SAND2020-2615C

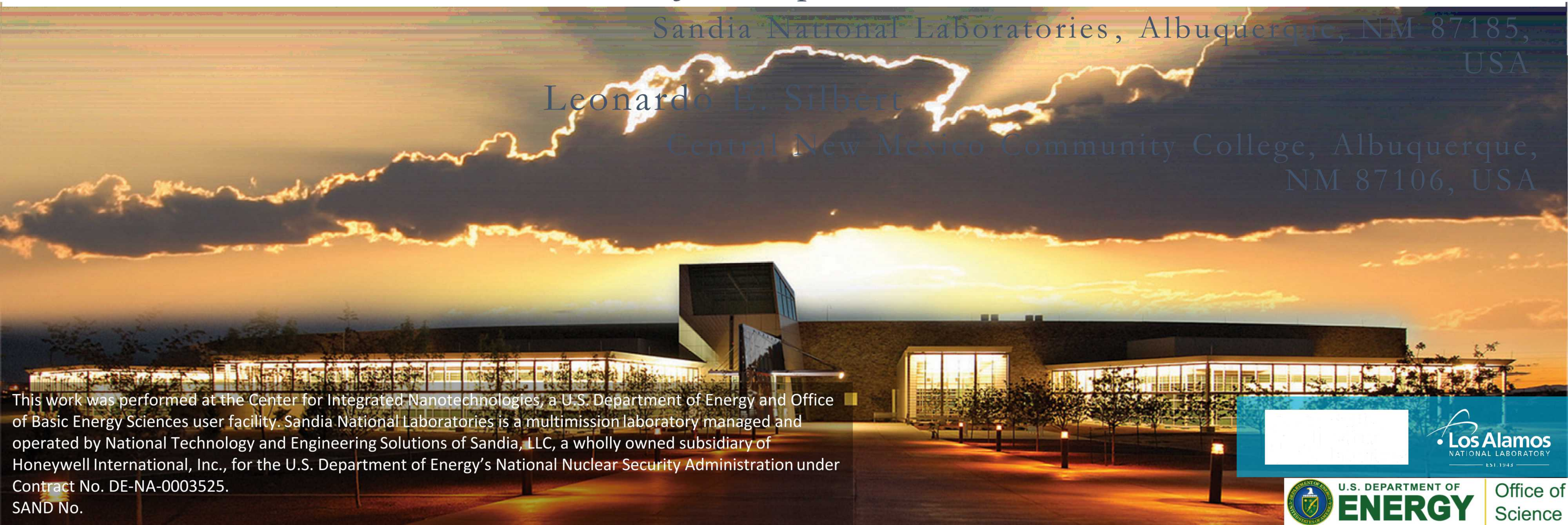
Granular packings with sliding, rolling and twisting friction

Andrew P. Santos, Ishan Srivastava, Dan S. Bolintineanu, Jeremy B. Lechman, Gary S. Grest, Steven J. Plimpton

Sandia National Laboratories, Albuquerque, NM 87185, USA

Leonardo E. Silbert

Central New Mexico Community College, Albuquerque, NM 87106, USA



This work was performed at the Center for Integrated Nanotechnologies, a U.S. Department of Energy and Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under Contract No. DE-NA-0003525.
SAND No.

Outline

- Rolling and twisting resistance background
- Constraint counting
- Contact model (spring-dashpot-slider)
- Packing methodology
- Impact on packing
- Conclusions and future studies

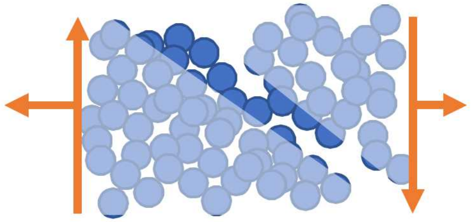
Background

Rolling and twisting resistance sources

- Load asymmetry built up by:
  - microslip and creep
  - inelastic deformation at contact area
  - roughness

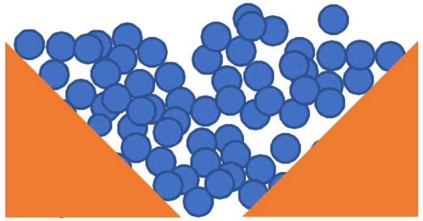
Rotational motion and friction in applications

Shear bands & extension



Bardet, J. P. (1994). *Mech. Mat.*, 18, 159–182.

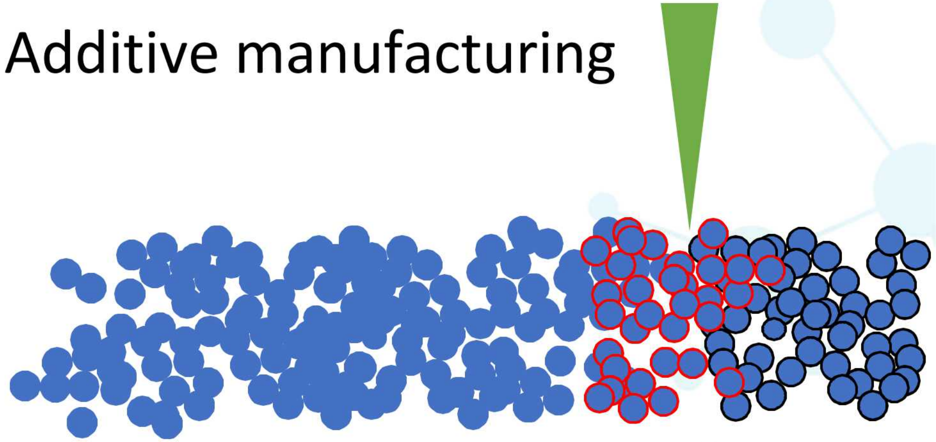
Hopper flow



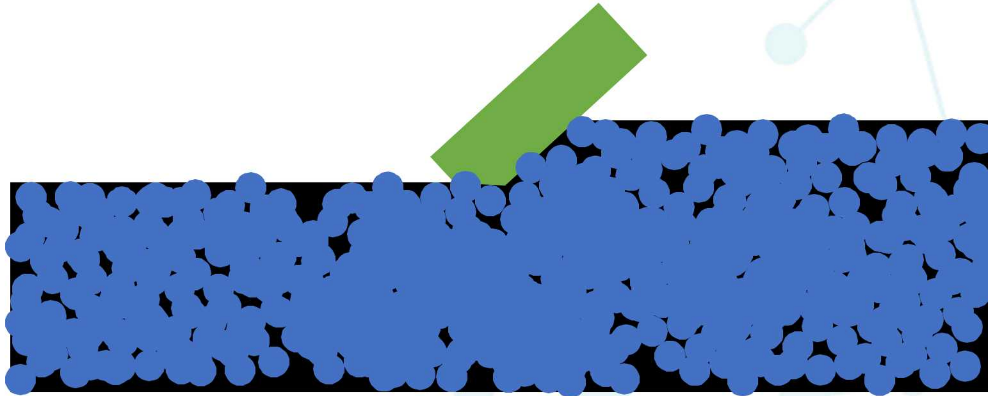
Mort, P. et al. (2015). *Powder Tech.*, 284, 571-584.

Applications for packing

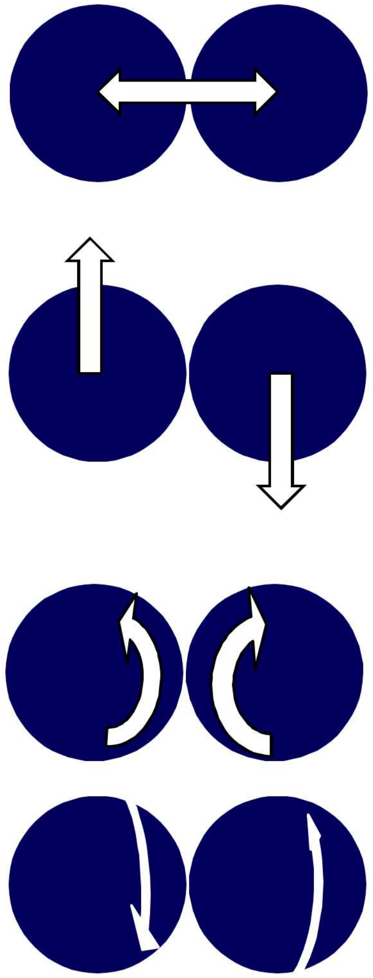
Additive manufacturing



Battery electrode printing



Constraint counting



$$N^{\text{eqn}} = \begin{cases} 6N, \text{if 3d, frictional} \\ 3N, \text{if 2d, frictional} \\ 3N, \text{if 3d, frictionless} \\ 2N, \text{if 2d, frictionless} \end{cases}$$

$$N^{\text{eqn}} = \frac{N^c}{2} N \langle Z \rangle$$ at jamming

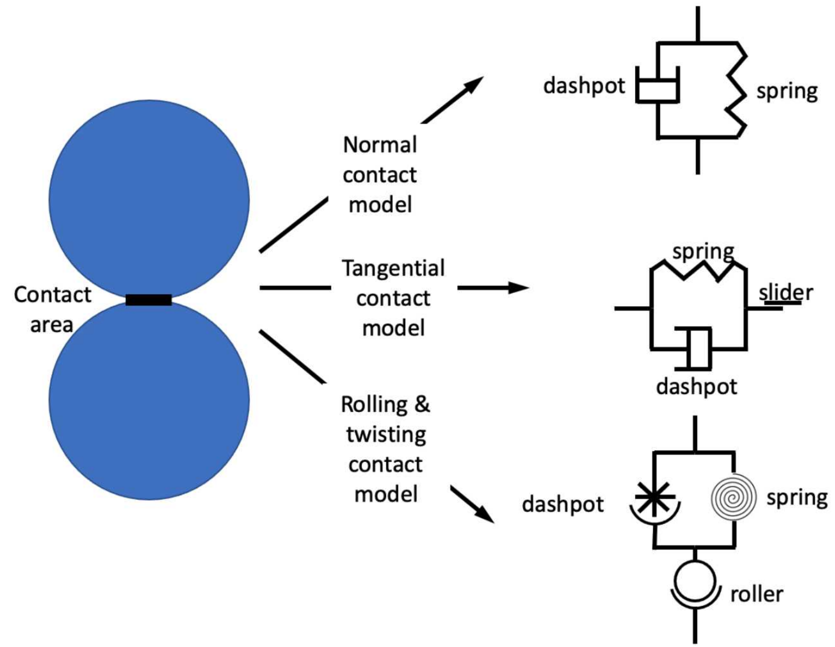
$$\langle Z \rangle = \frac{2N^{\text{eqn}}}{N^c N}$$ Avg. contacts/particle "coordination number"

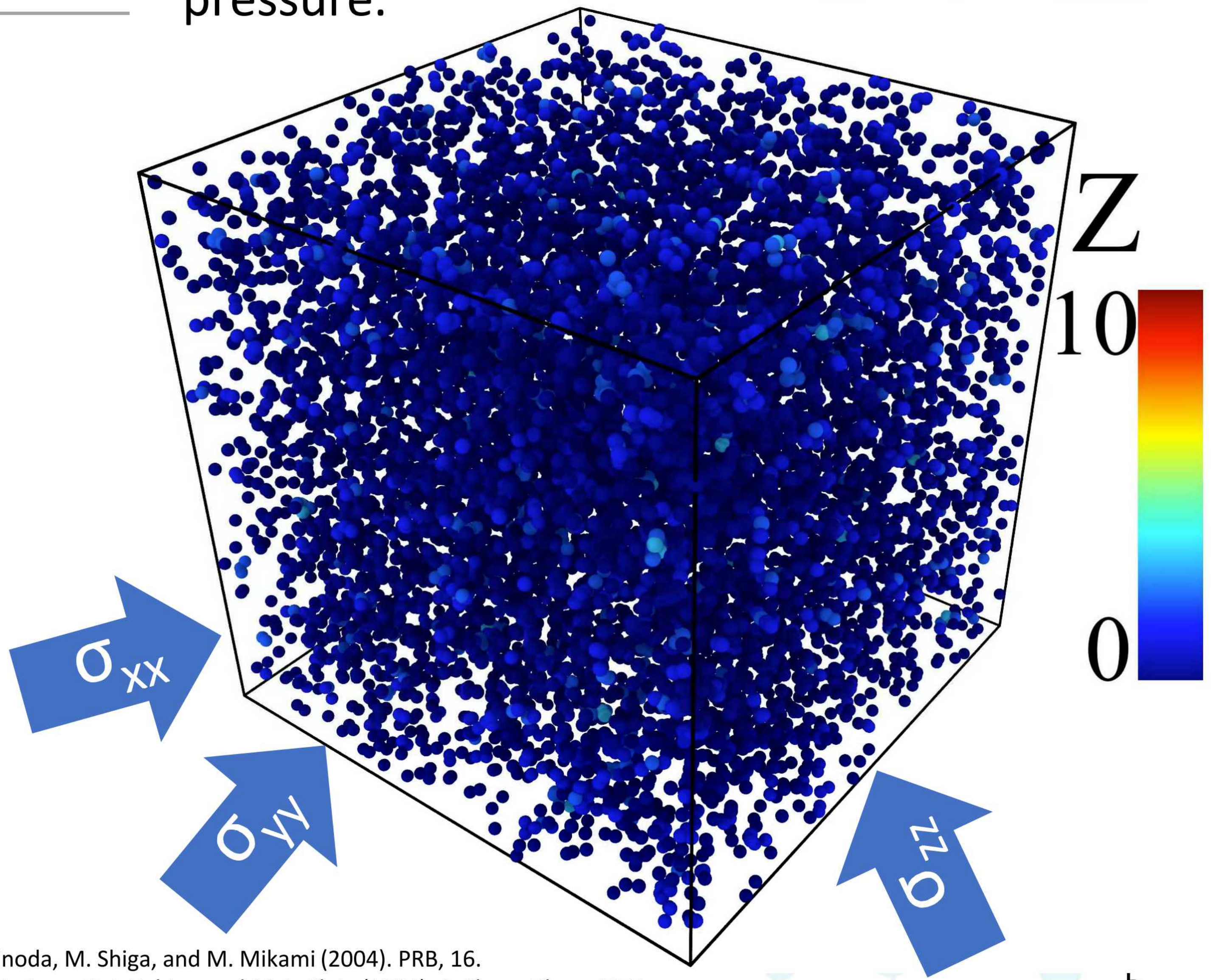
friction			3d		2d	
sliding	rolling	twisting	N^c	Z	N^c	Z
n	n	n	1	6	1	4
y	n	n	3	4	2	3
n	y	n	3	4	2	3
n	n	y	2	6	-	-
y	y	n	5	12/5	3	2
y	n	y	4	3	-	-
n	y	y	4	3	-	-
y	y	y	6	2	-	-

Methods and model

Packing protocol: specify pressure tensor and bring system to final state from a very low pressure.

Discrete element, particle-based modeling (DEM) (implemented within LAMMPS).

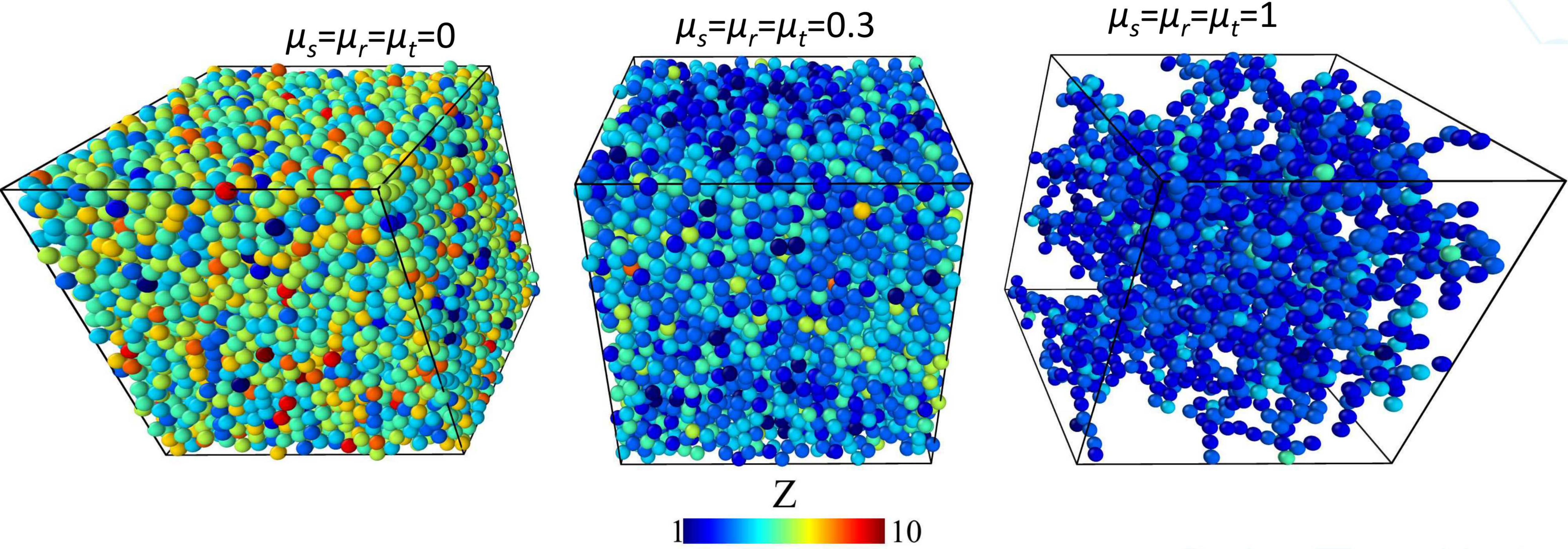




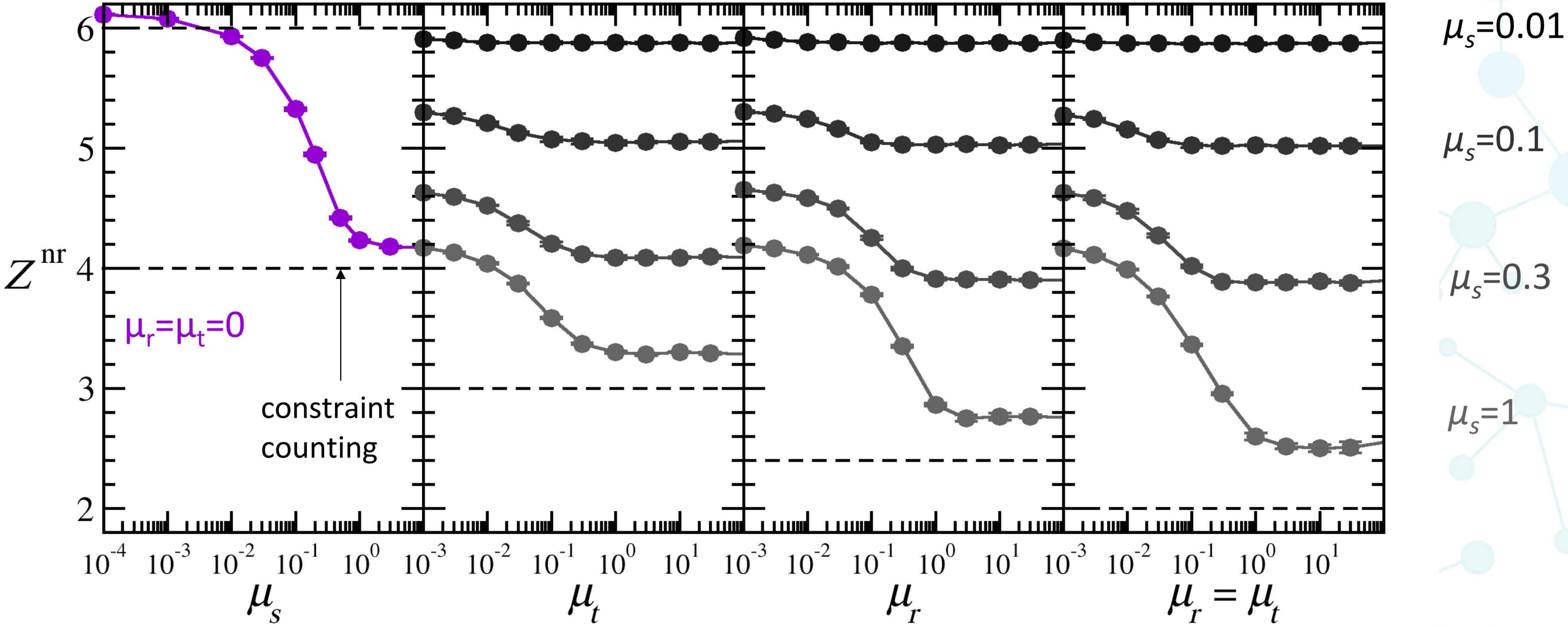
Plimpton S. (1995). *J. Comput. Phys.*, 117, 1-19.
Mindlin, R. D. (1949). *J. Appl. Mech., ASME* 16, 259-268.
Luding, S. (2008). *Granular matter*, 10(4), 235.

W. Shinoda, M. Shiga, and M. Mikami (2004). PRB, 16.
G. J. Martyna, D. J. Tobias, and M. L. Klein (1994). *J. Chem. Phys.*, 4177.
M. Parrinello and A. Rahman (1981). *J. Appl. Phys.*, 7182.

Microstructure



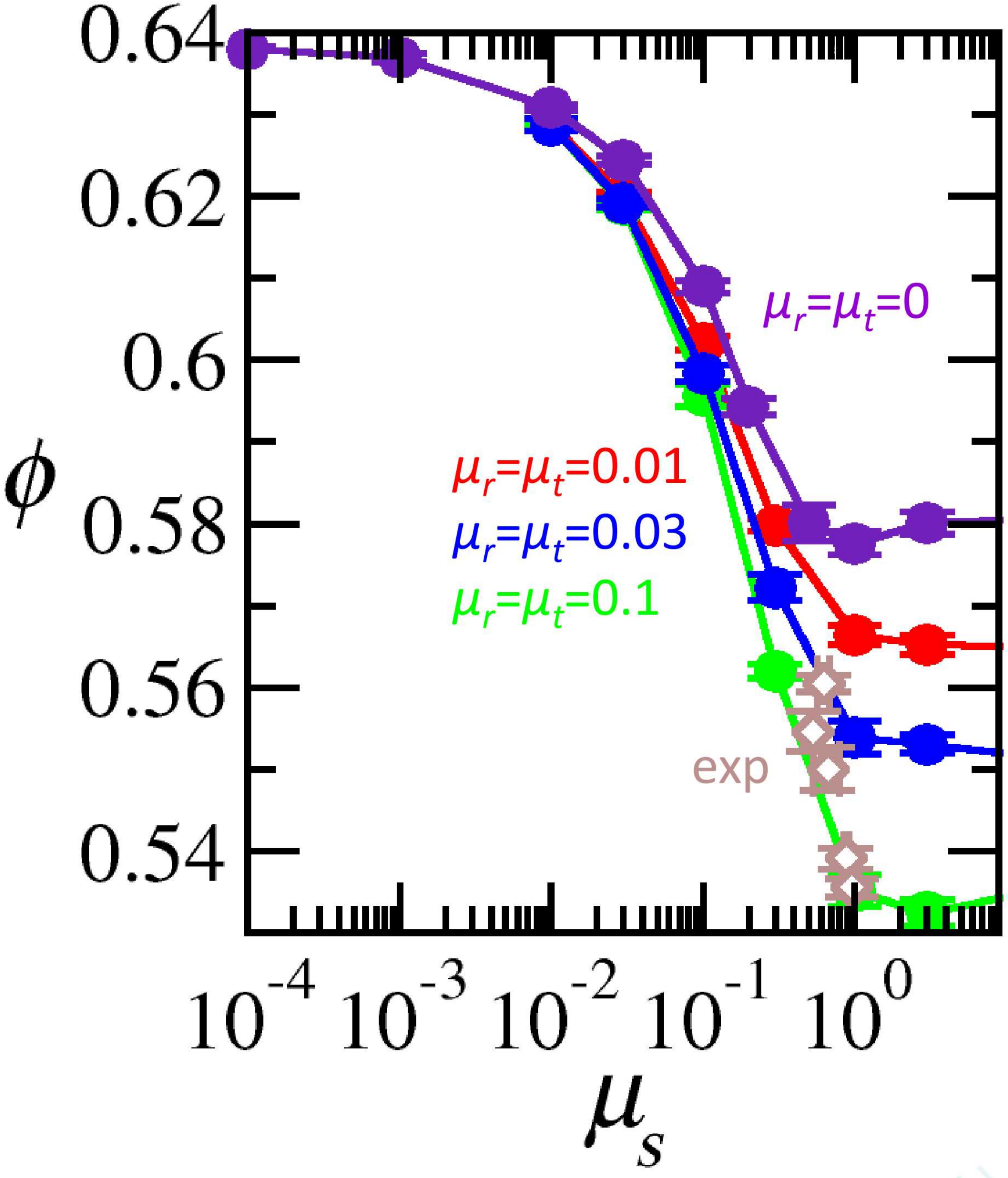
Coordination number



- Constraint counting under-predicts, but is affirmed by simlulations
- min(Z^{nr}) ~ 2.45

Volume fraction

- Experiments are matched when moderate rolling and twisting friction are included
- Rolling and twisting friction have little effect for low μ_s



Menon N. et al. (2010). *Soft Matter*, 6(13), 2925-2930

Conclusions

- Real packing volume fractions agree when $\mu_r \neq \mu_t \neq 0$
- Constraint counting predicts a decrease in Z from 6 to 2.5
- Rolling and twisting friction cause large changes in microstructure

Related and future work

Related

- Other packing protocols tested:
    - Over-compression
    - Gradual de-compression
    - Cyclical over-compression
- Pressure-controlled packing allows lower pressures
- Volume fraction can have non-monotonic dependence at low-pressure

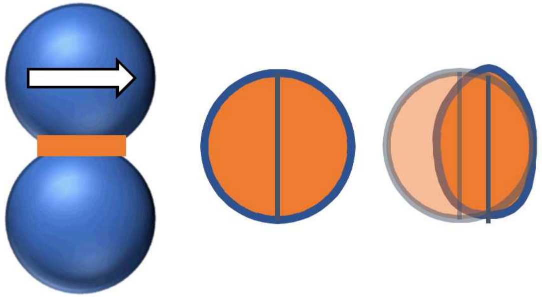
Future

- Rolling and twisting resistance on rheology
    - Incline plane
    - Rotating drum
    - Bulk-like applied shear stress
- Pressure-controlled packing of more realistic particle models:
    - Non-spherical
    - Cohesive
    - Deformable

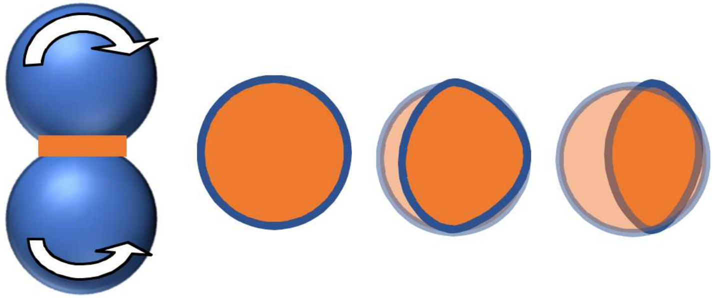
Resistance sources

Sliding resistance

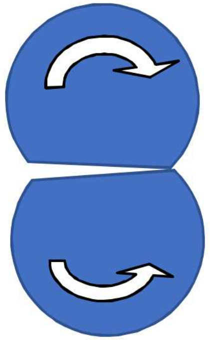
Microslip due to translational displacement



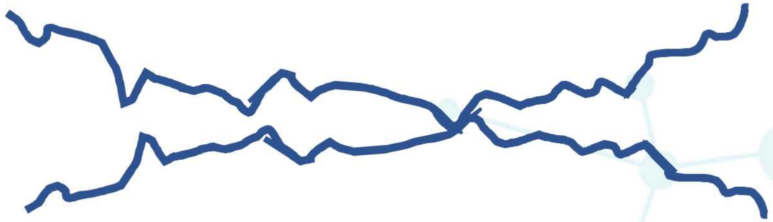
Rolling resistance



Microslip: pressure load asymmetry



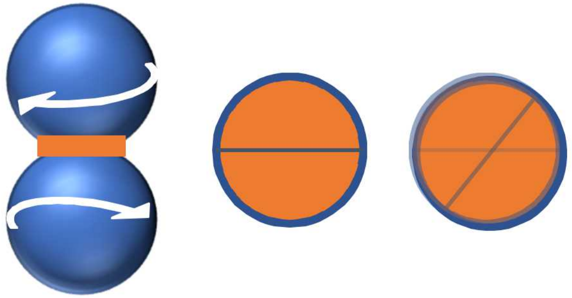
Inelastic deformation



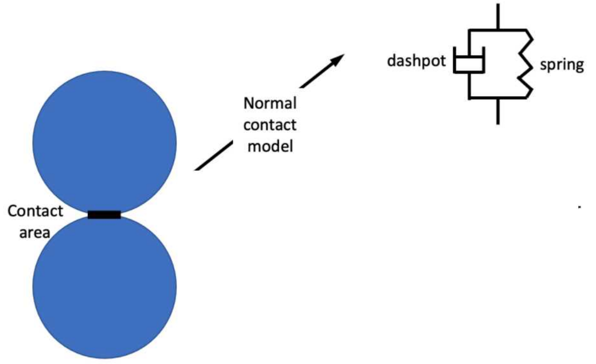
Roughness

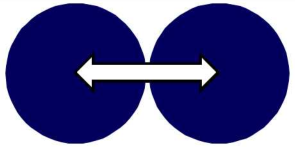
Twisting resistance

Microslip due to rotational displacement



Contact model





$$\mathbf{F}_{ij} = \mathbf{F}_n + \mathbf{F}_s + \mathbf{F}_r + \mathbf{F}_t$$
$$\mathbf{F}_n = k_n \delta_{ij} \mathbf{n}_{ij} - m_{\text{eff}} \gamma_n \mathbf{v}_n$$

$$\mathbf{v}_n = ((\mathbf{v}_j - \mathbf{v}_i) \cdot \mathbf{n})\, \mathbf{n}$$

m	k_m	γ_m
normal	1.0	0.5
sliding	1.0	0.5
rolling	1.0	0.5
twisting	1.0	0.5

$$\delta_{ij} = R_i + R_j - |\mathbf{r}_{ij}|$$

$$\xi_m = \int_{t0}^{t} \mathbf{v}_m(\tau) \mathrm{d}\tau$$

Usage

```
pair_style granular
pair_coeff 1 1 jkr 1000.0 50.0 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 20.0 tangential linear_history 300.0 1.0 0.1␣
↪rolling sds 200.0 100.0 0.1 twisting marshall
```

Mindlin, R. D. (1949). *J. Appl. Mech., ASME* 16, 259-268.
Luding, S. (2008). *Granular matter*, 10(4), 235.
Marshall, J. S. (2009). *J. Comput. Phys.*, 228(5), 1541-1561.
Derjaguin, B., et al. (1975). *J. Colloid Interf. Sci.*, 53(2), 314-326 .
Johnson, K. L., et al. (1971). *Proc. R. Soc. Lond. A*, 324(1558), 301-313.
Tsuji, Y., et al. (1992). *Powder Technol.*, 71(3), 239-250.

Packing methodology

Discrete element, particle-based modeling (DEM) (implemented within LAMMPS[a]).

Packing protocol: specify pressure tensor and bring system to final state from a very low pressure.

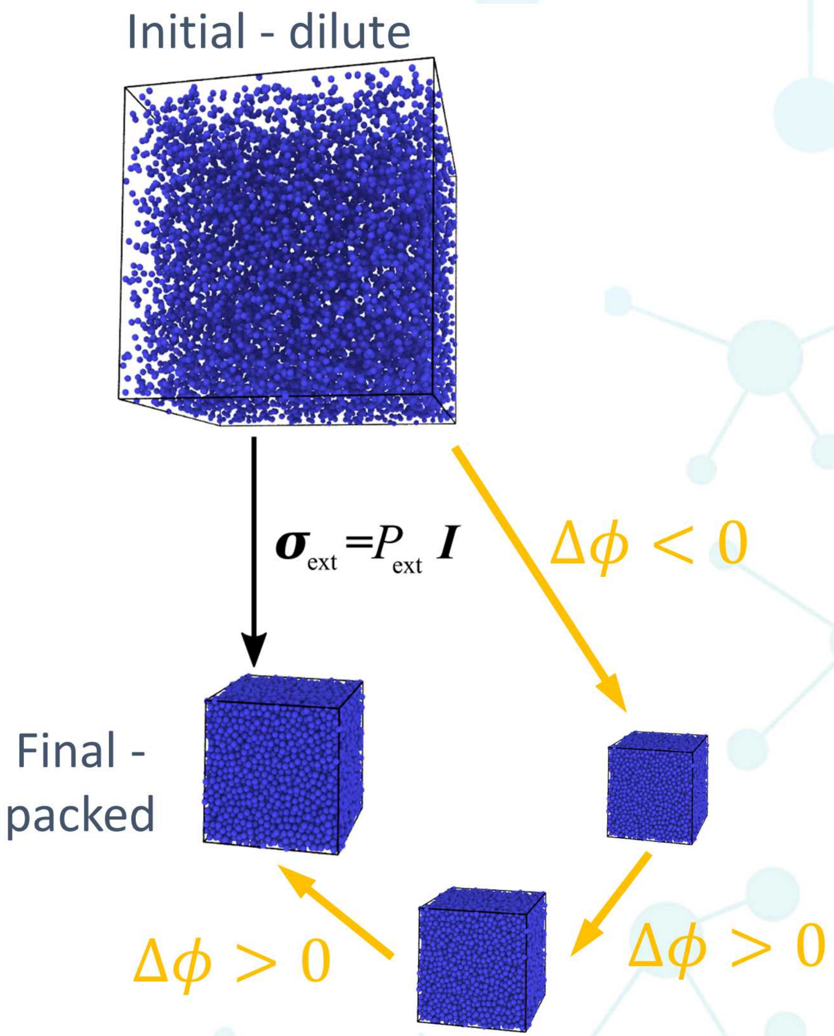
$$\dot{\mathbf{r}}_i = \frac{\mathbf{p}_i}{m_i} + \frac{\mathbf{p}_{\mathrm{box}}}{m_{\mathrm{box}}}\mathbf{r}_i$$

$$\dot{\mathbf{p}}_i = \mathbf{F}_i - \frac{\mathbf{p}_{\mathrm{box}} - \frac{1}{N_f}\mathrm{Tr}[\mathbf{p}_{\mathrm{box}}]}{m_{\mathrm{box}}}\mathbf{p}_i$$

$$\dot{\mathbf{h}} = \frac{\mathbf{p}_{\mathrm{box}}}{m_{\mathrm{box}}}\mathbf{h}$$

$$\frac{\dot{\mathbf{p}}_{\mathrm{box}}}{x_{\mathrm{drag}}} = V(\mathbf{P}_{\mathrm{int}} - \mathbf{I}P_a) - \mathbf{h}\Sigma\mathbf{h}^T + \frac{1}{N_f}\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{m_i}\mathbf{I}$$

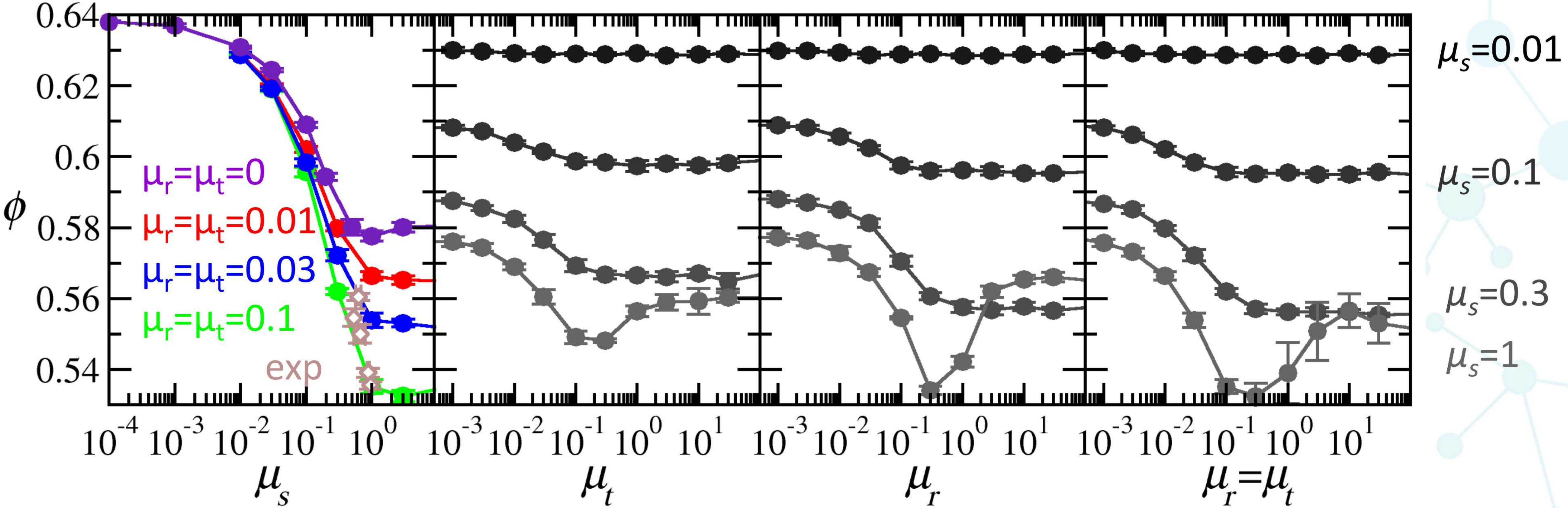
$$m_{\mathrm{box}} = NkTP_{\mathrm{damp}}^2$$



W. Shinoda, M. Shiga, and M. Mikami, PRB, 16, 2004.
G. J. Martyna, D. J. Tobias, and M. L. Klein, J. Chem. Phys., 4177, 1994.
M. Parrinello and A. Rahman, J. Appl. Phys., 7182, 1981.

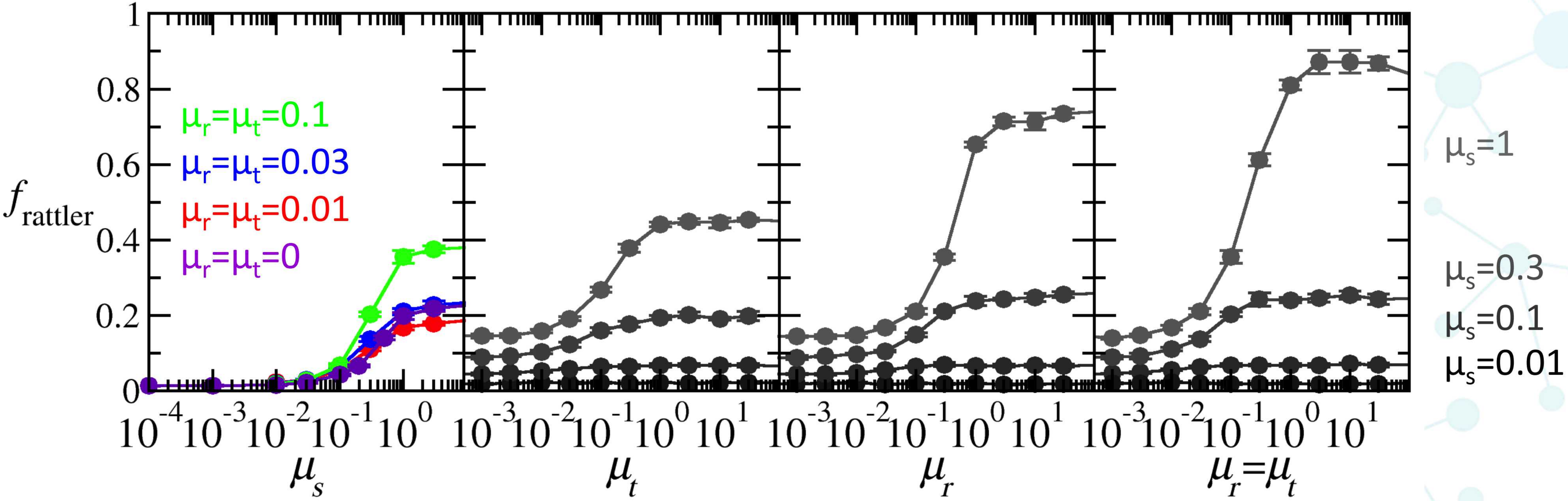
Menon N. et al. (2010). *Soft Matter*, 6(13), 2925-2930

Volume fraction



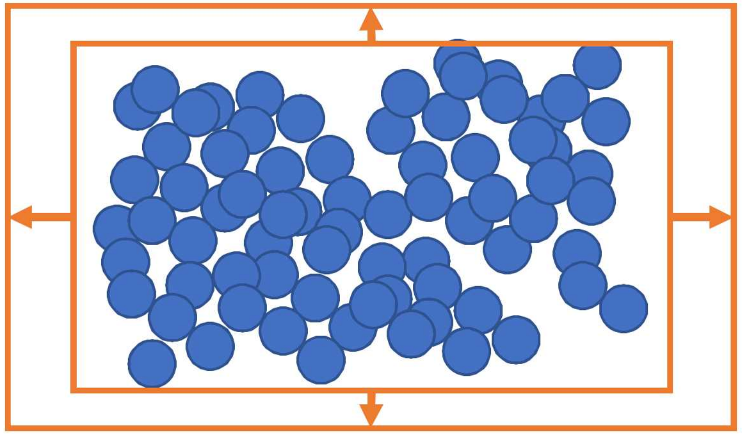
- Experiments are matched when moderate rolling and twisting friction are included
- Rolling and twisting friction have little effect for low μ_s
- ϕ minima at high $\mu_{s,r,t}$ may be due to large fraction of sliding contacts

Fraction of rattlers



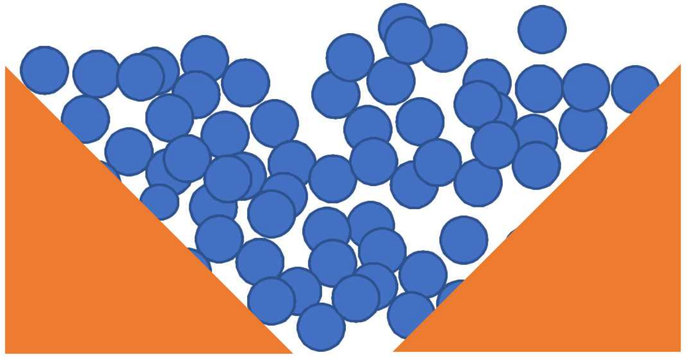
Background

Stress-dilatancy



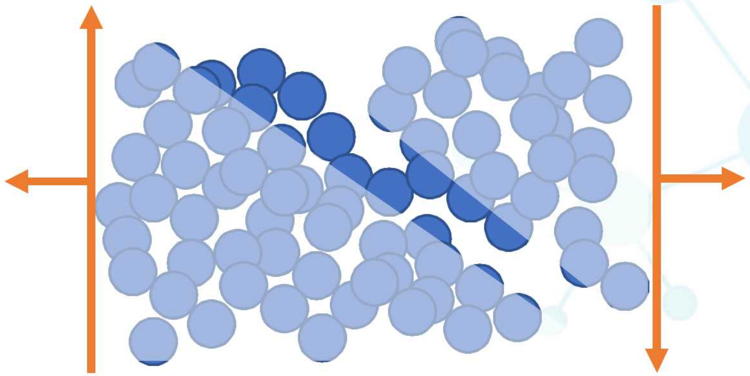
Liu, Y. et al. (2018). *Granular Matter*, 20, 12.

Hopper flow



Mort, P. et al. (2015). *Powder Tech.*, 284, 571-584.

Shear bands & extension



Bardet, J. P. (1994). *Mech. Mat.*, 18, 159–182.

<u>Sources for rolling and twisting resistance</u>

- Load asymmetry built up by:
  - microslip and creep
  - inelastic deformation at contact area
  - roughness

Outline

- Rolling and twisting resistance background
- Constraint counting
- Contact model (spring-dashpot-slider)
- Packing methodology
- Impact on packing
- Conclusions and future studies