jkr/rolling

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**Cohesion (DMT):**

\[ F_n = \left( \frac{4Ea^3}{3R} - 4\pi\gamma R \right) n \]

\[ \delta_N = \frac{a^2}{R} \]

**Rolling friction:**

\[ \tau_i = -\tau_j = Rn \times F_R \]

\[ F_R = -k_R \int_{t_0}^{t} v_L(\tau)d\tau - \eta_R v_L \]

\[ \|F_R\| \leq \mu_R \|F_n\| \]

\[ v_L = -R(\Omega_i - \Omega_j) \times n \]
2.) Triangulated surfaces, sphere-triangle and sphere-line interactions

```
pair_style tri/gran/hooke/history
pair_style line/gran/hooke/history

fix surface/global
```

Triangles/lines treated as particles, distributed across procs $\rightarrow$ ideal when $L_{\text{tri}} \sim L_{\text{sphere}}$, $N_{\text{tri}} \gg 1$

Triangles/lines belong to fix, each proc owns all tris/lines $\rightarrow$ ideal when $L_{\text{tri}} \gg L_{\text{sphere}}$, $N_{\text{tri}}$ small
Application: powder rheology

- Goal: calibrate DEM parameters based on powder dynamics experiments
- Freeman Technology FT4 rheometer: annular shear; measure force/torque for various impeller motions
Application: geosciences

- Hydraulic fracturing ("fracking") involves fracturing rock with high-pressure fluid
- Fractures are kept open with proppant particles
- Various proppant packing strategies:
  - Conventional: multi-layered, homogeneous
  - Partial monolayer
  - Heterogeneous, multi-layered (e.g. Schlumberger HiWAY)\(^1\)

→ Use DEM to **artificially** generate pack structures, study interplay of **mechanical stability** and **pack permeability**
Application: climate modeling

Sea ice: 2D granular material?

Herman, Geosci Model Dev., 2016

\[ x_{\text{hi}} - x_{\text{lo}} \sim \text{Time scale: } \sim 100 \text{ years} \]
QUESTIONS?