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# Rolling, Twisting and Cohesion in Granular Packings

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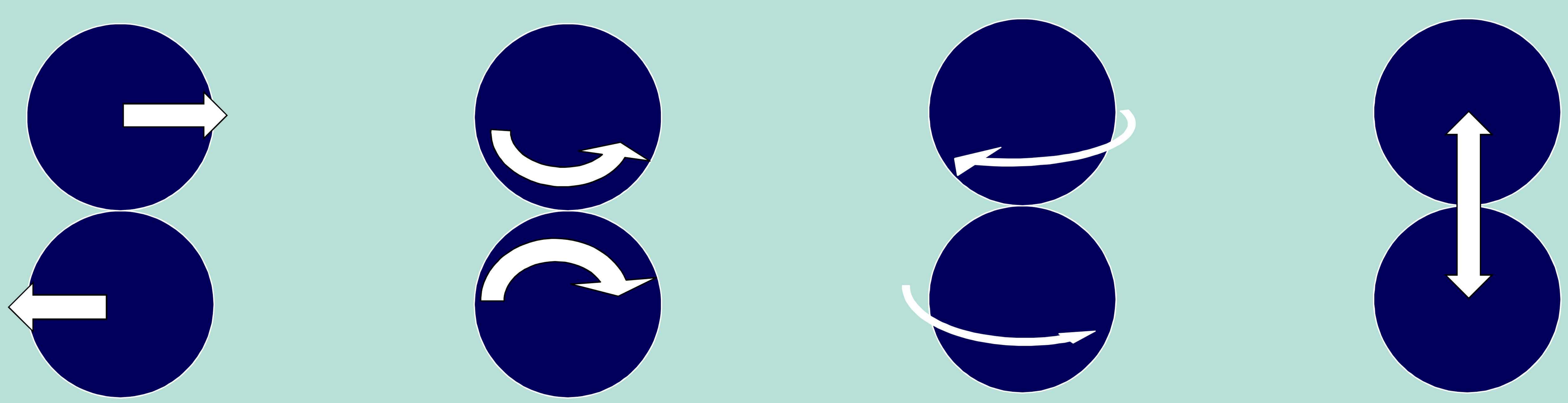
*Developers of new LAMMPS granular package

## New LAMMPS MD granular package



### Sliding friction

- Linear (w/ and w/o history)
- **Mindlin** (w/ rescale)[1]

### Rolling friction

- **Spring-daspot-slider**[2]

### Twisting friction

- **Spring-daspot-slider**[2]
- **Marshall**[3]

### Contact

- Hooke
- Hertz
- **Hertz/material**
- **DMT**[4]
- **JKR**[5]
- **Tsuji**[6]

Cohesion

### Types

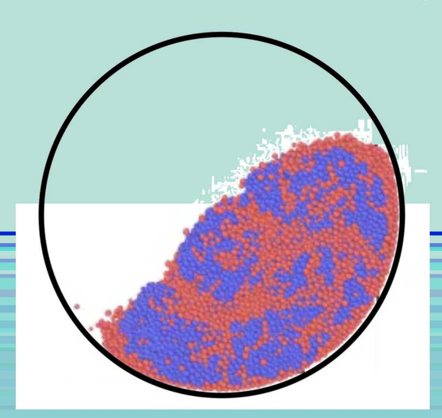


Figure 1: Snapshot from a rotating drum simulation with granular particles with two friction coefficients.

### Damping

- Mass_velocity
- Velocity
- Viscoeleastic
- **Tsuji**[6]

### Usage

```
pair_style granular
pair_coeff 1 1 hertz 10.0 5.0 tangential mindlin 80.0 0.5 0.5 rolling sds 50.0 2.0 0.5 twisting marshall
pair_coeff 2 2 dmt 10.0 5.0 0.3 1.0 tangential mindlin 80.0 0.5 0.1 rolling sds 50.0 2.0 0.1 twisting marshall
pair_coeff 1 2 dmt 10.0 5.0 0.3 1.0 tangential mindlin 80.0 0.5 0.1 rolling sds 50.0 2.0 0.1 twisting marshall
```

### Citations

[1]Mindlin, R. D. (1949). Compliance of elastic bodies in contact. J. Appl. Mech., ASME 16, 259-268
[2]Luding, S. (2008). Cohesive, frictional powders: contact models for tension. Granular matter, 10(4), 235
[3]Marshall, J. S. (2009). Discrete-element modeling of particulate aerosol flows. J. Comput. Phys., 228(5), 1541-1561
[4]Derjaguin, B., et al. (1975). Effect of contact deformations on the adhesion of particles. J. Colloid Interf. Sci., 53(2), 314-326
[5]Johnson, K. L., et al. (1971). Surface energy and the contact of elastic solids. Proc. R. Soc. Lond. A, 324(1558), 301-313
[6]Tsuji, Y., et al. (1992). Lagrangian numerical simulation of plug flow of cohesionless particles in a horizontal pipe. Powder Technol., 71(3), 239-250

## Effect of rolling friction on packing

### Motivation

Rolling friction has an important effect on packing and enables the reproduction of random loose packing volume fraction, see Figure A and C. Shear bands[d], pouring on a flat base, flow down an incline plane and other experimental phenomena demonstrate large regions with high rotation.

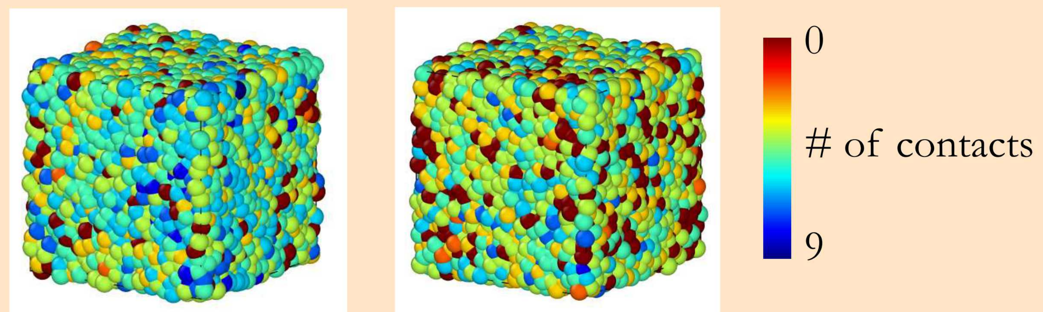



Figure A: Snapshots of packed granular system without ($\mu_r$=0, left) and with ($\mu_r$=1, right) rolling friction. Colors corresponds to number of contacts. Made with Ovito.

### Packing protocol

1. Randomly insert particles at $\phi$=0.1
2. Apply constant *NPH* with isotropic pressure
3. Stop at jamming criteria, $U_{kinetic}=1\times10^{-10}$

- Extrapolation to high $\mu_s$ is not needed

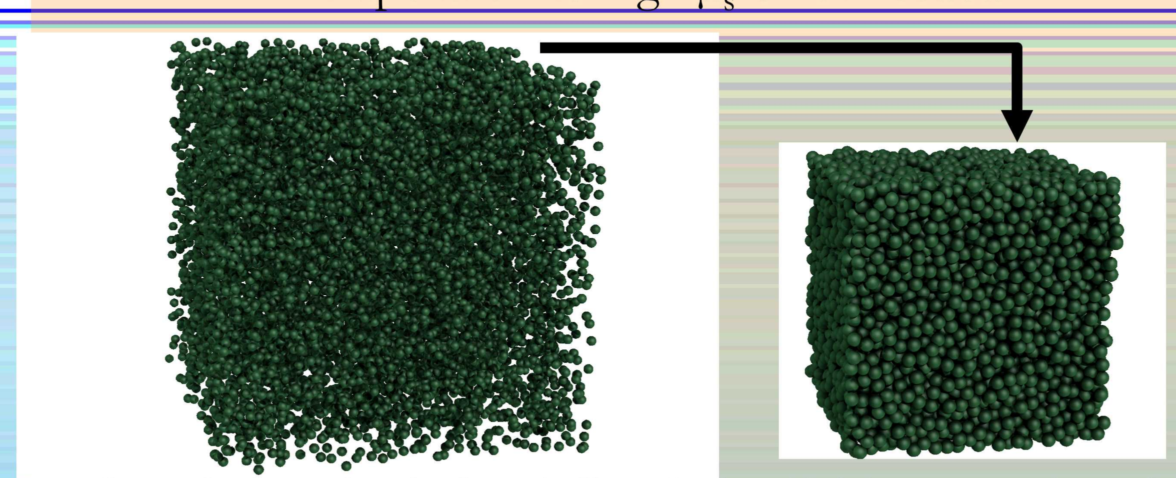


Figure B: Snapshot before (left) and after (right) compression of 10,000 slightly polydisperse granular particles. Made with PyMol.

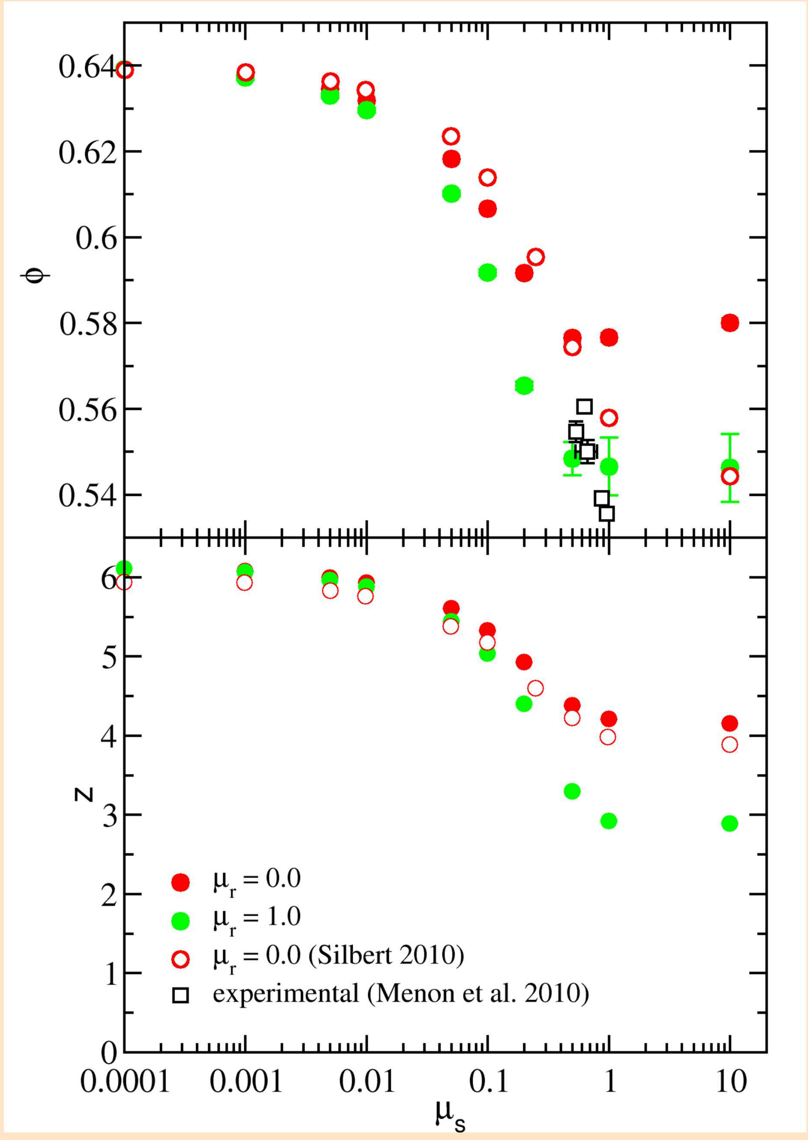



Figure C: The volume fraction ($\phi$) and coordination number (z) of packings as a function of sliding friction and rolling friction. The new DEM simulation protocol (solid symbols) are compared to Silbert 2010[a] simulations, and experiments performed by Menon et al.[c] (open symbols). Simulations were run with the new capabilities in LAMMPS[a].

### Model parameters

- $P = 1\times10^{-4}$, dt = 0.02
- $k_n$= 1.0, $k_t$= 1.0, $k_r$= $k_n/4$
- $\gamma_n$= 0.5 , $\gamma_t$=0.25 , $\gamma_r$= $\gamma_n/4$

### Citations

[a]Plimpton S. (1995). Fast Parallel Algorithms for Short-Range Molecular Dynamics. J. Comput. Phys., 117, 1-19
[b]Silbert L. (2010). Jamming of frictional spheres and random loose packing. Soft Matter, 6(13), 2918-2924
[c]Menon N. et al. (2010). Loose packings of frictional spheres. Soft Matter, 6(13), 2925-2930
[d]Bardet J. (1994). Observations on the effects of particle rotations on the failure of idealized granular materials. Mech. Mater., 18(2), 159-182

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