Powder spreading simulations and powder bed characterization for metal additive manufacturing

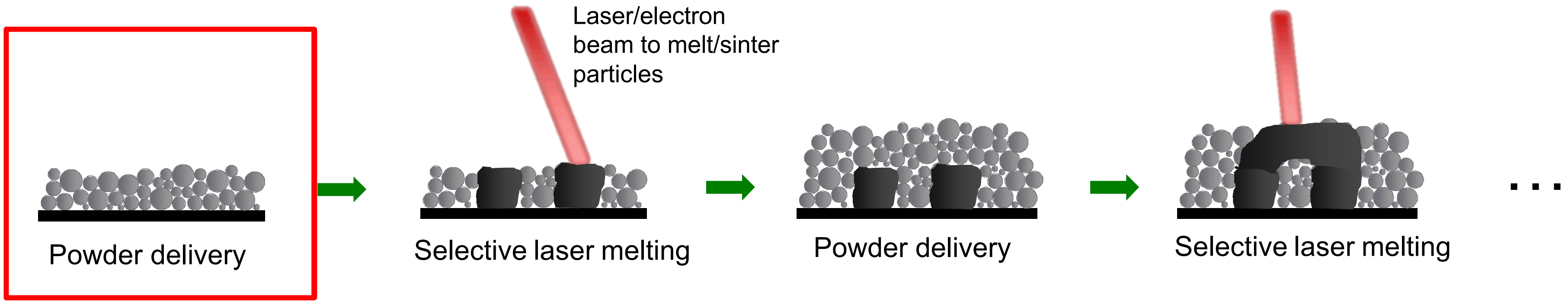
Dan S. Bolintineanu, Jeremy B. Lechman, Quintina Frink
Sandia National Laboratories
Albuquerque, NM

2016 Solid Freeform Fabrication Symposium

Aug 9, 2016

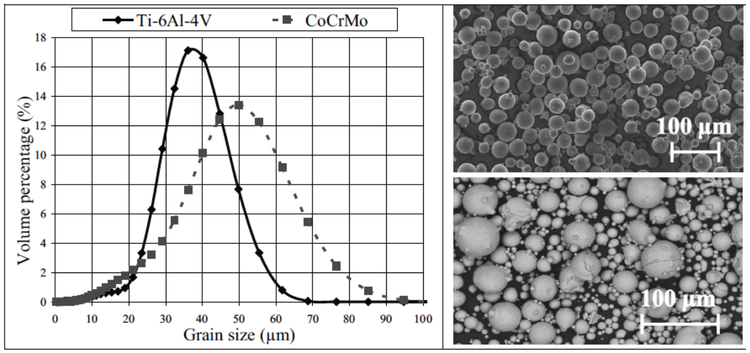
Background and Motivation

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

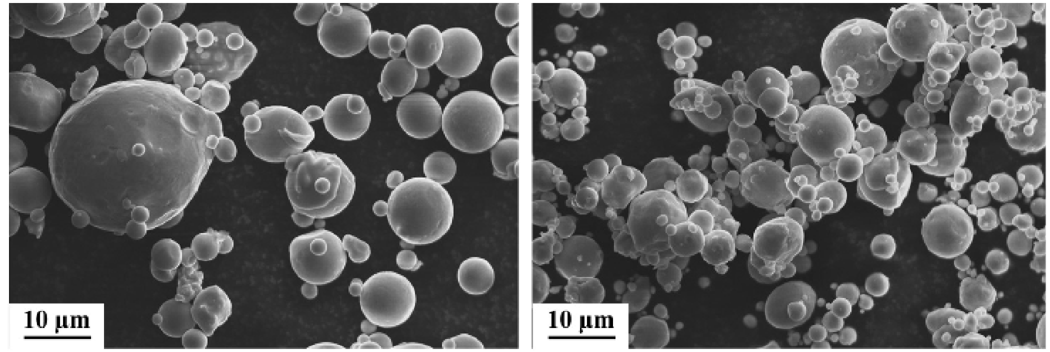


- Why study AM powder processing?
  - First step in AM powder bed process
    - Powder bed surface → laser interaction
    - Powder bed bulk packing →void formation, surface finish
  - Variability in powder properties due to vendor supply, powder recycling
    - Powder flow properties affect spreading quality, packing
  - Several key process length scales are comparable to individual particles

Typical powder characteristics



From Ref. 1



From Ref. 2

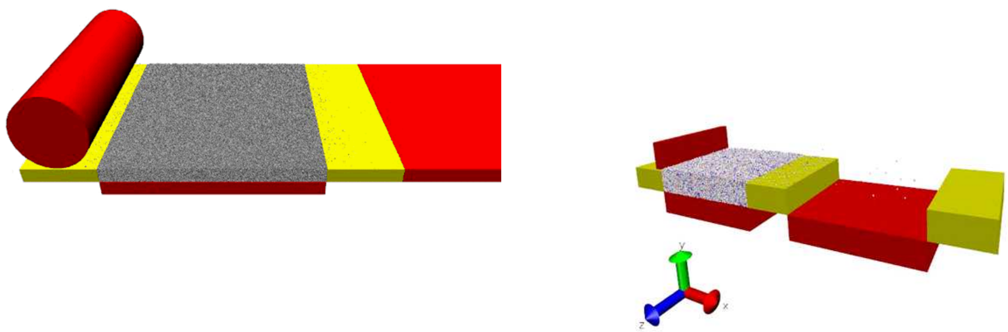
- Particle shape generally spherical, but aggregates are likely
- Typical particle diameter: 10-100 µm; polydispersity factor 4-5
- Powder layer thickness 30-150 µm, laser beam spot size 70-200 µm (ref. 1)

➡ Understanding powder bed structure at the scale of individual particles is important

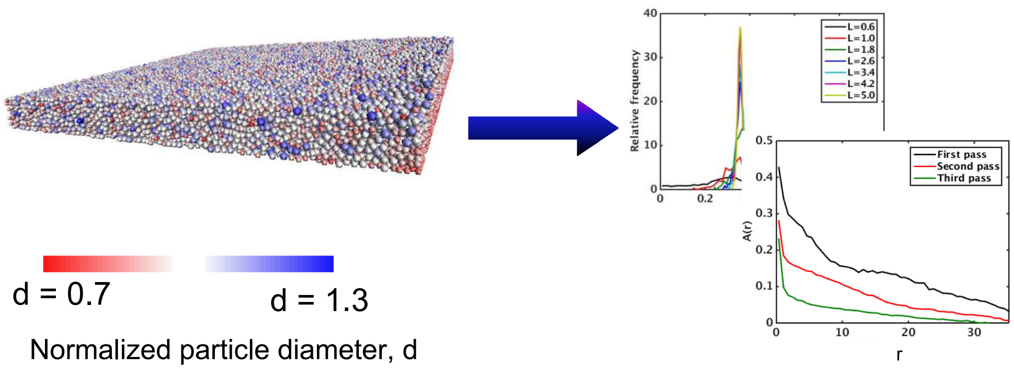
1. Vandenbroucke, B. and Kruth, J.P. *Rapid Prototyping Journal* 13 (2007): 196
2. Yadroitsev, I., et al. *Journal of Laser Applications* 25 (2013): 052003

Overview

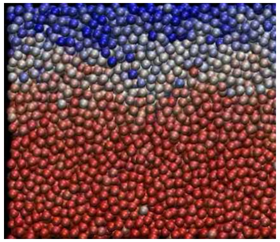
Powder spreading simulations (DEM)



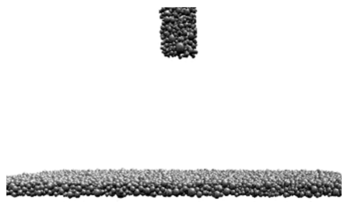
Statistical characterization of simulated powder beds



Powder flow characterization: combined simulations & experiments

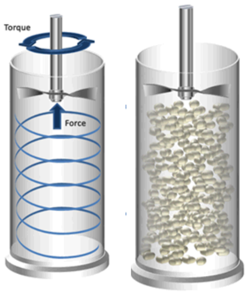


Simple shear



Angle of repose

Hall flow meter



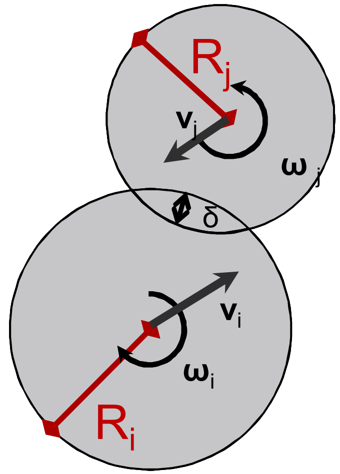
Powder rheology

Simulation methods: DEM

- **D**iscrete **E**lement **M**ethod (DEM): molecular-dynamics-like simulation of Newton's laws of motion for a collection of particles
- Forces/torques on particles computed from reduced-order contact mechanics models[1]:
  - Simple Hertzian normal force:

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

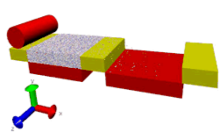
  - Tangential force: history dependent friction, damping
- LAMMPS simulation code[2]
  - Highly parallel via MPI
  - Recently added/in-progress features:



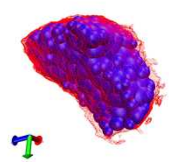
Collision:

$$\delta = R_i + R_j - \|\mathbf{r}_i - \mathbf{r}_j\| > 0$$

Triangulated walls



Geometric primitives for walls



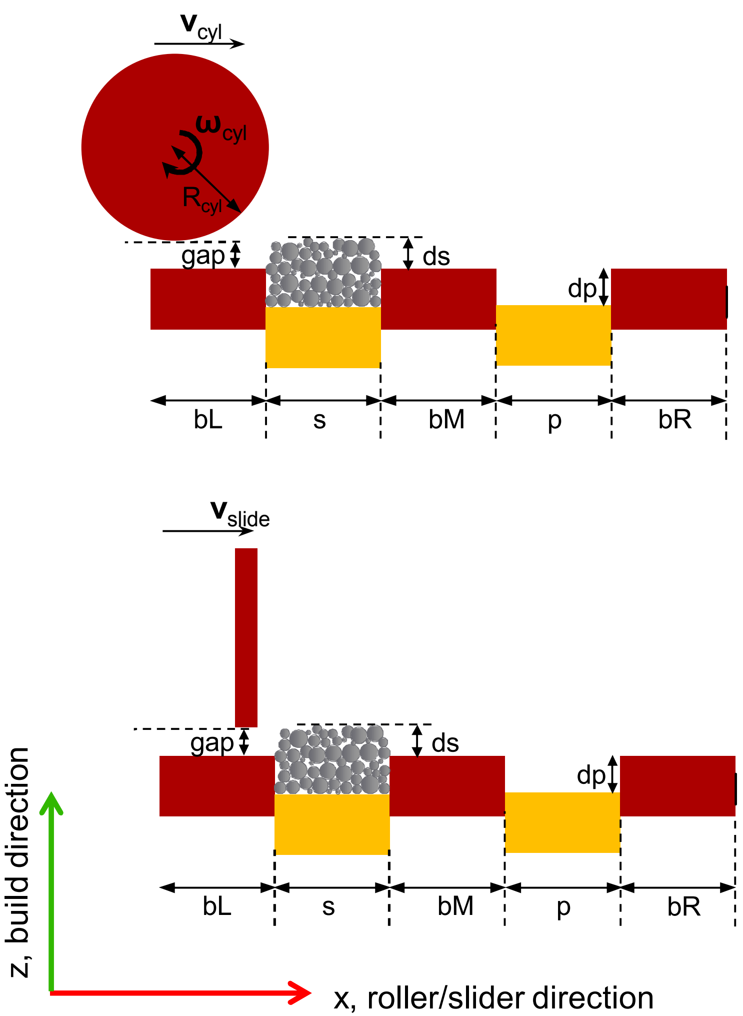
Non-spherical particles

Contact models for cohesion and rolling friction

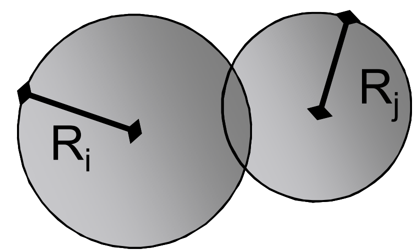
1. Cundall, PA and Strack, ODL. *Geotechnique* 29.1 (1979): 47-65.
2. Plimpton, S. J. *J Comput Phys* 117.1 (1995): 1-19. http://lammps.sandia.gov

Large parameter space!

Process-related



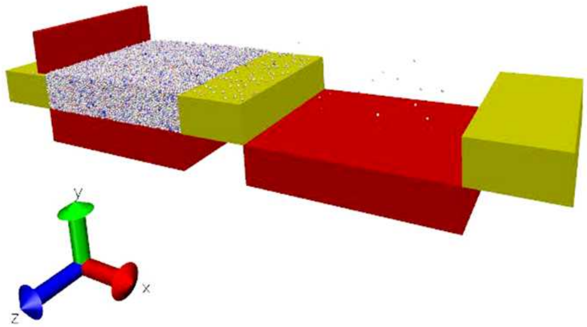
Particle-related

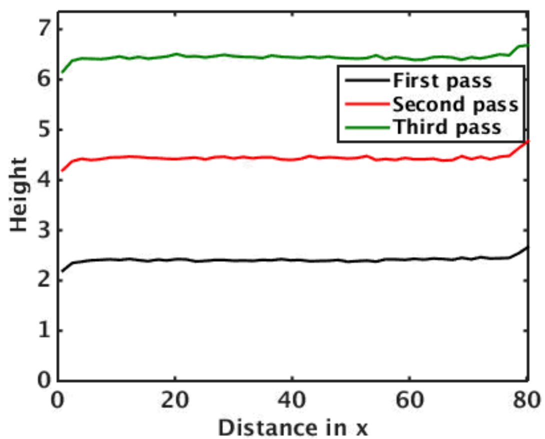


- Particle size/shape distribution
  - Type of distribution
  - Moments: mean, spread, skewness,etc.
  - Shape: asphericity, distribution, etc.
  - …
- Contact parameters
  - Stiffness, damping → relates to Young's modulus, contact models
  - Friction (sliding & rolling) → relates to particle surface characteristics, asphericity
  - Cohesion → particle surface energy
  - Different particle/particle, particle/wall parameters
  - …

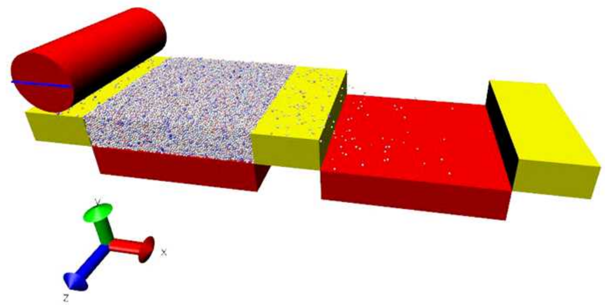
Effects of spreader type

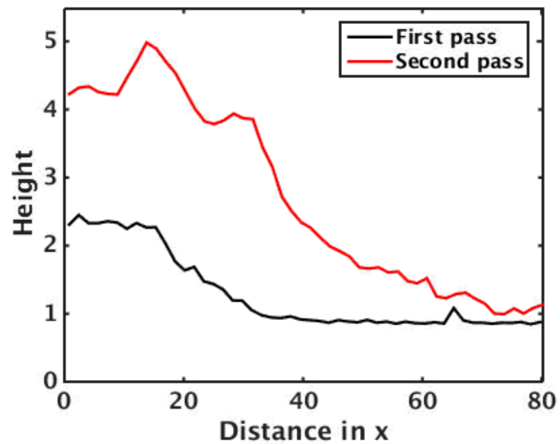
Slider



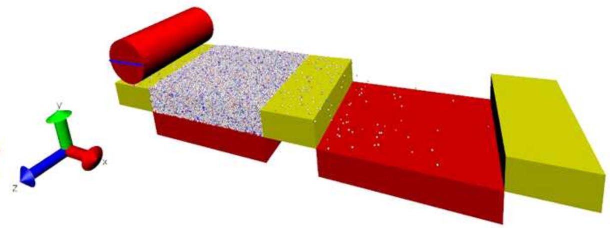


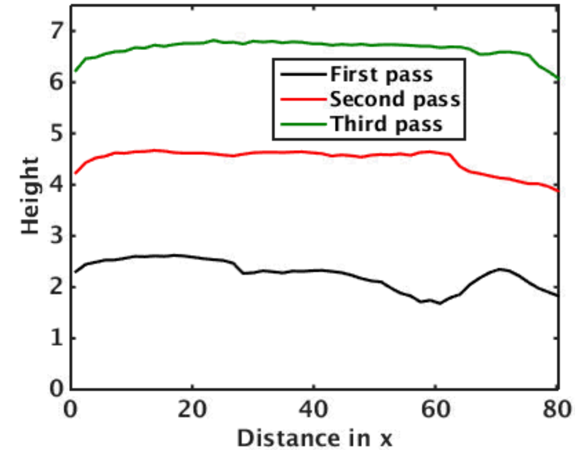
Roller, rotation in direction of translation (forward)





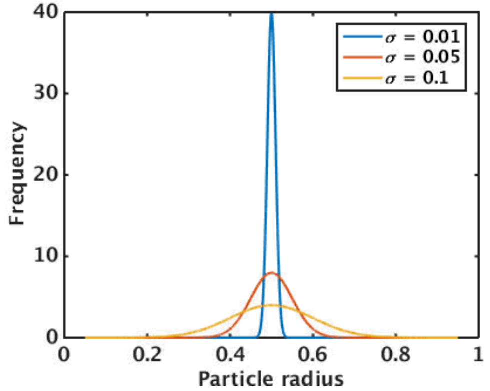
Roller, rotation against direction of translation (reverse)

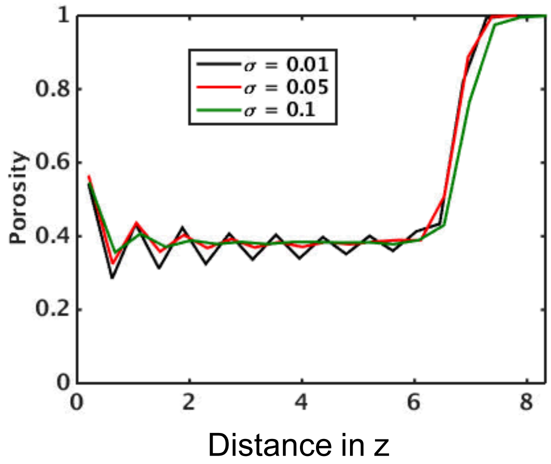




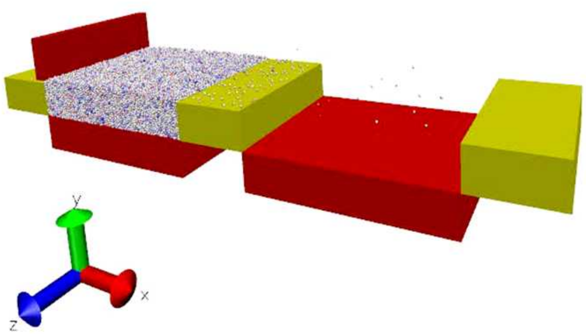
Effects of particle properties: size distribution

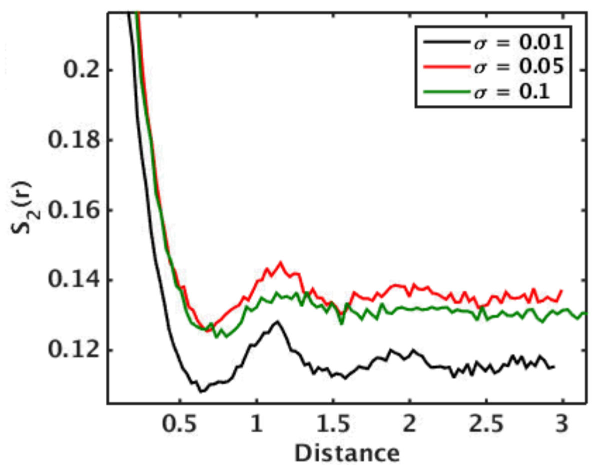
- Gaussian distributions, mean radius 0.5, vary σ
- Data shown for slider only





Layering order decreases with larger polydispersity. Small differences in mean porosity.

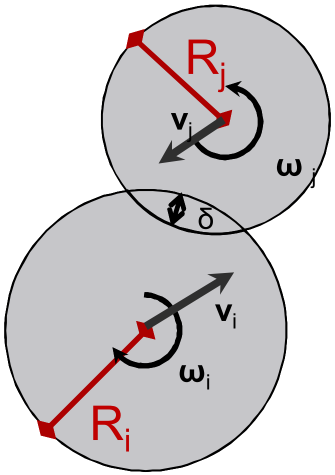




Less local structuring with larger polydispersity

Particle friction coefficient

Sandia National Laboratories



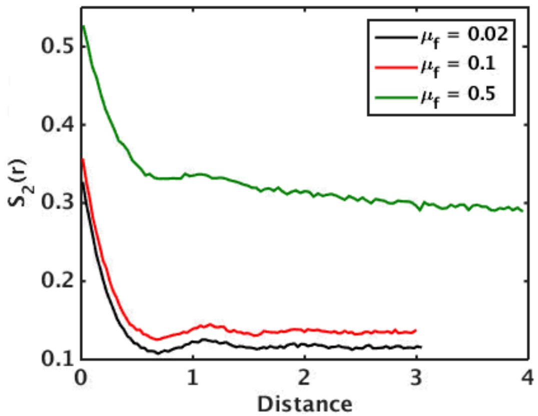
$$\mathbf{F}_t = \sqrt{R_e \delta}(-k_t \mathbf{u}_t - m_e \gamma_t \mathbf{v}_t)$$

$\mathbf{u}_t$ Total relative displacement during contact

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

Powder bed surface properties also affected, but notable differences in bulk packing structure:

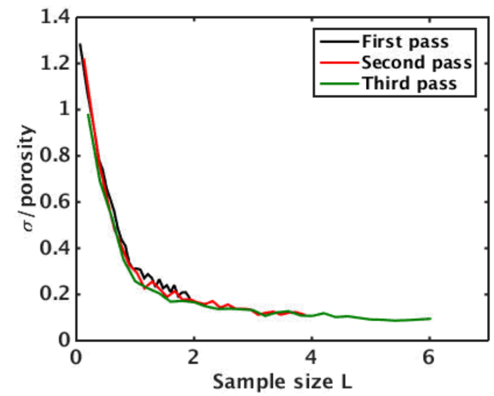
Two-point correlation function



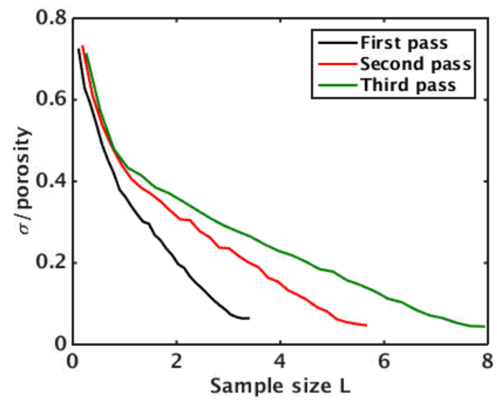
- General trends hold regardless of other process parameters

Coarseness

Low friction μ_f=0.1

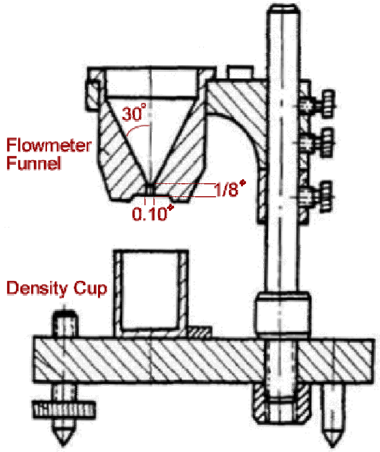


High friction μ_f=0.5



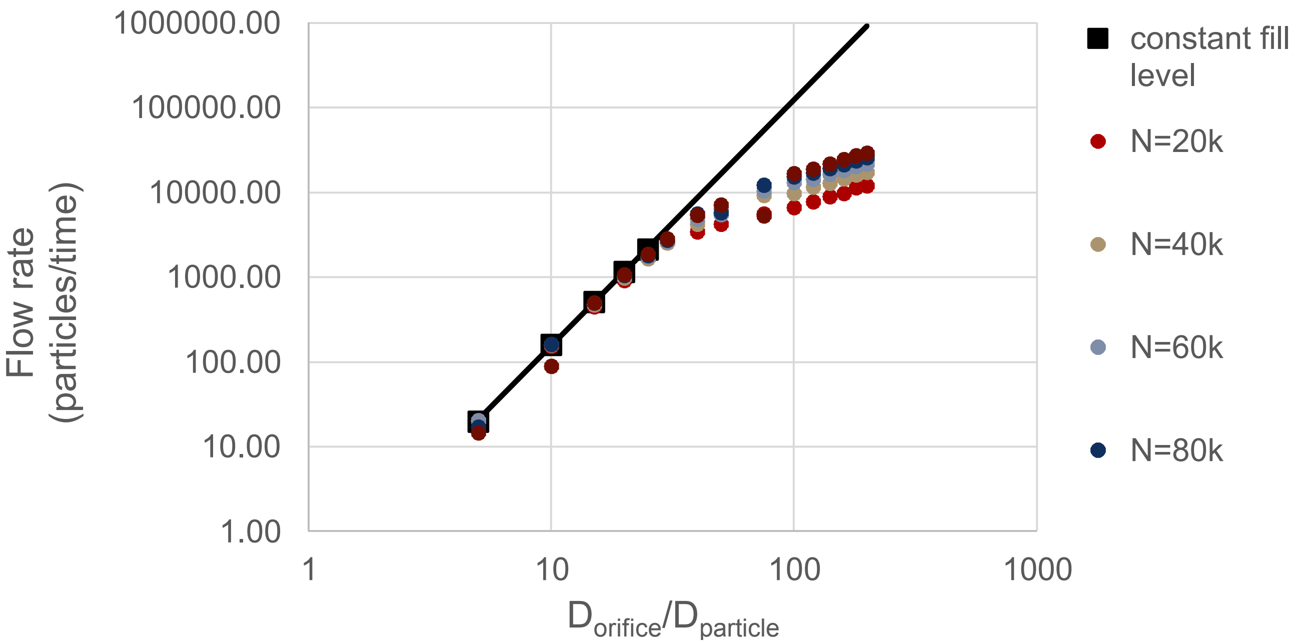
Characterizing AM powder flowability

- Dynamic/flow properties important to spreading
- Connection between DEM parameters and powder experiments
- Hall flowmeter: ASTM standard for measuring powder flowability
  - Time for 50 g of powder to drain from funnel
- Compare DEM simulations of Hall flowmeter to experiments, use data to parameterize simulations



Characterizing AM powder flowability

- Challenge: for AM powders, number of particles in DEM simulation of Hall flow is computationally prohibitive
  → Need to investigate scaling behavior!

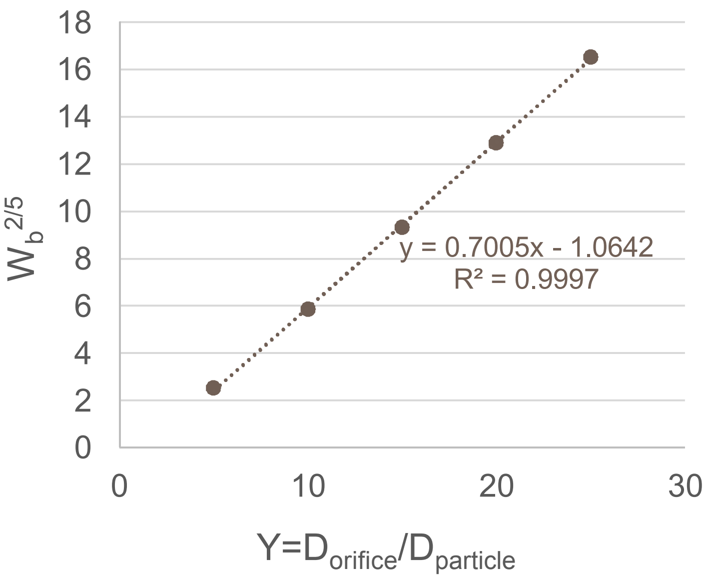


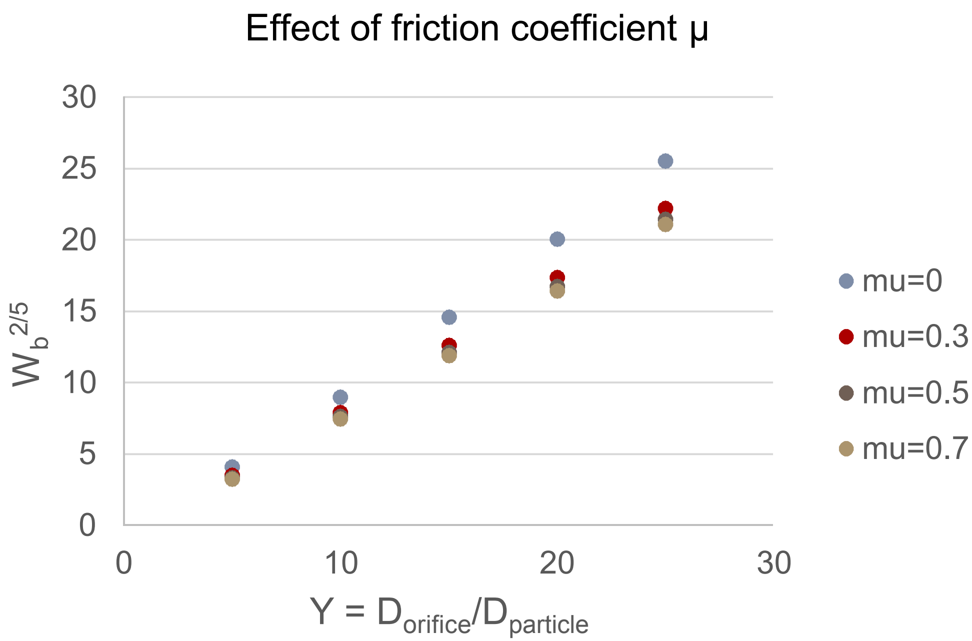
Characterizing AM powder flowability

Beverloo's equation[1]:

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

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



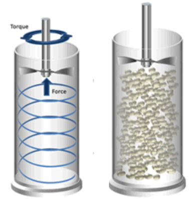


mu	k	C'
0	1.451	1.000
0.3	1.427	0.699
0.5	1.519	0.647
0.7	1.547	0.621

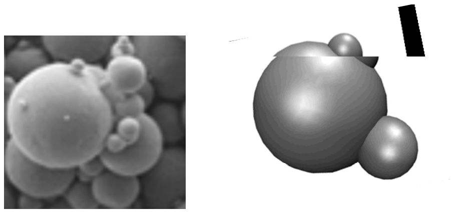
1. Beverloo, W. A et al. "The flow of granular solids through orifices." *Chemical Engineering Science* 15.3 (1961): 260-269.

Ongoing and future work

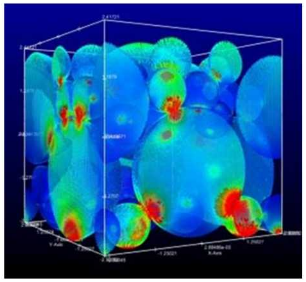
- Additional powder flow studies (simple shear, angle of repose, powder rheology)



- Powder deposition near/on rough surfaces representing partially manufactured part
- Particle shape variations, e.g. due to partial sintering

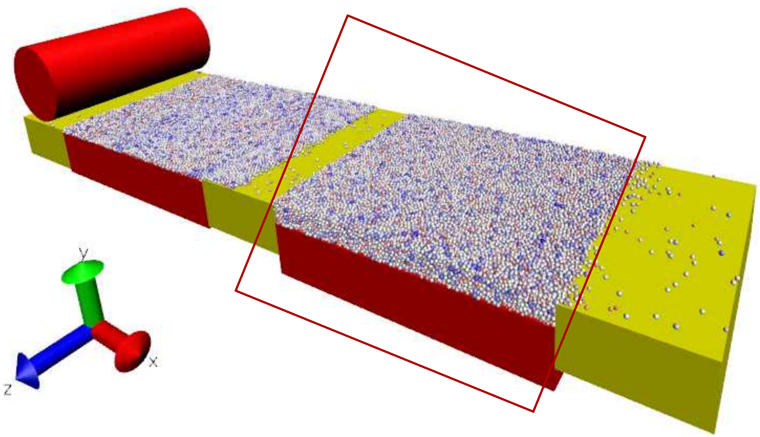


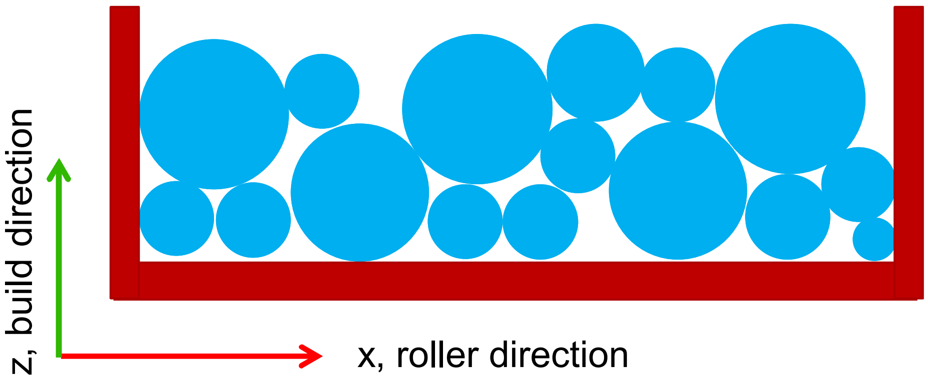
- Thermal transport modeling and coupling to melting/flow/solidification simulations



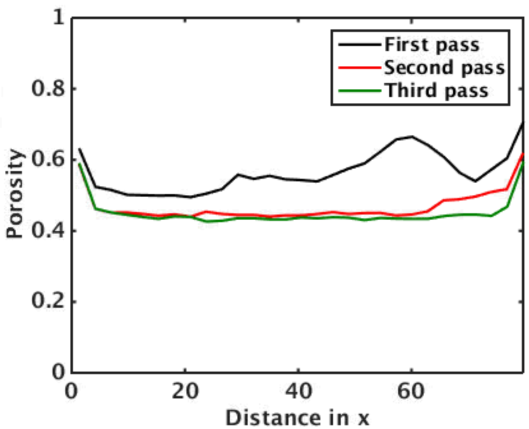
EXTRA SLIDES

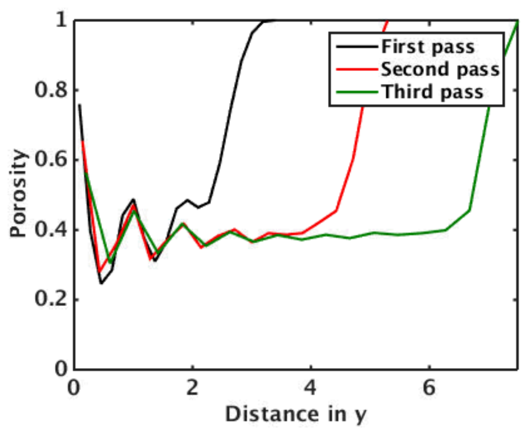
Descriptors of bulk powder bed



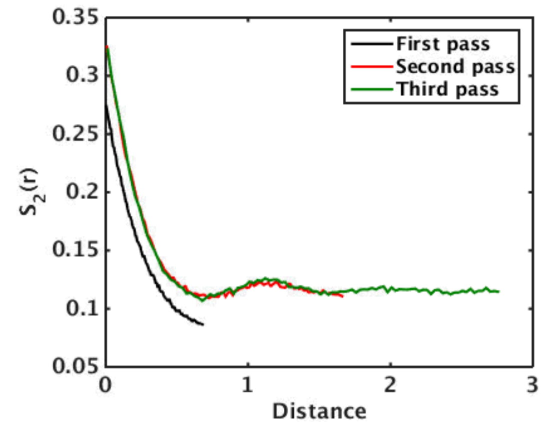


Porosity variation in x, y



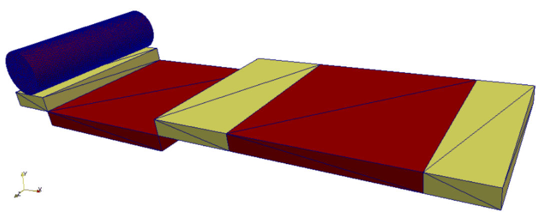


Pore space two-point correlation function



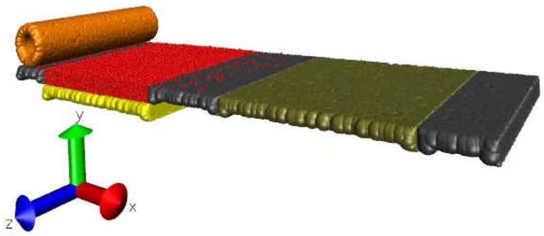
Simulations of powder spreading

- Several approaches to representing complex, moving boundaries in DEM



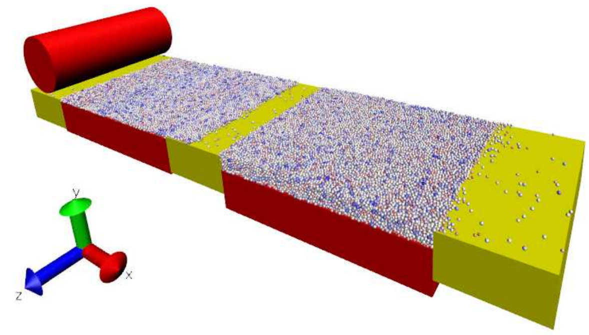
Surface triangle mesh[1]

- Poor computational performance
- Inaccurate forces where multiple triangles contact particles in curved walls (roller)



Clustered, overlapping spheres[2]

- Undesirable artificial roughness
- Inaccurate forces where multiple 'wall spheres' contact particles



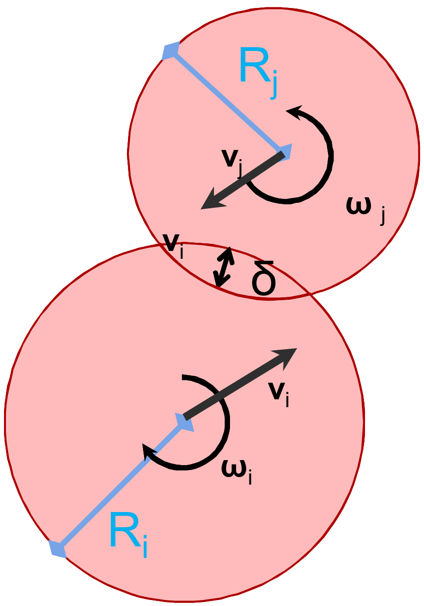
Geometry primitives[2]

- Slight inaccuracy in forces at corners
- Not general, but adequate for current work

1. Kloss and Goniva, *Supplemental Proceedings: Materials Fabrication, Properties, Characterization, and Modeling 2* (2011):781
2. **Plimpton, S. J. *J Comput Phys* 117.1 (1995): 1-19.** **http://lammps.sandia.gov**

Particle friction coefficient

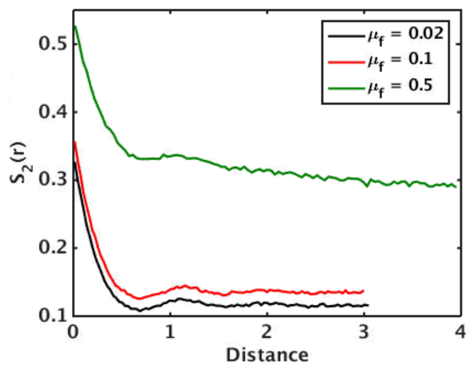
Powder bed surface properties also affected, but notable differences in bulk packing structure:



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

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

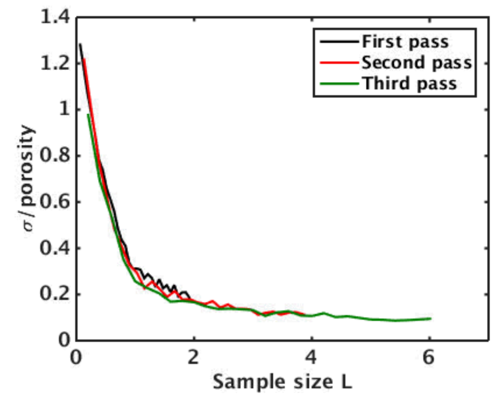
Two-point correlation function



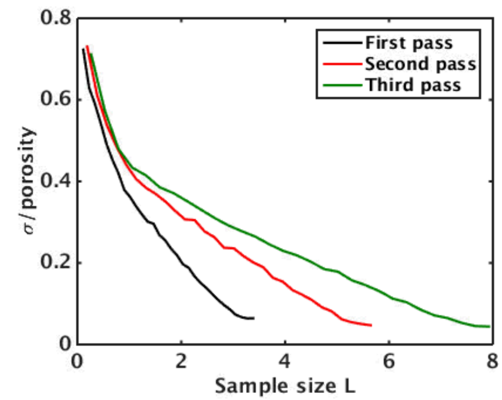
- Note that bulk porosity = $S_2(0)$
- Trends hold regardless of other process parameters

Coarseness

Low friction μ_f=0.1



High friction μ_f=0.5



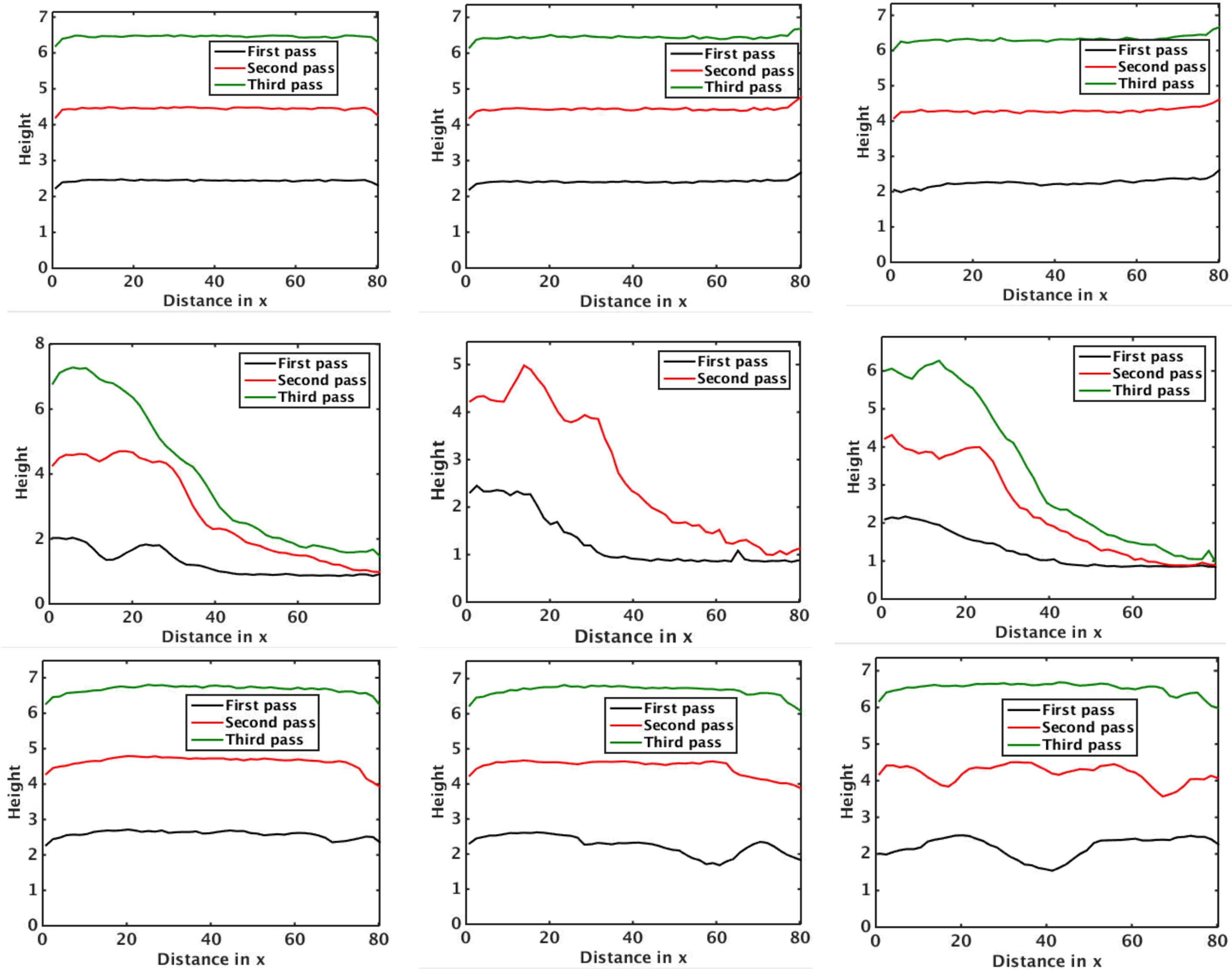
Effects of spreader speed

Increasing speed

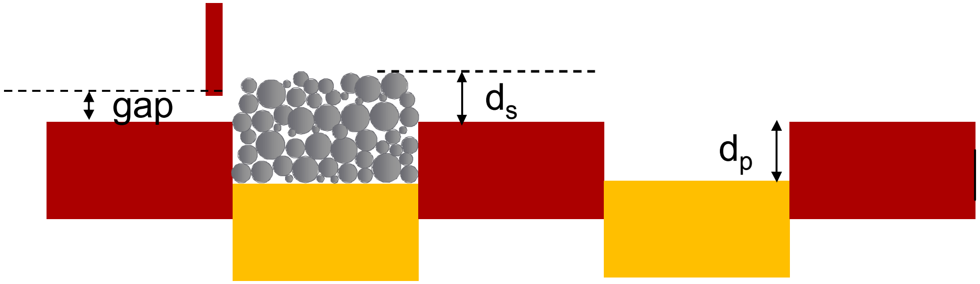
Slider

Roller
forward rotation

Roller
reverse rotation



Effects of powder layer thickness

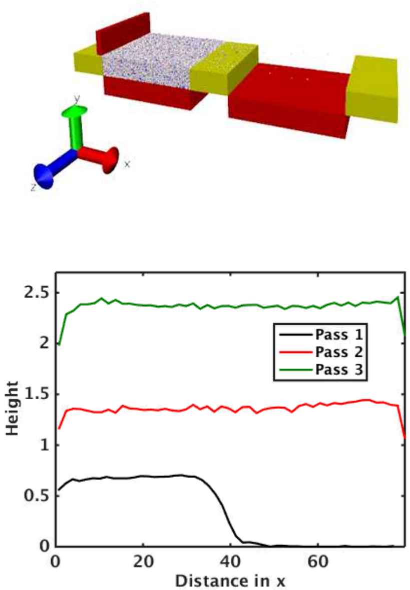


d_p: controls layer thickness

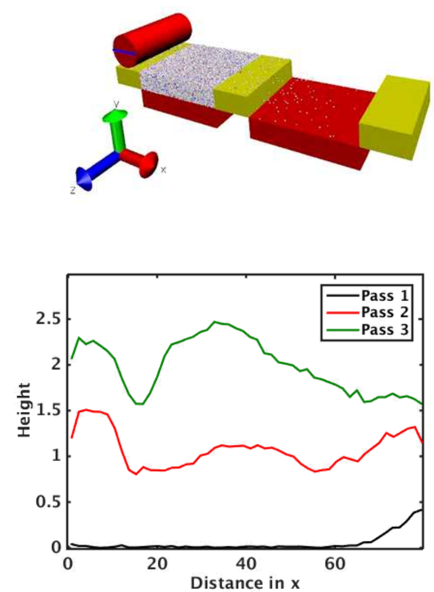
d_s: controls amount of powder

All previous data for **gap = 1.0, dp = 5.0, ds = 2.0**

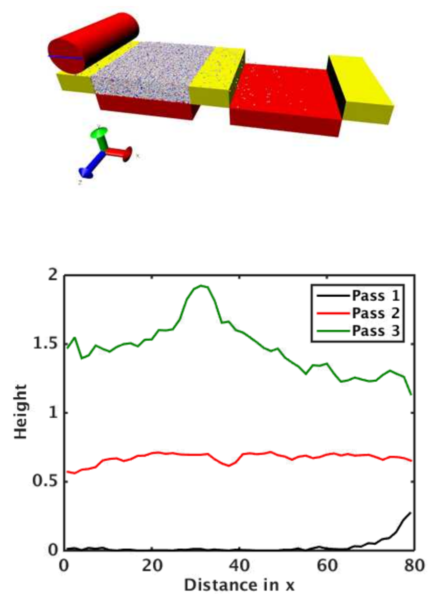
Slider
gap = 0, d_s = 1.5, d_p = 1.0



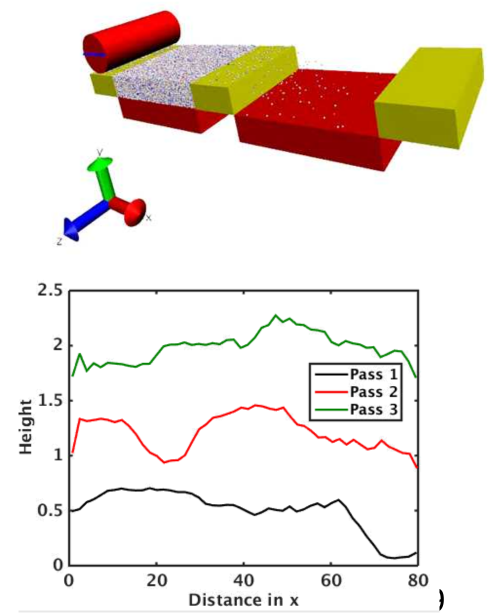
Roller/reverse
gap = 0, d_s = 1.5, d_p = 1.0



Roller/forward
gap = 0, d_s = 1.5, d_p = 1.0

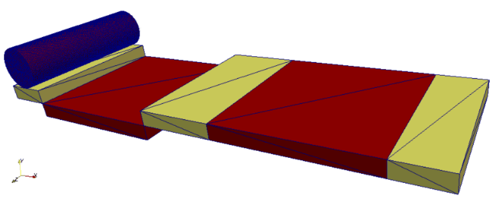


Roller/forward
gap = 0.5, d_s = 1.5, d_p = 1.0



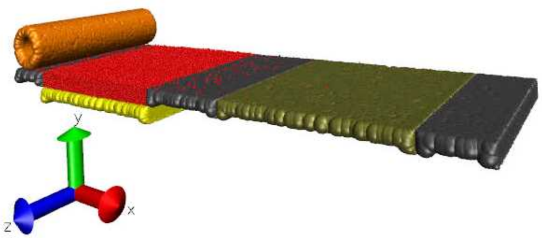
Simulation methods

- Several approaches to representing complex, moving boundaries in DEM:



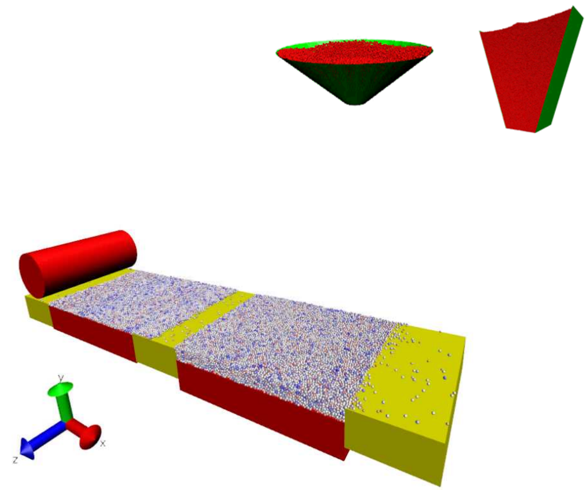
Surface triangle mesh[1]

- Poor computational performance for curved surfaces
- Inaccurate forces where multiple triangles contact particles



Clustered, overlapping spheres[2]

- Undesirable artificial roughness
- Potentially inaccurate forces where multiple 'wall spheres' contact particles

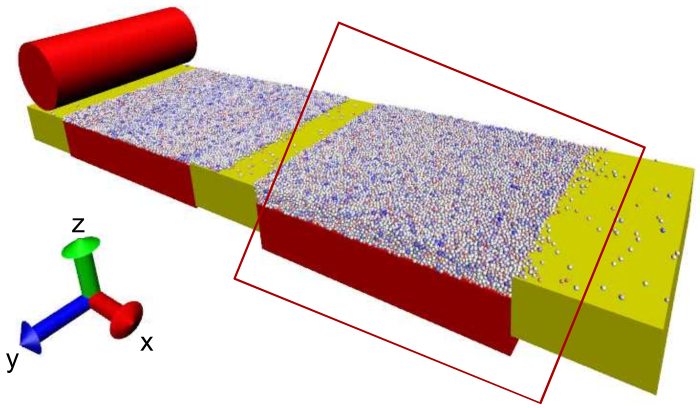


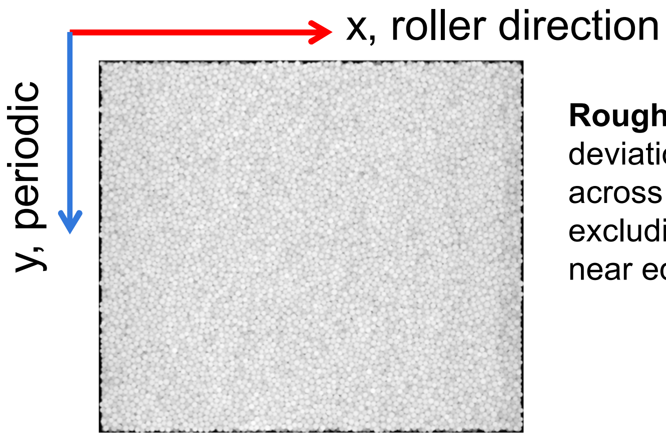
Geometry primitives[2]

- Not as general, but adequate for current work

1. Kloss and Goniva, *Supplemental Proceedings: Materials Fabrication, Properties, Characterization, and Modeling 2* (2011):781
2. Plimpton, S. J. *J Comput Phys* 117.1 (1995): 1-19. http://lammps.sandia.gov

Descriptors of powder bed surface

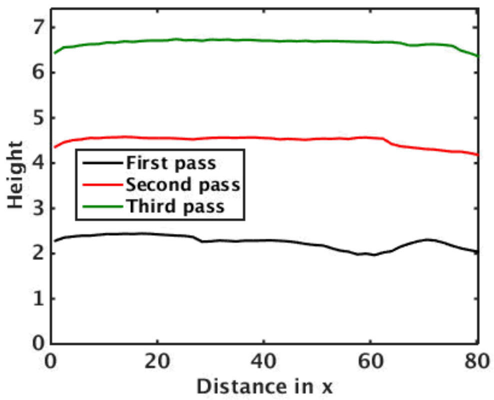




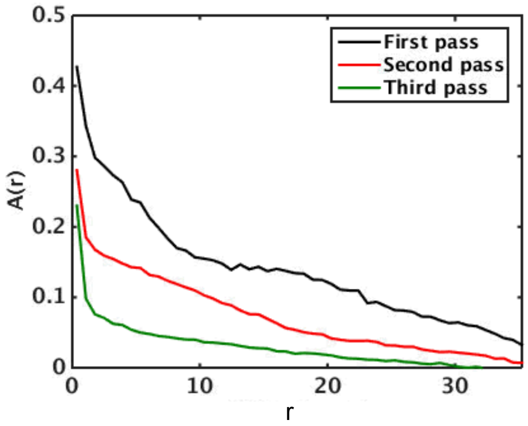
Roughness: standard deviation of height (σ) across entire pack, excluding small region near edges

Top view, grayscale intensity corresponds to height

Height profile: height averaged over z direction as a function of x



Height autocorrelation function:
A(r) = <(H(**x**)-μ) (H(**x**+**r**)-μ)>/ σ^2



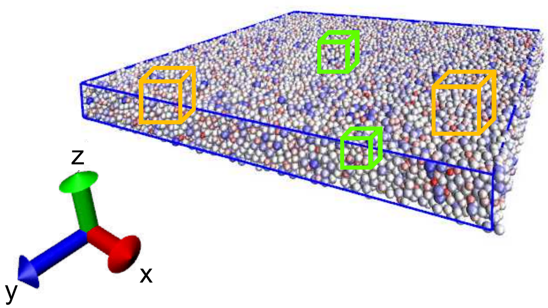
Descriptors of bulk powder bed

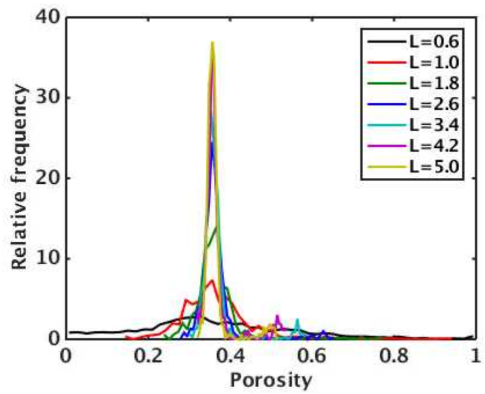
Sandia National Laboratories

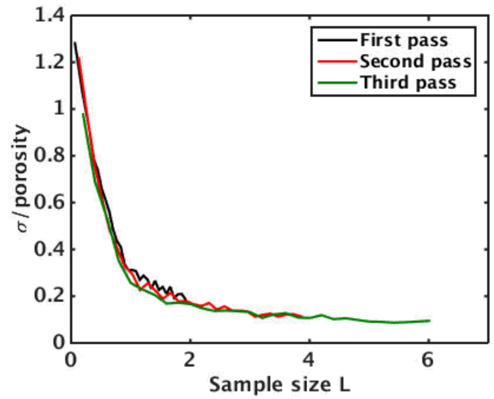
Porosity: mean value, spatial variation, etc.

Coarseness:

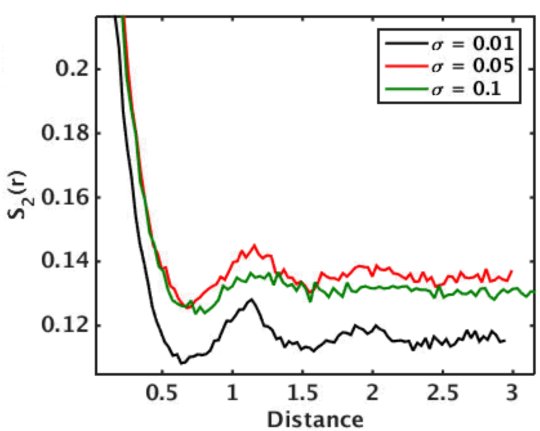
Cubic samples of side length L



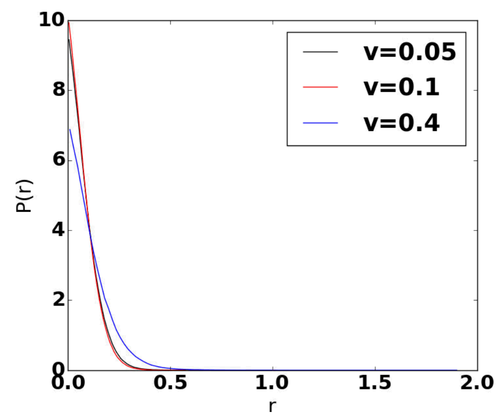




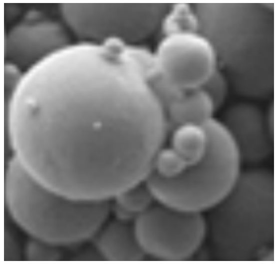
Two-point correlation function:

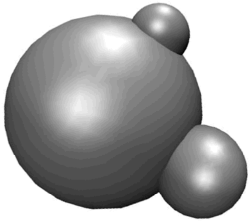


Pore size distribution function:

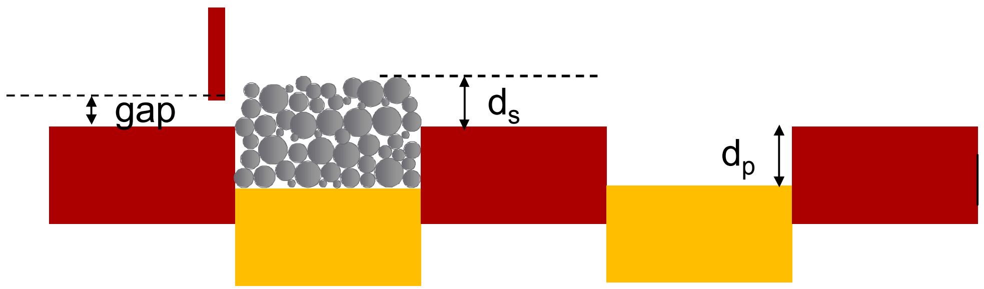


Effects of particle properties: particle shape





Effects of powder layer thickness

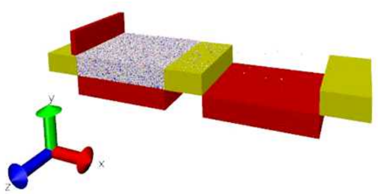


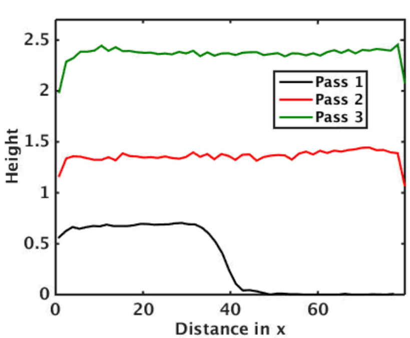
d_p: controls layer thickness

d_s: controls amount of powder

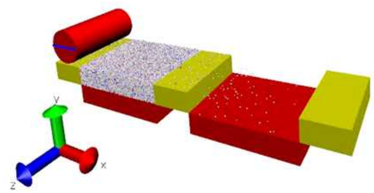
All previous data for **gap = 1.0, dp = 5.0, ds = 2.0**

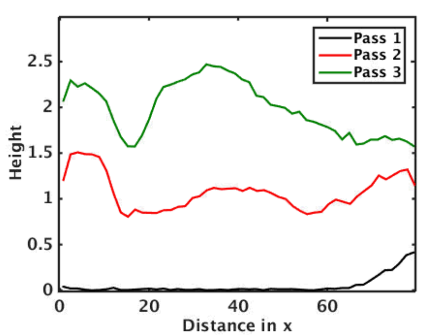
Slider
gap = 0, d_s = 1.5, d_p = 1.0



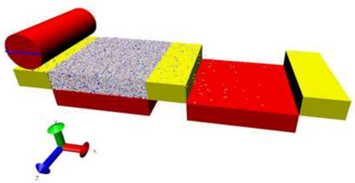


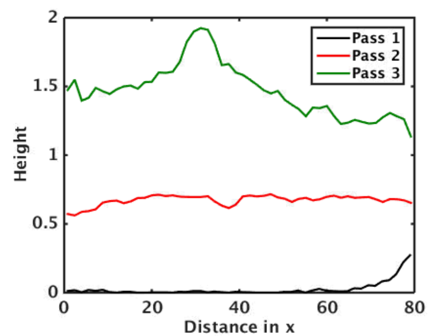
Roller/reverse
gap = 0, d_s = 1.5, d_p = 1.0



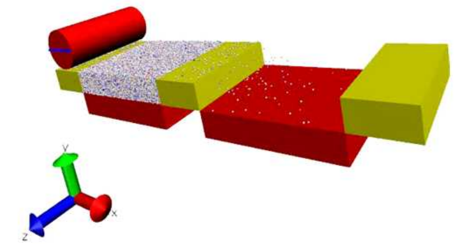


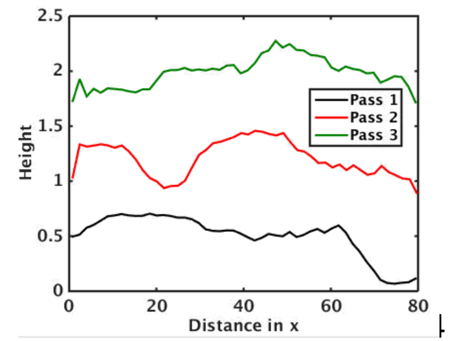
Roller/forward
gap = 0, d_s = 1.5, d_p = 1.0





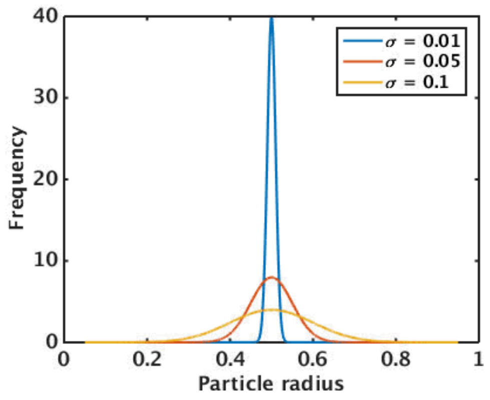
Roller/forward
gap = 0.5, d_s = 1.5, d_p = 1.0



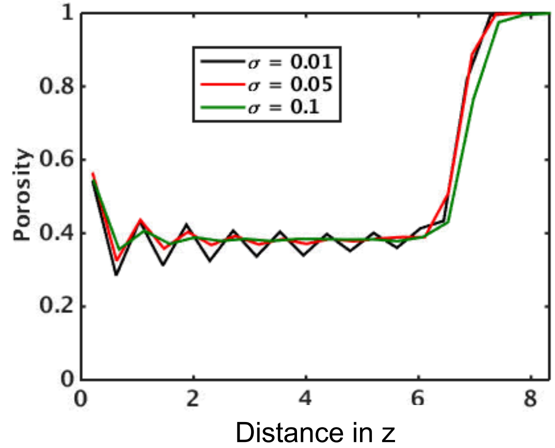


Effects of particle size distribution

- Gaussian distributions, mean radius 0.5, vary σ
- Data shown for slider only

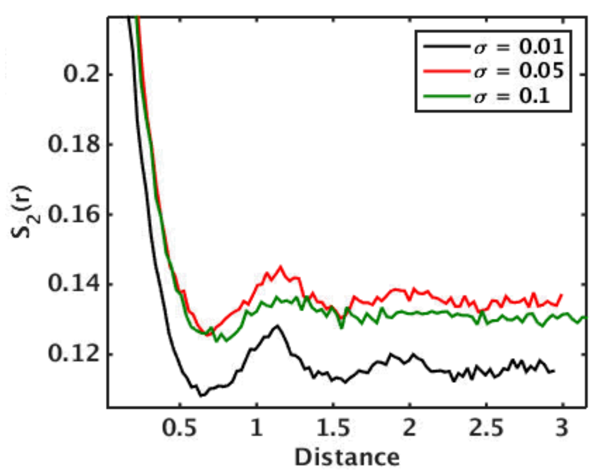


Porosity in the height direction, third pass of slider



Layering order decreases with larger polydispersity. Small differences in mean porosity.

Two-point correlation function



Less local structuring with larger polydispersity