SAND2016-1382C

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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

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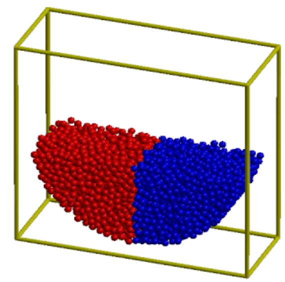
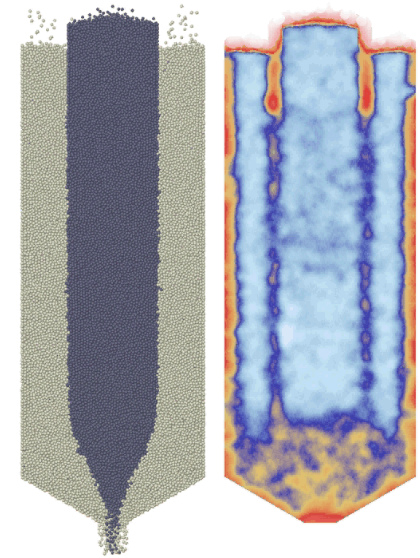
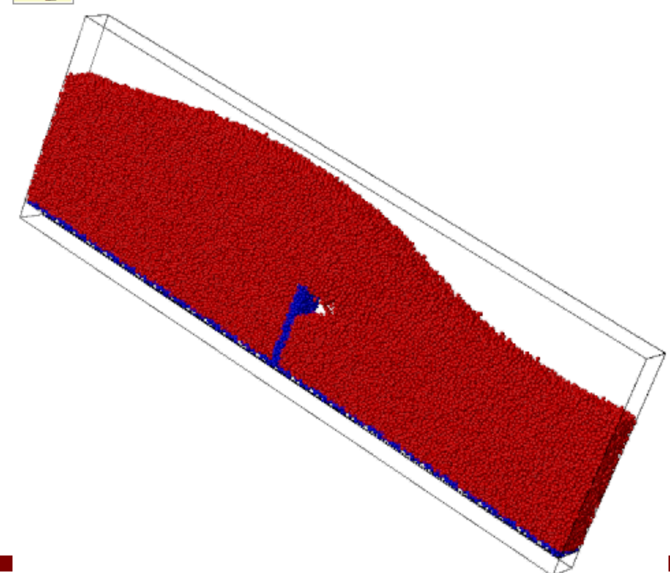
Background: Granular Simulations

- Discrete Element Method
  - Particle Dynamics (MD-like) method
- Inertial
  - Very rapid/dilute
    - Binary Collisions
    - Kinetic theory
  - Dense rapid/enduring contacts
    - Stresses scale with particle elasticity
    - Relatively high “Mach number”
  - Dense/collisional
    - Bagnold: $\sigma\ \alpha\ \gamma^2$
    - Distribution of collision times
    - Rheology becoming well established
- Quasistatic-Elastic
  - Slow, dense
  - Standard geomechanics
- Transitions
  - Failure criterion and flow rules
- Relationship between various geometries
  - Dense gravity driven
  - Dense boundary driven



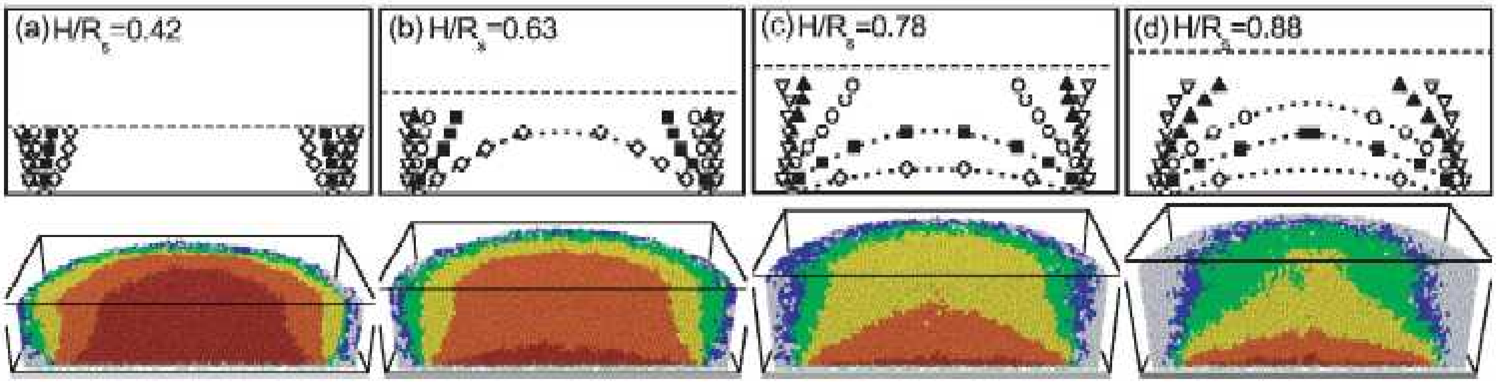




Silbert, Grest et al (2001) *Phys Rev E*, v. 64, p. 51302
Cheng, Lechman et al (2006) *Phys Rev Lett*, v. 96, p. 38001

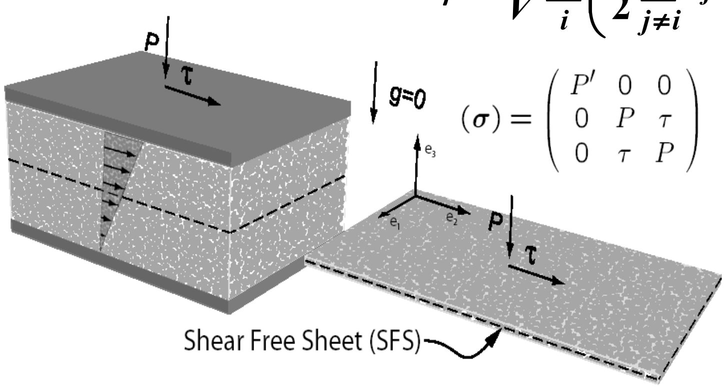
Quasi-static Granular Rheology

- Split-bottom Couette Cell
  - Quasistatic-Elastic, slow, dense, smooth
  - Validation of LAMMPS with MRI experiments for phenomenology of flow (with U. of Chicago)

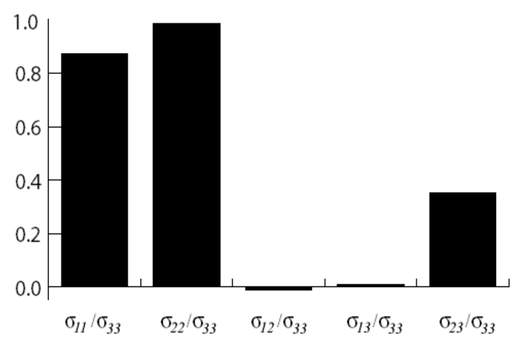


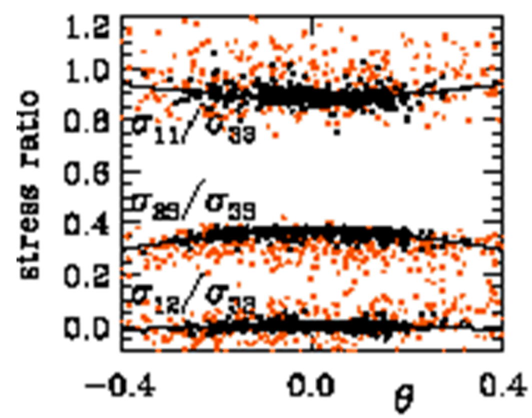
  - Theory for stresses in bulk flow (with U. of Leiden)

$$\sigma_{\alpha\beta} = \frac{1}{V}\sum_i \left(\frac{1}{2}\sum_{j\neq i} r_{ij}^{\alpha} F_{ij}^{\beta} + m_i (v_i^{\alpha} - \langle v^{\alpha} \rangle)(v_i^{\beta} - \langle v^{\beta} \rangle) \right)$$



$$(\sigma) = \begin{pmatrix} P' & 0 & 0 \\ 0 & P & \tau \\ 0 & \tau & P \end{pmatrix}$$





Meso-scale, particle-based applications

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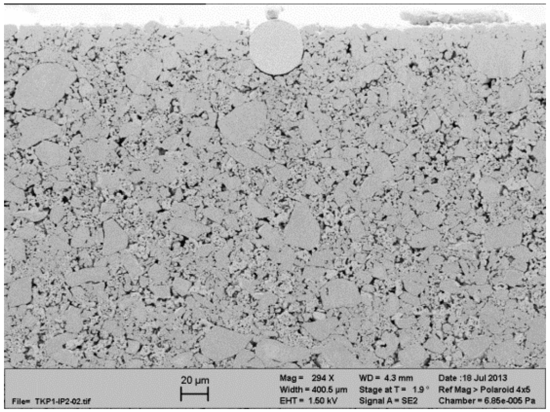
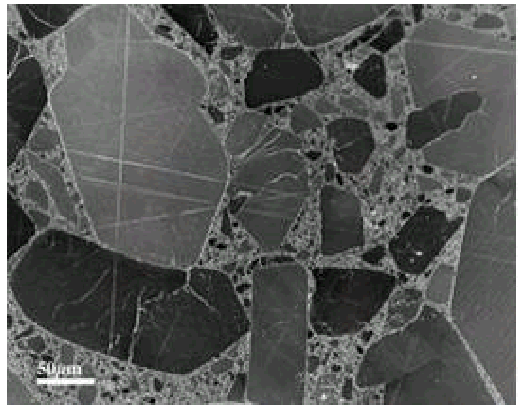
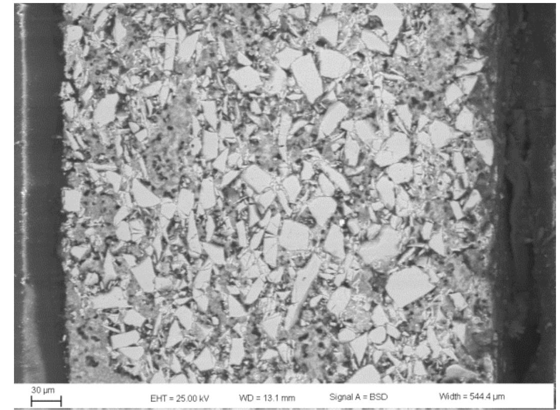
Need particle scale mod-sim capability to predict microstructure formation and properties

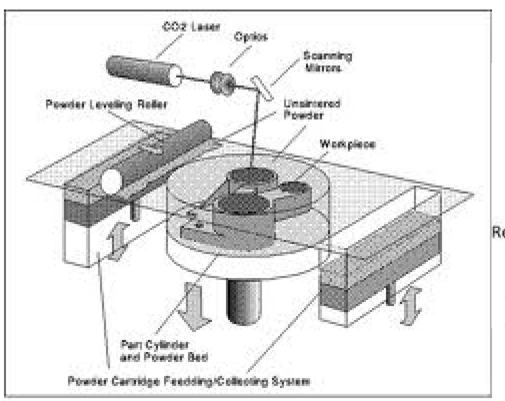




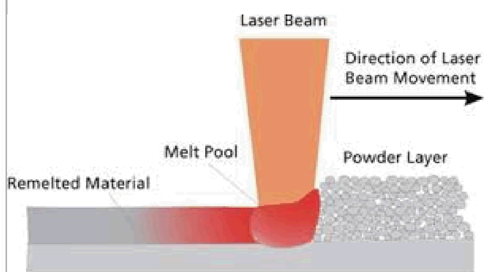


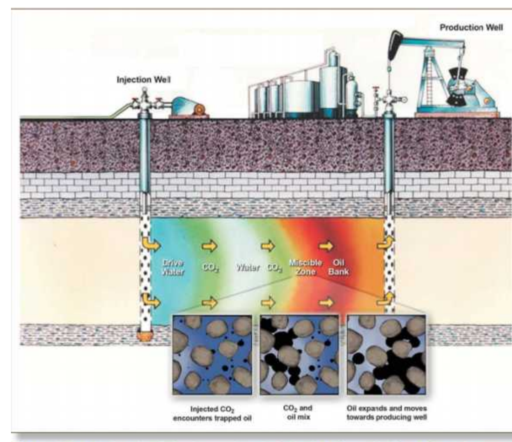
Energy storage: Battery electrodes

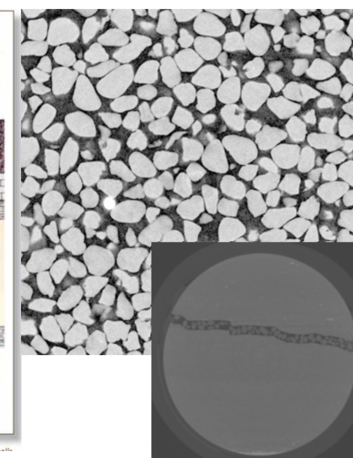
Energetic materials: phyrotechnics (dry powder), pbx's



A schematic drawing of an SLS process.





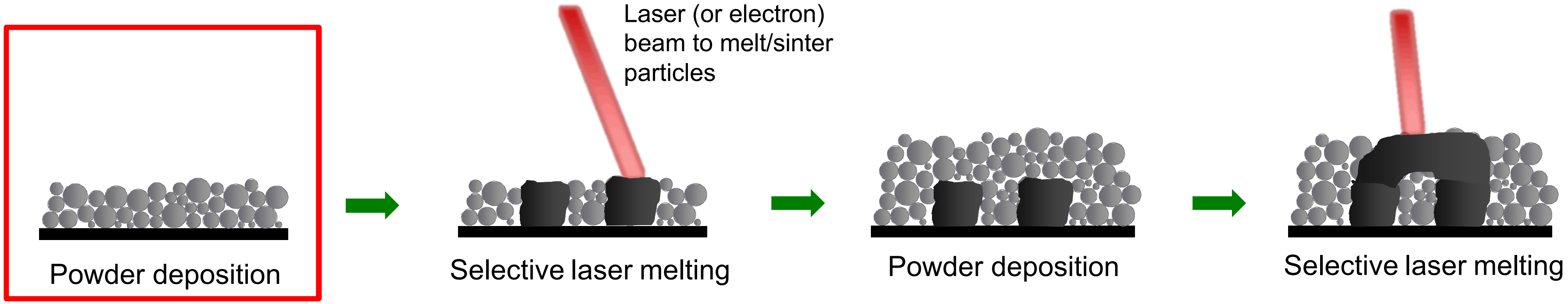


Additive Manufacturing: selective Laser melting/sintering

Waste repository: porous flow
Energy: fracking
Defense: Earth penetration

AM Powder-bed Process Motivation

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

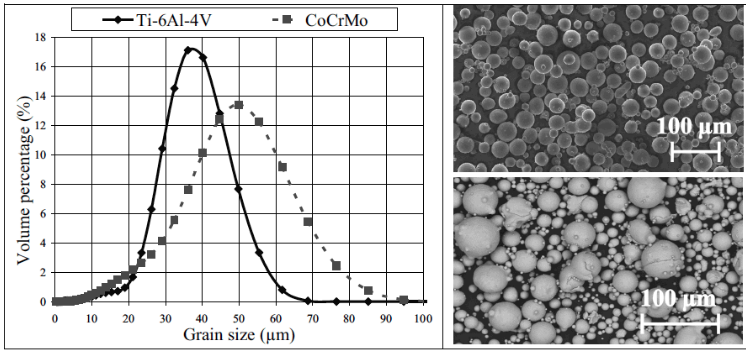


- Does powder matter?
  - 'Spreadability', even coverage are prerequisites for quality parts
  - **Surface structure** affects laser/powder bed interactions
  - **Bulk powder packing** affects defect formation/heterogeneity and surface finish of manufactured parts

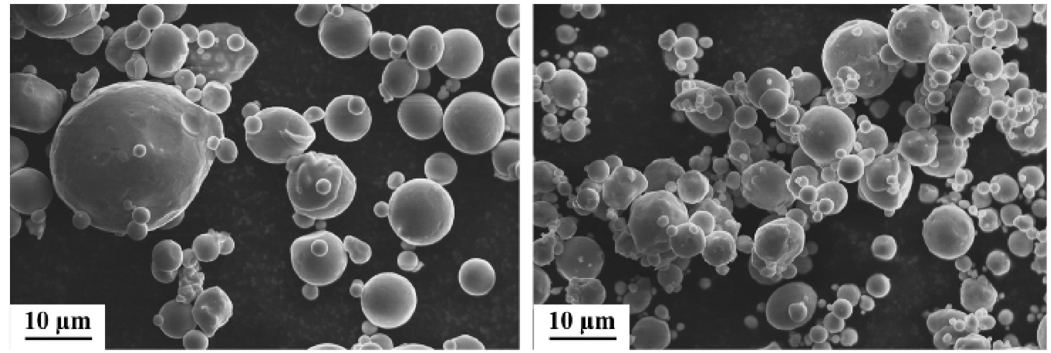
- Need to understand effects of **particle properties** and **powder process parameters**

- Models of laser interaction, powder melting/fusion depend on particle-scale structure

Typical powder characteristics



From Ref. 1



From Ref. 2

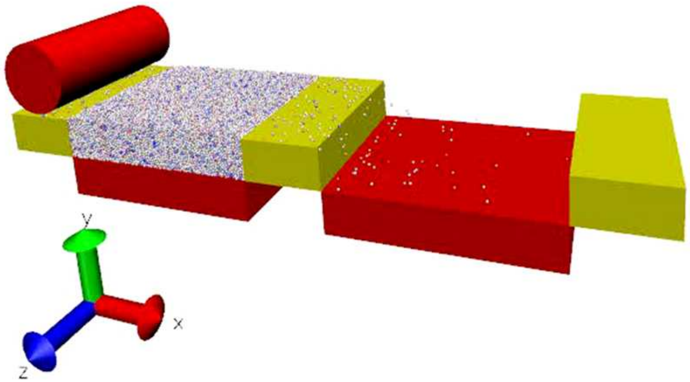
- Particle shape very close to spherical → well-suited for existing modeling capabilities
- Typical particle diameter: 10-100 µm; polydispersity factor 4-5
- Powder layer thickness 30-150 µm, laser beam spot size 70-200 µm (ref. 1)

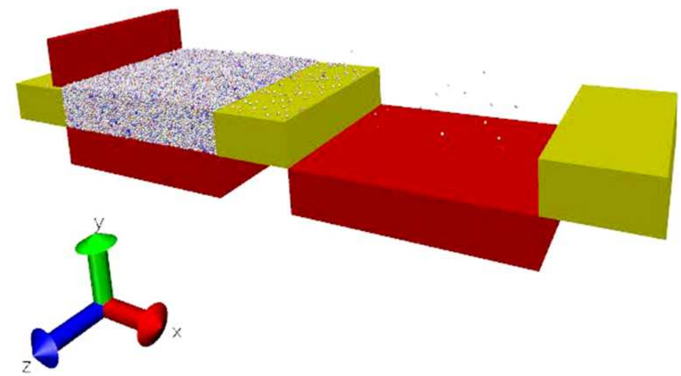
➡ Understanding powder bed structure at the scale of individual particles is important

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

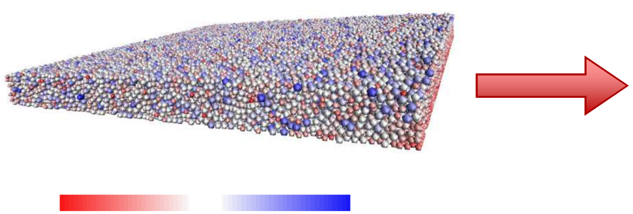
Overview

- Discrete Element Method (DEM) simulations of powder spreading (**LAMMPS**)





- Statistical characterization of resulting powder beds (static only)

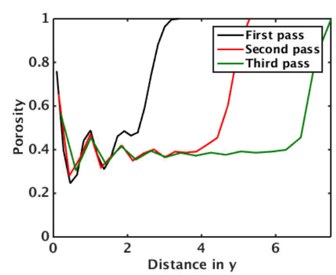


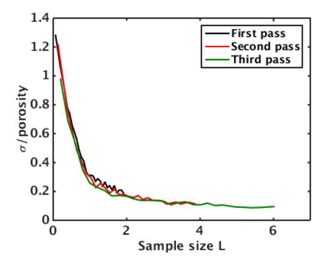
d = 0.7

d = 1.3

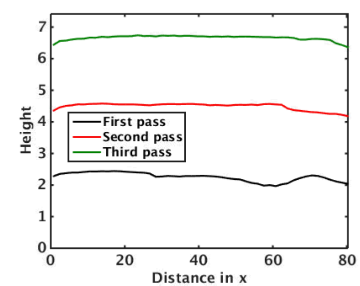
Particle diameter, d

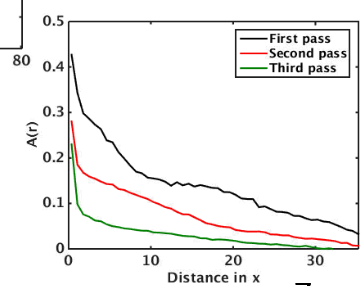
Bulk powder





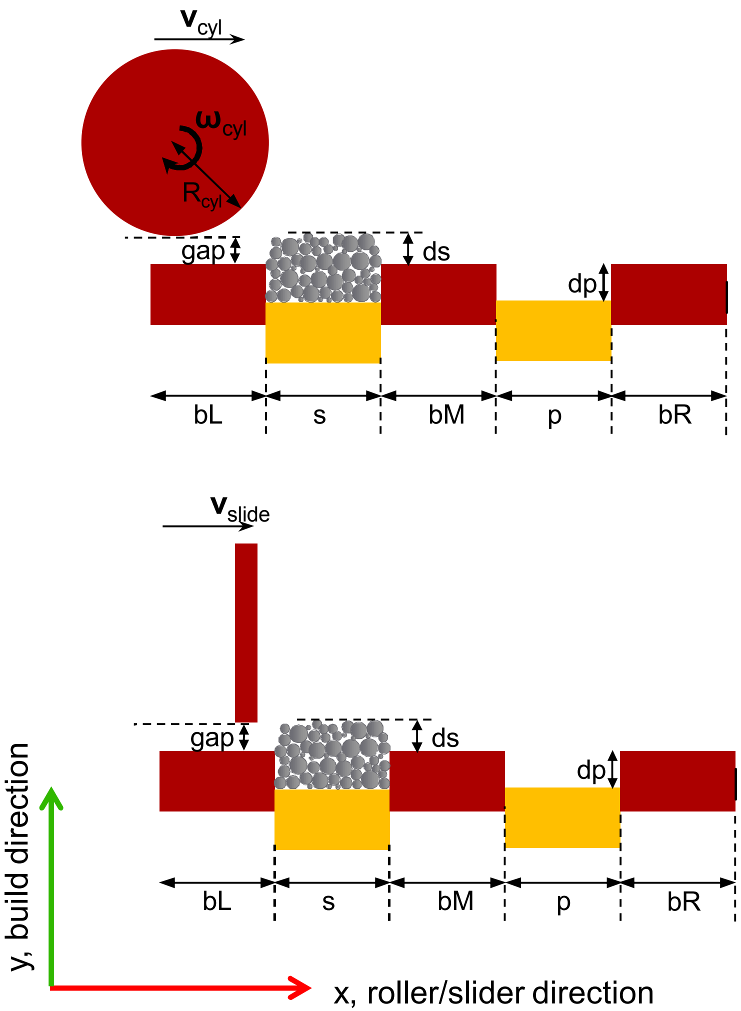
Powder bed surface



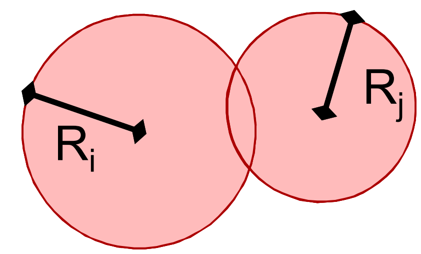


Large parameter space!

Process-related

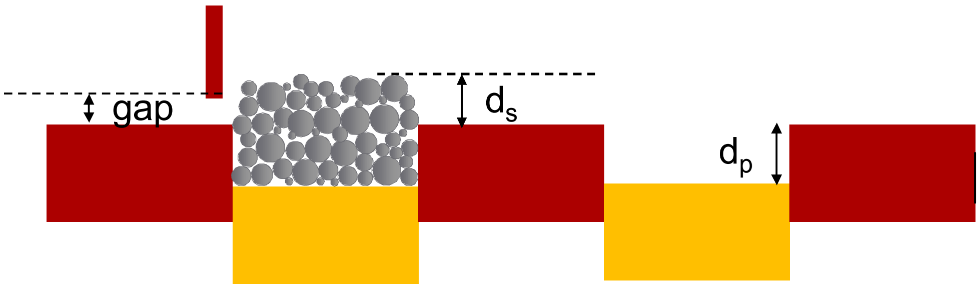


Particle-related



- Particle size distribution
  - Type of distribution
  - Mean, spread, skewness, …
- 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

Effects of powder layer thickness

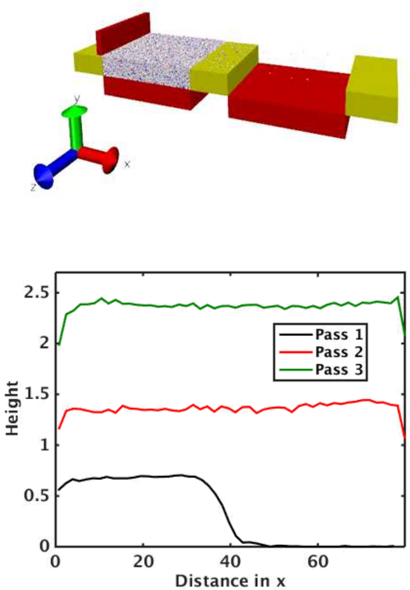


d_p: controls layer thickness

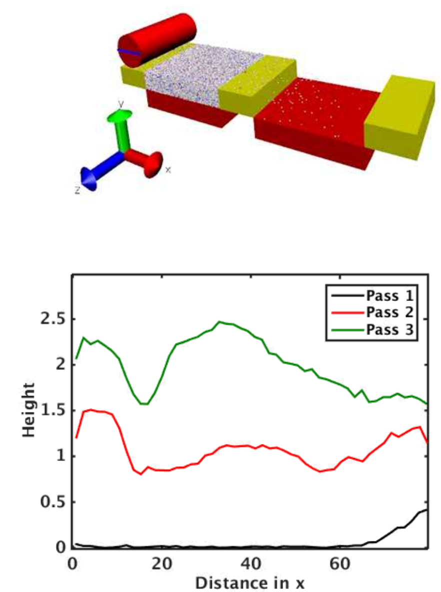
d_s: controls amount of powder

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

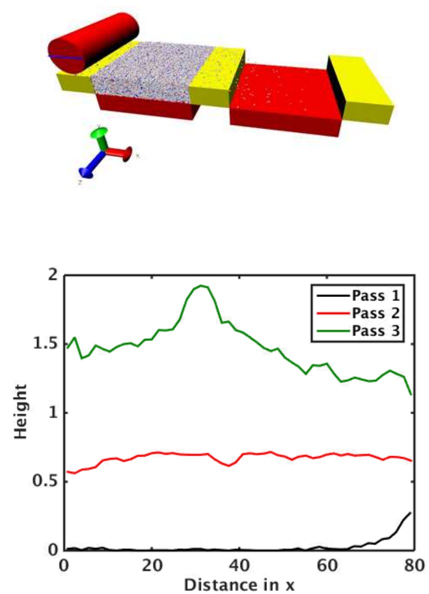
Slider
gap = 0, d_s = 1.5, d_p = 1.0



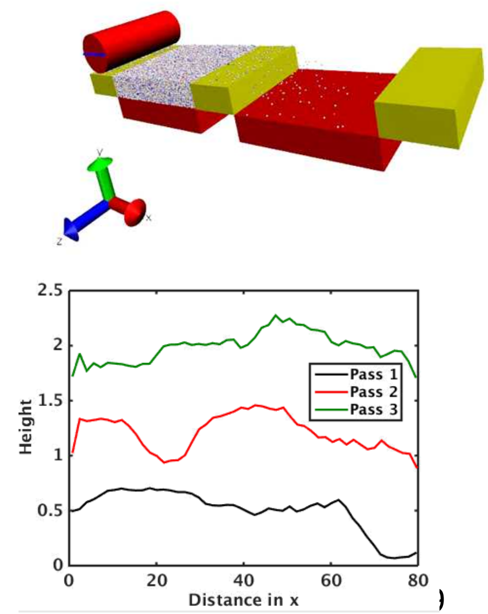
Roller/reverse
gap = 0, d_s = 1.5, d_p = 1.0



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

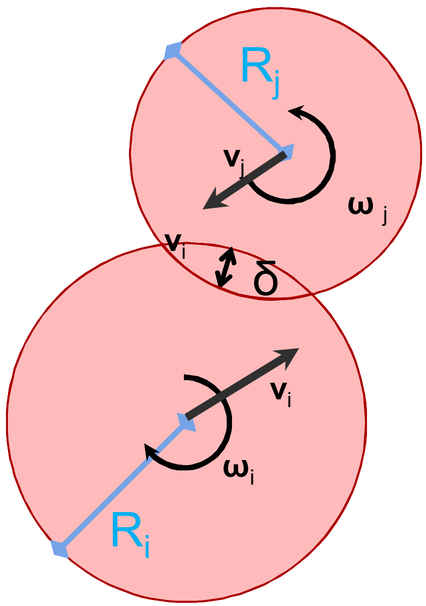


Roller/forward
gap = 0.5, d_s = 1.5, d_p = 1.0



Effect of particle friction coefficient

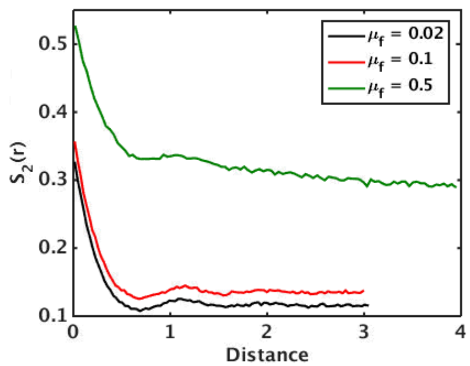
Powder bed surface properties also affected, but notable differences in bulk packing structure:



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

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

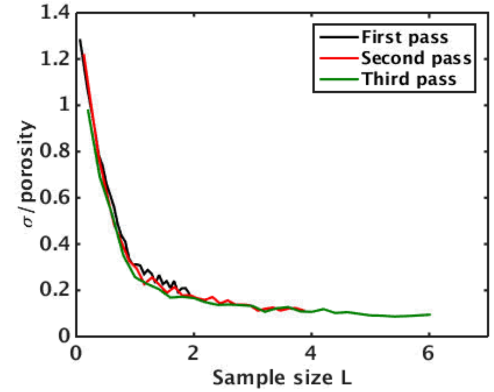
Two-point correlation function



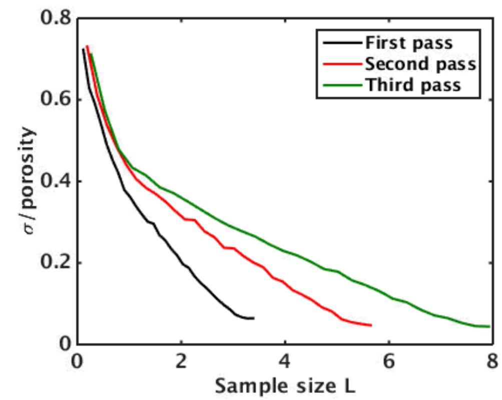
- Note that bulk porosity = $S_2(0)$
- Trends hold regardless of other process parameters

Coarseness

Low friction μ_f=0.1



High friction μ_f=0.5



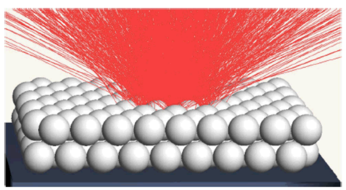
Ongoing/related work

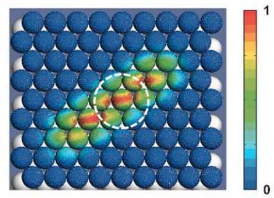
- Improvements to model fidelity through characterization of powder dynamics (‘flowability’)
  - Particle contact parameters: need to parametrize based on experimental data

Collaboration with NSC (Bryan Sartin, Ben Brown)
and possibly Freeman technologies (Jamie Clayton)

  - More realistic machine geometries/process parameters; spreading near/on top of partially manufactured parts

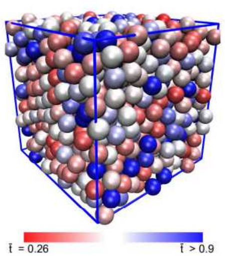
- Ray-tracing calculations to compute absorptivity of laser: collaboration with LLNL (Charles Boley and Sasha Rubenchik)

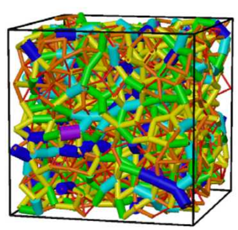


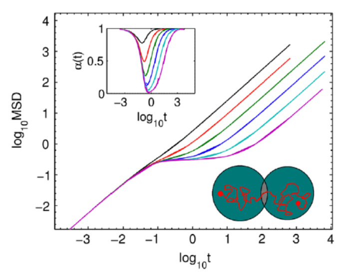


From Boley et al, Appl. Optics v 54, p 247 (2015)

- Calculations of conduction properties in particle packs (Jeremy Lechman, 1516), coupling to macroscale thermal models (Rick Givler, 1516)







From Bolintineanu, Lechman, et al, Phys Rev Lett v. 115, 088002 (2015)

- Coupling to mesoscale melting/flow models (Mario Martinez, 1516)

“Sticky” Particles: JKR/DMT Adhesion Theory

- Modify contact normal force for attraction
- Modify sliding criterion
  - Amonton’s Law

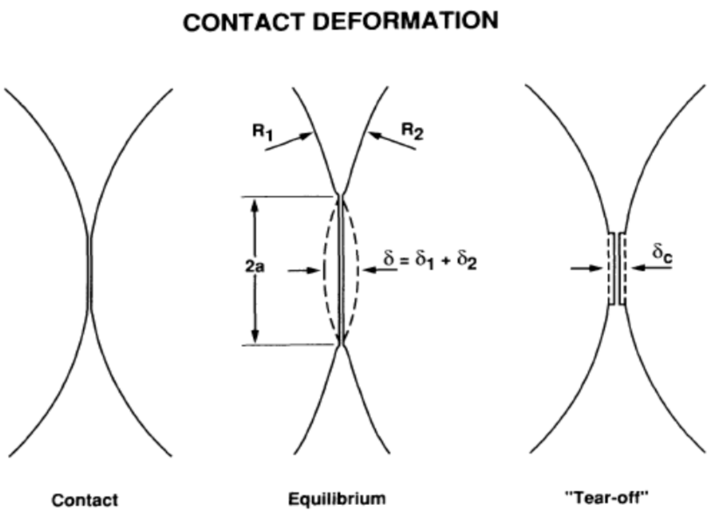
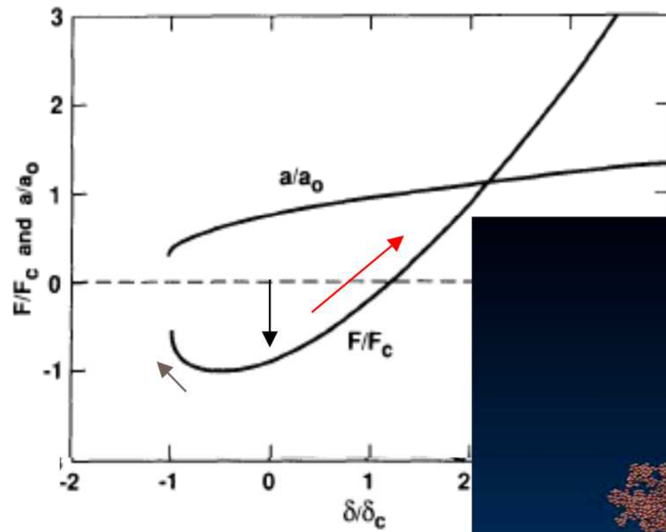
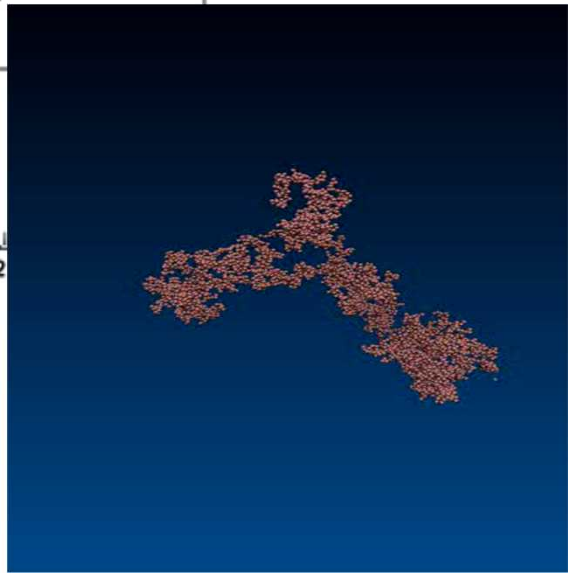


FIG. 2.—Schematic of the deformation during the collision process. At contact, a finite contact area is rapidly formed. This contact area grows in size during the compression and slowing down of the collision partners. Upon reversal of the collision process, the two grains will pull out a neck area, until they separate at a critical displacement, δ_c. See text for details.

From Chokshi, Tielens and Hollenbach (1993), ApJ





CHARACTERISTICS OF THE COLLISION PROCESS

Parameter	δ/δ_c	a/a_0	F/F_c	$U_T/F_c\,\delta_c$
Contact	0	$(2/3)^{2/3}$	$-8/9$	$-(8 \times 4^{2/3}/15)$
Equilibrium	$(4/3)^{2/3}$	1	0	$-(4 \times 6^{1/3})/5$
δ_{max} [a]	2.79	1.23	1.96	0
Tear-off..............	-1	$(1/6)^{2/3}$	$-5/9$	4/45

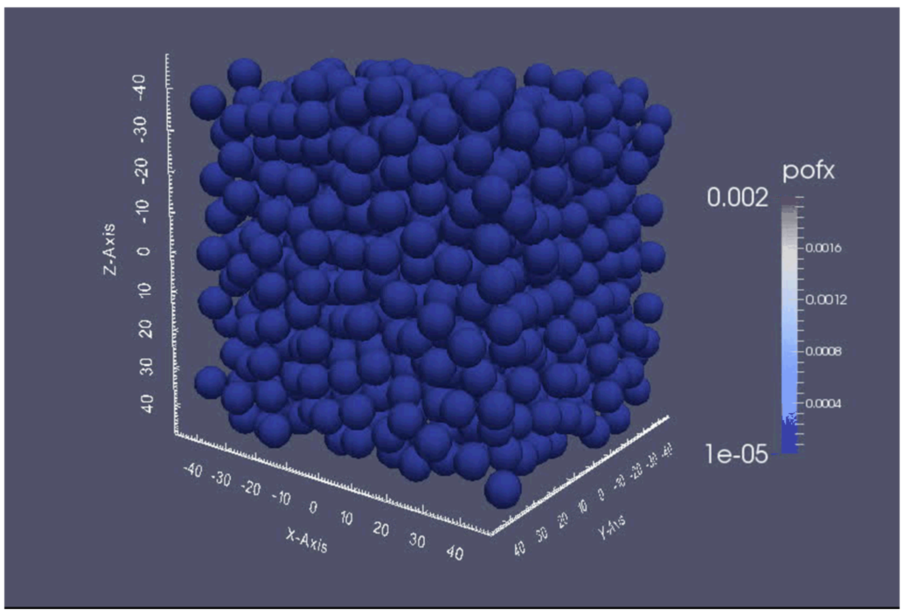
[a] Maximum compression, calculated assuming no initial velocity upon contact.

Simulate Markov Process on Contact Network

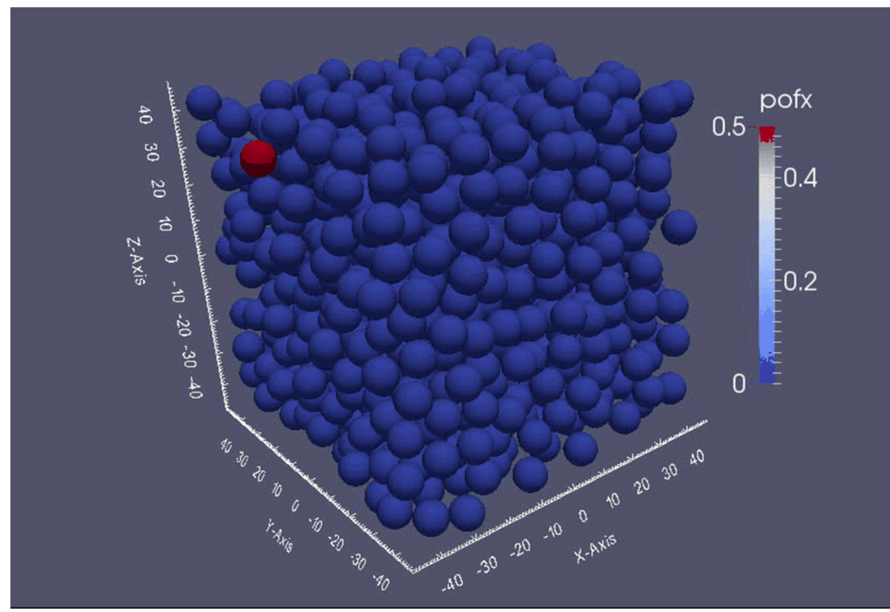
- Discretize Continuous-Time Equation

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

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



p = 0.0004



p = 0.00004

EXTRA SLIDES

The Multi-scale Transport Picture *through* Particulate Media

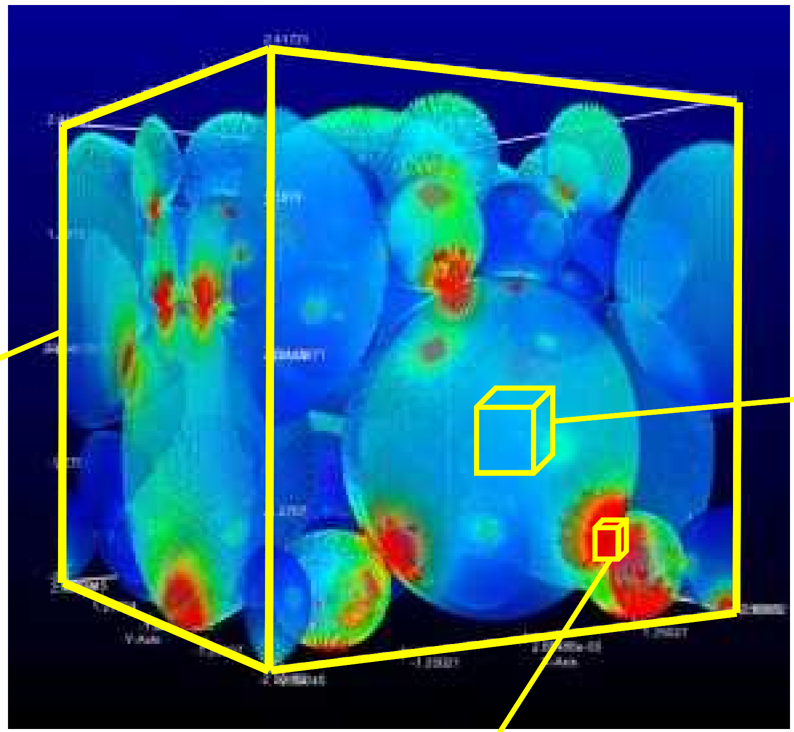
(1) Bulk, Macroscale
- Homogeneous
- “Continuum”
- Constant transport coef.

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

bridging

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

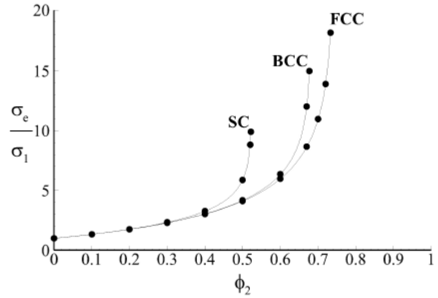
$$0 = \nabla \cdot \mathbf{q}(\mathbf{x}) = \nabla \cdot \left(K(\mathbf{x}) \nabla T(\mathbf{x}) \right)$$



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

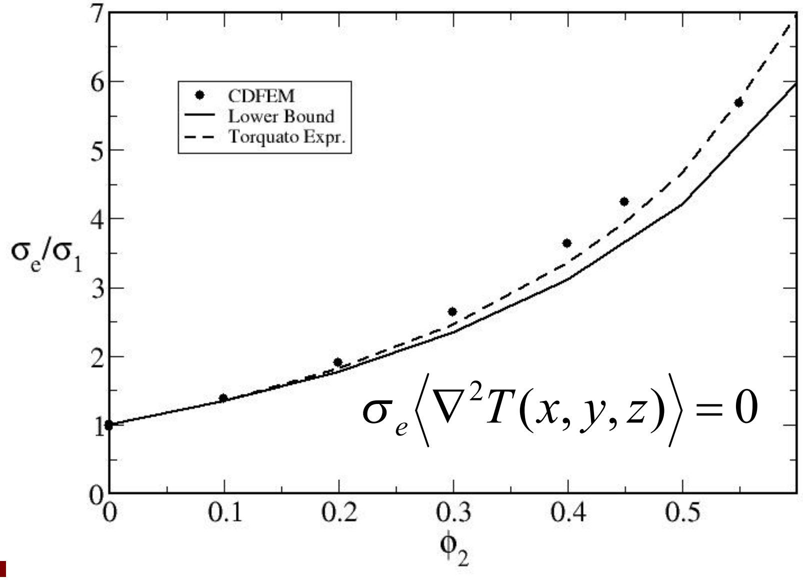
(4) Interfacial Scale
- Contact area, roughness, inter-diffusion
- Material types (e.g., phonon, electron dominated)

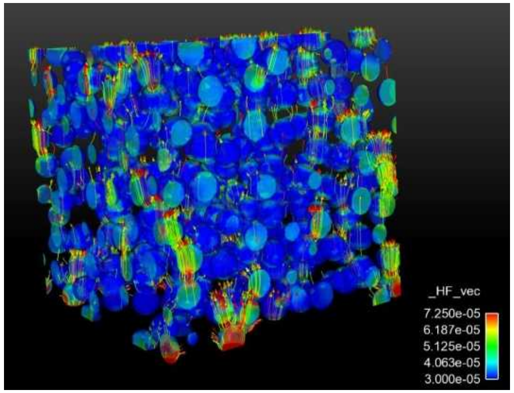
Effective Thermal Conductivity of Particle Dispersions

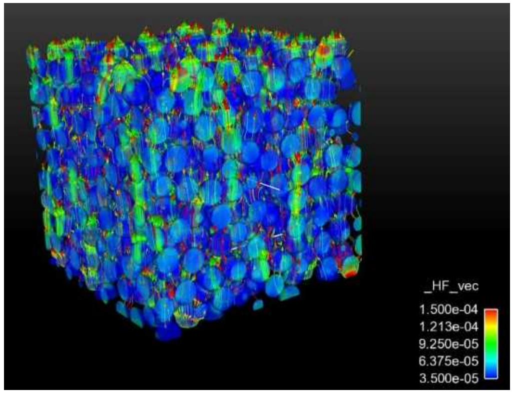


- Verification of CDFEM for Average thermal conductivity in static random dispersions
  - Particle configurations taken from Brownian Dynamics Simulations of Repulsive Colloids
  - Suspending fluid insulating, particles conductive (ratio of conductivities ~ 1000)

$$\left\langle \nabla \cdot \left(\sigma(x,y,z) \nabla T(x,y,z) \right) \right\rangle = 0$$







Exceedance Probability (Survival Function)

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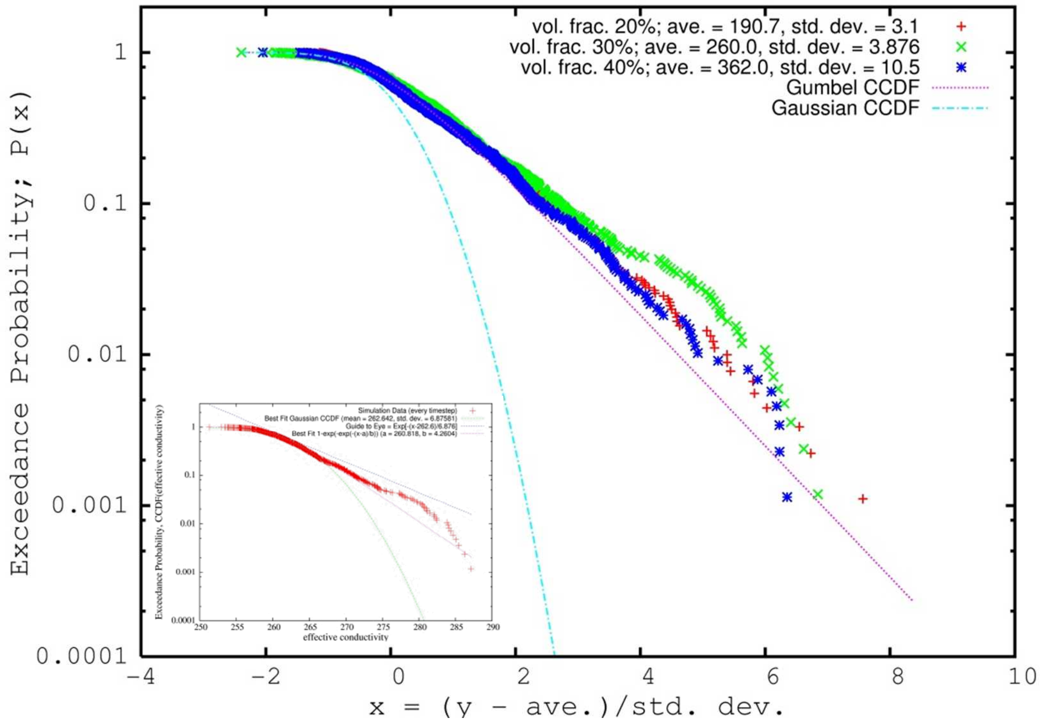
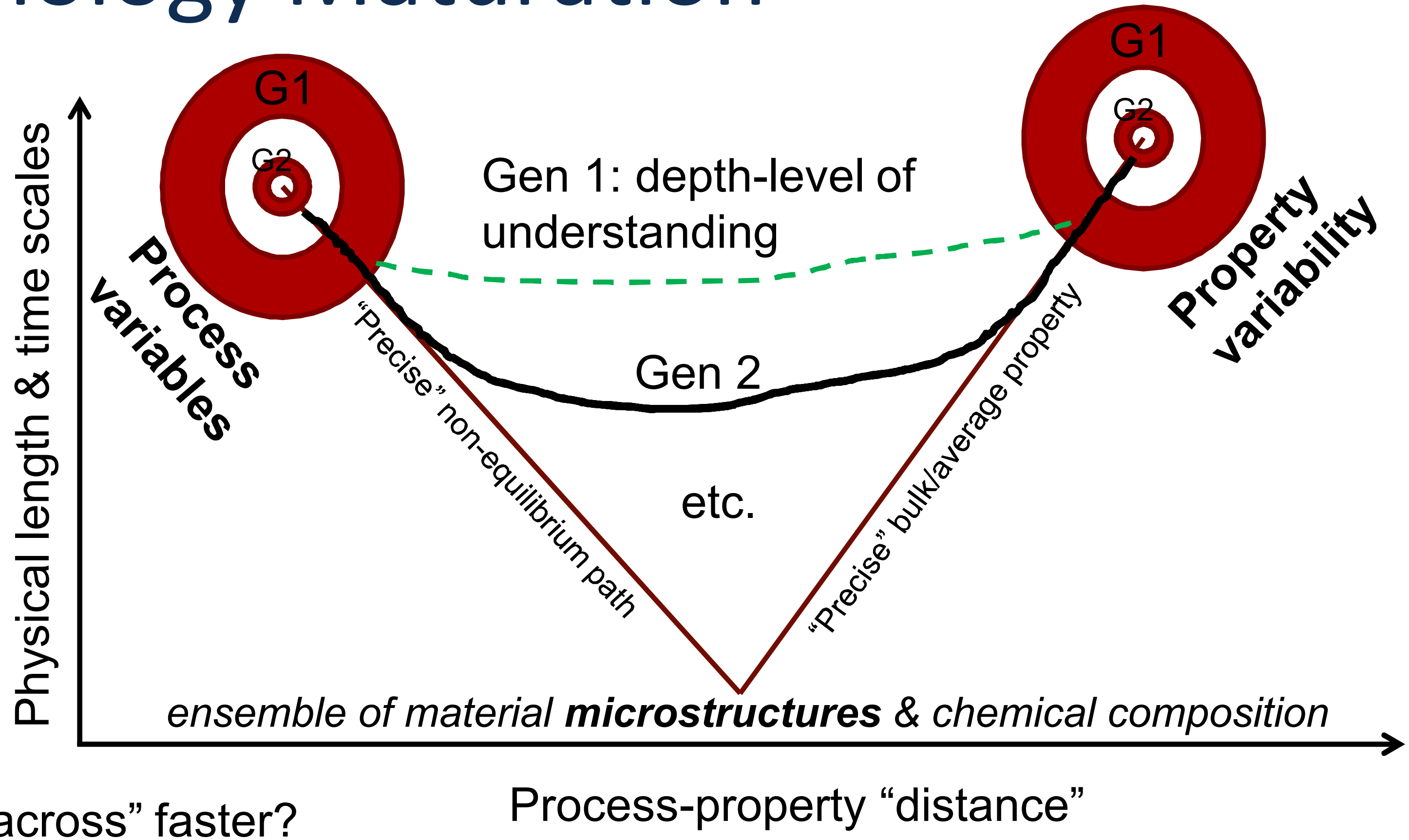
- **Based on sampling ~1000 μstructures**
  - "Aleatory" Uncertainty only
- What is "irreducible" about this uncertainty?
  - Note Gumbel distrib. and extreme-value-type statistics
    - "medium tailed", between Frechet and Wiebul
- What are sources of epistemic uncertainty?
    - Micro-structure resolution, thermal conductivity measurement

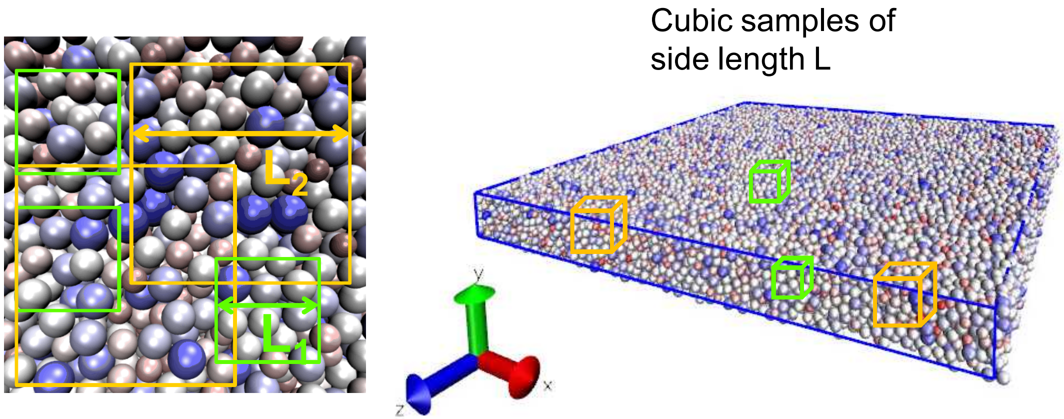


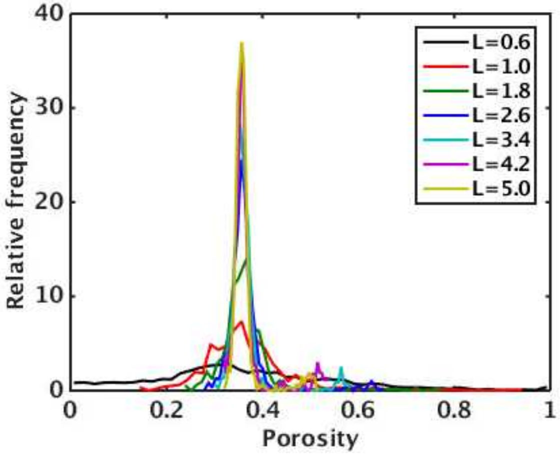
Process-Structure-Property and Technology Maturation



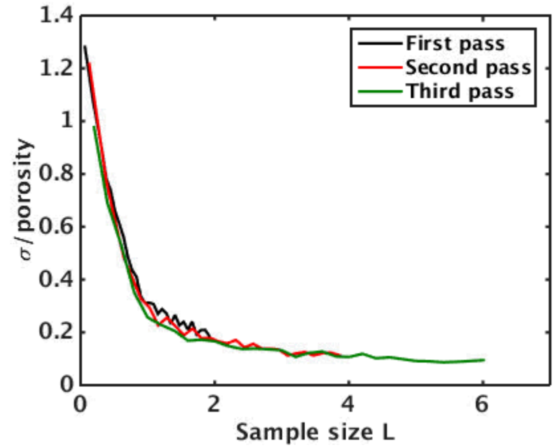
- Want to go "across" faster?
  - Determines time to solution/delivery
- Want to go "deeper" faster?
  - Determines time to innovation
- Want to go "around"/iterate faster?
  - Determines rate of "cycle of learning"

Descriptors of bulk powder bed: ‘coarseness’



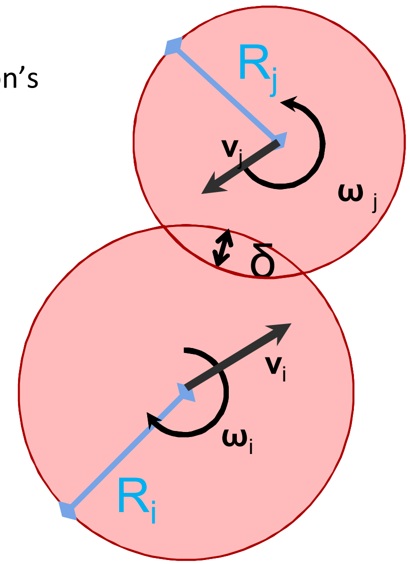


- For given size L, take many sub-samples, compute distribution of porosity
- Plot L vs standard deviation of porosity at each sub-sample size



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:

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

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

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

- 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

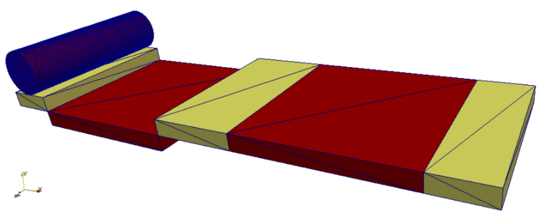
Total force: $\mathbf{F}_{i,tot} = m_i\mathbf{g} + \sum_j(\mathbf{F}_{n,ij} + \mathbf{F}_{t,ij})$

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.

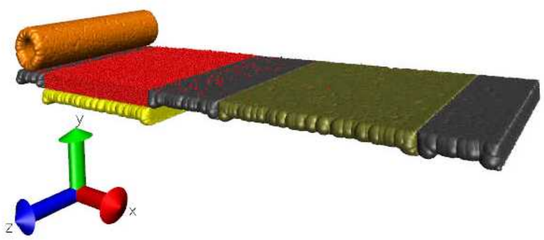
Simulations of powder spreading

- Several approaches to representing complex, moving boundaries in DEM



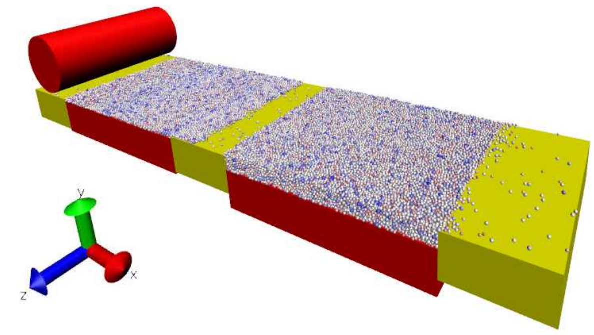
Surface triangle mesh[1]

- 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

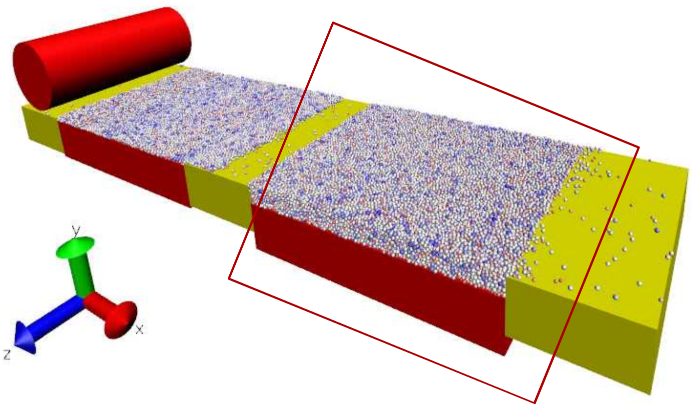


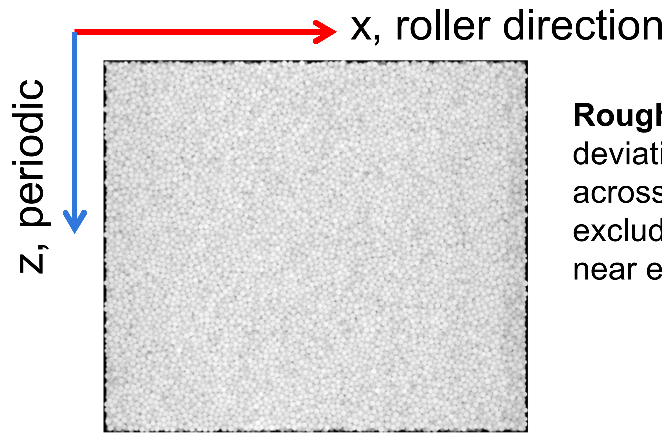
Geometry primitives[2]

- 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**

Descriptors of powder bed top surface

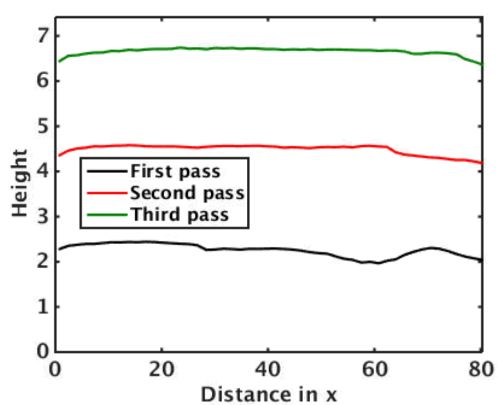




Roughness: standard deviation of height (σ) across entire pack, excluding small region near edges

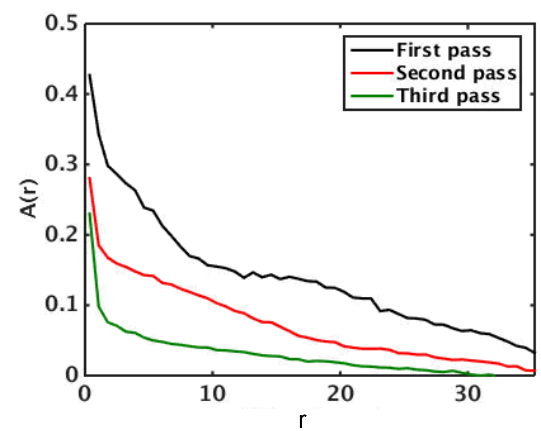
Top view, grayscale intensity corresponds to height

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

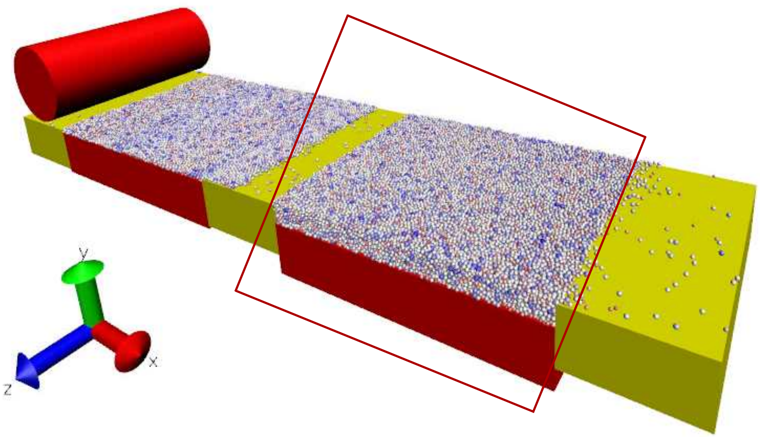


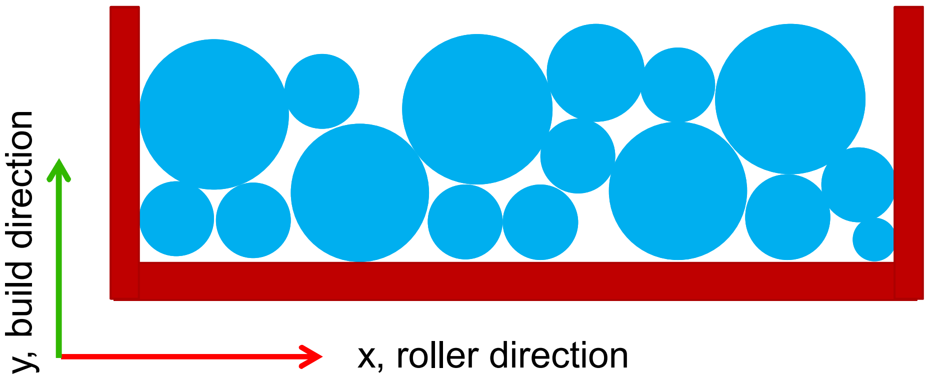
Height autocorrelation function:

$A(r) = \langle (H(\mathbf{x})-\mu)\,(H(\mathbf{x}+\mathbf{r})-\mu) \rangle / \sigma^2$

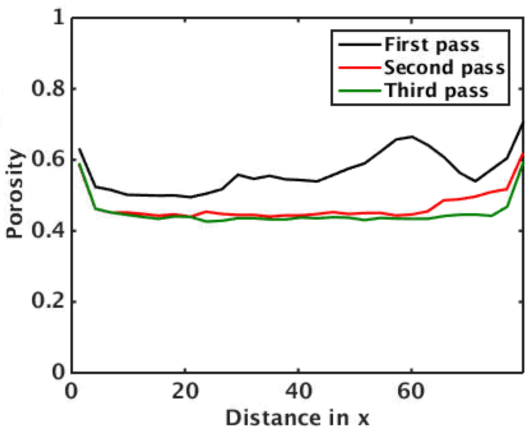


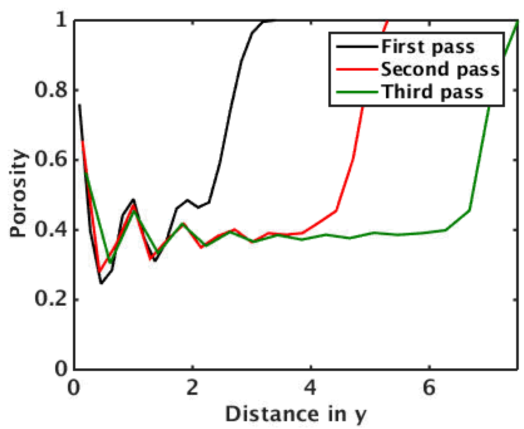
Descriptors of bulk powder bed



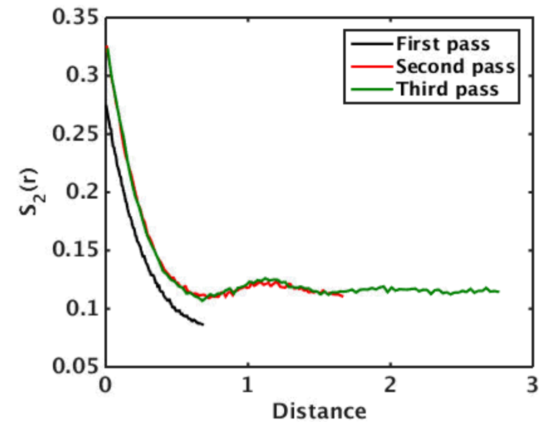


Porosity variation in x, y





Pore space two-point correlation function



Effects of spreader speed

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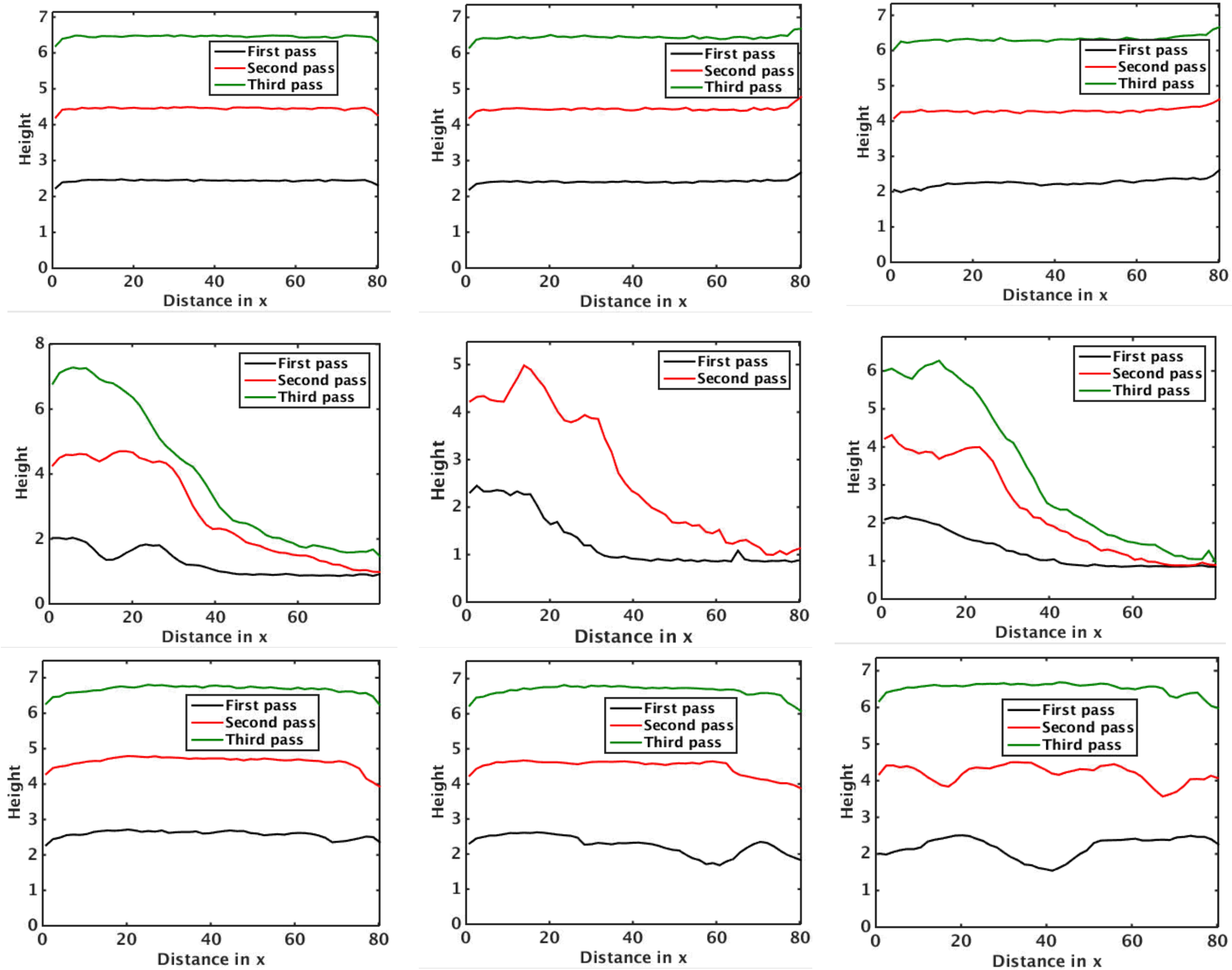
Increasing speed

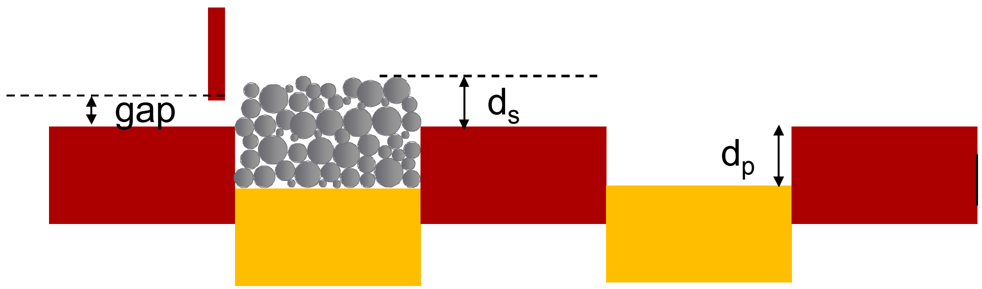
Slider

Roller
forward rotation

Roller
reverse rotation



Effects of powder layer thickness

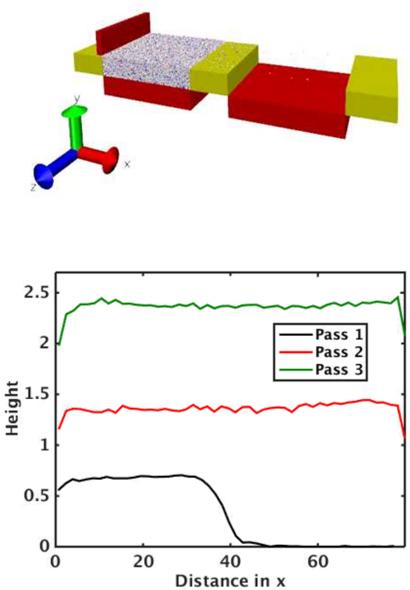


d_p: controls layer thickness

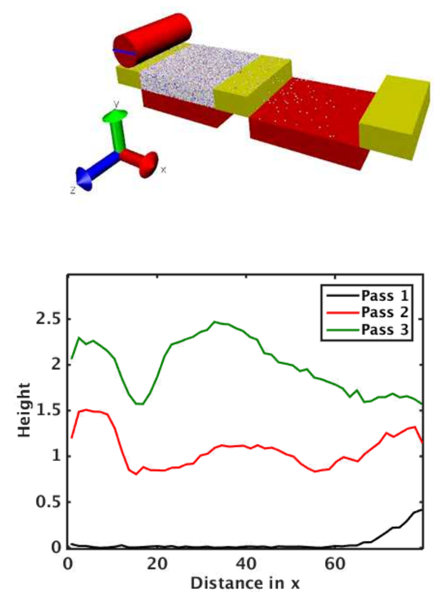
d_s: controls amount of powder

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

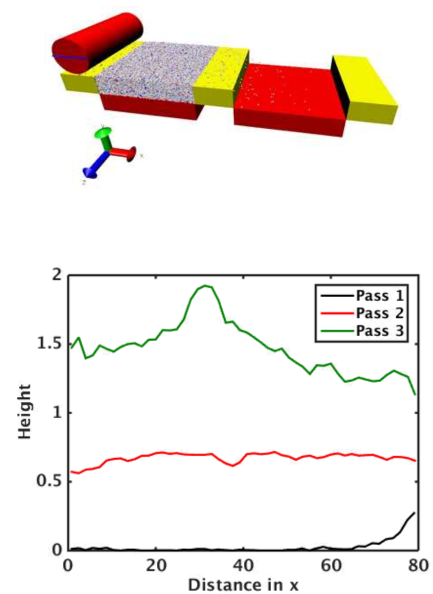
Slider
gap = 0, d_s = 1.5, d_p = 1.0



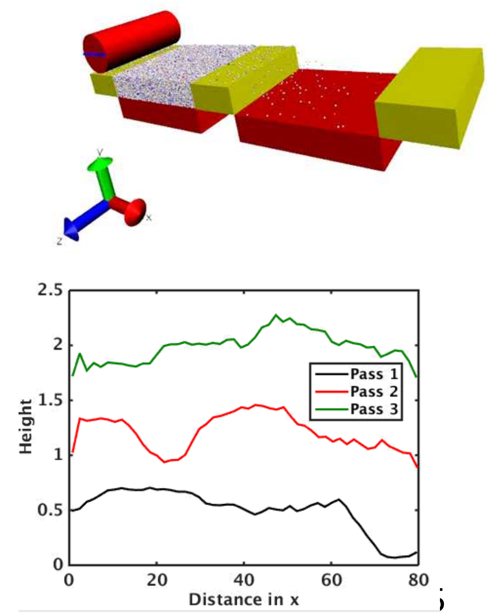
Roller/reverse
gap = 0, d_s = 1.5, d_p = 1.0



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

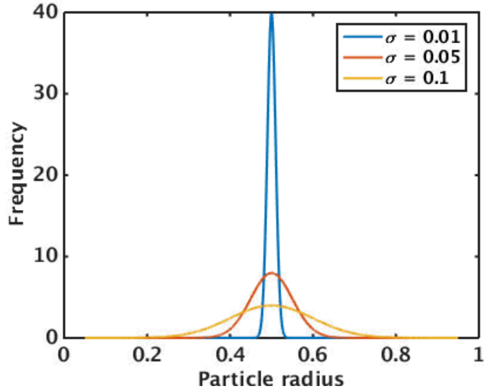


Roller/forward
gap = 0.5, d_s = 1.5, d_p = 1.0

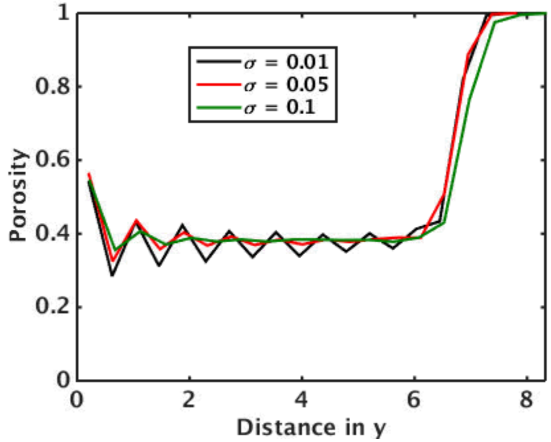


Effects of particle size polydispersity

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

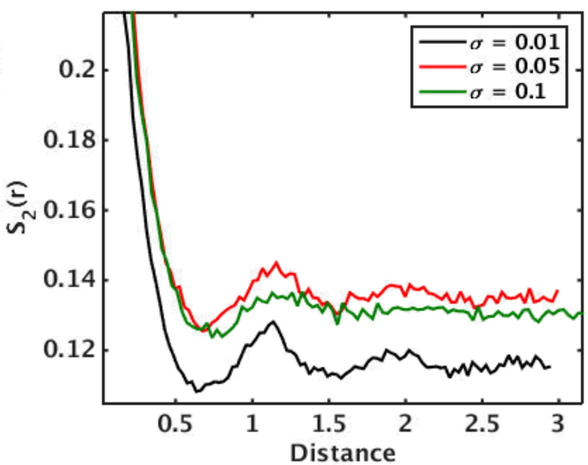


Porosity in the height direction, third pass of slider



Layering order decreases with larger polydispersity. Only slight differences in mean porosity.

Two-point correlation function



Less local structuring with larger polydispersity

Effects of spreader type

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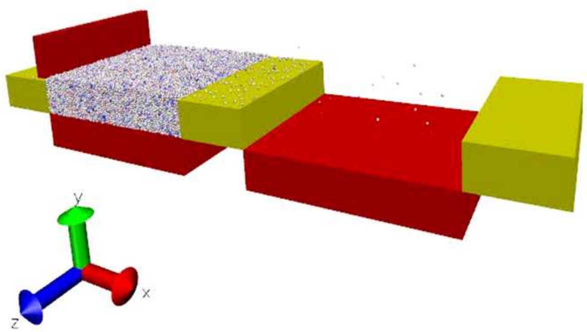
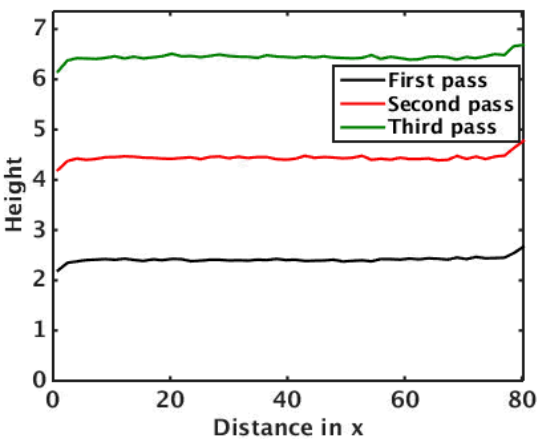
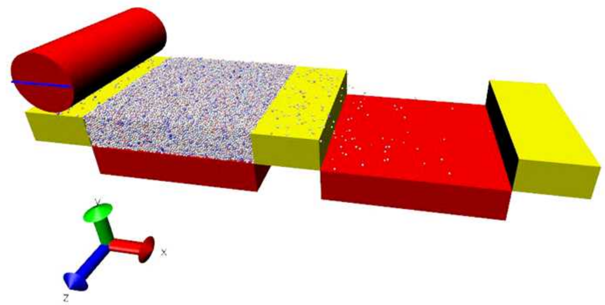
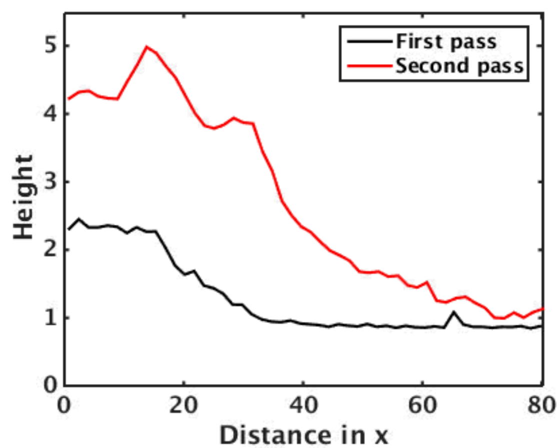
Slider





Roller, rotation in direction of translation (forward)





Roller, rotation against direction of translation (reverse)