Sandia National Laboratories

Granular simulations with LAMMPS: enhanced contact models and applications to powder rheology

PRESENTED BY

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U.S. DEPARTMENT OF ENERGY NNSA

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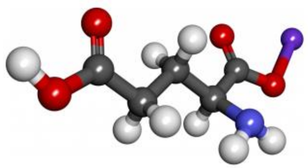
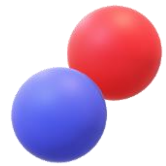
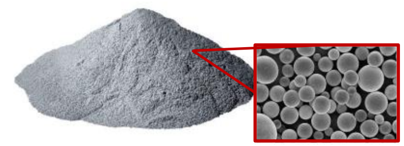
What is ‘granular’?

Molecular Dynamics vs. Granular (aka Discrete Element Method)







Molecular Dynamics

Length scale ~ molecular
System size >> atom size

Point particles: update position, velocity

```
atom_style atomic, full, etc.
fix nve, fix npt, etc.
```

Long-range, conservative interactions

```
pair_style lj/cut, ...
```

Simple boundaries, representative sample, equilibrium

```
boundary ppp,
boundary ppf + fix wall/*
fix nve, fix npt, ...
```

Granular

Length scale >> molecular
System size >> atom size

Finite-sized particles: update position, velocity, angular velocity; potentially non-spherical

```
atom_style sphere
fix nve/sphere, fix nph/sphere,
etc.
```

Contact interactions, dissipative

```
pair_style gran/hooke,
pair_style granular
```

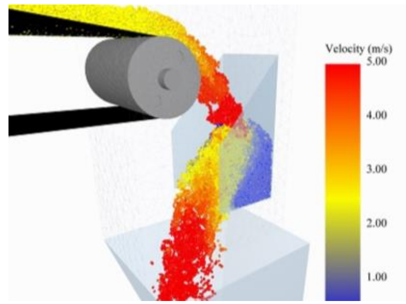
Complex (moving) boundaries, sometimes model full system, non-equilibrium

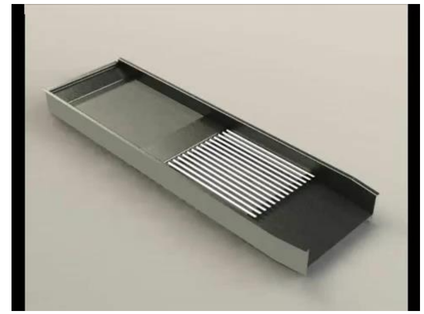
```
fix wall/gran/region, fix gravity,
...
```

Granular/DEM simulations

Well-established in geomechanics (Cundall and Strack, 1979), mining industry, pharma, particle technologies

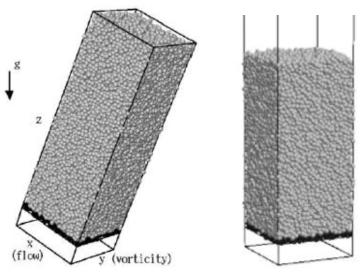
Many DEM codes: EDEM, Yade, PFC 2D/3D, MercuryDPM, **LIGGGHTS**



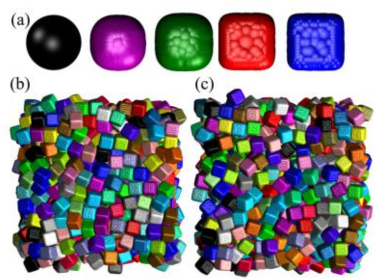


From EDEM youtube channel:
https://www.youtube.com/watch?v=er2i_pl8NQ0

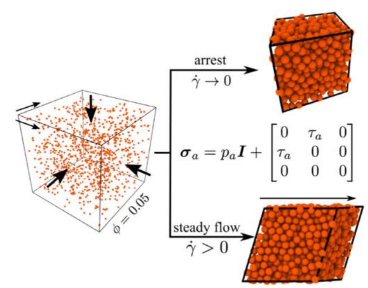
LAMMPS users: fundamental physics of particle packing and flow (Grest, Silbert, Landry, Lechman, …)



Silbert et al, PRE, 2001

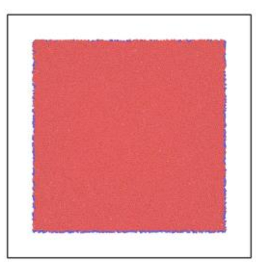


Salerno et al, PRE, 2018



Srivastava et al, PRL 2019

More exotic applications: sea ice dynamics for climate modeling, asteroid collisions



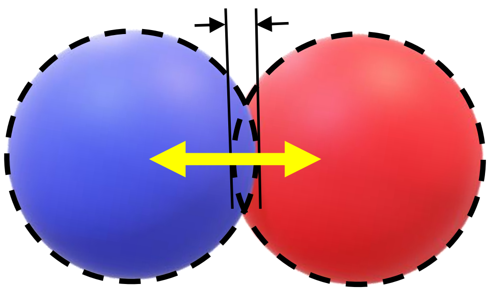
Tancredi et al, 2012

Granular models

```
pair_style gran/hooke
pair_style gran/hooke/history
pair_style gran/hertz/history
```

Normal component of force:

$$\delta = R_i + R_j - \|\mathbf{r}_i - \mathbf{r}_j\| > 0$$

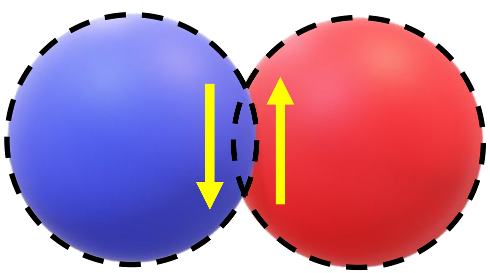


$$\mathbf{F}_n = \underbrace{k_n \sqrt{R}\delta^{3/2}\mathbf{n}}_{\text{Hertz theory (1880s)}} - \underbrace{\gamma_n \sqrt{R\delta}\mathbf{v}_n}_{\text{Viscoelastic solution}}$$

Hertz theory (1880s)

Viscoelastic solution
(Brilliantov et al, PRE, 1996)

Tangential component of force: additional force, torque

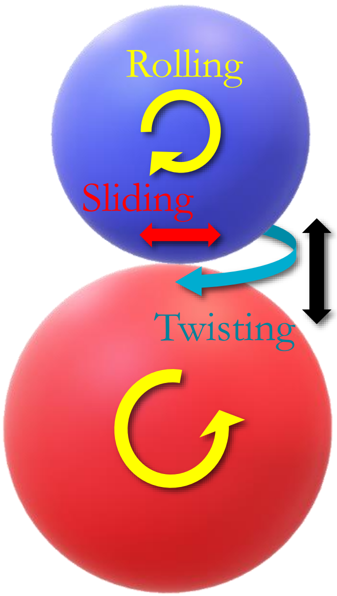


Coulomb friction criterion

$$\mathbf{F}_t = -\min(\mu_t F_{n0}, \| - k_t \xi + \mathbf{F}_{t,damp}\|)\mathbf{t}$$

$$\xi = \int_{t0}^{t} \mathbf{v}_{t,rel}(\tau) d\tau$$

New capability: `pair_style granular`



Normal model choices: hooke, hertz, hertz/material, jkr, dmt
Damping: velocity, mass_velocity, viscoelastic, tsuji
Tangential: linear_nohistory, linear_history, mindlin, mindlin_rescale
Rolling: none, sds
Twisting: none, sds, marshall

E.g. JKR:

$$\mathbf{F}_{ne,jkr} = \left(\frac{4Ea^3}{3R} - 2\pi a^2\sqrt{\frac{4\gamma E}{\pi a}}\right)\mathbf{n}$$

$$\delta = a^2/R - 2\sqrt{\pi\gamma a/E}$$

<u>Old syntax:</u>

```
pair_style gran/hertz/history 3e5 1e5 1e3 1e3 0.3 1
pair_coeff * *
```

<u>New syntax:</u>

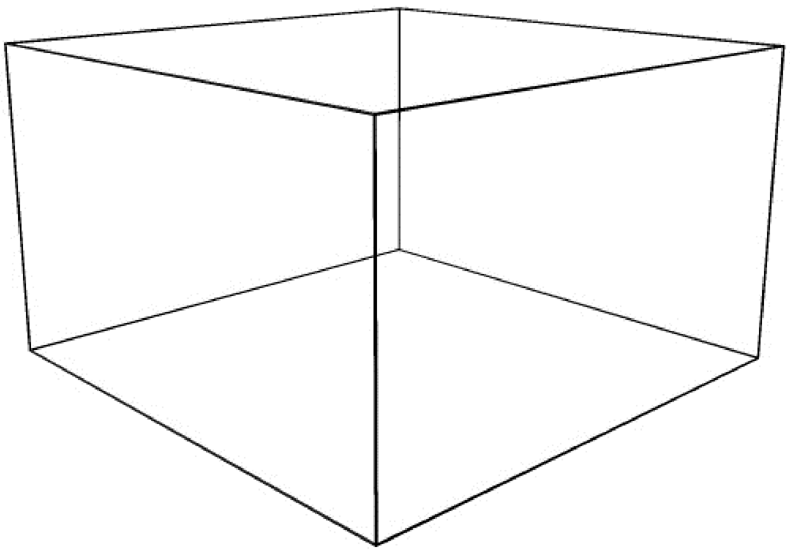
```
pair_style granular
pair_coeff * * hertz 3e5 1e3 tangential mindlin 1e5 1e3 0.3

pair_style granular
pair_coeff * * hertz/material 1e8 0.3 0.3 tangential mindlin_rescale NULL 1.0 0.4 damping tsuji

pair_style granular
pair_coeff 1 * jkr 1000.0 500.0 0.3 10 tangential mindlin 800.0 1.0 0.5 rolling sds 500.0 200.0 0.5 twisting marshall
pair_coeff 2 2 hertz 200.0 100.0 tangential linear_history 300.0 1.0 0.1 rolling sds 200.0 100.0 0.1 twisting marshall
```

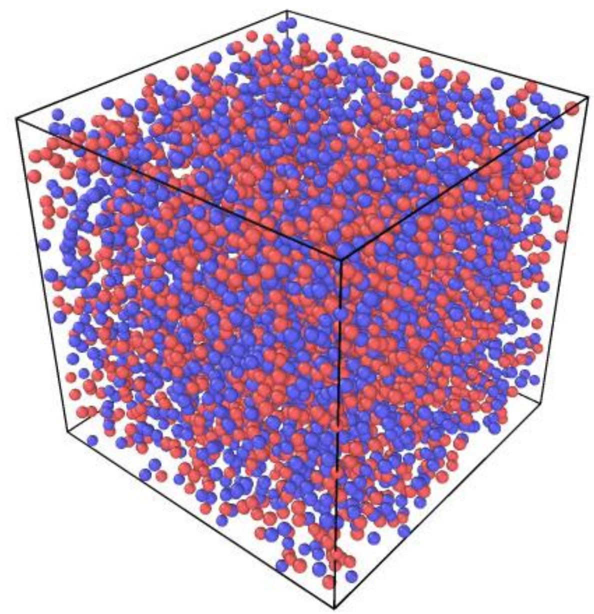
New capability: `pair_style granular`

Pouring 3 different particle types with varying cohesion and rolling friction:



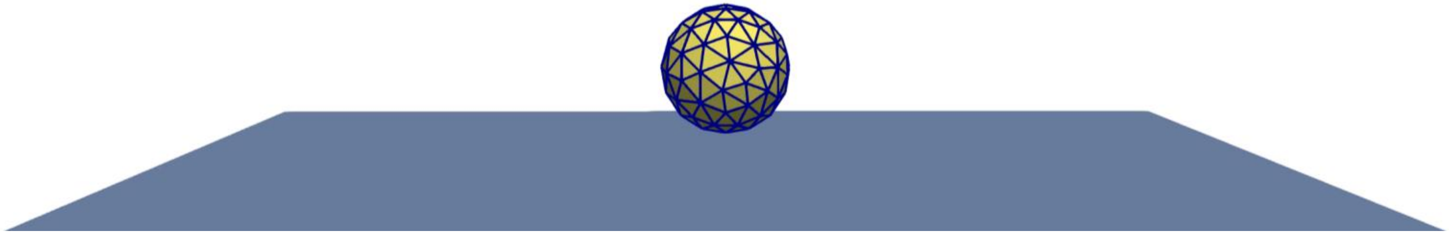
Red: high cohesion, high rolling friction
Blue: mildly cohesive, moderate rolling friction
Yellow: no cohesion, no rolling friction

Cohesive and non-cohesive particles with Langevin dynamics:

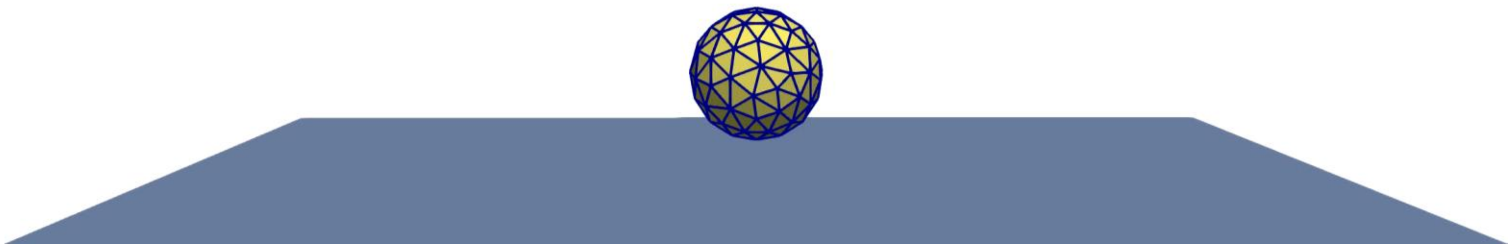


Red: high cohesion, high rolling friction
Blue: no cohesion

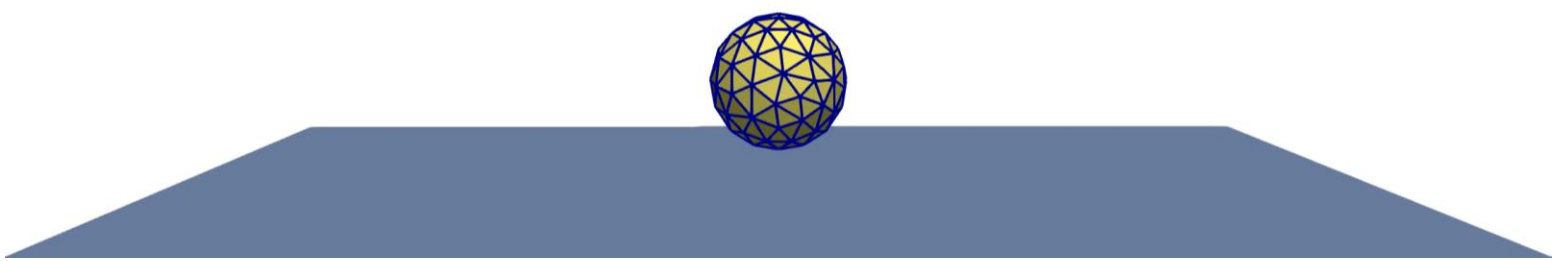
No sliding friction:



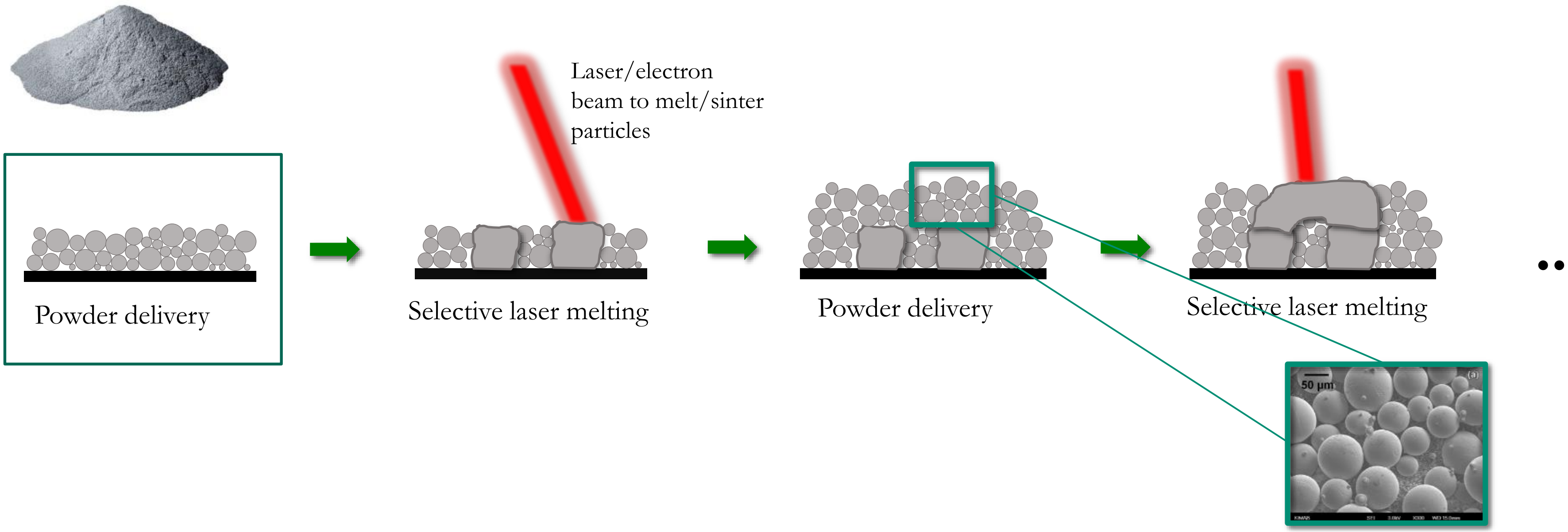
Sliding friction, no rolling friction:



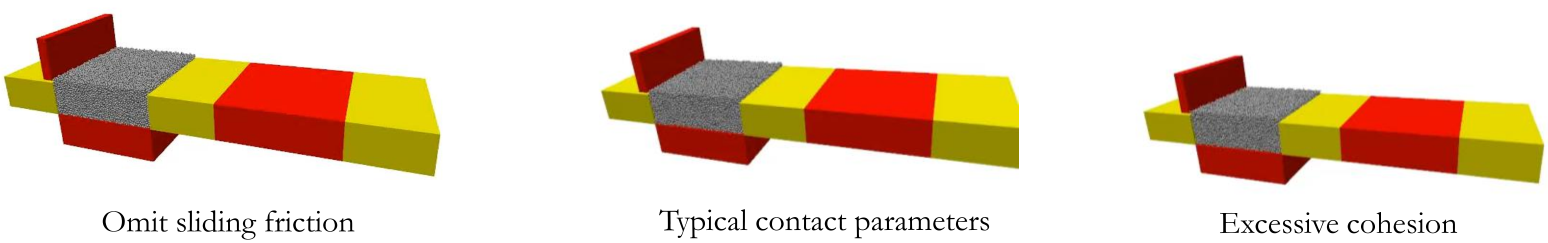
Sliding friction, rolling friction:

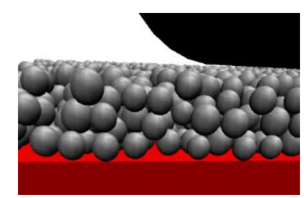


Motivating application: additive manufacturing



Strondl et al, *JoM* 2015.

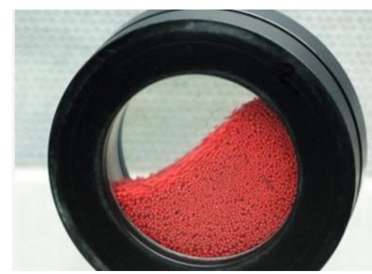
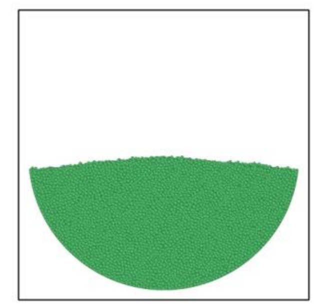




Need to understand powder spreading, powder flow

Calibration of DEM models: powder flow tests

Goals:
1. Calibrate/validate contact model parameters
2. Understand relationship between particle-scale parameters, various flow index tests, and spreading characteristics

Anton-Paar rheometer, Freeman Tech. FT4 rheometer, etc.

→ Measure torque as a function of RPM, depth

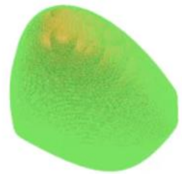
Granutools Granudrum

→ Measure angle as a function of RPM

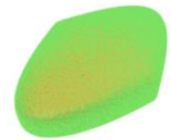
Other recent LAMMPS/granular capabilities

Clustered, overlapping spheres to represent arbitrary particle shapes (Silbert, Salerno)

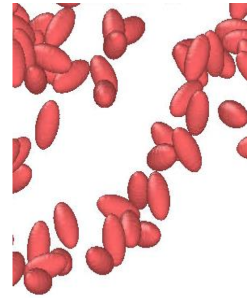
```
pair_style gran* +
fix/rigid
```

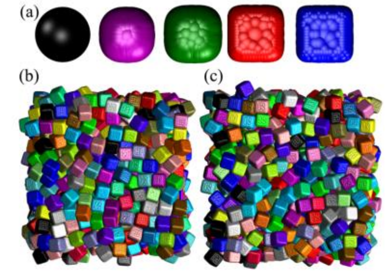


N=200 spheres



N=2000

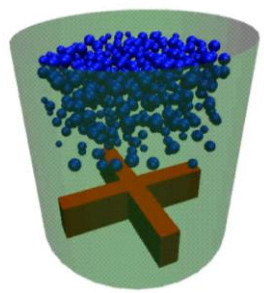


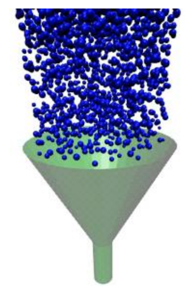


Salerno et al, PRE, 2018

Complex boundaries built from LAMMPS regions:

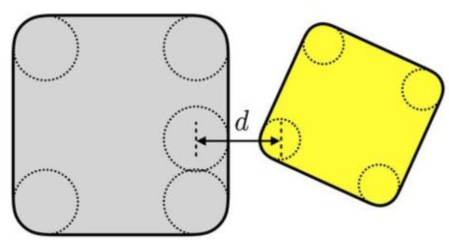
```
fix wall/gran/region
```

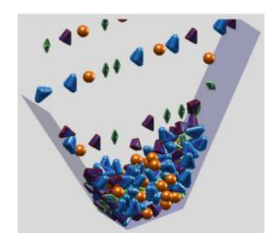




Non-spherical particles via rounded polygons/polyhedra:

```
atom_style body
pair_style body/rounded/polygon
Pair_style body/rounded/polyhedron
```





Nguyen and Plimpton, Comp Phys Comm 2019
Wang, Yu, Langston, Fraige, Granular Matter, 2011

QUESTIONS?