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Investigating Flowability of AM Powders via DEM

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Sandia National Laboratories

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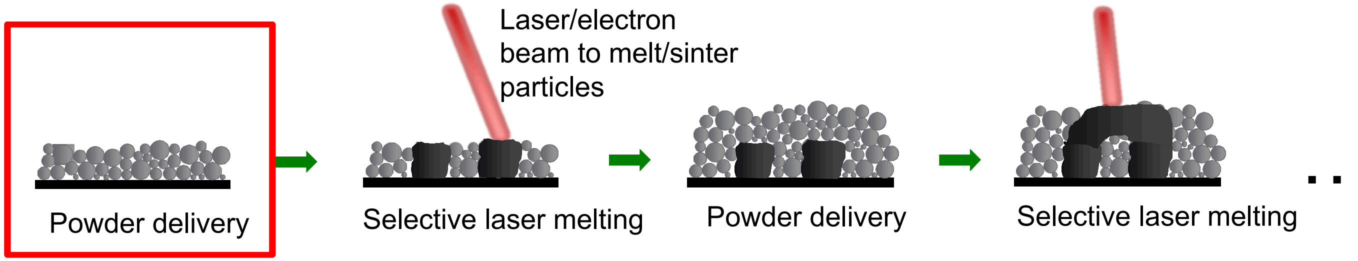
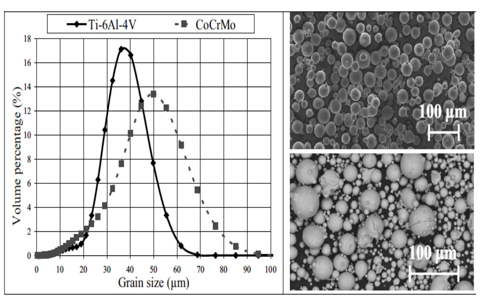
Background and Motivation

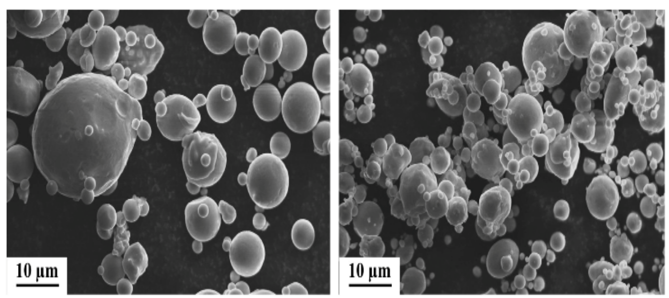
Layer-by-layer powder bed fusion processes (e.g. SLM/SLS):



- First step in AM powder bed process
  - Powder bed surface can affect laser interaction; power bed packing can affect void formation, surface finish, thermal properties
  - Informs downstream process models
- Variability in powder properties due to vendor supply, powder recycling
- Several key process length scales are comparable to individual particles:



From Ref. 1



From Ref. 2

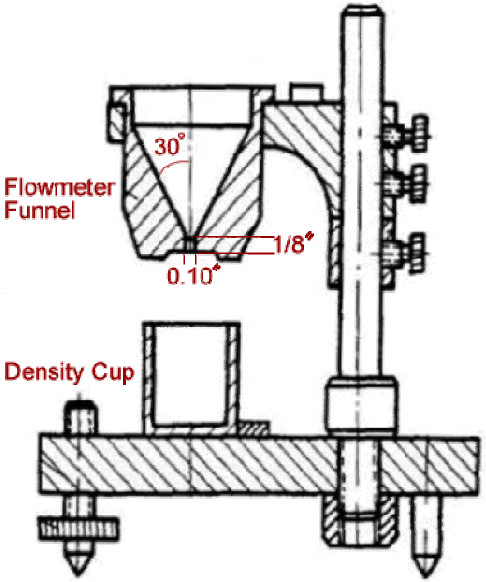
Typical particle diameter: 10-100 µm

Powder layer thickness 30-150 µm
Laser beam spot size 70-200 µm (ref. 1)

1. Vandenbroucke, B. and Kruth, J.P. *Rapid Prototyping Journal* 13 (2007): 196
2. Yadroitsev, I., et al. *Journal of Laser Applications* 25 (2013): 052003

Characterizing Flow: Hall Flowmeter

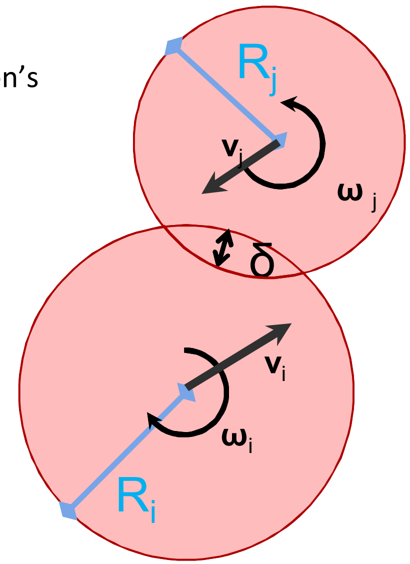
- ASTM standard measurement of "flowability"
  - Hall flow rate, $FR_H = t$ s/50g, where t is time it takes to flow 50g of powder
  - Gives index number to classify powders
  - Designed for metal powder & powder mixture
  - Must flow without any aid



ASTM Standard B213, 2013, "Flow Rate of Metal Powders Using the Hall Flowmeter Funnel," ASTM International, West Conshohocken, PA, 2013, DOI: 10.1520/B0213-13, www.astm.org

Numerical Simulations

- **D**iscrete **E**lement **M**ethod (DEM): molecular-dynamics-like simulation of Newton's laws of motion for a collection of particles
- Collision: $\delta = R_i + R_j - \|\mathbf{r}_i - \mathbf{r}_j\| > 0$
- Standard approach to compute forces/torques: spring-dashpot, aka Cundall-Strack[1]



- Normal contact force:

$$\mathbf{F}_n = \sqrt{R_e\delta}(\underbrace{k_n\delta\mathbf{n}_{ij}}_{\text{Elastic force due to deformation (Hertzian case here)}} - \underbrace{m_e\gamma_n\mathbf{v}_n}_{\text{Dissipative force (associated with coefficient of restitution < 1)}})$$

k_n, γ_n Constants related to material properties

$$R_e = R_iR_j/(R_i + R_j)$$
$$m_e = m_im_j/(m_i + m_j)$$
$$\mathbf{n}_{ij} = (\mathbf{r}_i - \mathbf{r}_j)/\|\mathbf{r}_i - \mathbf{r}_j\|$$
$$\mathbf{v}_n = ((\mathbf{v}_i - \mathbf{v}_j)\cdot\mathbf{n}_{ij})\mathbf{n}_{ij}$$

- Tangential contact force

$$\mathbf{F}_t = \sqrt{R_e\delta}(-k_t\mathbf{u}_t - m_e\gamma_t\mathbf{v}_t)$$

$$\mathbf{v}_t = (\mathbf{v}_i - \mathbf{v}_j) - \mathbf{v}_n - (R_i\omega_i + R_j\omega_j)\times\mathbf{n}_{ij}$$

Truncated such that $\|\mathbf{F}_t\| \leq \|\mu\mathbf{F}_n\|$

$\mathbf{u}_t$ Relative tangential displacement; throughout duration time *t* of contact: $\frac{d\mathbf{u}_t}{dt} = \mathbf{v}_t - \frac{\mathbf{u}_t\cdot\mathbf{r}_{ij}}{r_{ij}^2}$

μ Coefficient of friction

Total force: $\mathbf{F}_{i,tot} = m_i\mathbf{g} + \sum_j(\mathbf{F}_{n,ij} + \mathbf{F}_{t,ij})$

Total torque: $\tau_{i,tot} = -\frac{1}{2}\sum_j \mathbf{r}_{ij}\times\mathbf{F}_{t,ij}$

1. Cundall, P. A., and Strack, O. D. L. *Geotechnique* 29.1 (1979): 47-65.

Questions

Can we use Hall Flowmeter to parametrize particle properties in DEM simulations?

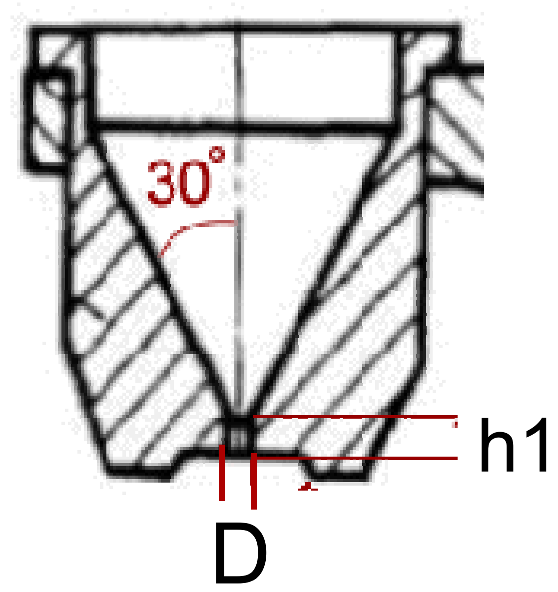
Complication 1: DEM simulations are limited in size. Can we relate the two size scales?

Complication 2: What does Hall Flowmeter really measure?

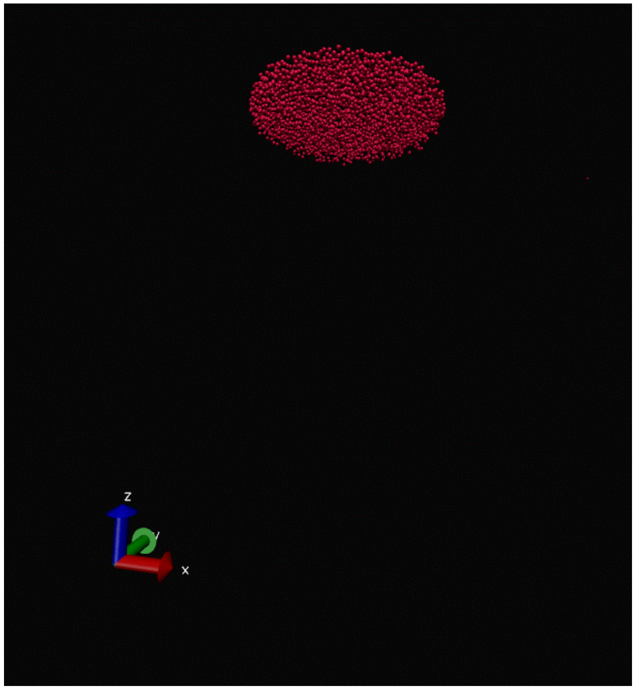
Can we use DEM simulations to gain insight into the physics of particle flow in Hall Flowmeter funnel?

Simulation Setup

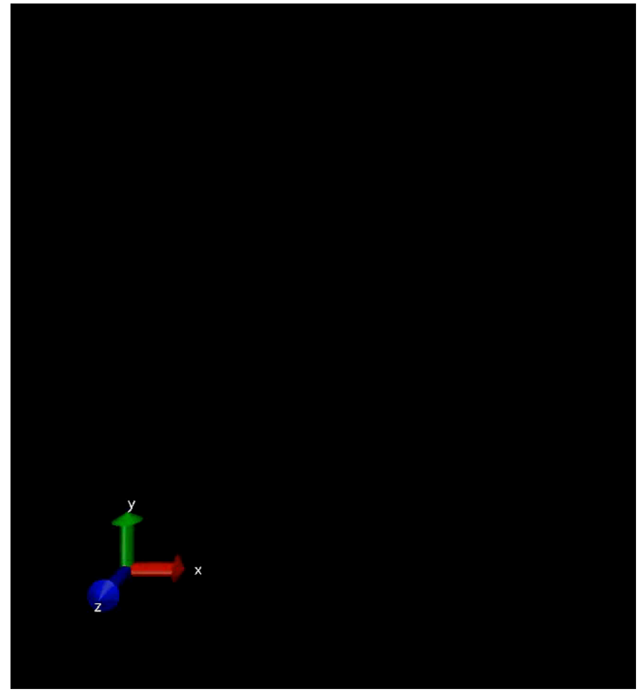
- Funnel dimensions
  - Non-dimensionalized: based on particle size, d
  - R = orifice diameter / particle diameter, D/d
- Actual Hall Flowmeter
  - If the powder is 10 microns, then R = 254
  - If 25.4 microns, R = 100
- Vary particle properties
  - μ=[0,1], γ=[0,~900]
- Fill funnel
  - Obstruct orifice, randomly place particles, let fall/settle under gravity
- Amount of powder (50g in ASTM standard)
  - Fixed number of particles for R=5 to 200
  - "constant fill level", R=5 to 25



DEM Simulation of Hall Flowmeter

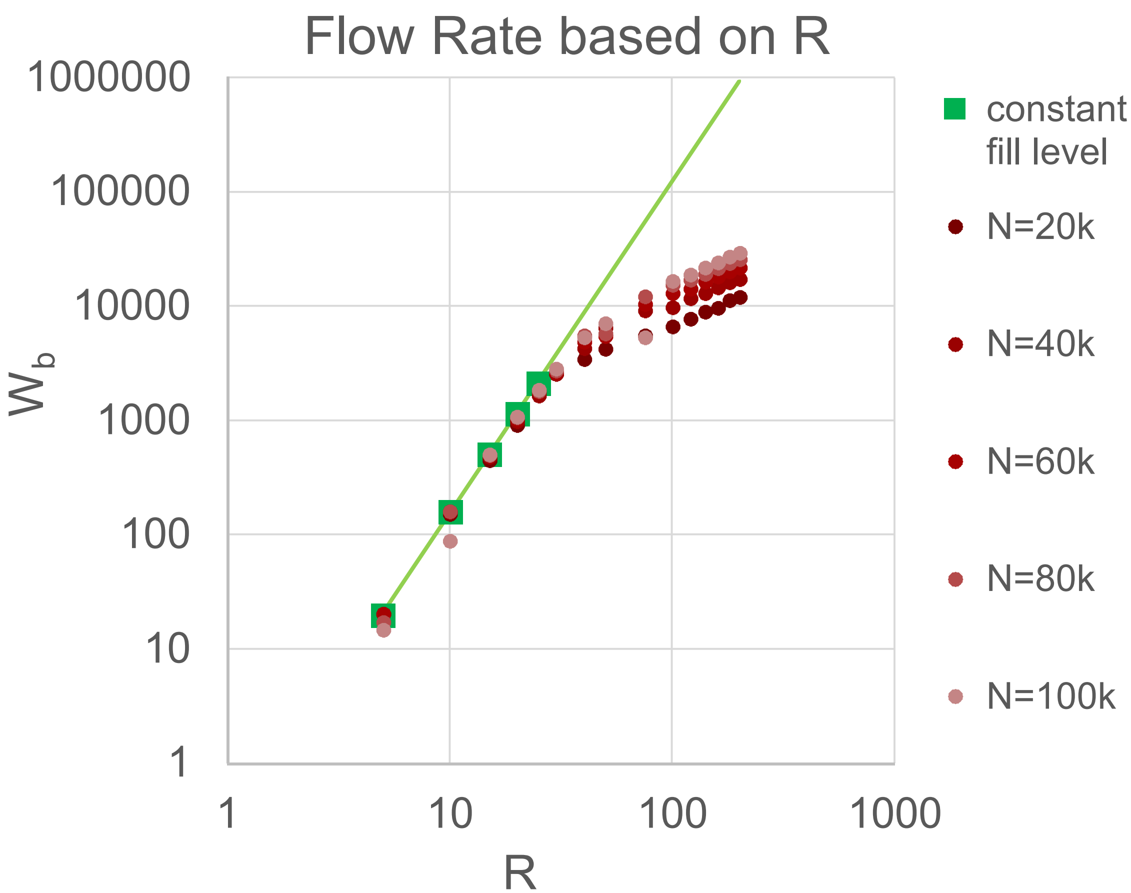


“standard model” –
no rolling friction, no cohesion



With rolling friction and cohesion

Funnel to Particle Scale



$$W_b = \frac{total\ particles\ discharged}{discharge\ time}$$

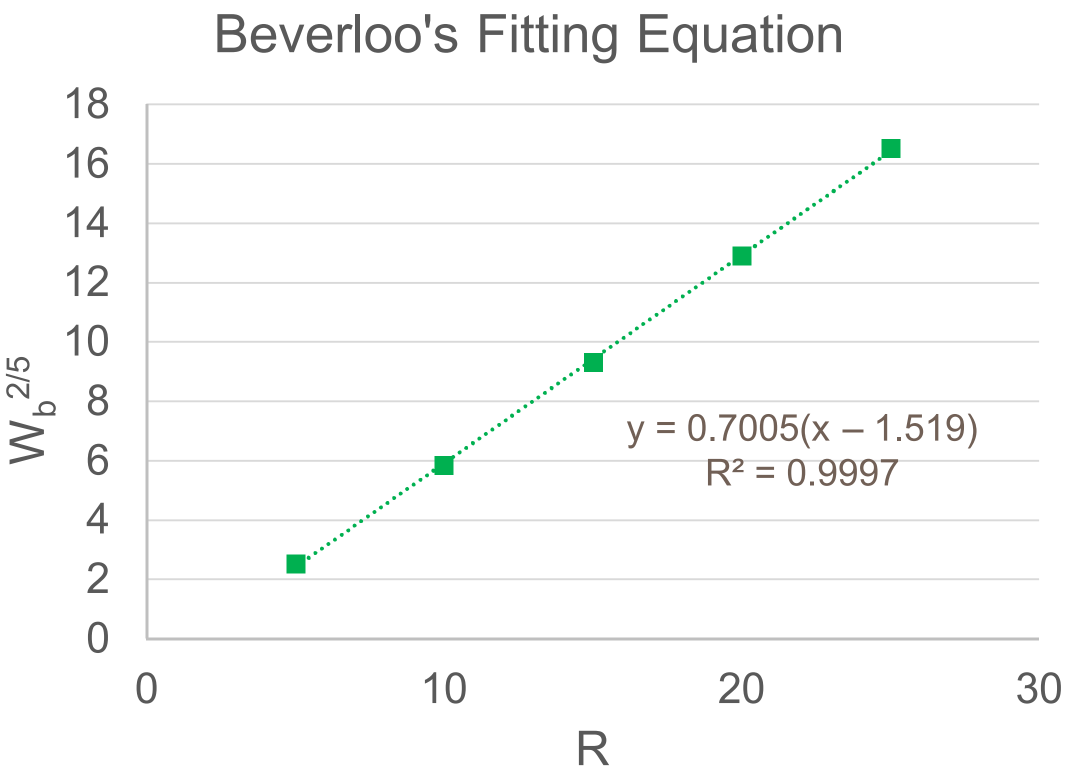
$$\mathrm{R} = \frac{orifice\ diameter\ D_o}{particle\ diameter\ d}$$

Power Law Behavior: Beverloo Law

$$W = C\rho_{bulk}\sqrt{g}(D-kd)^{5/2}$$
$$W \propto D^{5/2}$$

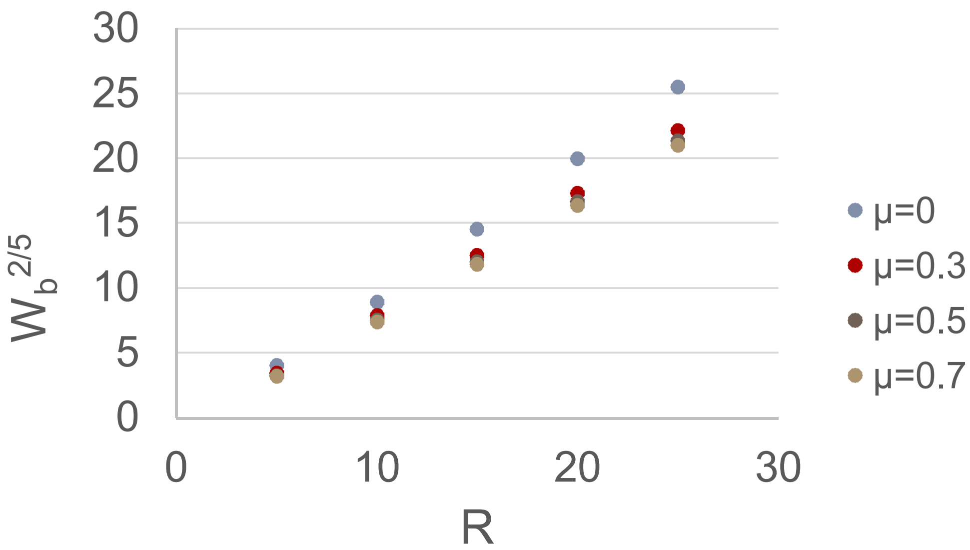
$$W_b^{2/5} = C'^{2/5}(R-k),$$
where d=1

C'=0.411
k=1.52



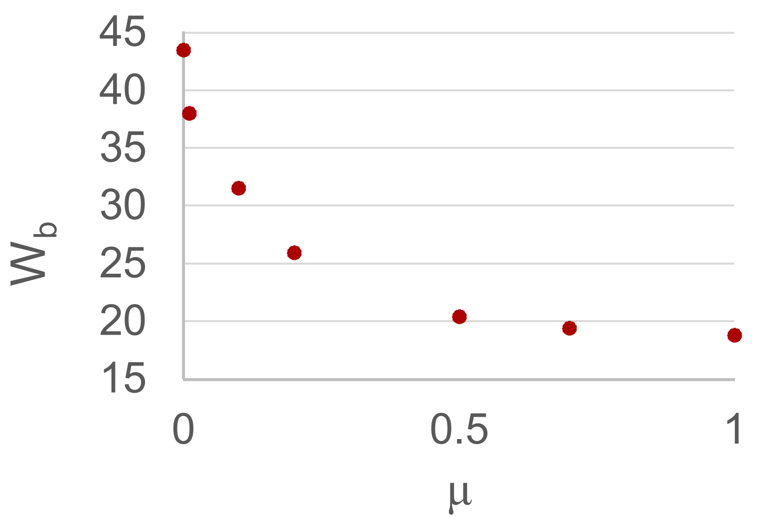
W A Beverloo, H A Leniger, J Van De Velde, "The flow of granular solids through orifices," Chem. Eng. Sci., 15, 260 (1961), DOI: 10.1016/0009-2509(61)85030-6

Friction Coefficient μ



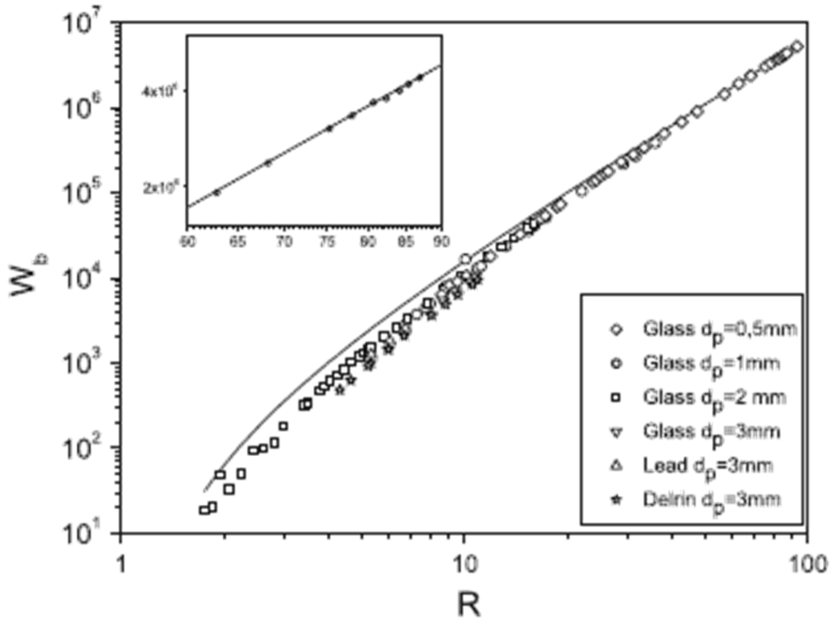
$$W_b^{2/5} = C'^{2/5}(R - k),$$

μ	k	C'
0	1.450526	1.000374
0.3	1.42666	0.699256
0.5	1.519102	0.647292
0.7	1.547243	0.621375

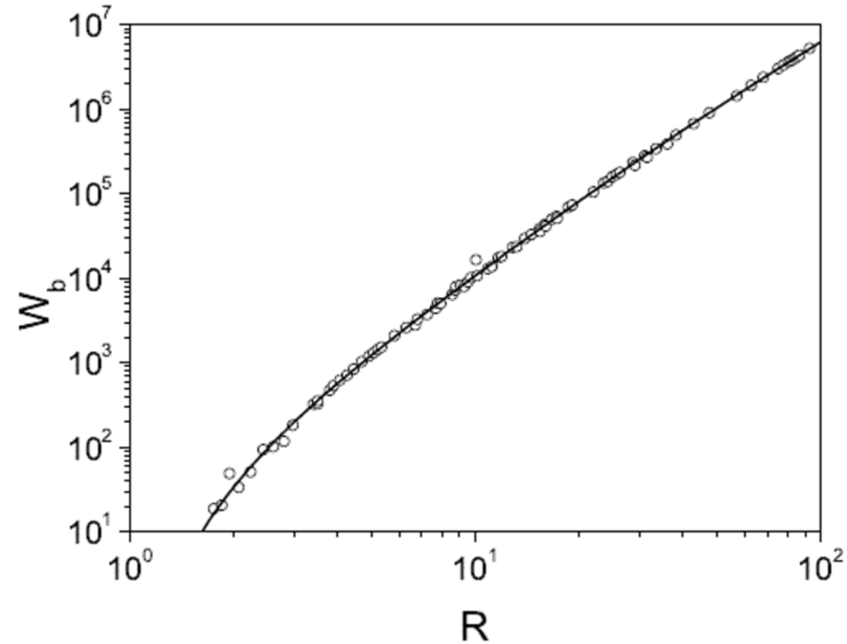


FQ33

Mankoc et al: Beverloo at Small R



$$W_b = C'(1 - \frac{1}{2}e^{-b(R-1)})(R-1)^{5/2}$$



Mankoc et al.'s (2007) experiments on glass beads:

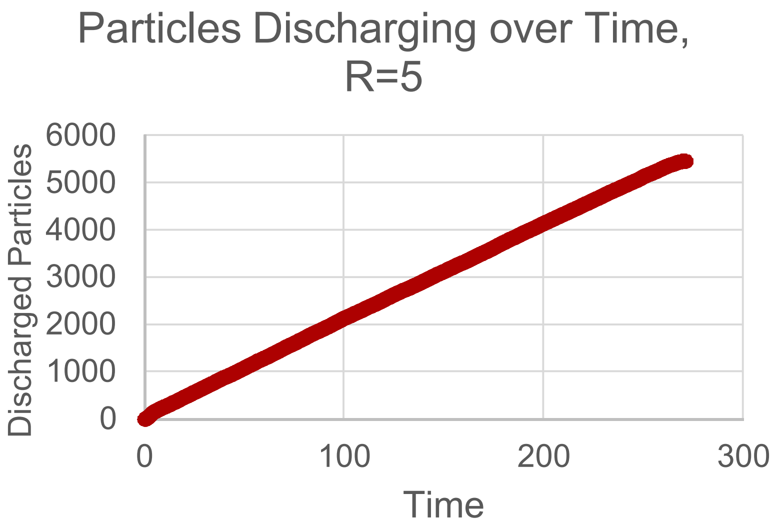
- k = 1d (where W_b must go to zero)
- b ~ 0.05 = $\frac{1}{20d}$

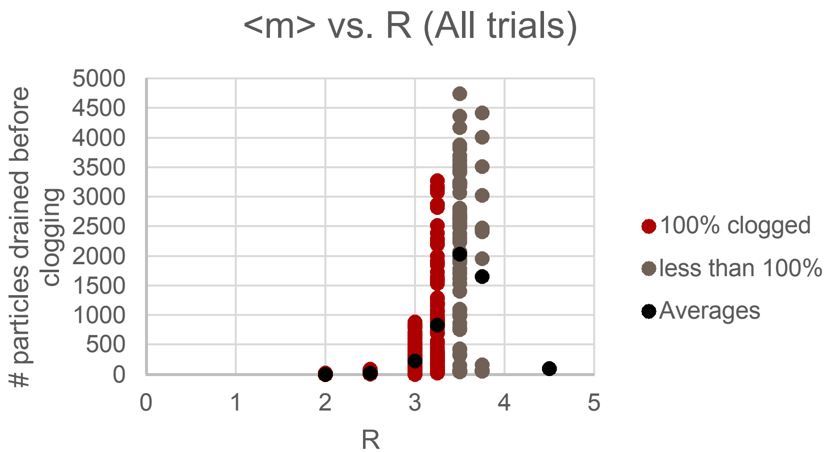
Mankoc, C., Janda, A., Arévalo, R. et al. Granular Matter (2007) 9: 407. doi:10.1007/s10035-007-0062-2

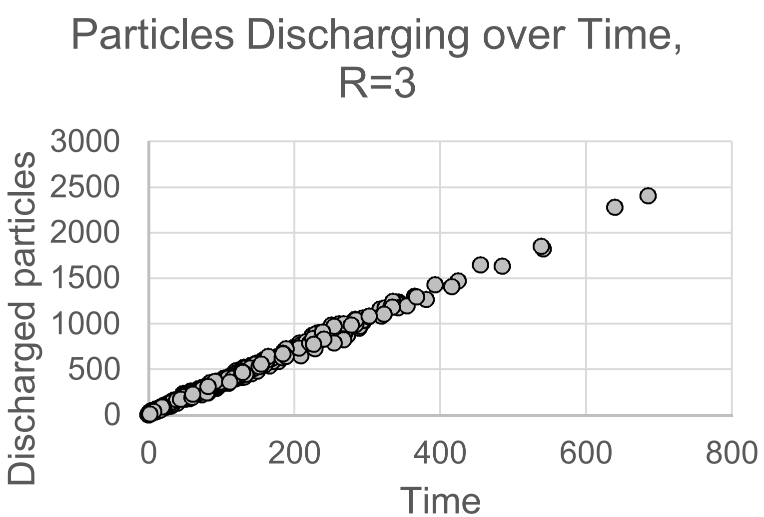
FQ33 thought it's about both R>5 (no jamming) and limited range of R?
Frink, Quintina, 8/9/2016

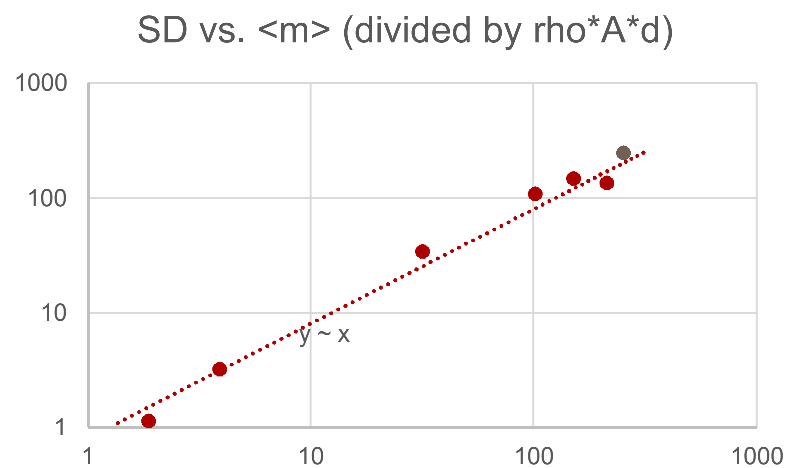
Intermittency

- Flow when R is small









C. C. Thomas and D. J. Durian, Phys. Rev. E 94, 022901

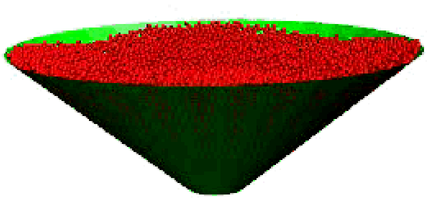
Conclusion

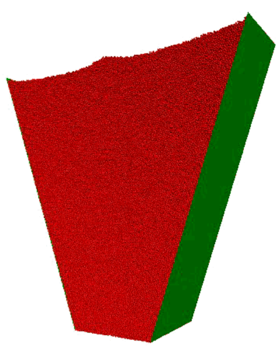
- Equations of Beverloo et al and Mankoc et al with modification could be used to parametrize particle properties in DEM simulations
- Relationships between flow rate, orifice size, and friction needed to predict flow rate for the orifice size chosen
  - The influences of other parameters on flow rate need to be explored further
- Statistics of flow for small orifices give more insight to powder behavior

EXTRA SLIDES

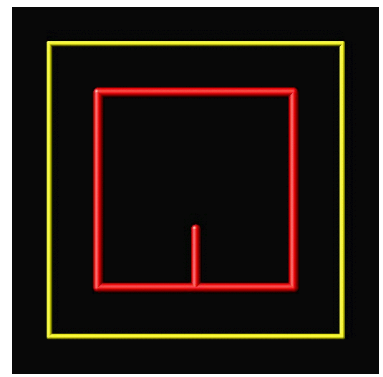
LAMMPS: Complex moving boundaries for granular interactions

fix wall/region/gran – build walls using primitive ‘region’ shapes:



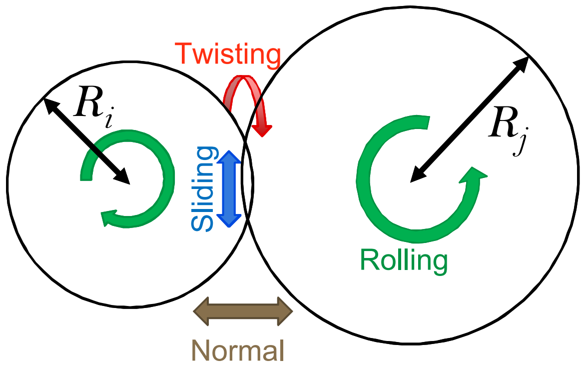


Pair style sphere/line (2D) and sphere/tri (3D)



In progress

Granular contact models



Geometry/kinematics

$\mathbf{r}_i$, $\mathbf{r}_j$: positions
$\mathbf{v}_i$, $\mathbf{v}_j$: translational velocities
$\boldsymbol{\Omega}_i$, $\boldsymbol{\Omega}_j$: angular velocities
a: area of contact*

$$\delta = R_i + R_j - \|\boldsymbol{r}_i - \boldsymbol{r}_j\|$$

$$\boldsymbol{n} = (\boldsymbol{r}_i - \boldsymbol{r}_j)/\|\boldsymbol{r}_i - \boldsymbol{r}_j\|$$

$$R = \frac{1}{1/R_i + 1/R_j} = \frac{R_i R_j}{R_i + R_j}$$

$$\boldsymbol{v}_R = \boldsymbol{v}_i - \boldsymbol{v}_j$$

$$\boldsymbol{v}_t = \boldsymbol{v}_R - (\boldsymbol{v}_R \cdot \boldsymbol{n})\boldsymbol{n}$$

Relative sliding velocity:

$$\boldsymbol{v}_{tR} = \boldsymbol{v}_t - (R_i\boldsymbol{\Omega}_i + R_j\boldsymbol{\Omega}_j) \times \boldsymbol{n}$$

Relative twisting 'velocity':

$$\Omega_T = (\boldsymbol{\Omega}_i(\tau) - \boldsymbol{\Omega}_j(\tau)) \cdot \boldsymbol{n}$$

Relative rolling velocity:

$$\boldsymbol{v}_L = -R(\boldsymbol{\Omega}_i - \boldsymbol{\Omega}_j) \times \boldsymbol{n}$$

***a* depends on contact model!**

Material properties

m_i, m_j: masses
E_i, E_j: elastic moduli
G_i, G_j: shear moduli
ν_i, ν_j : Poisson's ratios

$$E = \left(\frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j}\right)^{-1} \quad G = \left(\frac{2-\nu_i}{G_i} + \frac{2-\nu_j}{G_j}\right)^{-1}$$

(isotropic: $2G(1+\nu) = E$)

γ_i : adhesion energy
e_i : coefficient of restitution
k_N, k_S, k_T, k_R: normal, sliding, twisting, rolling stiffness
η_N, η_S, η_T, η_R : normal, sliding, twisting, rolling dissipation
μ_S, μ_T, μ_R : sliding, twisting, rolling friction coefficients

Hertz: $k_N = 4Ea/3$
Mindlin: $k_S = 8Ga$
Brilliantov: $\eta_N = \gamma_D m$, $\gamma_D = f(e)$
Tsuji: $\eta_N = f(e)(mk_N)^{1/2}$

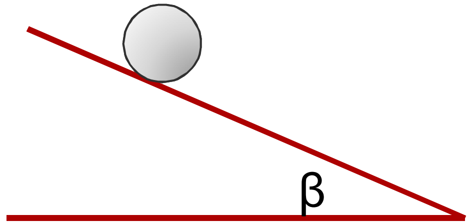
$\eta_S = \eta_N$
$k_T, \eta_T, \mu_T = f(k_S, \eta_S, \mu_S, a)$

	gran/hertz	dmt/rolling	jkr/rolling
Normal elastic (spring)	$\boldsymbol{F}_n = k_n\sqrt{R}\delta^{3/2}\boldsymbol{n}$	$\boldsymbol{F}_n = \left(\frac{4Ea^3}{3R} - 4\pi\gamma R\right)\boldsymbol{n}$ $\delta_N = a^2/R$ $F_{\text{pulloff}} = -4\pi\gamma R$	$\boldsymbol{F}_n = \left(\frac{4Ea^3}{3R} - 2\pi a^2\sqrt{\frac{4\gamma E}{\pi a}}\right)\boldsymbol{n}$ $\delta_N = a^2/R - 2\sqrt{\pi\gamma a/E}$ $F_{\text{pulloff}} = -3\pi\gamma R$
Normal dissipative (dashpot)	$-\eta_n\boldsymbol{v}_R \cdot \boldsymbol{n}$	$-\eta_n\boldsymbol{v}_R \cdot \boldsymbol{n}$ Option for η_N based on Tsuji or Brilliantov	$-\eta_n\boldsymbol{v}_R \cdot \boldsymbol{n}$ Option for η_N based on Tsuji or Brilliantov
Sliding elastic[1]	$\boldsymbol{F}_S = -k_S\int_{t0}^{t}\boldsymbol{v}_{tR}(\tau)\mathrm{d}\tau$	$\boldsymbol{F}_S = -k_S\int_{t0}^{t}\boldsymbol{v}_{tR}(\tau)\mathrm{d}\tau$	$\boldsymbol{F}_S = -k_S\int_{t0}^{t}\boldsymbol{v}_{tR}(\tau)\mathrm{d}\tau$
Sliding dissipative	$-\eta_T\boldsymbol{v}_{tR}$	$-\eta_T\boldsymbol{v}_{tR}$	$-\eta_T\boldsymbol{v}_{tR}$
Sliding frictional	$\|\boldsymbol{F}_S\| \leq F_{\text{S,crit}}$ $F_{\text{s,crit}} = \mu_S\|\boldsymbol{F}_n\|$	$\|\boldsymbol{F}_S\| \leq F_{\text{S,crit}}$ $F_{\text{s,crit}} = \mu_S\|\boldsymbol{F}_n\|$	$\|\boldsymbol{F}_S\| \leq F_{\text{S,crit}}$ $F_{\text{s,crit}} = \mu_S(\|\boldsymbol{F}_n\| + F_{\text{pulloff}})$
Rolling elastic[2]		$\boldsymbol{F}_R = -k_R\int_{t_0}^{t}\boldsymbol{v}_L(\tau)\mathrm{d}\tau$	$\boldsymbol{F}_R = -k_R\int_{t_0}^{t}\boldsymbol{v}_L(\tau)\mathrm{d}\tau$
Rolling dissipative		$-\eta_R\boldsymbol{v}_L$	$-\eta_R\boldsymbol{v}_L$
Rolling frictional		$\|\boldsymbol{F}_R\| \leq F_{\text{R,crit}}$ $F_{\text{R,crit}} = \mu_R\|\boldsymbol{F}_n\|$	$\|\boldsymbol{F}_R\| \leq F_{\text{R,crit}}$
Twisting elastic[3]		$M_t = -k_Q\int_{t_0}^{t}\Omega_T(\tau)\mathrm{d}\tau$	$M_t = -k_Q\int_{t_0}^{t}\Omega_T(\tau)\mathrm{d}\tau$
Twisting dissipative		$-\eta_Q\Omega_T$	$-\eta_Q\Omega_T$
Twisting frictional		$M_t \leq -M_{t,\text{crit}}\Omega_T/\|\Omega_T\|$ $M_{\text{t,crit}} = \frac{2}{3}aF_{\text{s,crit}}$	$M_t \leq -M_{t,\text{crit}}\Omega_T/\|\Omega_T\|$ $M_{\text{t,crit}} = \frac{2}{3}aF_{\text{s,crit}}$

1,2,3: Integrals must be carried out to remove effects of rigid body rotation/twisting of contacting pair
2: $\mathbf{F}_R$ is a 'pseudo-force', resulting only in torque $R\mathbf{n} \times \mathbf{F}_R$

Effects of contact parameters

Sliding and rolling friction coefficients $\mu_{S,}$ μ_R

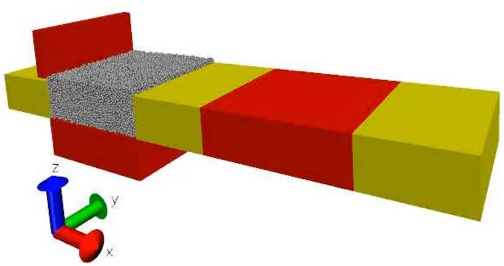


μ_S, μ_R = tan(β), where β is angle at which sliding/rolling begins

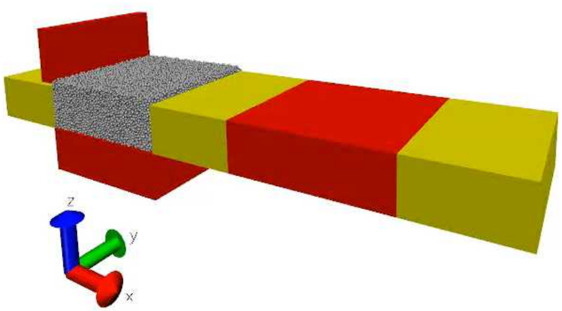
Typically $0 < \mu_S, \mu_R < 1$, but any value is physically possible.

γ (cohesion): energy of cohesion of metals ~ 1-2 J/m^2

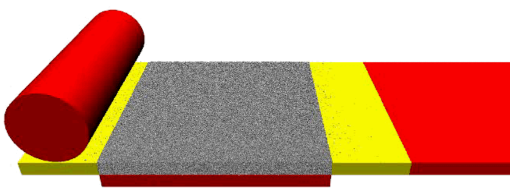
Preserve ratio of repulsive force to cohesive force $E_Y R/\gamma \rightarrow \gamma \sim O(1)$ in dimensionless units



Very high cohesion
Moderate friction



No cohesion
Moderate rolling and sliding friction



No cohesion
Moderate sliding friction
No rolling/twisting friction

Representing Granular Shapes

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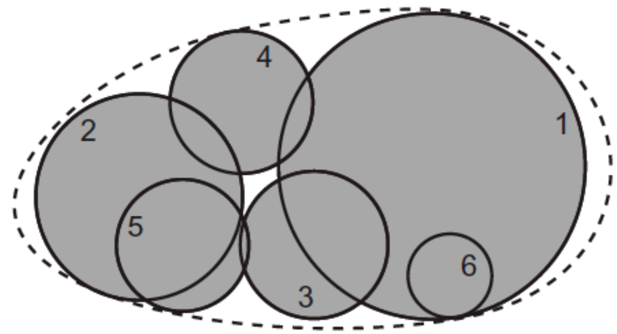
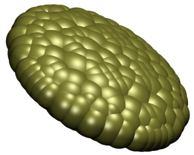
Clustered
Overlapping
Sphere

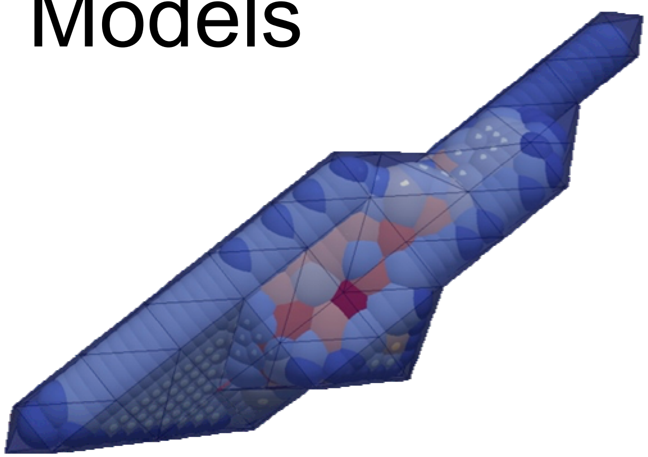


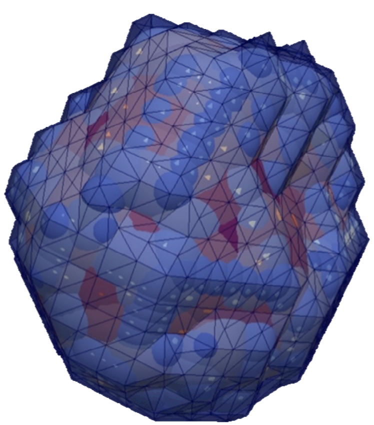
(f)

Garcia, X., et al. *Géotechnique* (2009).



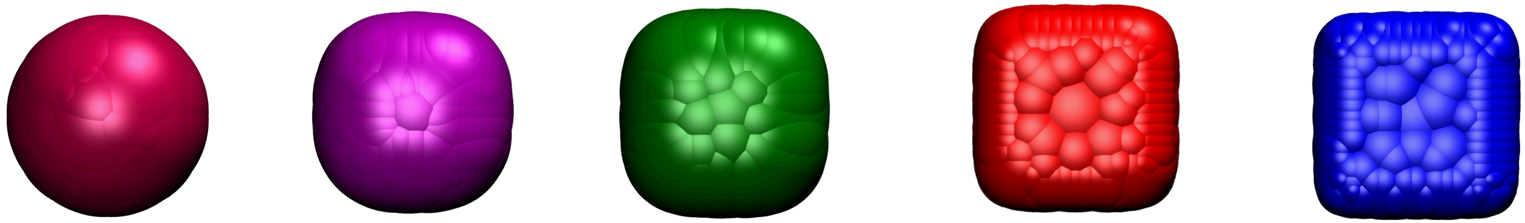
LAMMPS DEM Models



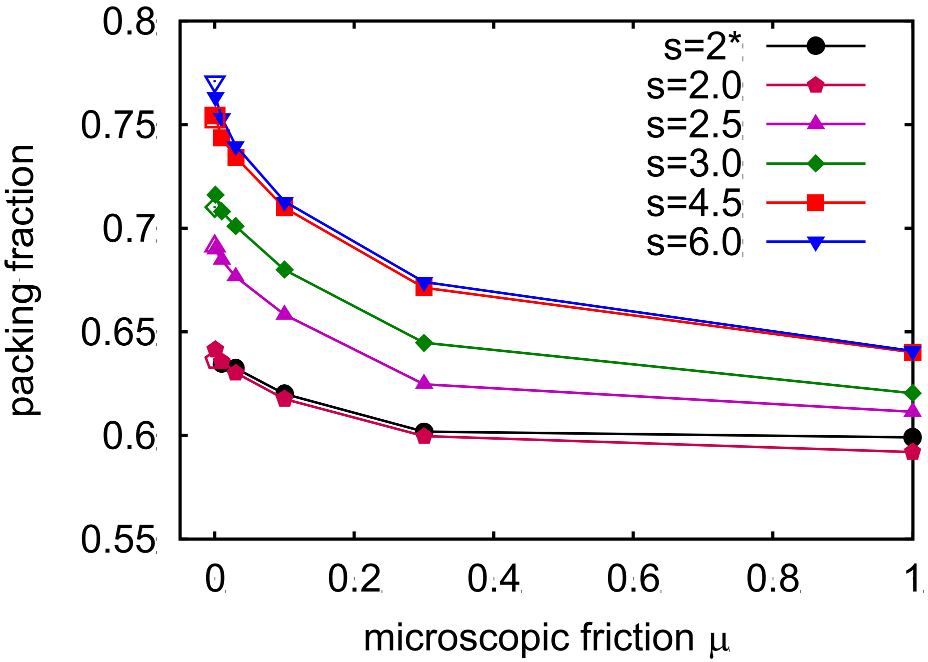


Packing

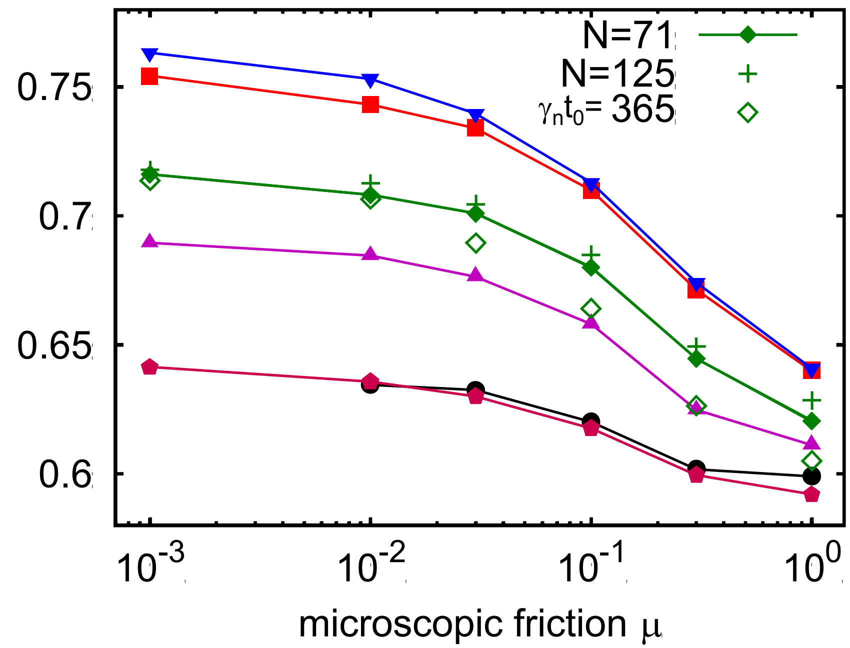
s=2.0 s=2.5 s=3.0 s=4.5 s=6.0



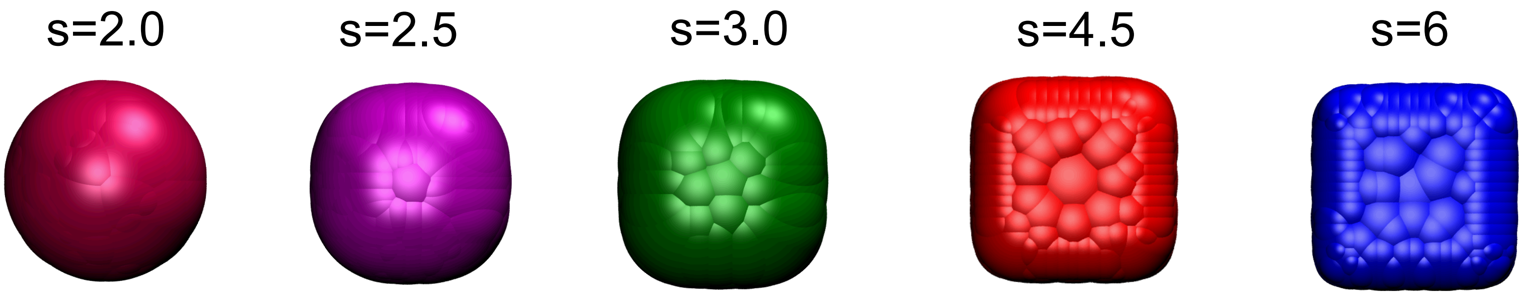
Jiao, Y., Stillinger, F. H., & Torquato, S. *PRE* (2010) open, $\mu = 0.0$



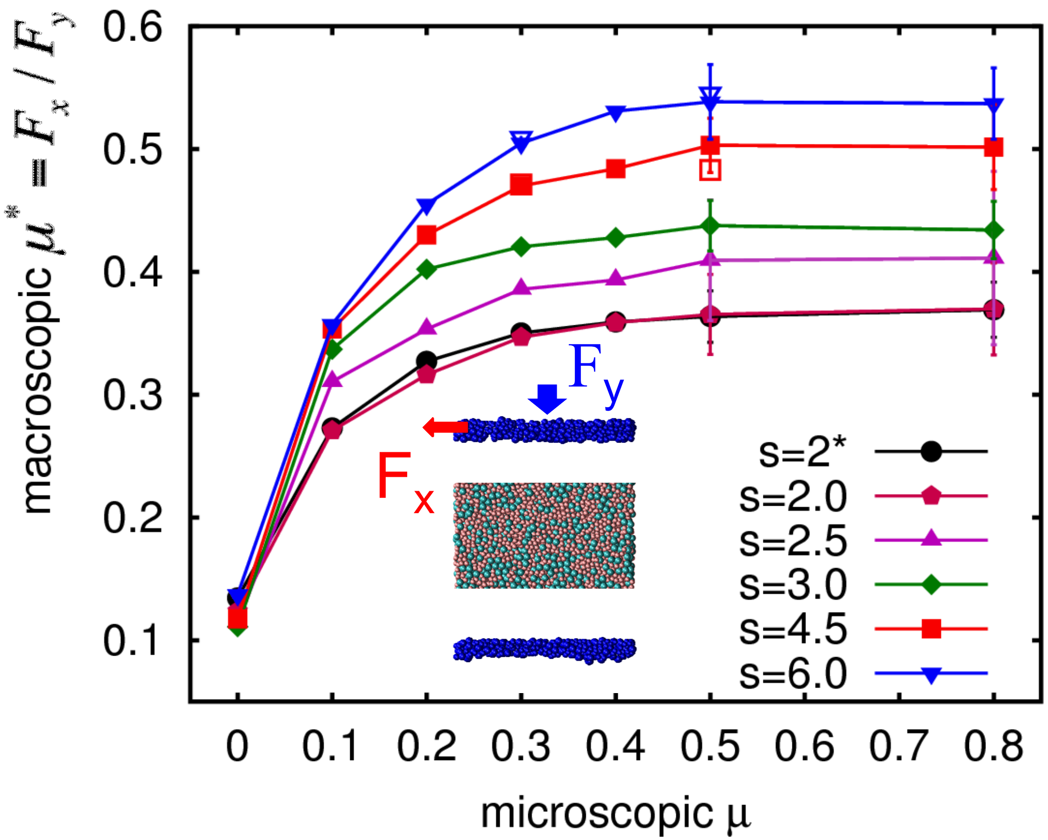
LES, *Soft Matter* (2010) $s = 2^*$



Bulk Rheology



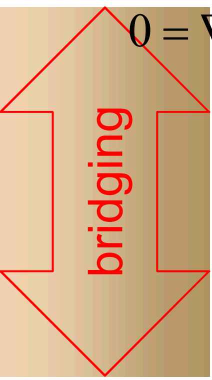
- Identical zero-friction (microscopic) limit
- Monotonic in shape parameter **s** for *$\mu > 0$*
- Saturates 0.3 > *$\mu > 0.5$*
- *μ** saturation value 0.36 – 0.54

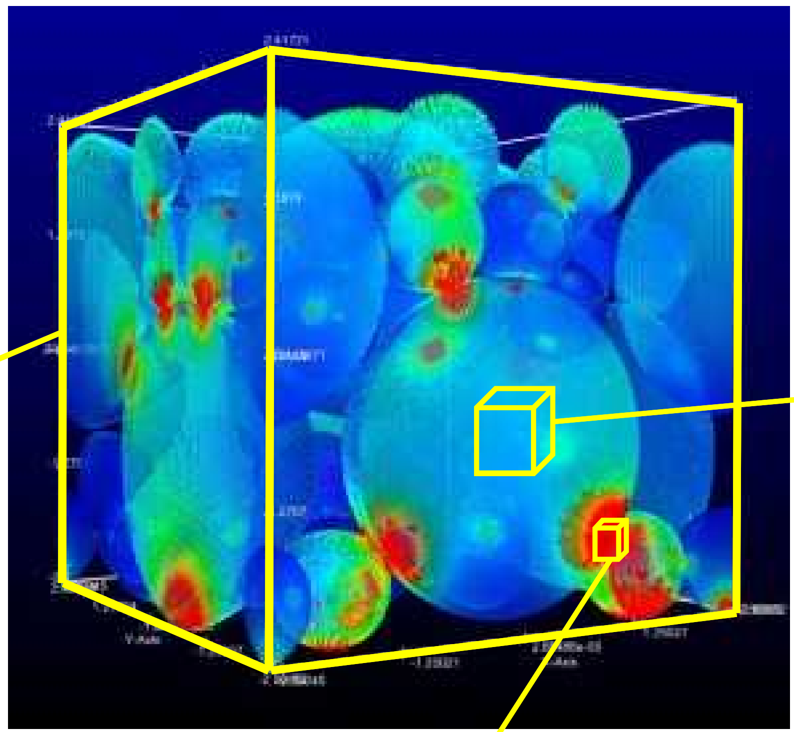


The Multi-scale Transport Picture *through* Particulate Media

(1) Bulk, Macroscale
- Homogeneous
- “Continuum”
- Constant transport coef.

$$0 = \nabla \cdot \mathbf{q}(\mathbf{x}) = K_{eff} \nabla \cdot \langle \nabla T(\mathbf{x}) \rangle$$





(2) Particle-Particle (Meso-structure) Scale
- Inhomogeneous
- “Discrete”; Disordered
- “Anomalous” transport

$$0 = \nabla \cdot \mathbf{q}(\mathbf{x}) = \nabla \cdot \left(K(\mathbf{x}) \nabla T(\mathbf{x}) \right)$$

(3) Sub-particle materials structure
- Crystal structure
  - Anisotropy
  - defects, impurities, etc.
- Polycrystalline
  - Grain boundaries

(4) Interfacial Scale
- Contact area, roughness, inter-diffusion
- Material types (e.g., phonon, electron dominated)

"Coarse-graining" Workflow: Discretizing the Mesoscale

- Continuum percolation-type viewpoint + Spectral Graph Theory

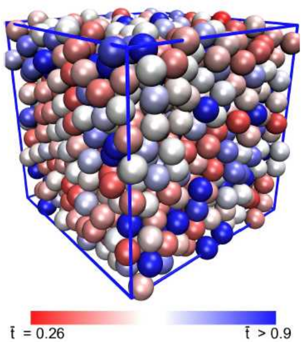
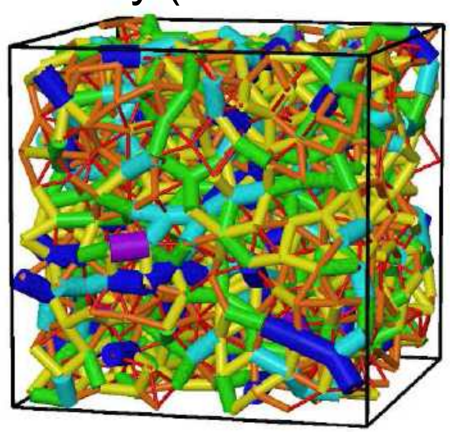


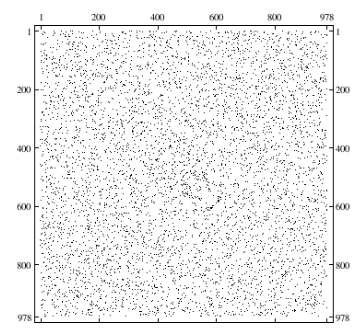
Image stack, or simulated μstructure

Determine segmentation: clustering (similarity relation, e.g., greyscale) & connectivity (distinction relation, e.g., proximity relation)



graph of contact network

Determine: edge weights (interfacial resolution and physics models)



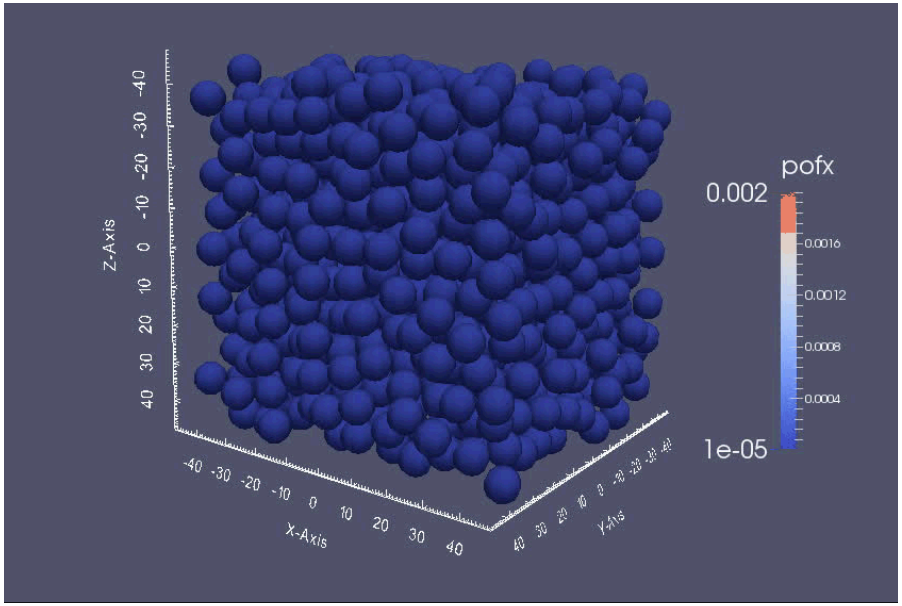
Graph Laplacian, Transition Rate Matrix, Transition Probability Matrix, …

Simulate Markov Process on Contact Network

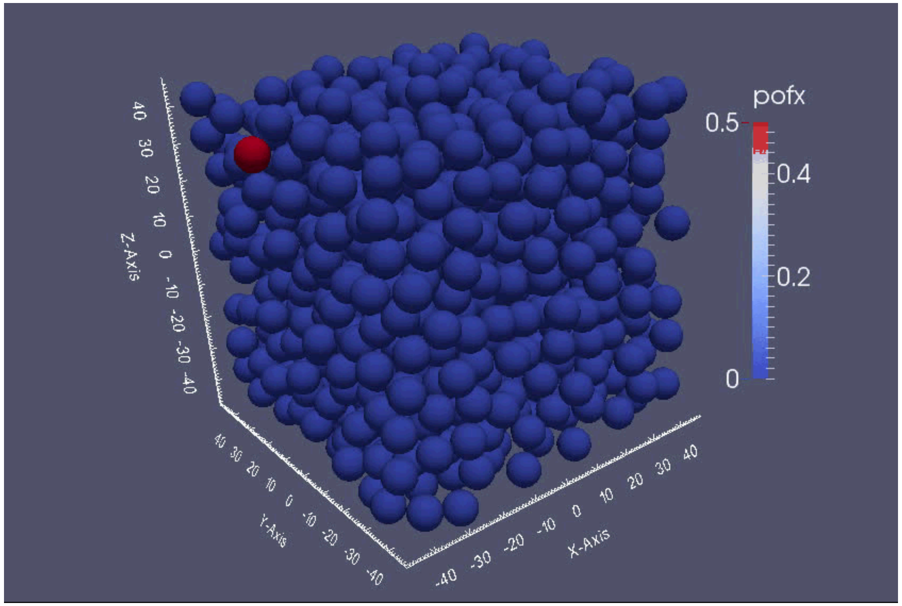
- Discretize Continuous-Time Equation

$$\frac{\partial \mathbf{P}(t)}{\partial t} = \mathbf{WP}(t) \Rightarrow \begin{cases} \mathbf{P}_{n+1} = \mathbf{MP}_n \\ \mathbf{M} = \mathbf{I} + \Delta t \mathbf{W} \end{cases}$$

  - I.C. $\mathbf{P}_0 = \hat{\mathbf{e}}_1 \quad \left\|\hat{\mathbf{e}}_1\right\| = 1$
  - Periodic B.C.'s



p = 0.0004



p = 0.00004