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Simulations of powder bed formation for additive manufacturing

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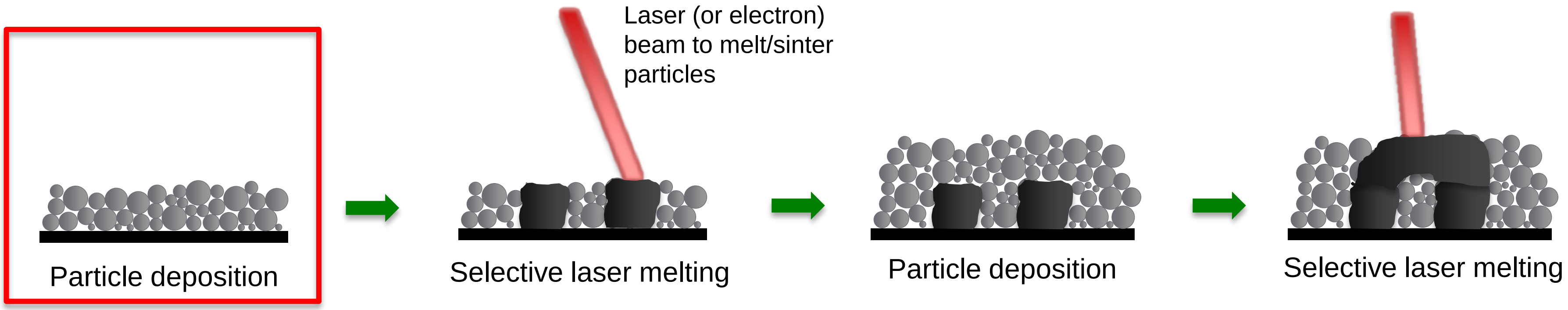
U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Background and Motivation

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

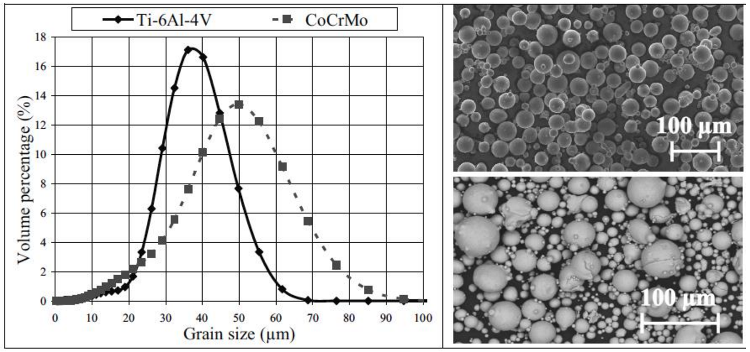


- Does powder bed structure matter?
  - **Surface structure** may affect laser/particle bed interactions
  - **Bulk powder packing** may affect defect formation and surface finish of manufactured parts

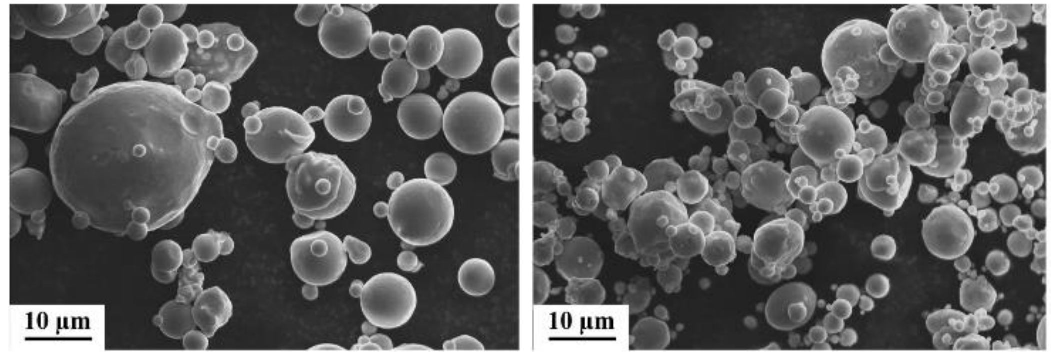
- Need to understand effects of **particle properties** and **powder process parameters** on powder bed structure

- Models of laser interaction, powder fusion depend on effective powder bed properties **and their variability** → tied to particle-scale structure

Typical powder characteristics



From Ref. 1



From Ref. 2

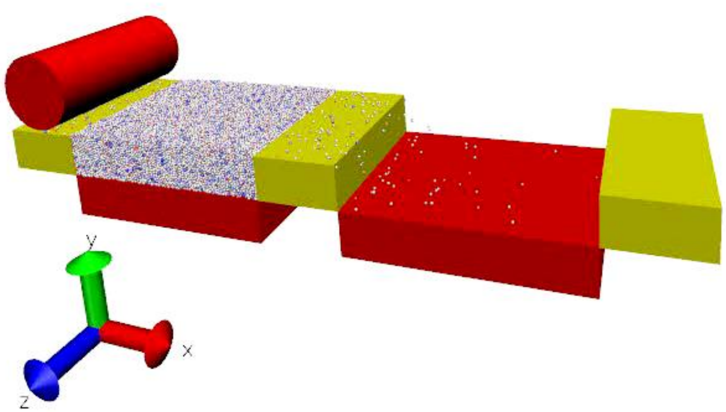
- Particle shape very close to spherical → well-suited for existing modeling capabilities
- Typical particle diameter: 10-100 μm; polydispersity factor 4-5
- Powder layer thickness 30-150 μm, laser beam spot size 70-200 μm (ref. 1)

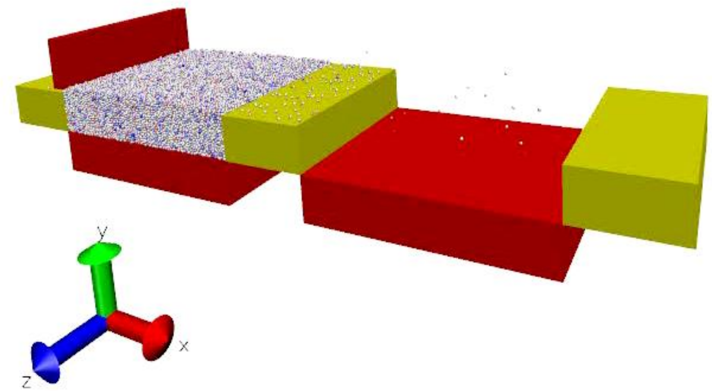
Understanding powder bed structure at the scale of individual particles is important

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

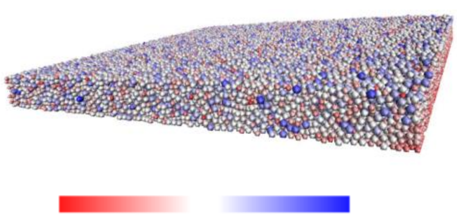
Overview

- Discrete Element Method (DEM) simulations of powder spreading





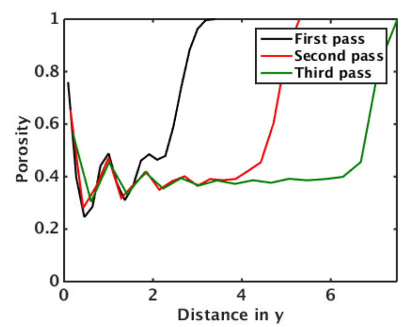
- Statistical characterization of resulting powder beds (static only)

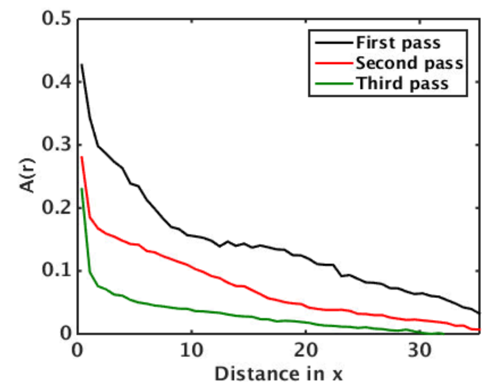


d = 0.7

d = 1.3

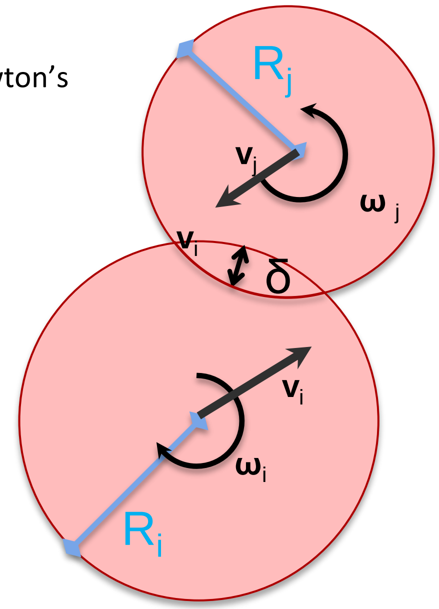
Particle diameter, d





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
- 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:

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

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

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

- Tangential contact force

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

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

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

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

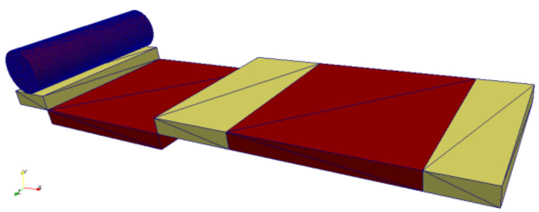
μ Coefficient of friction

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

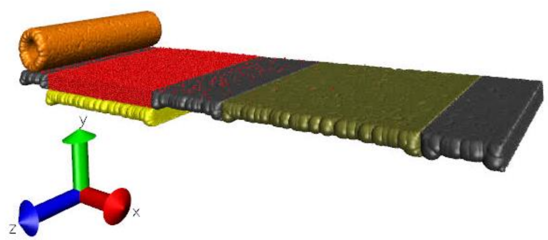
Total torque: $\tau_{i,tot} = -\frac{1}{2}\sum_j \mathbf{r}_{ij}\times\mathbf{F}_{t,ij}$

Simulations of powder spreading

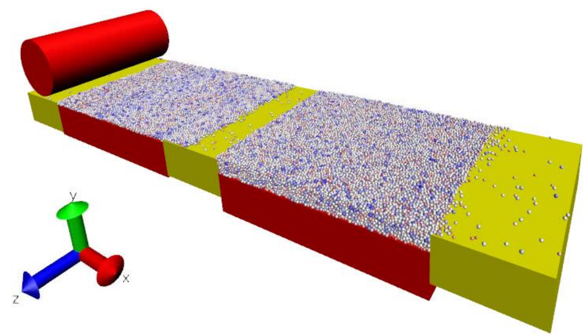
- Goal is not an exact match to actual process, but to capture key features, length scale ratios and overall trends.
- Several approaches to representing complex, moving boundaries in DEM



Surface triangle mesh (LIGGGHTS code)



Clustered, overlapping spheres



Geometry primitives

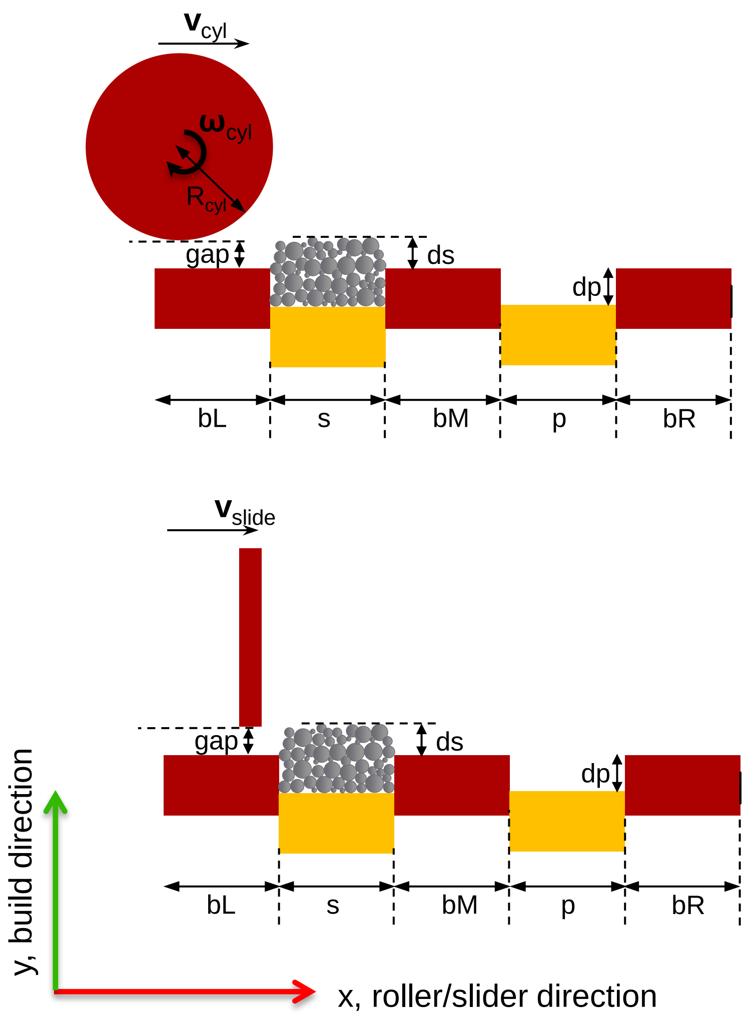
- Poor computational performance
- Inaccurate forces where multiple triangles contact particles

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

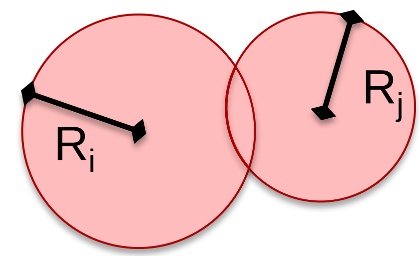
- Slight inaccuracy in forces at corners
- Not general, but adequate for current work

Large parameter space!

Process-related

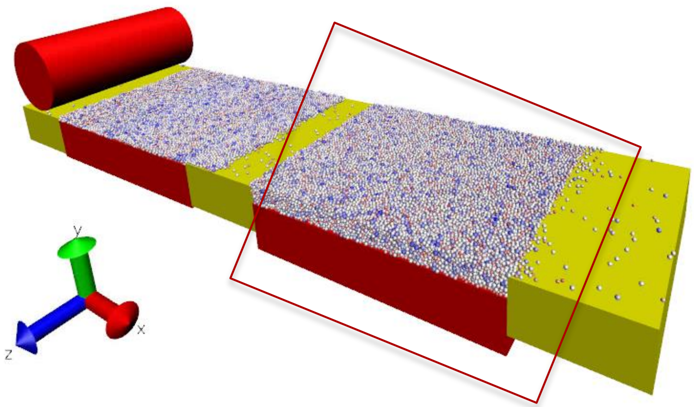


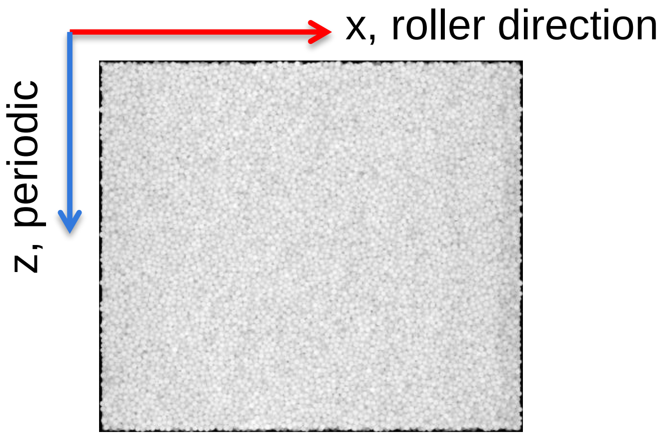
Particle-related



- Particle size distribution
  - Type of distribution
  - Overall spread
- Contact parameters
  - Stiffness, damping → relates to Young's modulus, contact mechanics
  - Friction → relates to surface characteristics
  - Cohesion → in progress!
  - Note: contact parameter sets can be different for particle-particle and particle-wall contact

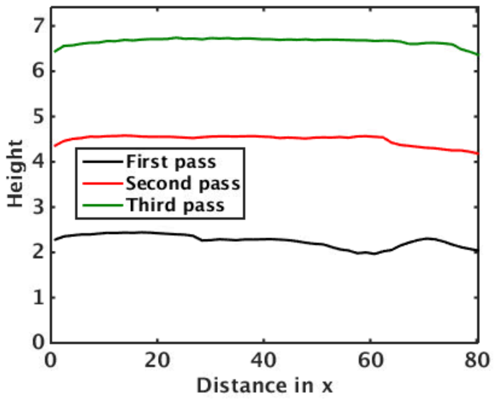
Descriptors of powder bed top surface





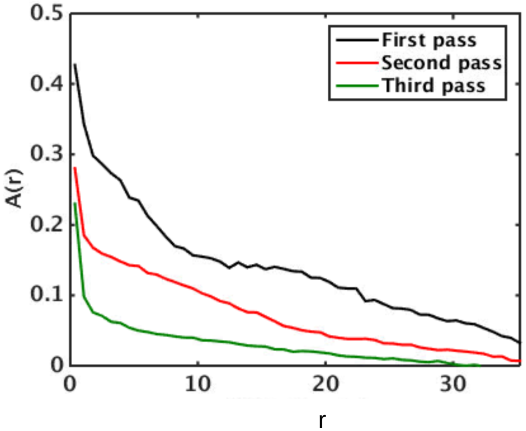
Top view, grayscale intensity corresponds to height

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

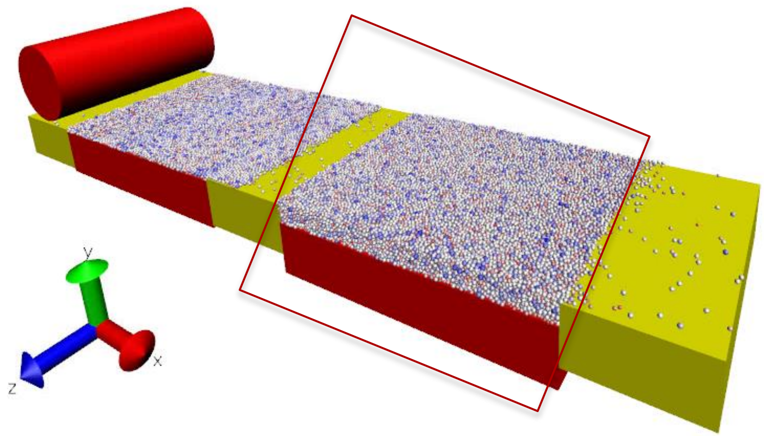


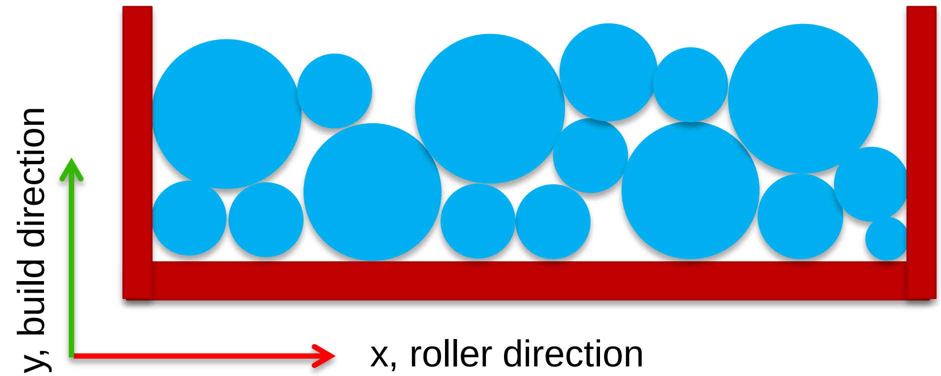
Roughness: standard deviation of height (σ) across entire pack, excluding small region near edges

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

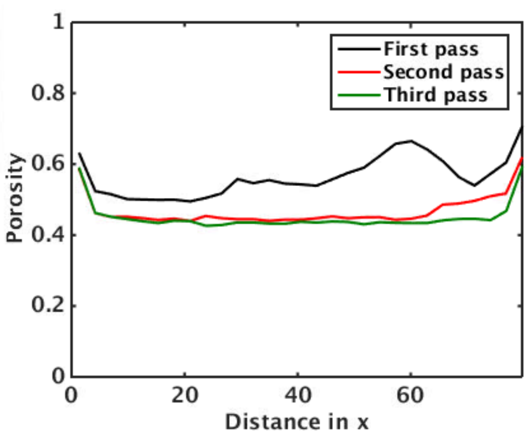


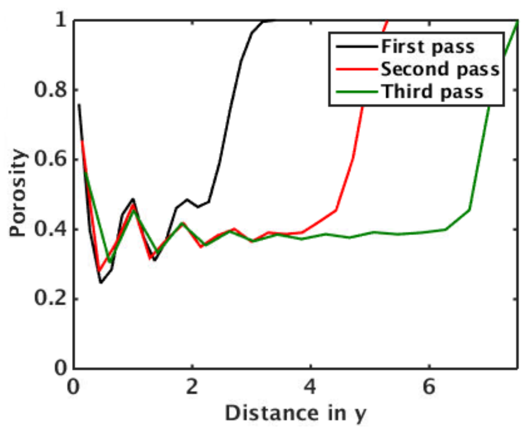
Descriptors of bulk powder bed



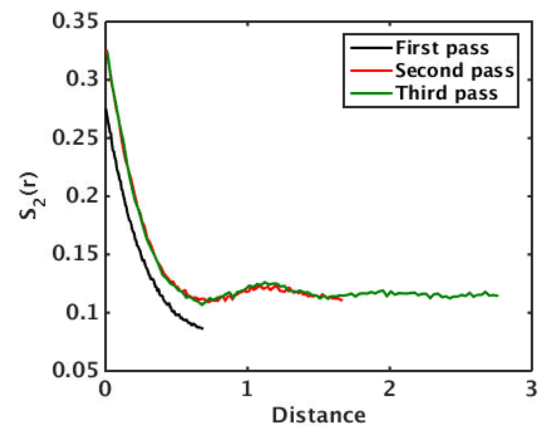


Porosity variation in x, y

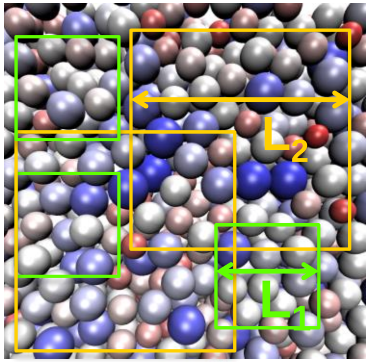




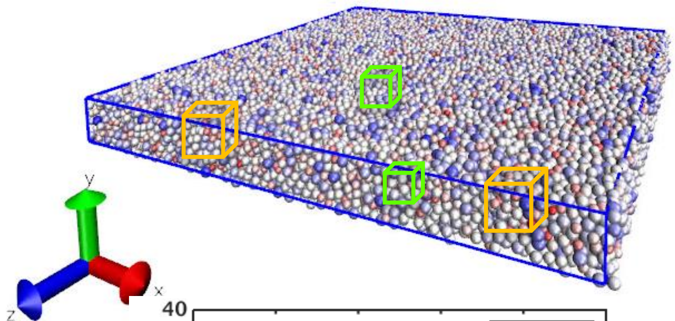
Pore space two-point correlation function



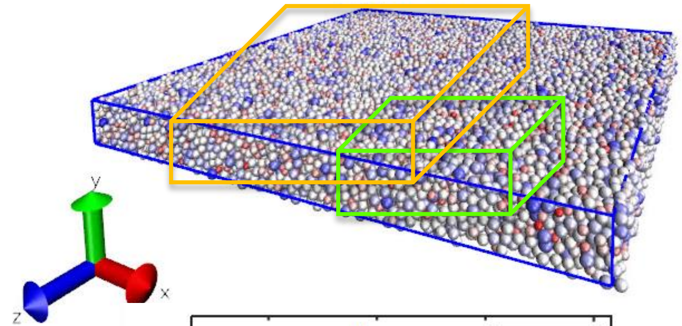
Descriptors of bulk powder bed: ‘coarseness’



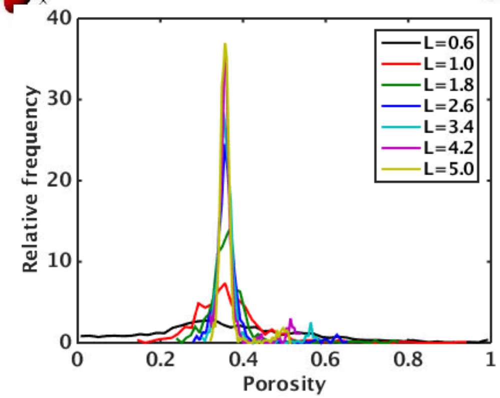
Cubic samples of side length L

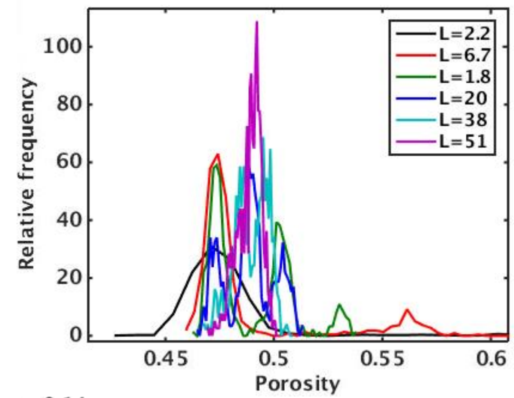


Full-thickness samples, lateral dimension L

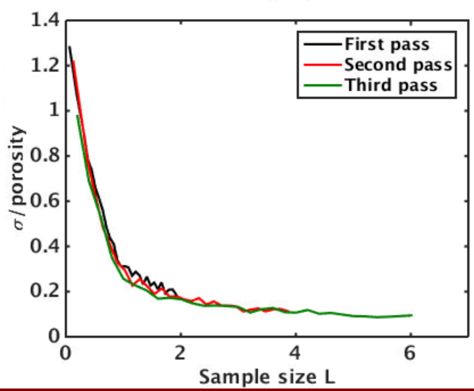


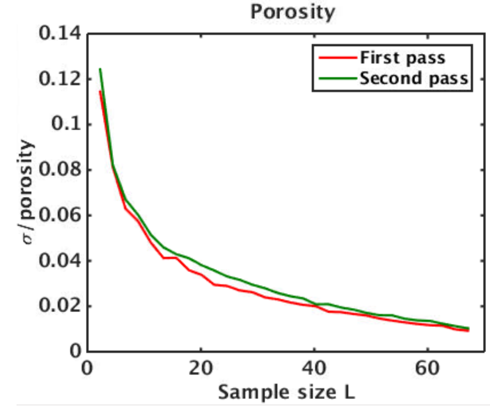
- For given size L, take many sub-samples, compute distribution of porosity





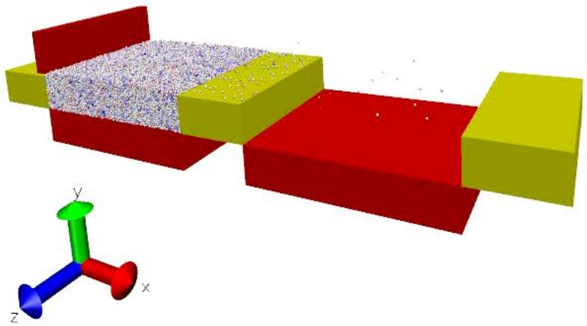
- Plot L vs standard deviation of porosity at each sub-sample size

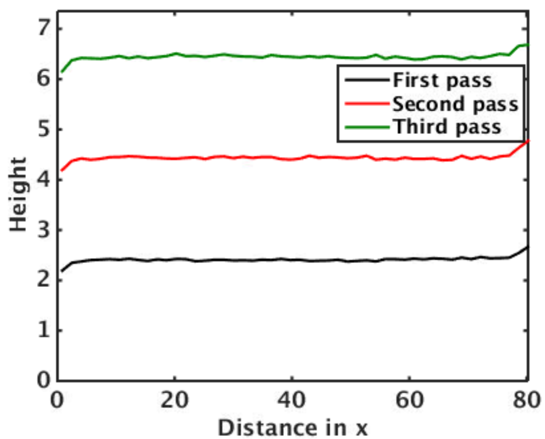




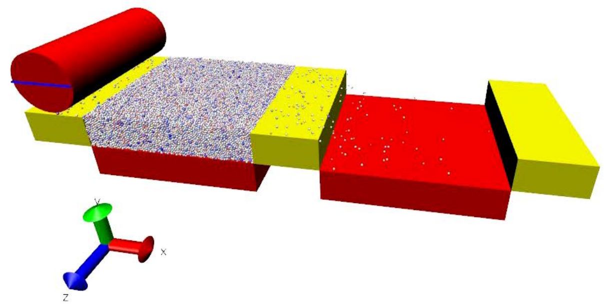
Effects of spreader type

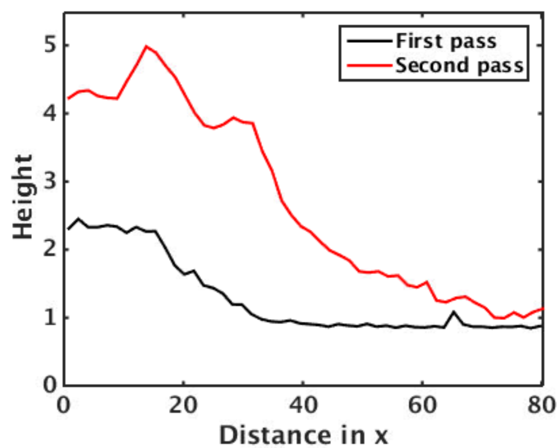
Slider



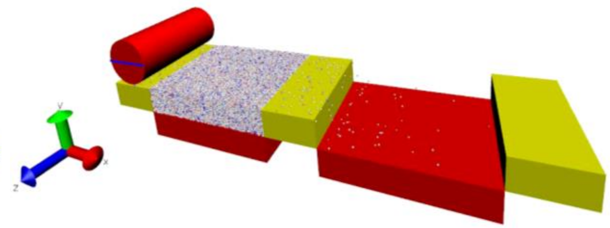


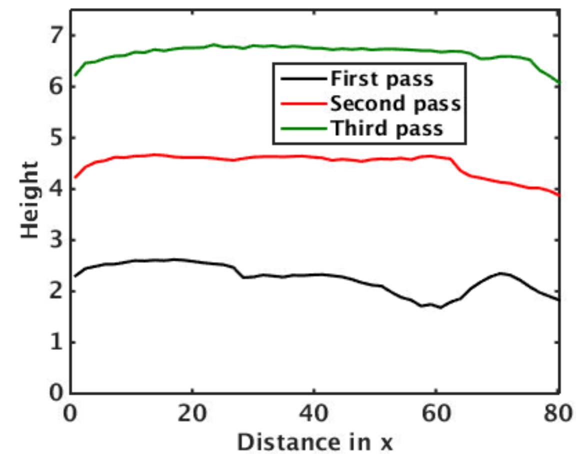
Roller, rotation in
direction of translation (forward)





Roller, rotation against
direction of translation (reverse)





Effects of spreader speed

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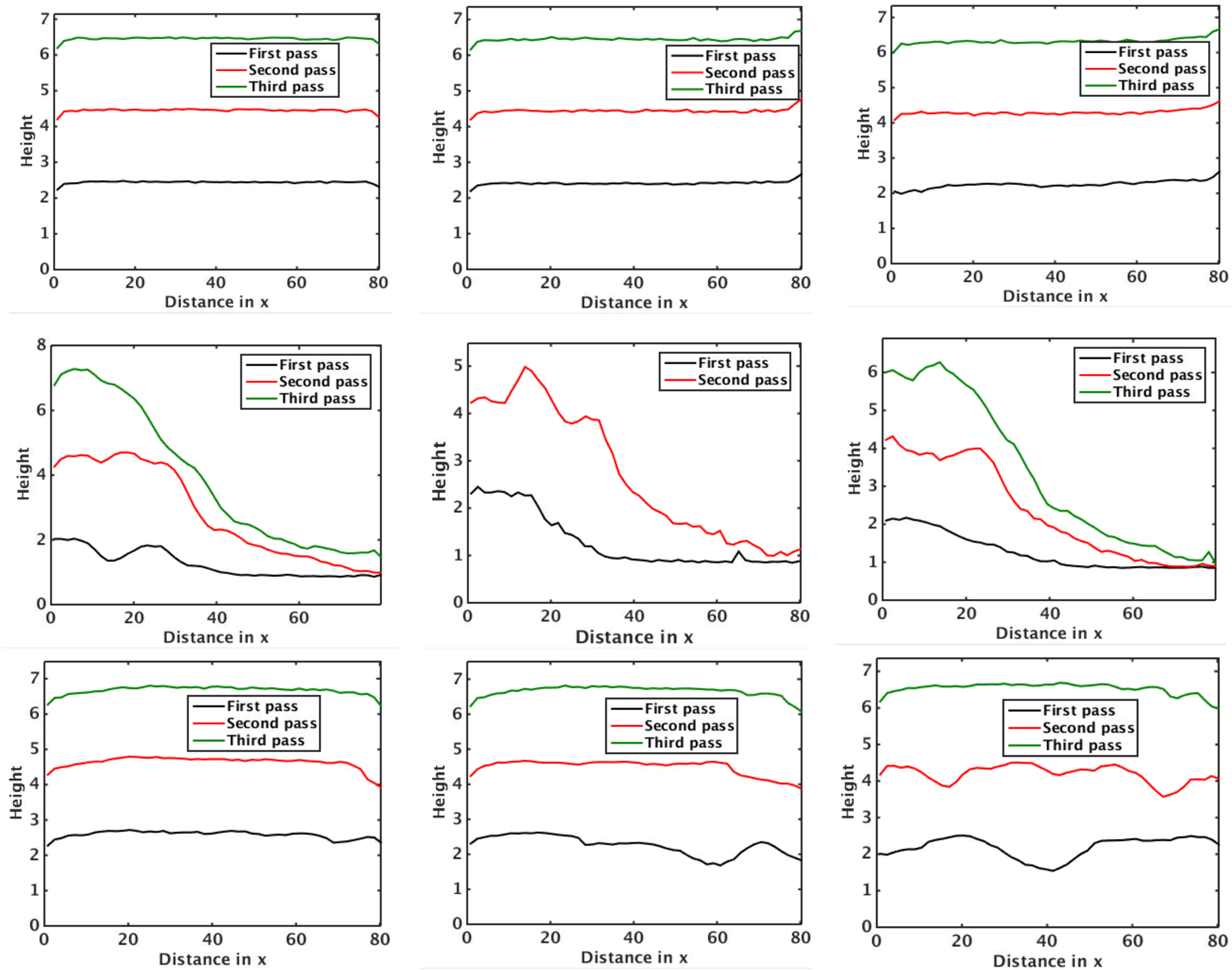
Increasing speed

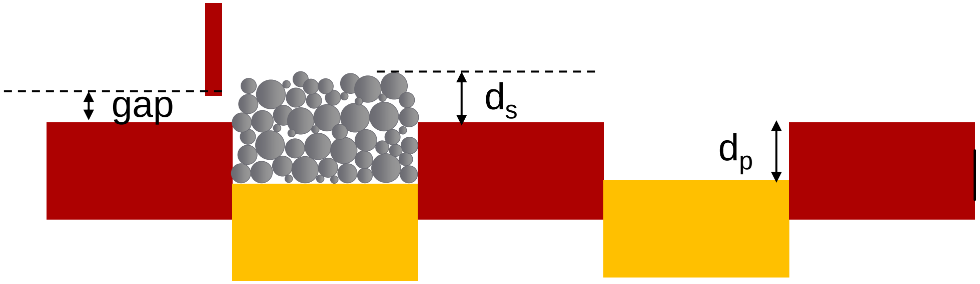
Slider

Roller forward rotation

Roller reverse rotation



Effects of powder layer thickness

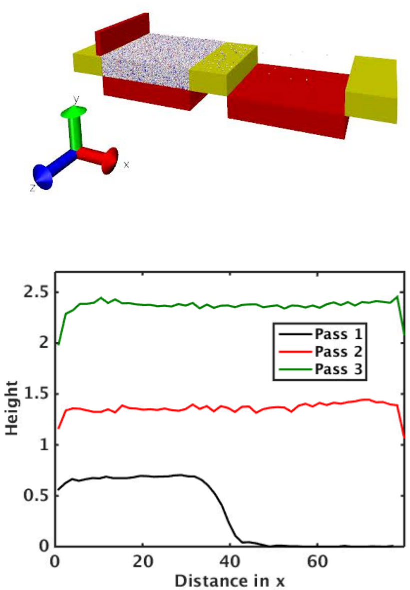


d_p: controls layer thickness

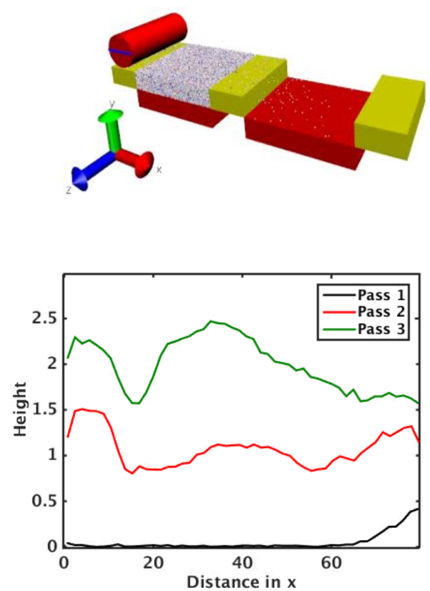
d_s: controls amount of powder

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

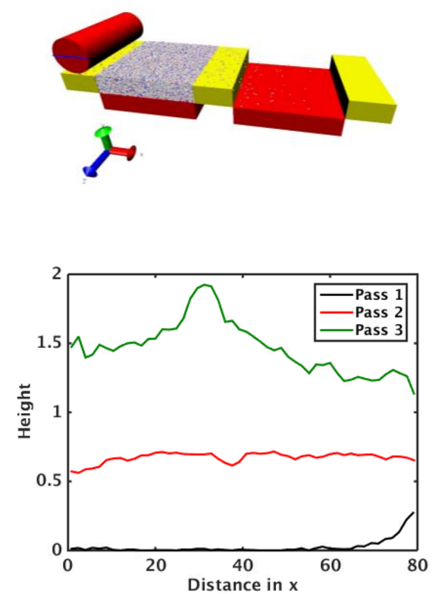
Slider
gap = 0, d_s = 1.5, d_p = 1.0



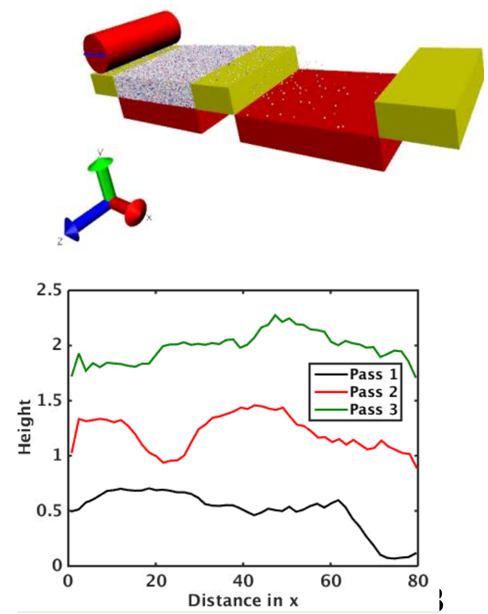
Roller/reverse
gap = 0, d_s = 1.5, d_p = 1.0



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

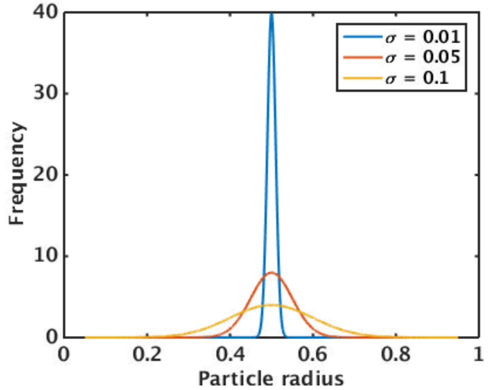


Roller/forward
gap = 0.5, d_s = 1.5, d_p = 1.0

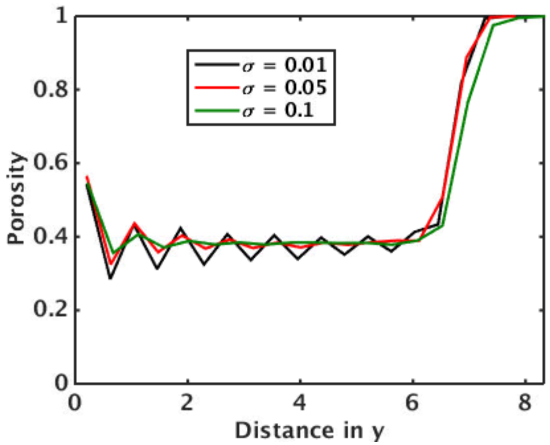


Effects of particle size polydispersity

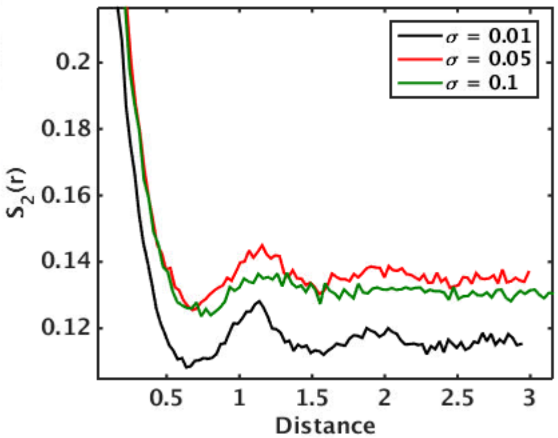
- Gaussian distributions, mean radius 0.5, vary σ
- Data shown for slider only



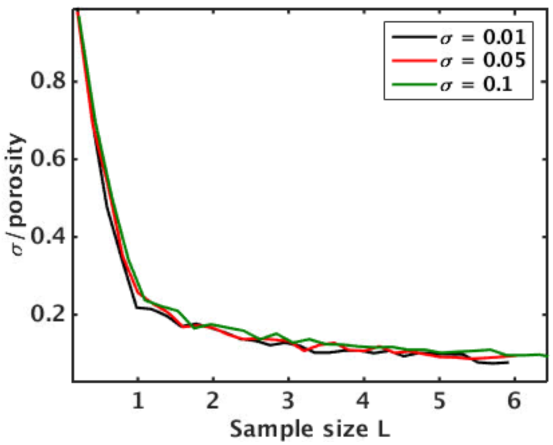
Porosity in the height direction, third pass of slider



Two-point correlation function



Coarseness



Layering order decreases with larger polydispersity. No large differences in mean porosity,

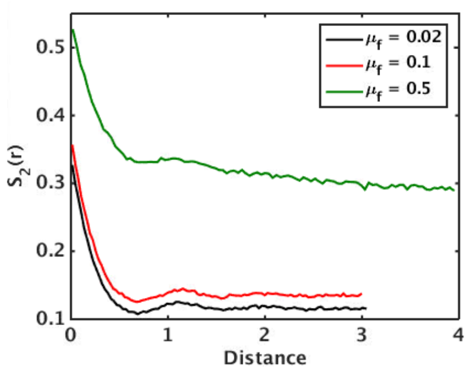
Less local structuring with larger polydispersity

Surprisingly, little or no effect on coarseness

Particle friction coefficient

Surface properties also affected, but notable differences in bulk packing structure:

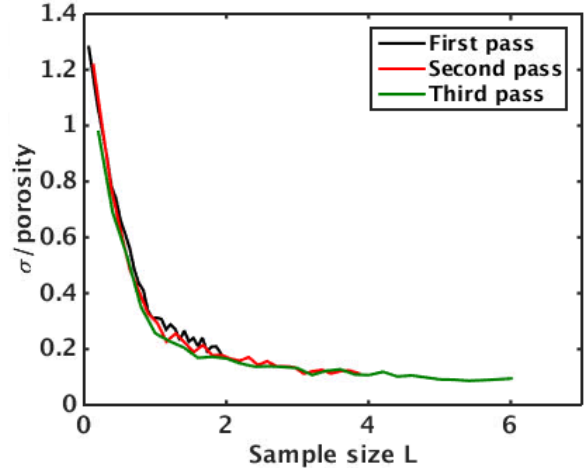
Two-point correlation function



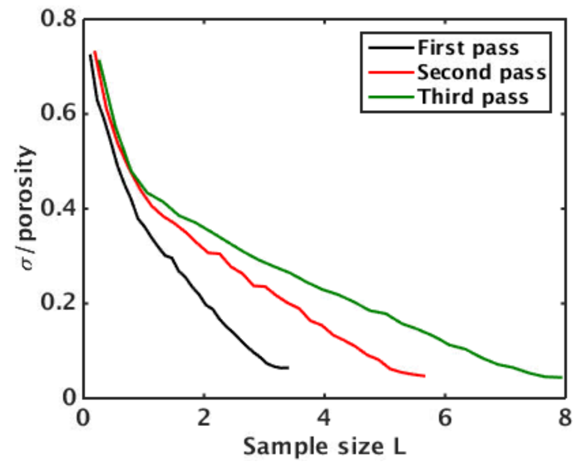
- Note that bulk porosity = $S_2(0)$
- Trends hold regardless of other process parameters

Coarseness

μ_f=0.1



μ_f=0.5



Summary

- Spreader geometry, configuration and speed control quality of powder bed surface
  - Slider generally more robust, roller in reverse rotation better than forward rotation
  - Bulk packing (below surface) not strongly affected by spreader parameters

- Particle properties control bulk packing (as well as powder bed surface)
  - Higher friction → higher porosity, increased heterogeneity
  - Larger polydispersity results in more homogeneous packing

Future work

- Include **particle cohesion**, rolling friction, more realistic geometries

- Adjust particle contact parameters based on experimental flowability data (e.g. angle of repose, Hall flowmeter)

- Look at powder deposition near partially manufactured part

- Ray-tracing calculations for laser-power bed interaction (with LLNL)

- Coarse-grained calculations of thermal conductivity in particle packs, coupling to macroscale thermal models