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Discrete element modeling of powder spreading and flow for metal additive manufacturing

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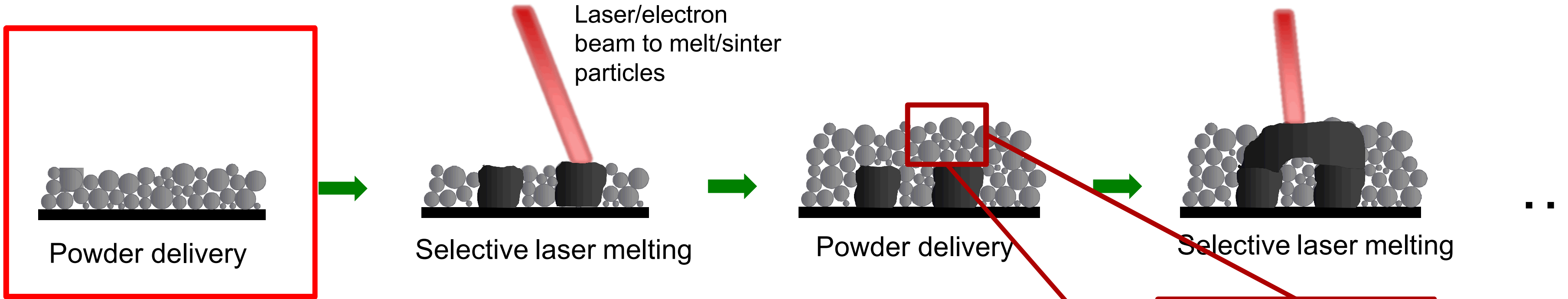
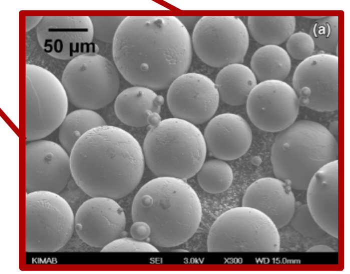
Background and Motivation

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





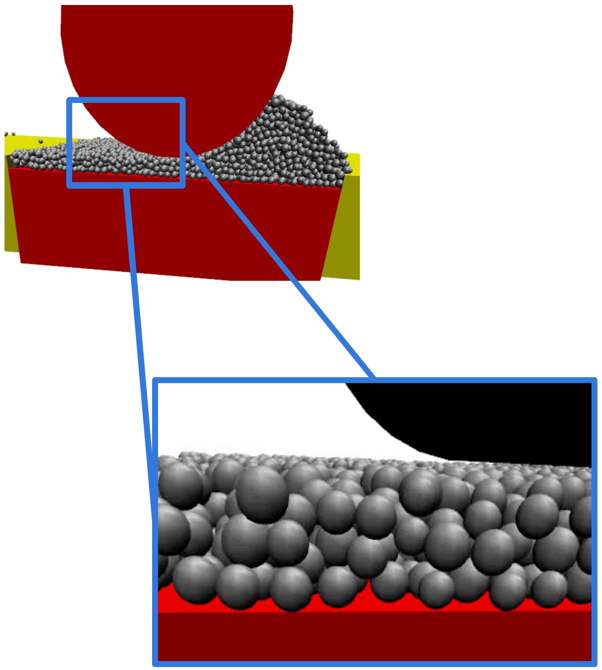
- Powder bed **surface** affects laser interaction
- Powder bed **bulk packing** affects void formation, surface finish
- **Variability in powder properties** due to e.g. vendor supply, powder recycling
- Some key length scales:
  - Layer thickness ~ 30-100 µm
  - Laser spot size ~100-200 µm
  - Particle diameter ~ 10-100 µm
  - Material defects ~ 100 µm

→ Understanding powder at scale of individual particles is important!

1. Strondl et al, *JoM* 2015.

Simulation method:
Discrete **E**lement **M**ethod (DEM)

Layer thickness ~ particle diameter
→ continuum models (e.g. μ(I) rheology) inherently unsuitable



Method of choice: DEM

Advantages:
- Captures individual particle dynamics
- Can handle polydispersity, shape variations, complex geometries
- Material properties captured by contact parameters

Disadvantages:
- Computationally expensive
- **Difficult to parametrize**

Simulation method:
Discrete **E**lement **M**ethod (DEM)

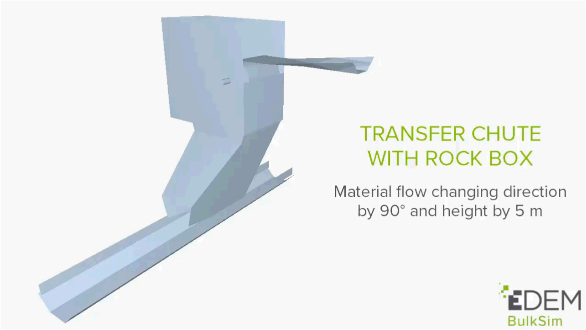
Molecular dynamics-like method:

- Particles modeled explicitly (position, velocity, angular velocity)
- Integrate collective dynamics:

$$\mathbf{F}_i = m_i \frac{d^2 \mathbf{r}_i}{dt} \qquad \tau_i = I_i \frac{d^2 \mathbf{w}_i}{dt} \qquad i = 1, ..., N \qquad N \approx 10^5 - 10^6$$

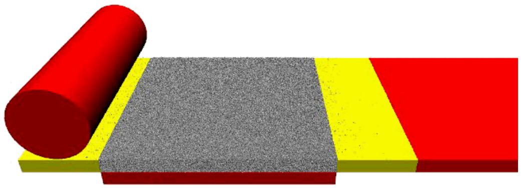
- Forces/torques computed at contact based on <u>reduced order models</u>

Well-established for 'large' particle applications (e.g. mining, pharmaceutical)



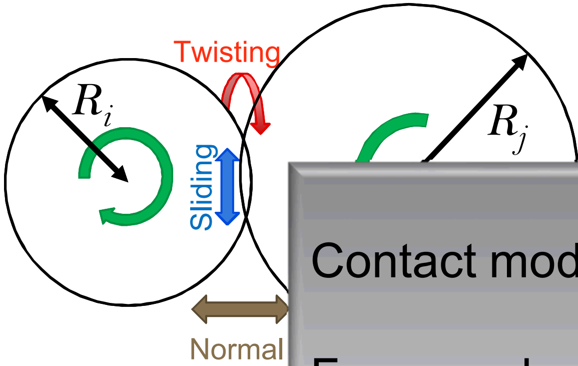
From EDEM youtube channel

Much more challenging for fine/cohesive powders!



http://lammps.sandia.gov

Granular contact models



Contact models are complicated!

Focus on key physics and associated parameters:

1. Cohesion → relates to surface chemistry, morphology
2. Friction → relates to surface morphology, micromechanics

Consider both particle/particle and particle/wall interactions

Geometry/kinematics

$\mathbf{r}_i, \mathbf{r}_j$: positions
$\mathbf{v}_i, \mathbf{v}_j$: translational velocities
$\mathbf{\Omega}_i, \mathbf{\Omega}_j$: 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!**

k_N, k_S, k_T, k_R: normal, sliding, twisting, rolling stiffness
$\eta_N, \eta_S, \eta_T, \eta_R$: normal, sliding, twisting, rolling dissipation
μ_S, μ_T, μ_R : sliding, twisting, rolling friction coefficients

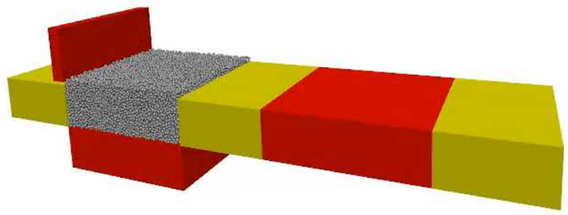
Hertz: $k_N = 4Ea/3$
Mindlin: $k_S = 8Ga$
Brilliantov: $\eta_N = \gamma_D m$, $\gamma_D = f(e)$
Tsuji: $\eta_N = f(e)(mk_N)^{1/2}$

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

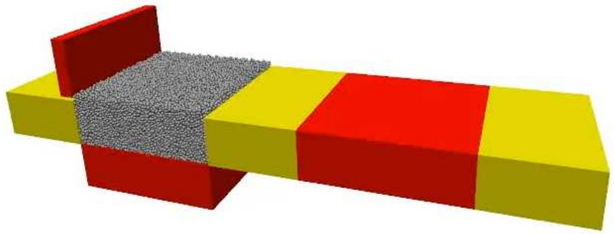
	gran/hertz	dmt/rolling	jkr/rolling
Normal elastic (spring)	$\boldsymbol{F}_n = k_n\sqrt{R}\delta^{3/2}\boldsymbol{n}$	$\boldsymbol{F}_n = \left(\frac{4Ea^3}{3R} - 4\pi\gamma R\right)\boldsymbol{n}$ $\delta_N = a^2/R$ $F_{\text{pulloff}} = -4\pi\gamma R$	$\boldsymbol{F}_n = \left(\frac{4Ea^3}{3R} - 2\pi a^2\sqrt{\frac{4\gamma E}{\pi a}}\right)\boldsymbol{n}$ $\delta_N = a^2/R - 2\sqrt{\pi\gamma a/E}$ $F_{\text{pulloff}} = -3\pi\gamma R$
Normal dissipative			$\boldsymbol{v}_R \cdot \boldsymbol{n}$ …or η_N based on Tsuji or …v
			$-k_S\int_{t0}^{t}\boldsymbol{v}_{tR}(\tau)\mathrm{d}\tau$
			$\eta_T\boldsymbol{v}_{tR}$
			$\| \leq F_{\text{S,crit}}$ $= \mu_S(\|\boldsymbol{F}_n\| + F_{\text{pulloff}})$
			$-k_R\int_{t_0}^{t}\boldsymbol{v}_L(\tau)\mathrm{d}\tau$
			$\boldsymbol{v}_L$
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 $R\mathbf{n} \times \mathbf{F}_R$

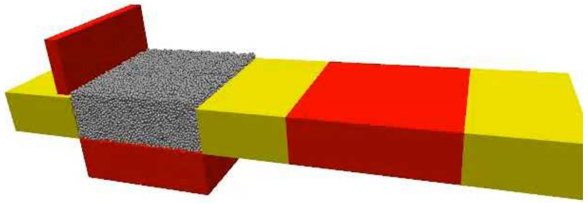
Granular contact models



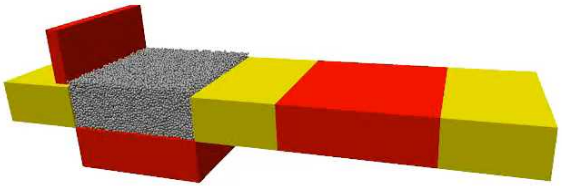
No rolling friction



No sliding friction

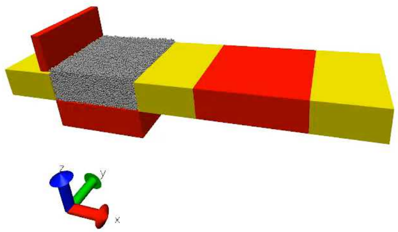


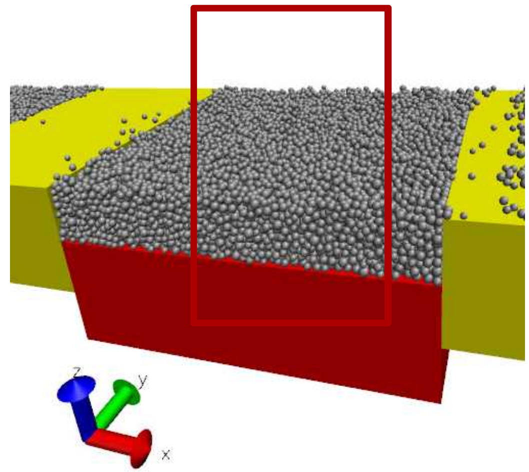
No particle-particle cohesion

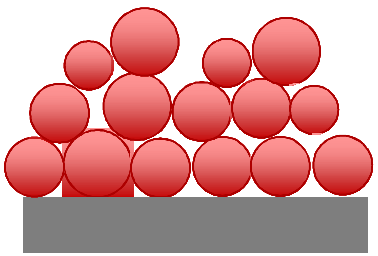


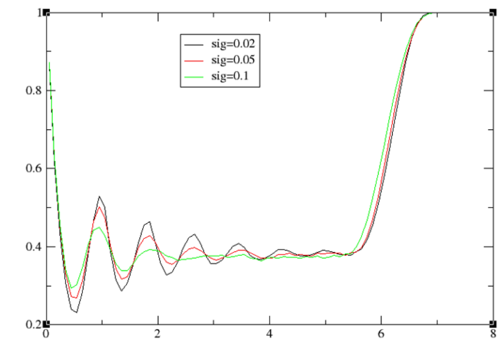
Very high particle-particle cohesion

Analysis of packed beds

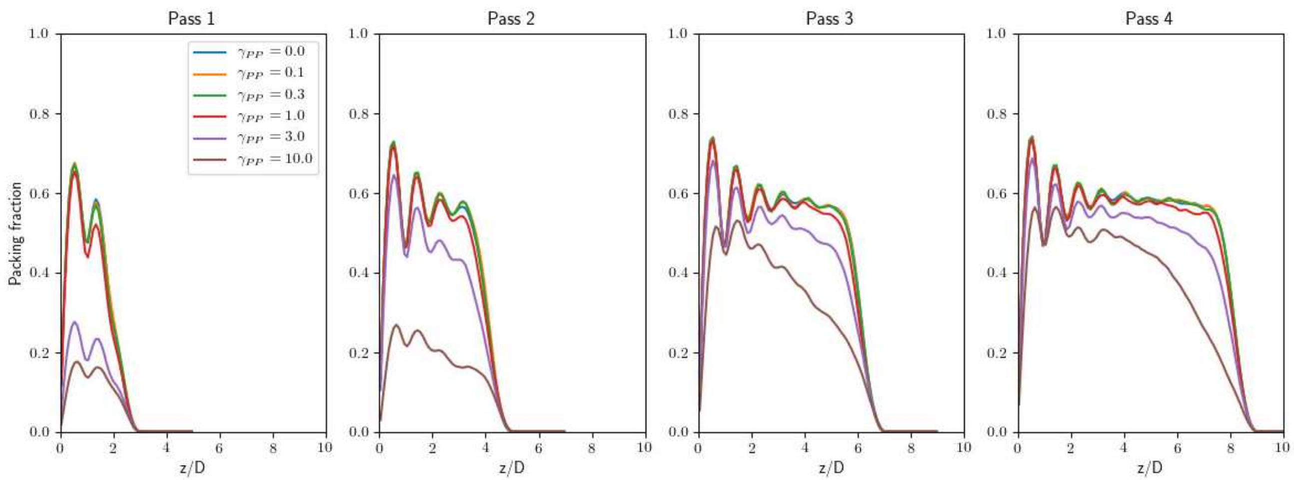






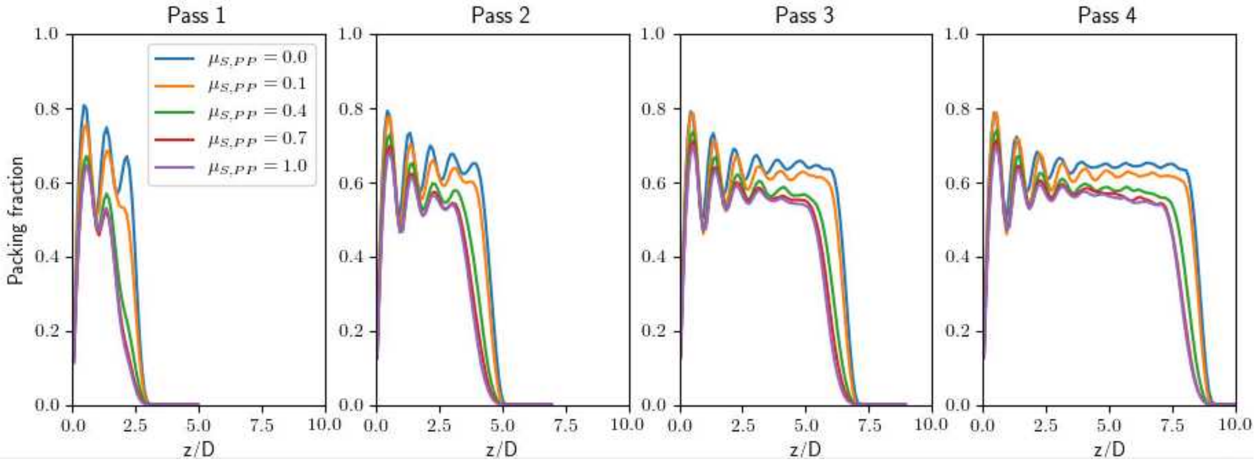


Effect of particle-particle cohesion γ_{PP}:

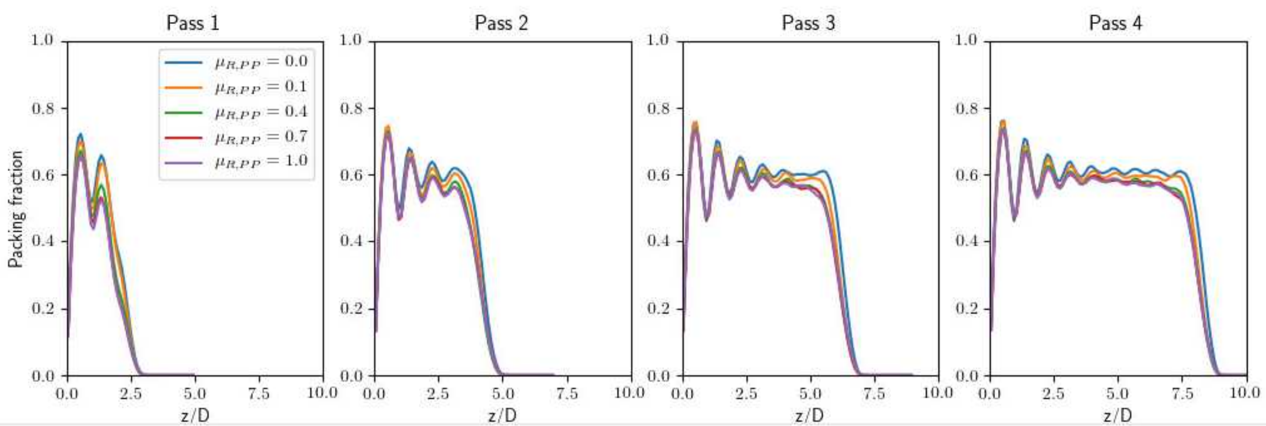


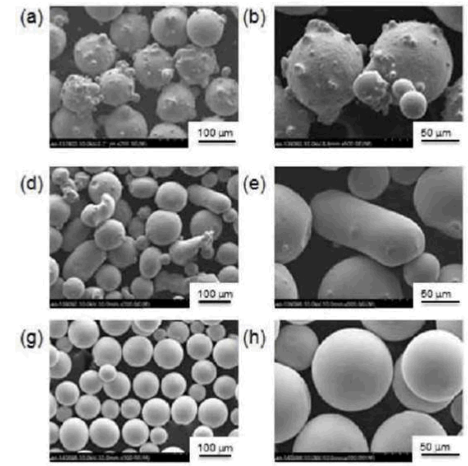
Analysis of packed beds

Effect of sliding friction coefficient $\mu_{S,PP}$



Effect of rolling friction coefficient $\mu_{R,PP}$

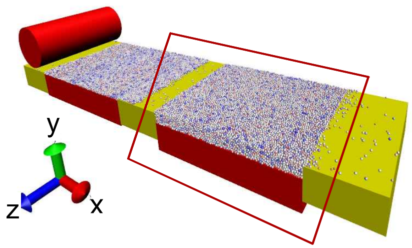




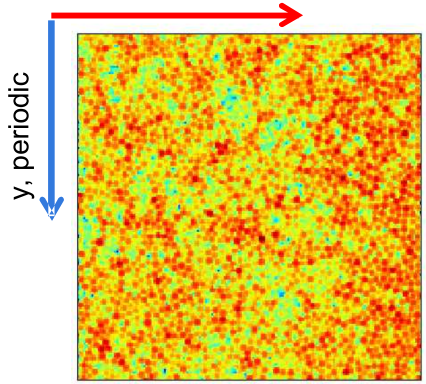
a/b: gas atomisation - d/e: rotary atomisation - g/h: Plasma rotating electrode process [1]

Strondl et al, *JoM* 2015.

Analysis of powder bed surface

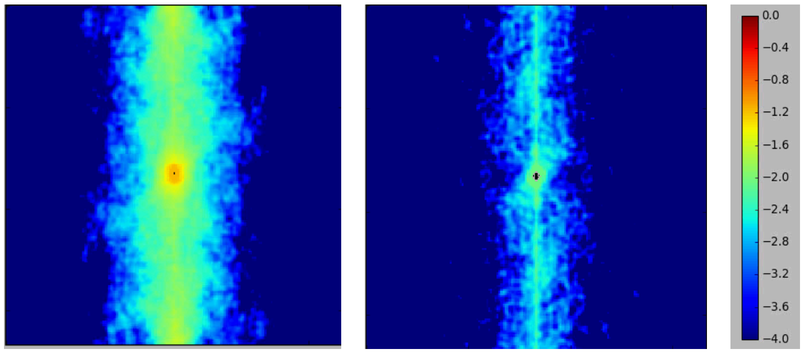


$$H(\boldsymbol{x})$$



$$ACF\big(h(\boldsymbol{x})\big) = \langle h(\boldsymbol{x}' + \boldsymbol{x})(h(\boldsymbol{x}')\rangle$$

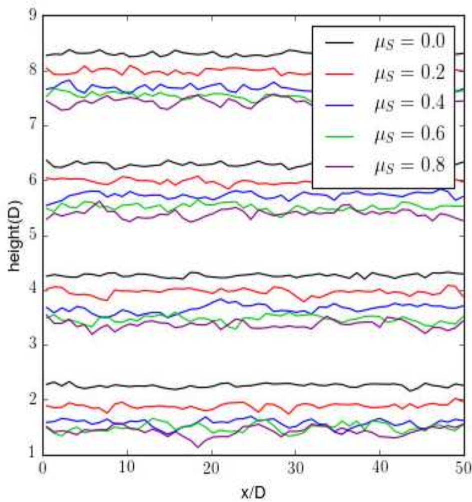
$$h(\boldsymbol{x}) = (H(\boldsymbol{x}) - \langle H(\boldsymbol{x})\rangle)/\sigma_{H(x)}$$

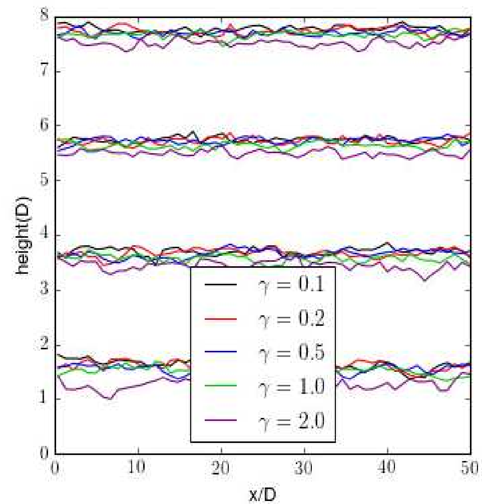


Slider, 4 passes

Roller, 4 passes

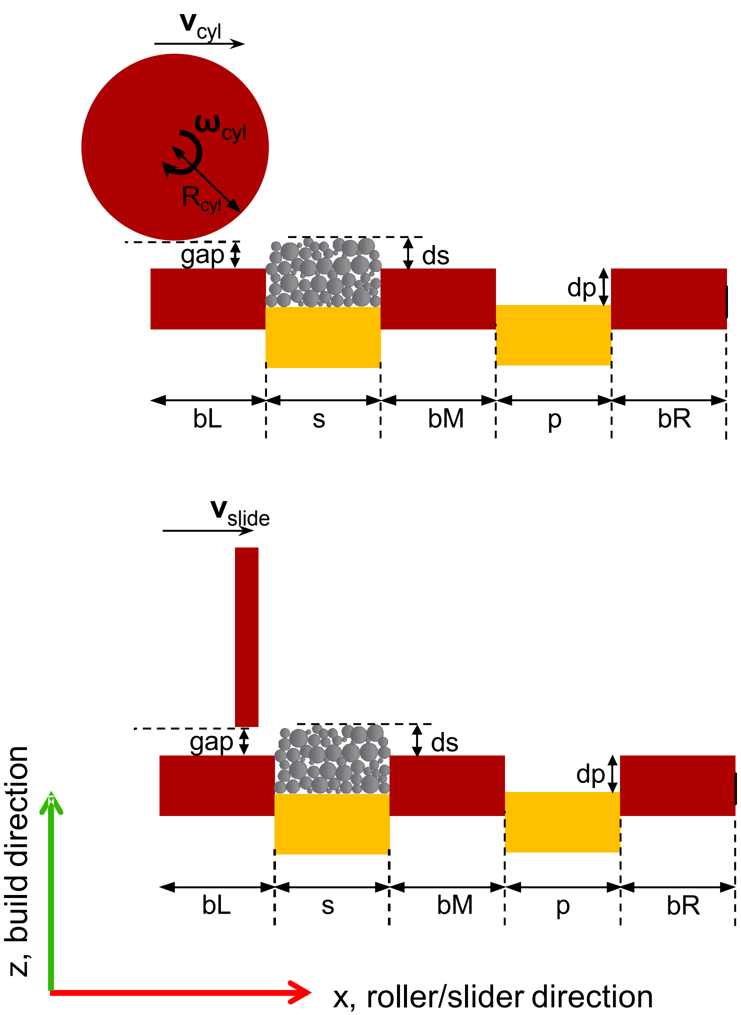
Height as a function of x:



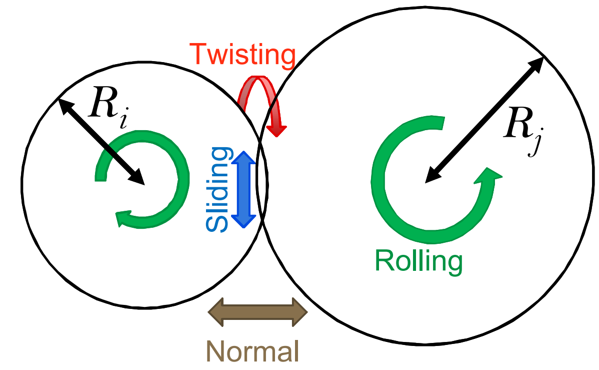


Large parameter space!

Process-related



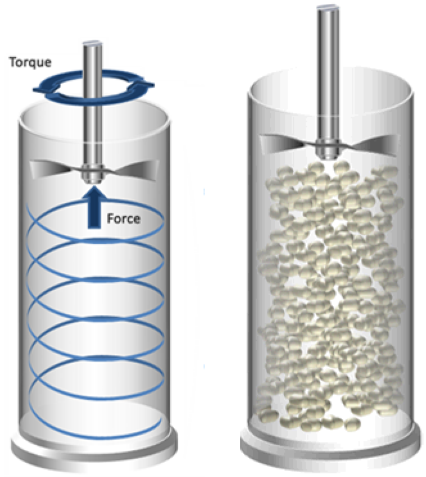
Particle-related

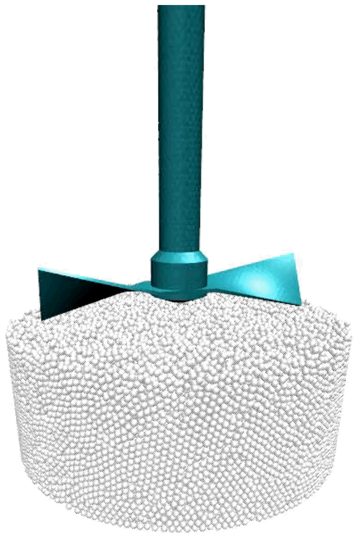


- **Particle size /shape distribution**
- Contact parameters
  - **Contact model form**
  - Stiffness, damping → actual values (e.g. E_Y=200 GPa for steel) lead to prohibitively small time stepping, only need to be sufficiently high so that $\delta << R$
  - **Friction** (sliding, rolling, twisting) → relates to particle surface morphology
  - **Cohesion** → particle surface morphology, chemistry
  - Different for particle/particle, particle/wall contact

Toward model calibration

- Direct measurement of particle-scale parameters extremely difficult
- Goal: calibrate DEM parameters based on powder dynamics experiments
- One option: Freeman Technology FT4 rheometer: measure force/torque for various impeller motions





QUESTIONS?