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Flowability, Spreadability, and Segregation

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AM Powder Flow Modeling Workshop

Austin, TX

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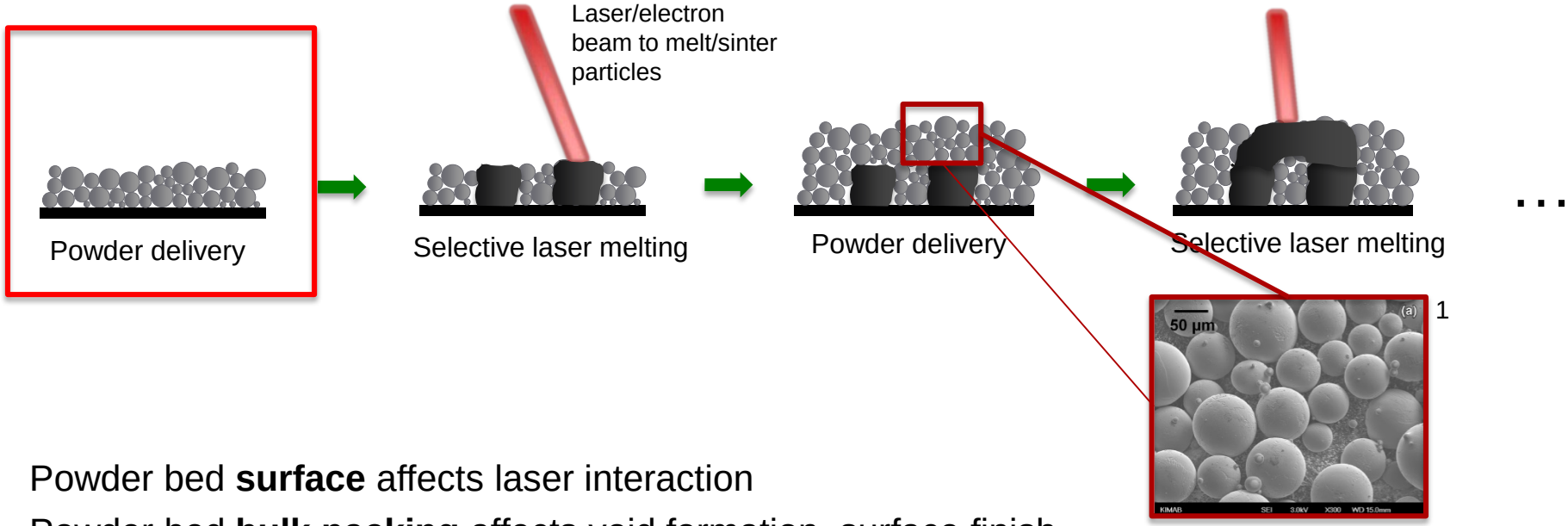
Background and Motivation

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 process length scales:
  - Layer thickness ~ 30-100 µm
  - Laser spot size ~100-200 µm
  - Particle diameter ~ 10-100 µm

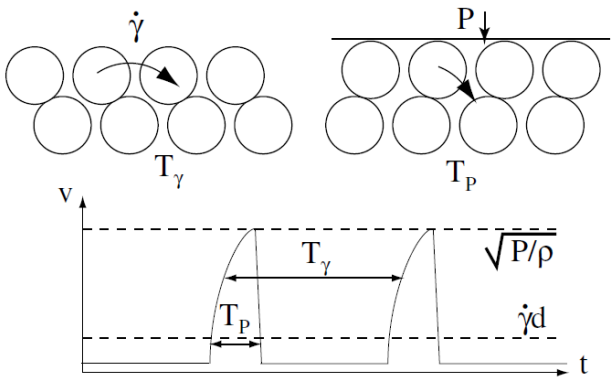
Understanding powder at scale of individual particles is important!

DEM

1. Strondl et al, *JoM* 2015.

Flowability

- Ease of flow? An index measure, or a material property?
- Dry, dense granular (cohesionless) flow
  - Hopper Flow (Beverloo), rotating drum, inclined plane (Bagnold, Savage), Couette
  - GDR MiDi (*Eur. Phys. J. E* 14, 341-365 (2004))
    - $\mu(I)$ theory linking quasistatic and inertial regimes
    - Bulk flow. h >> d



$$\mu_{\text{eff}} = \frac{\tau}{P}$$

$$I = \frac{\dot{\gamma} d}{\sqrt{P/\rho}}$$

Fig. 7. Schematic showing the physical meaning of the typical time of deformation T_γ and the confinement timescale T_P.

- Other transport mechanisms
  - Pneumatic, Vibration

Bulk Flow Current State of the Art

- mu(I) theory linking quasistatic and inertial regimes
  - Bulk flow, h >> d
    - Can relate internal structure to bulk (Asema and Radjai *PRL*,)
    - Can use in continuum models (e.g., Ionescu et al. *J. of Non-Newt. Fluid Mech.* 219 (2015) 1–18)
    - Can use derive a thin film limit (more later)

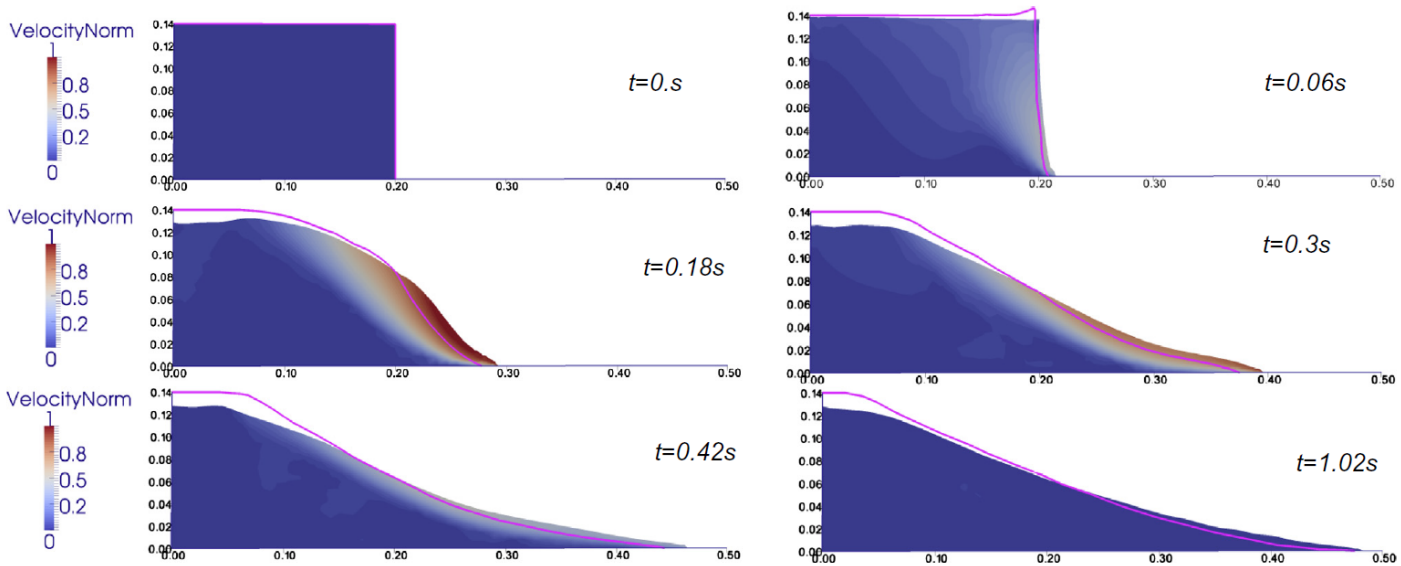


Fig. 2. Simulation using variable viscosity $\eta(\|\boldsymbol{D}\|, p)$ (i.e. $\mu(I)$): Comparison of the simulated granular mass and the experimental results (pink line) at different times for granular collapse over a horizontal plane ($\theta = 0°$). The colors represent the distribution of the norm of the computed velocity field $|\boldsymbol{u}|$ (in m/s). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Emerging Trends

- Current issues being worked out
  - "nonlocal"/cooperative effects, fluctuations and correlations
  - Boundary conditions
  - Particle size/shape distributions
  - Cohesion, e.g., Berger et al. *EPL*, **112** (2015) 64004
    - "simple" models – central forces
    - role of long range attraction – Parteli et al. *Sci. Rep.*, 4 (2014), 6227

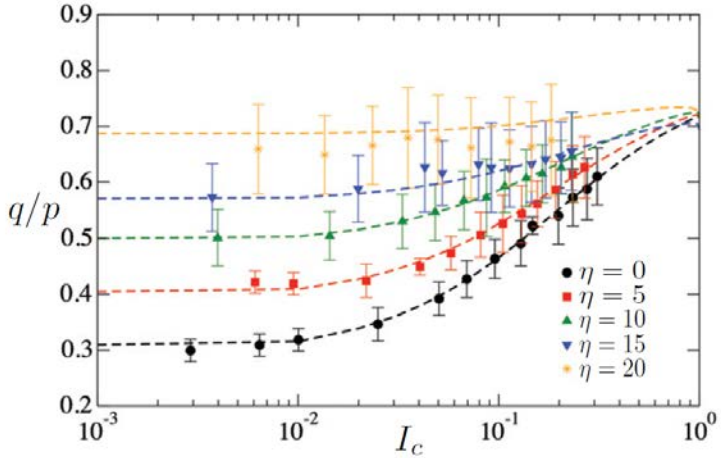


Fig. 7: (Color online) Normalized shear stress as a function of the cohesive inertial number. The lines represent analytical estimates for each value of the adhesion index; see text.

$$\eta = \frac{f_c}{\sigma_n \langle d \rangle}$$

$$I_c = \dot{\gamma}\langle d \rangle \left(\frac{\rho}{\sigma_n + \alpha f_c / \langle d \rangle} \right)^{1/2} = \frac{I}{(1+\alpha\eta)^{1/2}}$$

Research Needs

- Material characterization for flow modeling
  - Particle description
    - Shape
    - Composition
      - Changes, e.g., oxidation kinetics
    - Surfaces – structure, composition
  - Particle-particle interactions
    - Long-range van der Waals, tribology of contacts
  - Index tests
    - Relevance to varying conditions, types of flow – very thin flow
    - Hall Flow, flowdex, rotating drum, rheometers, …
      - Model selection, parameter estimation, and calibration
      - Model validation and uncertainty quantification
  - Measure "mu" and "c" in limit of no confining stress
    - Van der Waals attraction/adhesion, humidity, electrostatics, …
  - Role of air, etc.

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

Spreadability Background

- For “thin flows” shallow flow equations have been developed
  - Depth-integrated mass and momentum balance
    - Assume mu(I) rheology
    - Erodable bed needs closure model
  - Use shallow flow approximation: h/R << 1
  - But for continuum, i.e. PDE, description of balance laws to hold
    - d/h << 1
- What about if h = d, or h = <d>?
  - Metered by narrow gap and moving boundary
  - Flow/deposition over, around complex shapes
  - Limited to no work?
  - DEM models ideal

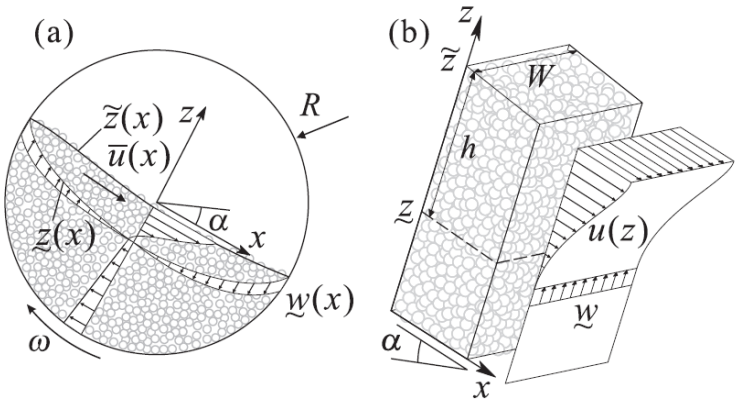
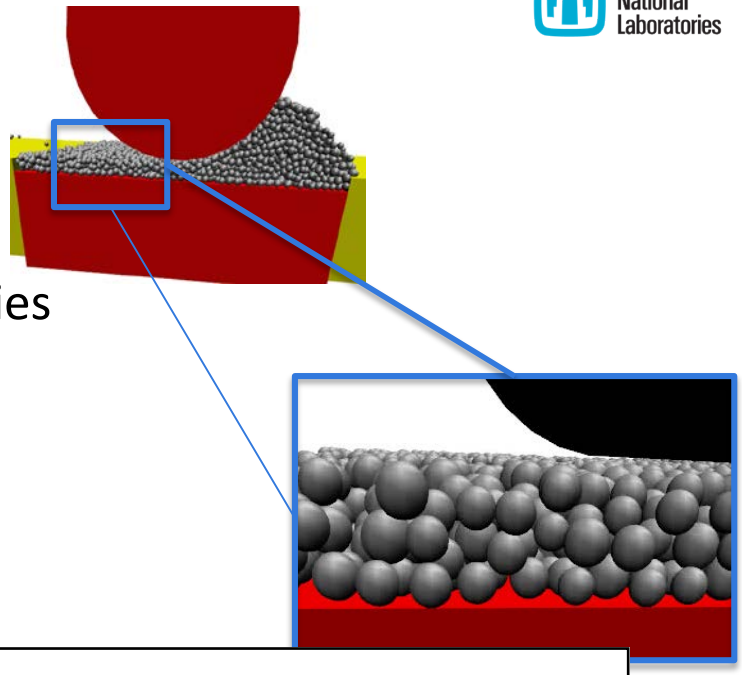


FIG. 1. Definition sketch: (a) Overview; (b) local cutaway.

Hung, et al. *Physical Review E* **93**, 030902(R) (2016)

Spreadability

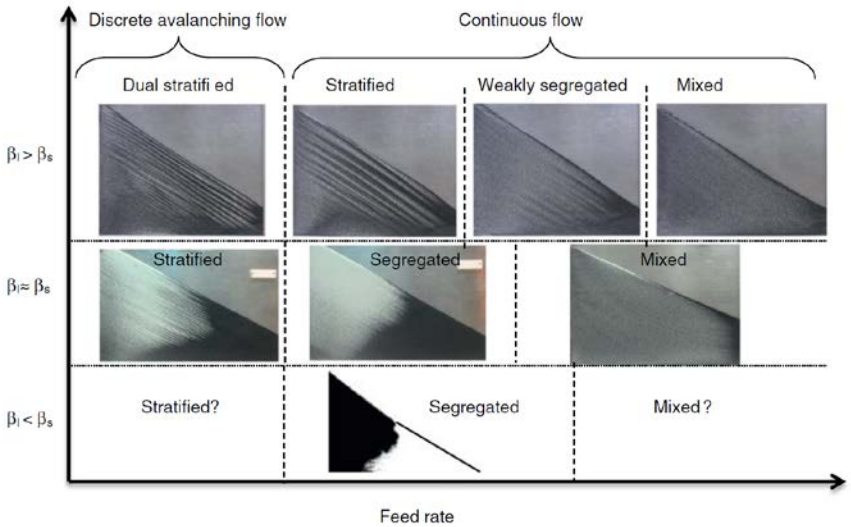
- Application of DEM to AM
  - Free surface, erodible bed
  - B.C.'s for packing in complicated geometries
  - Cohesion: $\frac{\rho g d^2}{\pi \gamma}$~ O[10^-4]
    - Cooperativity due to cohesion
- Compositional changes in powder
  - Contamination
- What is a good spread?
  - No "dewetting"
  - Surface roughness
  - Packing (in/around build, subsurface)
  - Powder mixedness
- What powder characteristics determine a good, reliable spread?

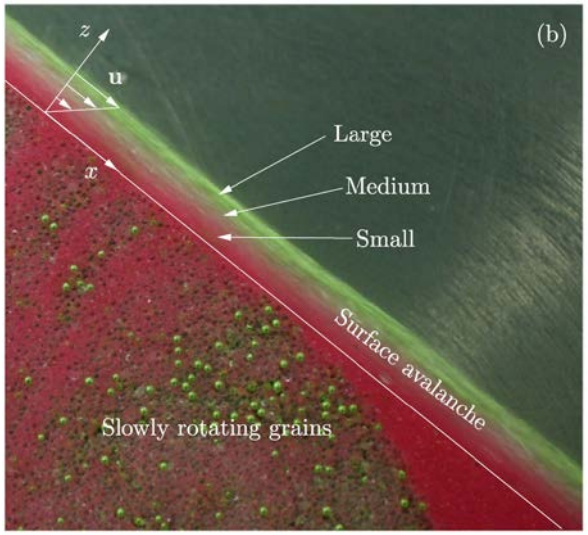


Stratification

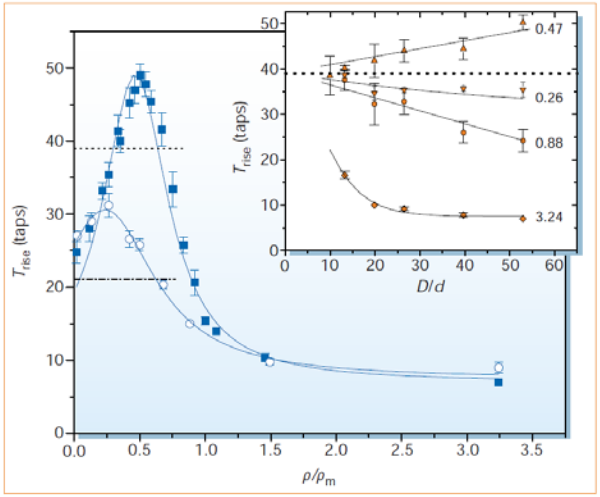
- Size, shape, density segregation
  - Shallow flows – heaps, silos, rotating drums
    - Gravity driven: kinetic sieving
      - Mixture theory (mostly binary, high concentration)
      - Depth averaged equations have been formulated

Fan et al. *Powder Tech.* 312 (2017)





Gray et al. *C. R. Physique* 16 (2015)

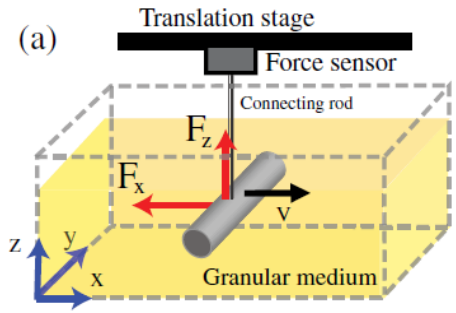


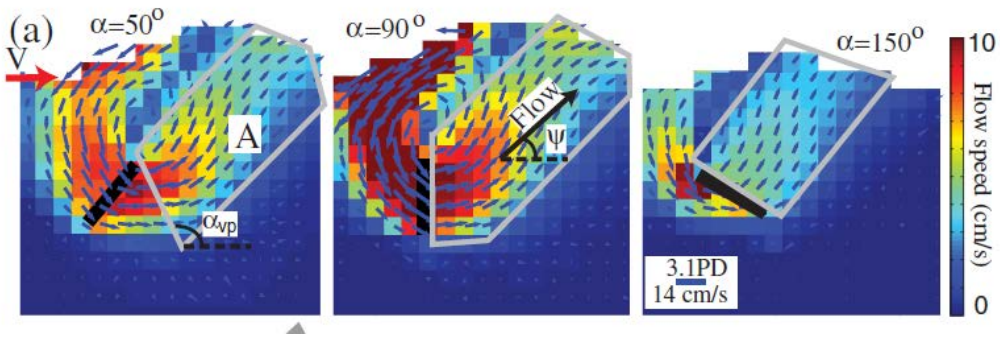
  - Shear induced
  - Other mechanisms -- Role of air
- Brazil Nut effect – role of air?

  Mobius *et al. Nature* **414**, 270 (2001)

Emerging trends

- Connections to fluids and suspensions
  - Drag induced lift (Ding et al. *PRL* 106, 028001 (2011))





  - Safman Lift in flowing grains (van der Vaart et al. cond-mat.soft https://arxiv.org/pdf/1705.06803.pdf)
    - Dilute concentration of large particles

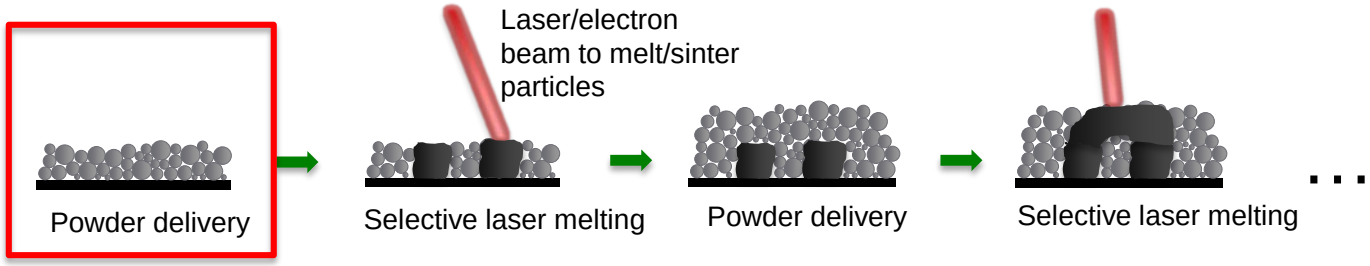
Research Needs

- Flow on/into/around complex, confined domains
  - Effects on feature fineness, surface roughness
- Reuse/recycle
  - Old + new powder mixing/blending – handling, storage, transport
  - Compositional variability
    - Size/shape, cohesion – segregation
- Multimaterial
  - Characterization of particle interactions and dynamics
  - Characterization of segregation/stratification for relevant materials
  - B.Y.O.P?
- Particles sticking on surface
  - Internal works – powder charging, dispensing, deposition, re-use
  - Cleaning/Contamination
- Gas pressure/flow, vibration…

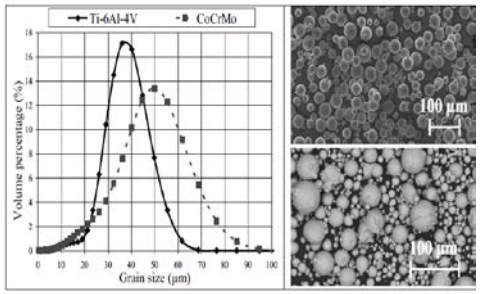
EXTRA SLIDES

Background and Motivation

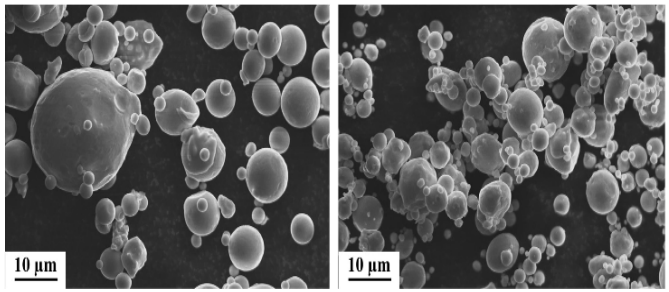
Layer-by-layer powder bed fusion processes (e.g. SLM/SLS):



- 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

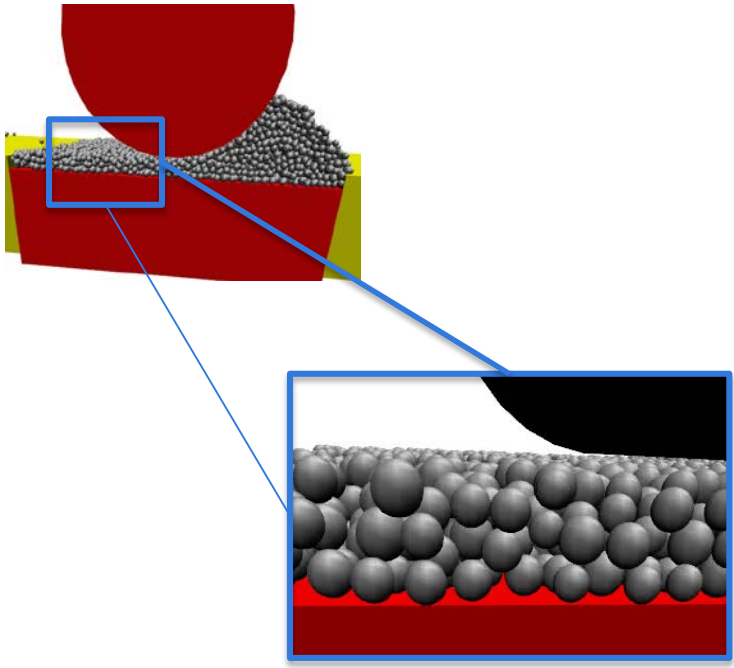
Powder layer thickness 30-150 μm
Laser beam spot size 70-200 μm (ref. 1)

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

Discrete Element Method (DEM)

Layer thickness ~ particle diameter

Method of choice: DEM
→Explicitly solve collective dynamics of large number of particles
→ Collisions treated using reduced order contact models

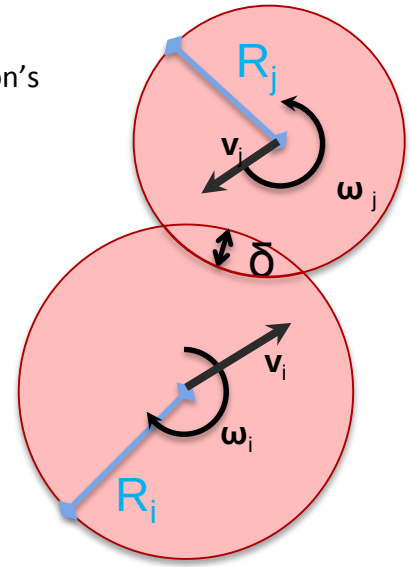


Advantages:
- Captures individual particle dynamics
- Can handle polydispersity, shape variations, complex geometries
- Material properties captured by contact parameters

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

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:

$$\mathbf{F}_n = \sqrt{R_e \delta}(\underbrace{k_n \delta \mathbf{n}_{ij}}_{} - \underbrace{m_e \gamma_n \mathbf{v}_n}_{})$$

Elastic force due to deformation (Hertzian case here)

Dissipative force (associated with coefficient of restitution < 1)

k_n, γ_n Constants related to material properties

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

- 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: $\frac{d\mathbf{u}_t}{dt} = \mathbf{v}_t - \frac{\mathbf{u}_t \cdot \mathbf{r}_{ij}}{r_{ij}^2}$

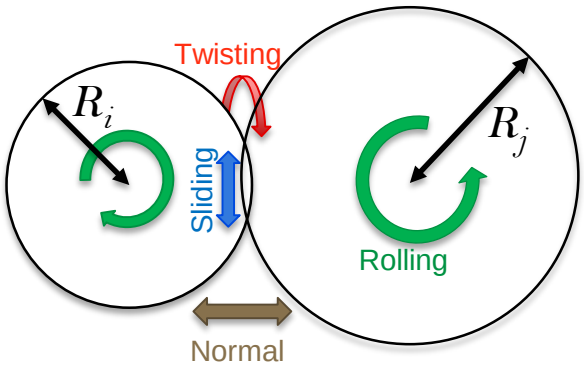
μ Coefficient of friction

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.

Granular contact models



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!**

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	$\|\boldsymbol{F}_S\| \le F_{\text{S,crit}}$ $F_{\text{s,crit}} = \mu_S \|\boldsymbol{F}_n\|$	$\|\boldsymbol{F}_S\| \le F_{\text{S,crit}}$ $F_{\text{s,crit}} = \mu_S \|\boldsymbol{F}_n\|$	$\|\boldsymbol{F}_S\| \le F_{\text{S,crit}}$ $F_{\text{s,crit}} = \mu_S(\|\boldsymbol{F}_n\| + F_{\text{pulloff}})$
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		$\|\boldsymbol{F}_R\| \le F_{\text{R,crit}}$ $F_{\text{R,crit}} = \mu_R \|\boldsymbol{F}_n\|$	$\|\boldsymbol{F}_R\| \le F_{\text{R,crit}}$
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		$M_t \le -M_{t.\text{crit}}\Omega_T/\|\Omega_T\|$ $M_{\text{t,crit}} = \frac{2}{3}aF_{\text{s,crit}}$	$M_t \le -M_{t,\text{crit}}\Omega_T/\|\Omega_T\|$ $M_{\text{t,crit}} = \frac{2}{3}aF_{\text{s,crit}}$

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**n** X $\mathbf{F}_R$