Multiscale Modeling in Granular Flow

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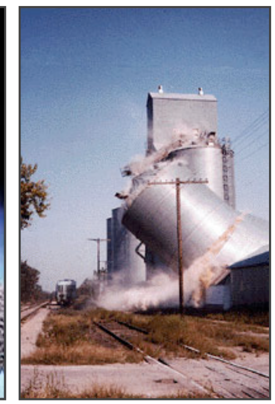
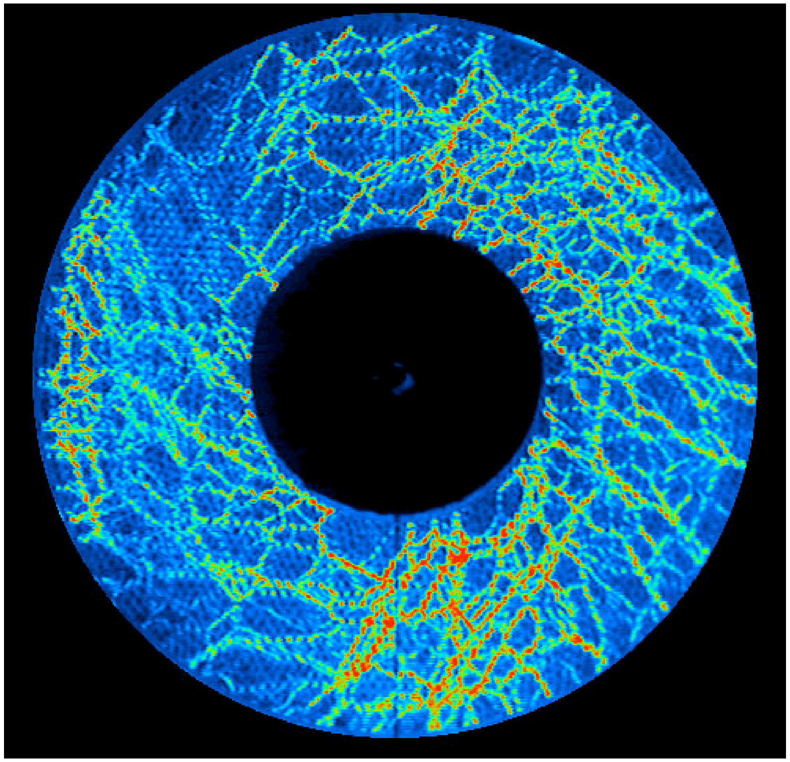


Problems modeling granular materials

- Particle discreteness:
  - Force chains
  - Difficulty defining material quantities
  - Inelastic collisions
- Solid-like and liquid-like behavior
- Numerically ill-posed continuum models



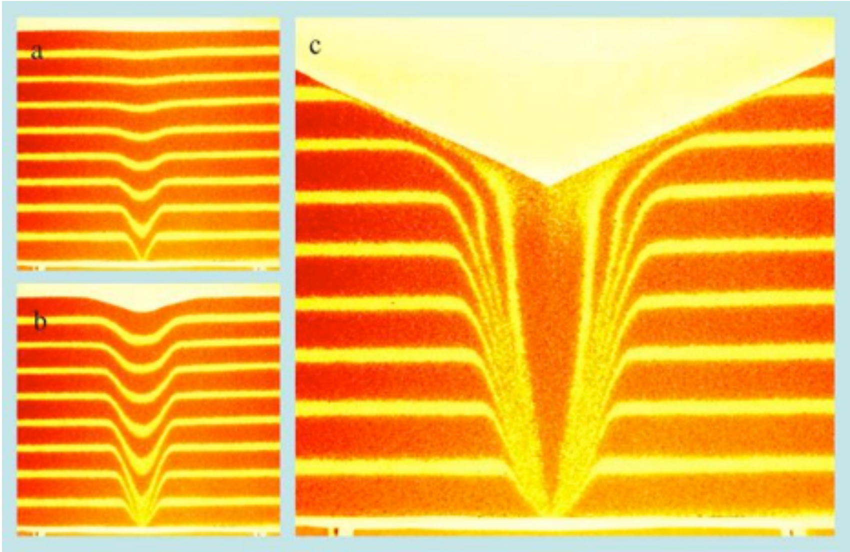
Force chains in a 2D shear cell

Majumdar and Behringer, Nature **435**, 1079 (2005).

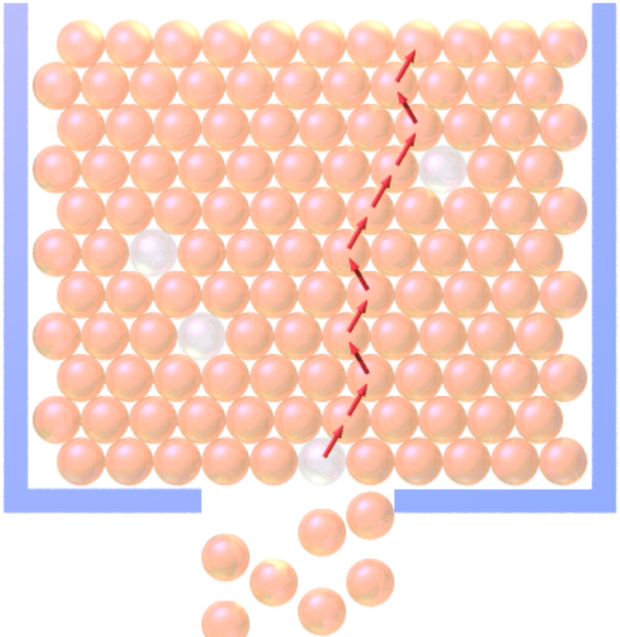
Smooth flow fields / Diffusive behavior

- Despite force chains, granular materials often exhibit smooth average flows
- Some, like granular drainage, suggest a diffusing object
- Only candidate in literature is a “void” of empty space – gives an unrealistic microscopic picture

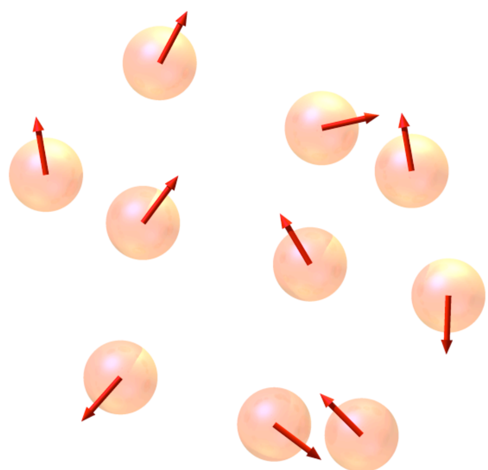
J. Mullins, *Stochastic theory of particle flow under gravity*, J. Appl. Phys. **43**, 665 (1972).

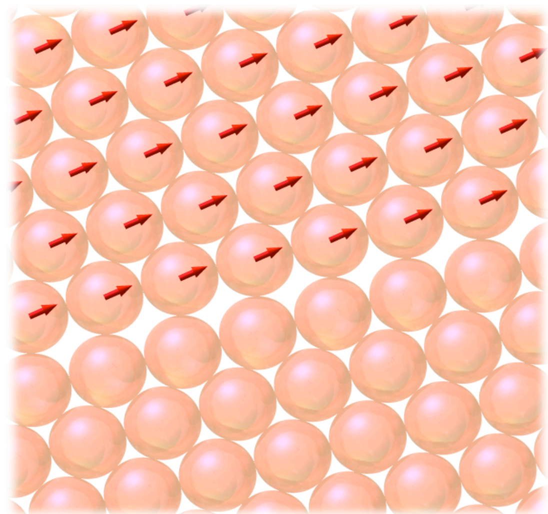


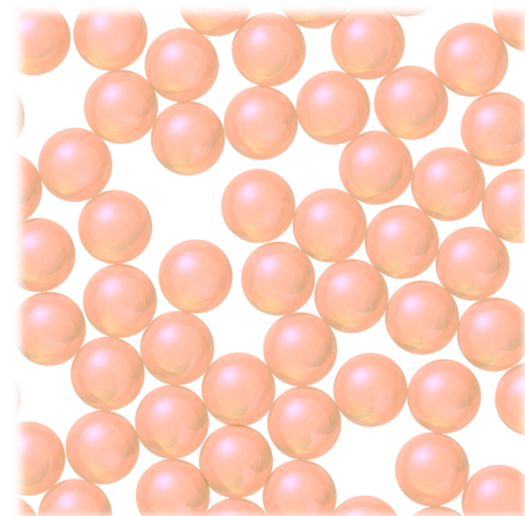
Kudrolli and Samadani, Clark University



Microscopic flow mechanism







Gas

Dilute, random "packing"

• Boltzmann's kinetic theory
• Sudden randomizing collisions

Crystal

Dense, ordered packing

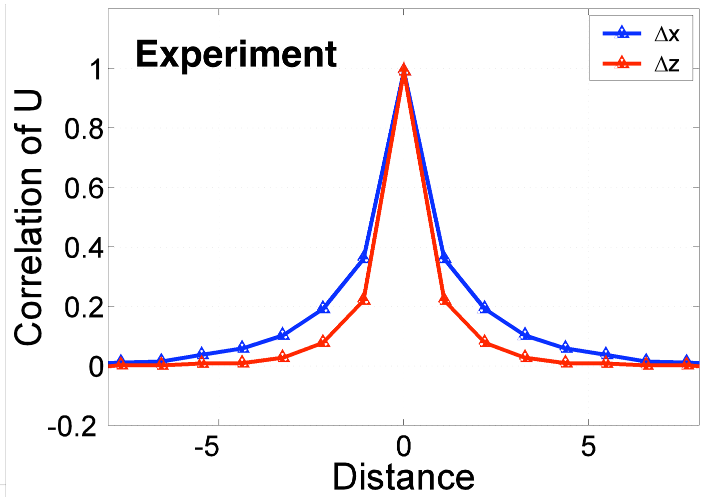
· Vacancy/interstitial diffusion
· Dislocations and defects

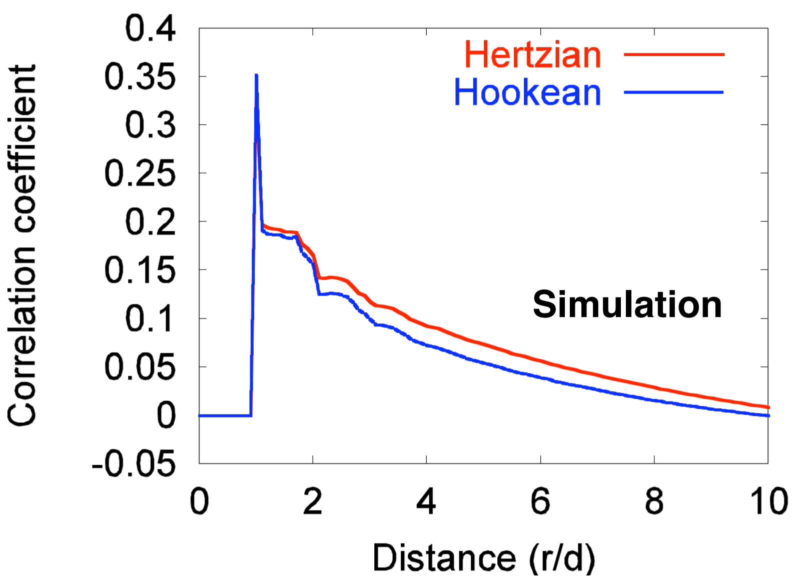
Granular

Dense, random packing

· Long lasting many-body contacts
· Unclear microscopic model

Velocity correlations

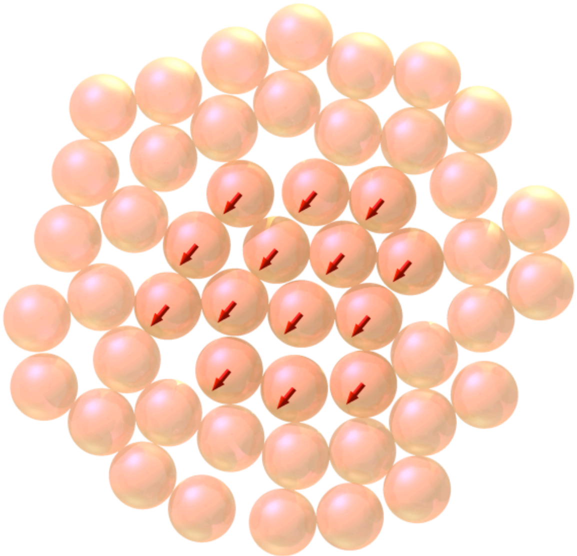




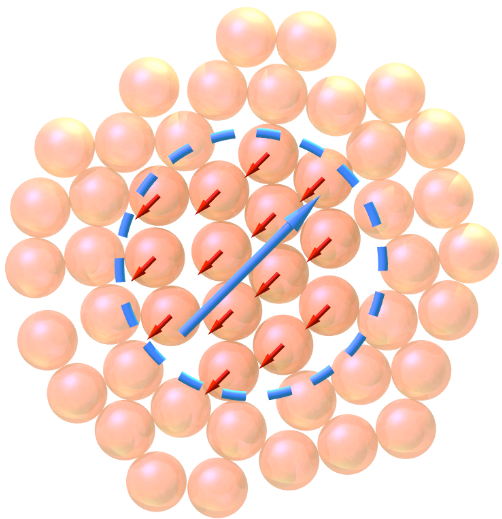
- Local velocity correlations

$$C(r) = \frac{\langle \mathbf{u}(0)\mathbf{u}(r)\rangle}{\sqrt{\langle \mathbf{u}(0)^2\rangle\langle \mathbf{u}(r)^2\rangle}}$$

- Suggests *correlated* motion



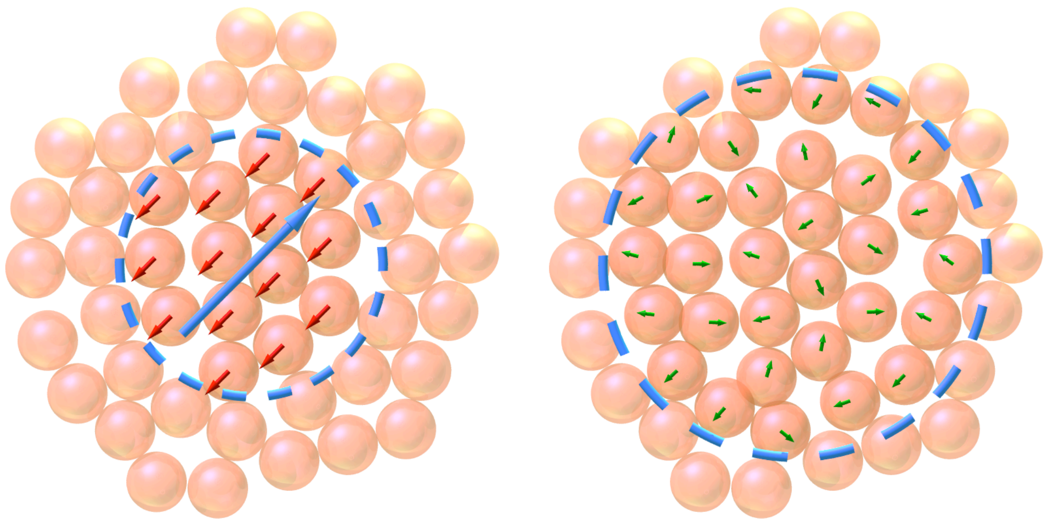
Spot model with relaxation



- An extended region of slightly enhanced interstitial volume
- Spots cause correlated displacements of passive, off-lattice particles within range

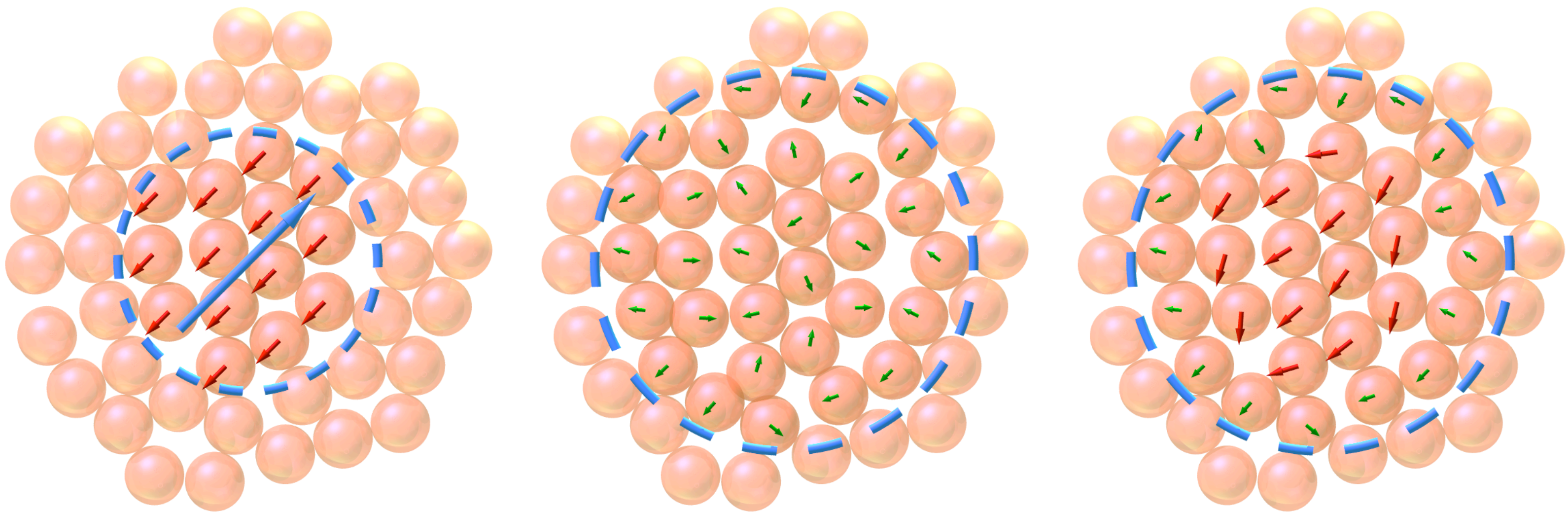
M.Z. Bazant, *The Spot Model for random-packing dynamics*, Mech. Mat. **38**, 717 (2005).

Spot model with relaxation



- Apply elastic relaxation to all particles within range
- All overlapping particles experience a correcting normal displacement

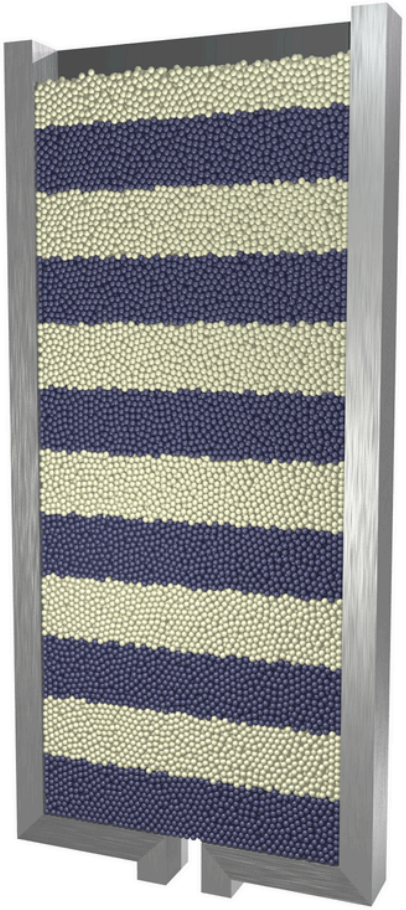
Spot model with relaxation



- The combination is a bulk spot motion, while preserving packings
- Not clear *a priori* if this will produce realistic flowing random packings

Brute-force simulation of granular flow

- Parallel Discrete Element Method (DEM) simulation:
  - Model particles according to Newton's Laws
  - Particles treated as soft spheres
  - History-dependent contacts
- Good quantitative match to experiment



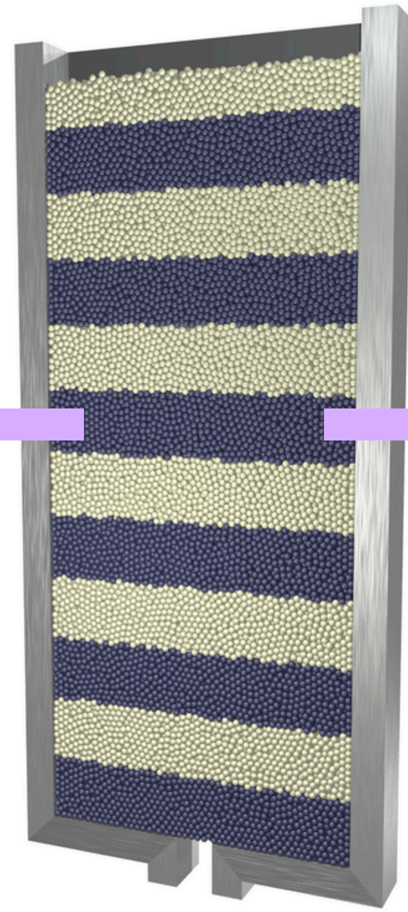
(55000 particles poured into a container of size 50*d* by 8*d* by 110*d*)

L.E. Silbert *et al.*, Phys Rev E, **64**, 051302 (2001).
J.W. Landry *et al.*, Phys Rev E, **67**, 041303 (2003).
C.H. Rycroft *et al.*, Phys Rev E, **74**, 021306 (2006).
http://lammps.sandia.gov/

Two very different simulations

DEM

- Particles drained from a circular orifice $8d$ across
- Snapshot recorded at fixed intervals
- Run on 24 processors



Initial packing of 55000 poured particles from DEM

Spot

- Spots introduced at orifice
- Event driven
- Spots move upwards and do random walk horizontally
- Calibrate free parameters from DEM

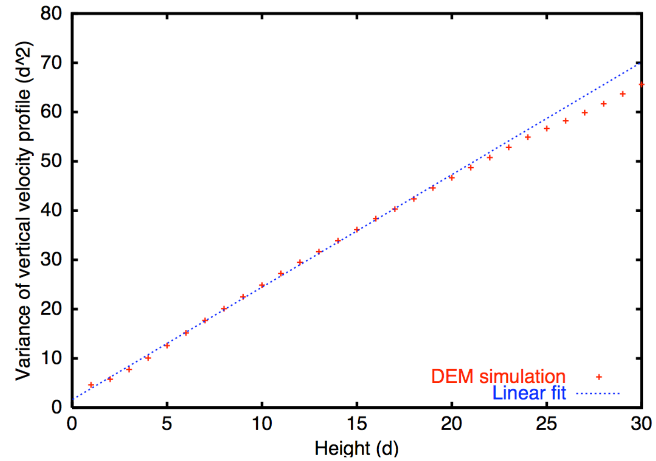
Calibration of spot simulation

- Systematically calibrate three parameters from DEM:
  - Spot radius R_s
    (from velocity correlations)
  - Spot volume V_s
    (from particle diffusion)
  - Spot diffusion rate b
    (from velocity profile width)

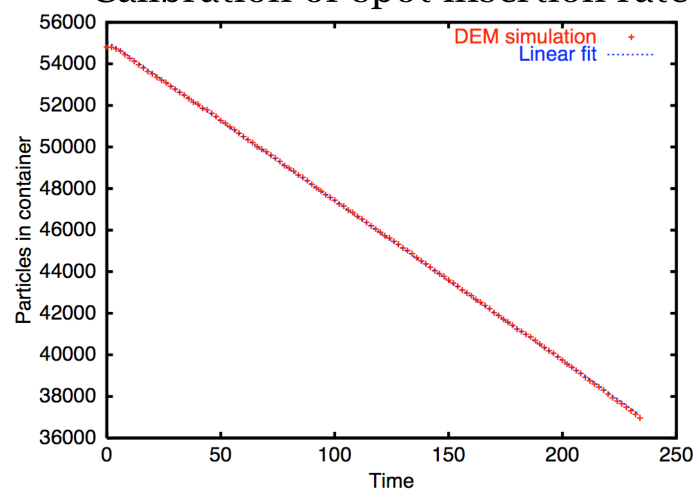
- Two more parameters to capture time dependence:
  - Spot insertion rate
    (from flow rate)
  - Spot velocity
    (from density drop)

Rycroft *et al.*, *Dynamics of Random Packings in Granular Flow*, Phys. Rev. E **73**, 051306 (2006).

Calibration of diffusion rate



Calibration of spot insertion rate



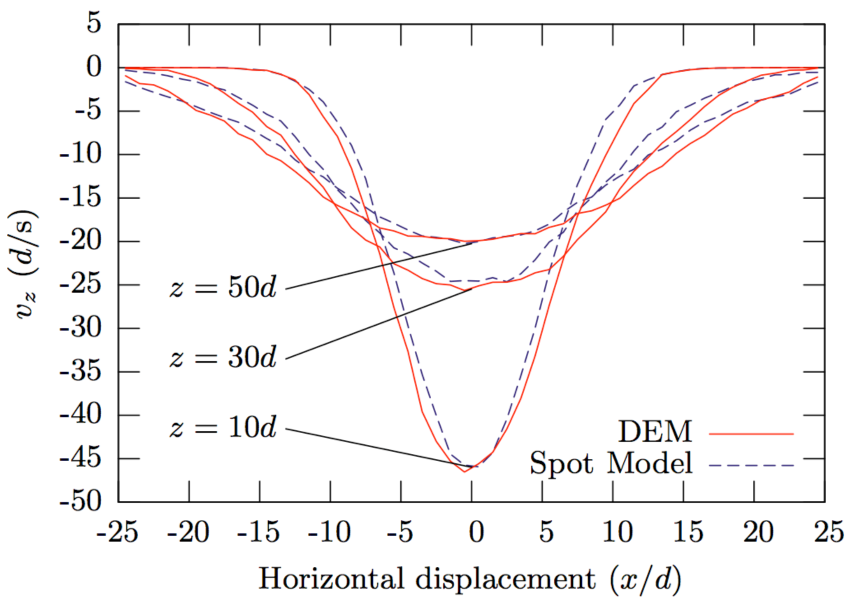
Spot / DEM comparison

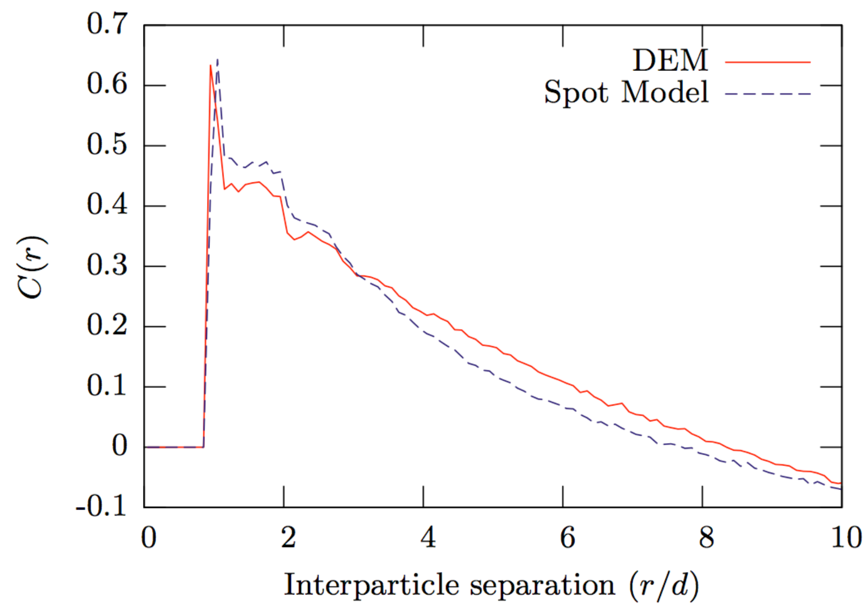
- Calibrated parameters:
  - $R_s = 2.6d$
  - $V_s = 0.2V_p$
  - $b = 1.14d$
- Spot model gives factor of 100 speedup
- No mechanics, only geometry

DEM simulation
(3 days, 24 processors)

Spot simulation
(8 hours, single processor)

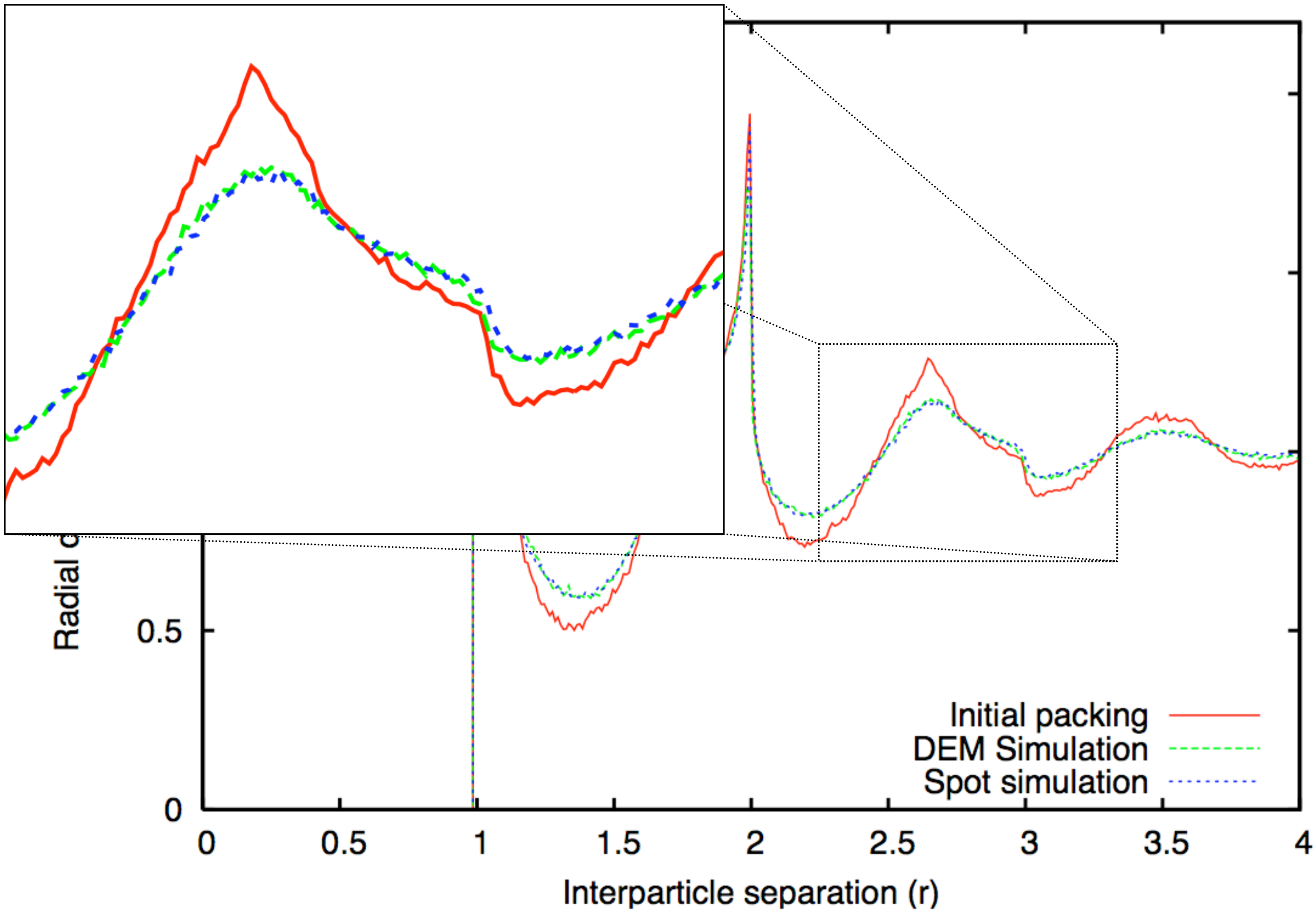
Velocity profiles and correlations



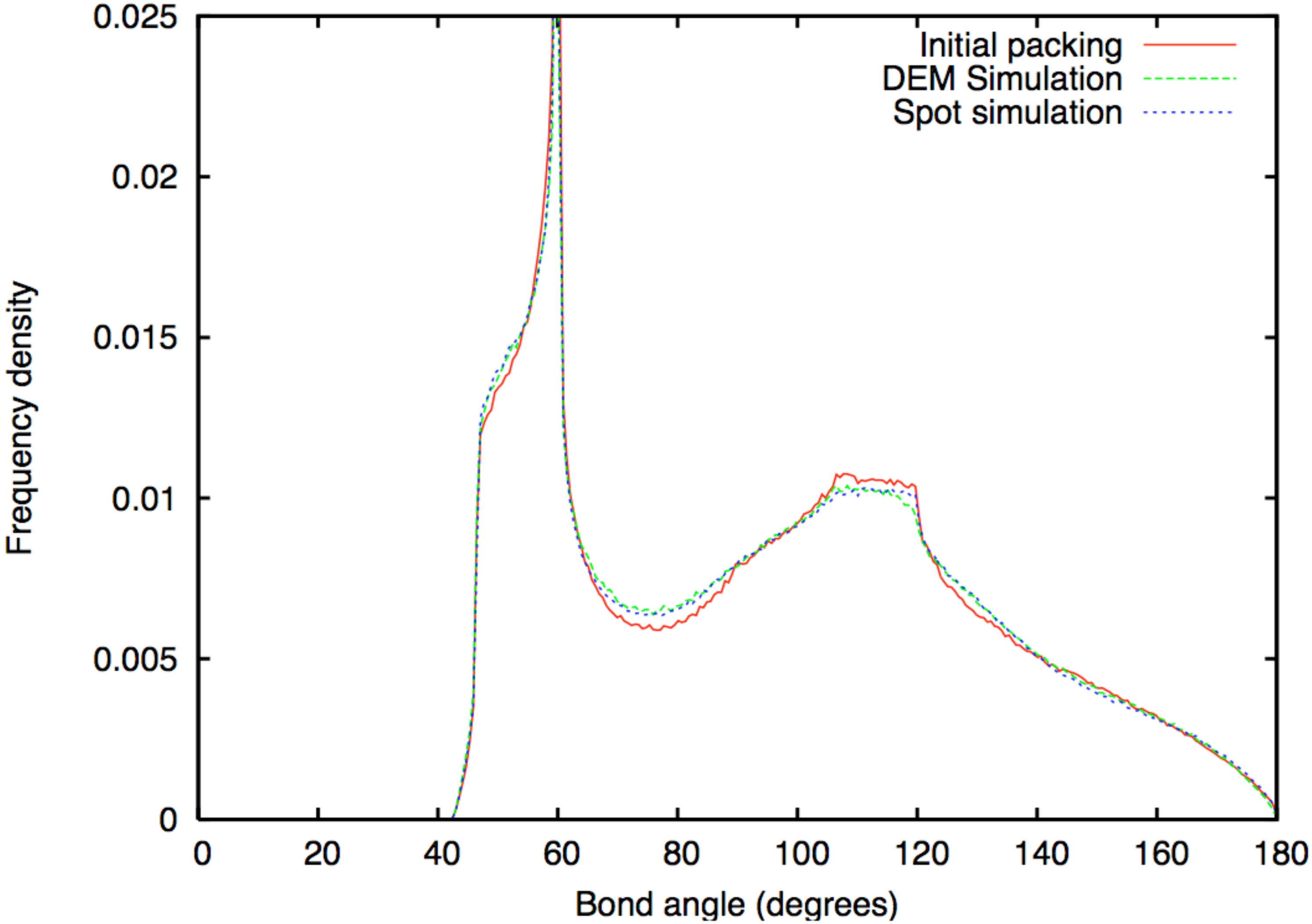


- Some parameters calibrated, but very good match of functional forms to DEM
- Velocity profile more plug-like at z=50d

Microscopic packing statistics



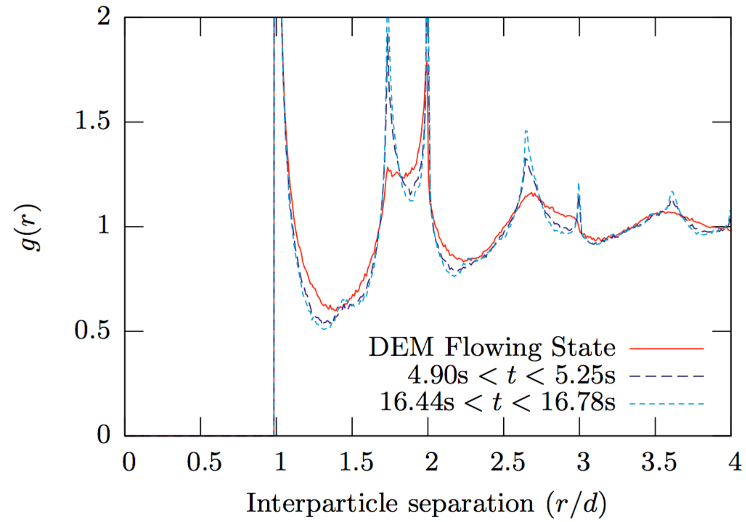
Bond angles



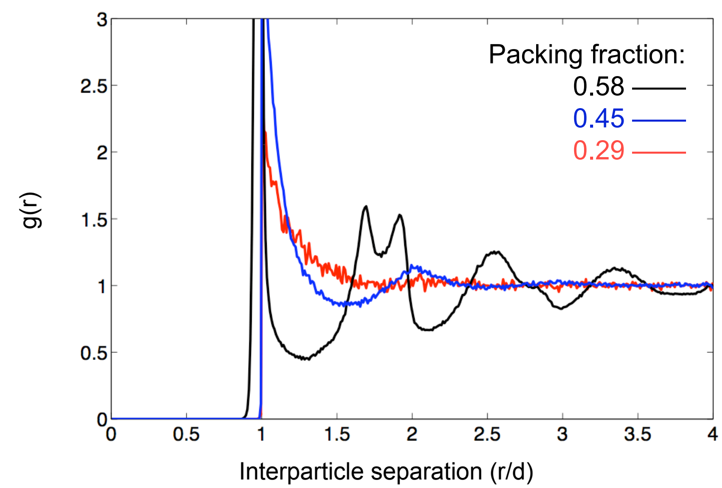
Initial packing
DEM Simulation
Spot simulation
Frequency density
Bond angle (degrees)
0.025
0.02
0.015
0.01
0.005
0
0
20
40
60
80
100
120
140
160
180

Random packing studies

- Taller silos, longer times
  - Reaches statistical steady state
  - Spot algorithm never breaks down
  - More local ordering at long times
  - Smaller step size reduces deviation from DEM



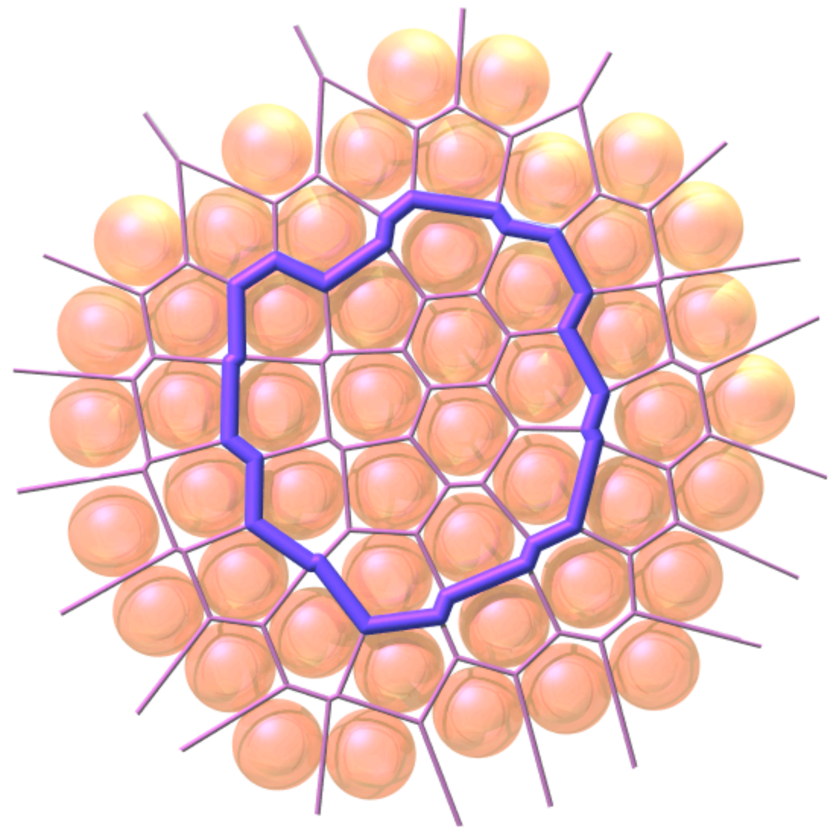
- Unbiased spot diffusion in a periodic cell (J. Palacci)
  - Also reaches steady state, largely independent of initial conditions
  - New simulation method for generating hard sphere systems



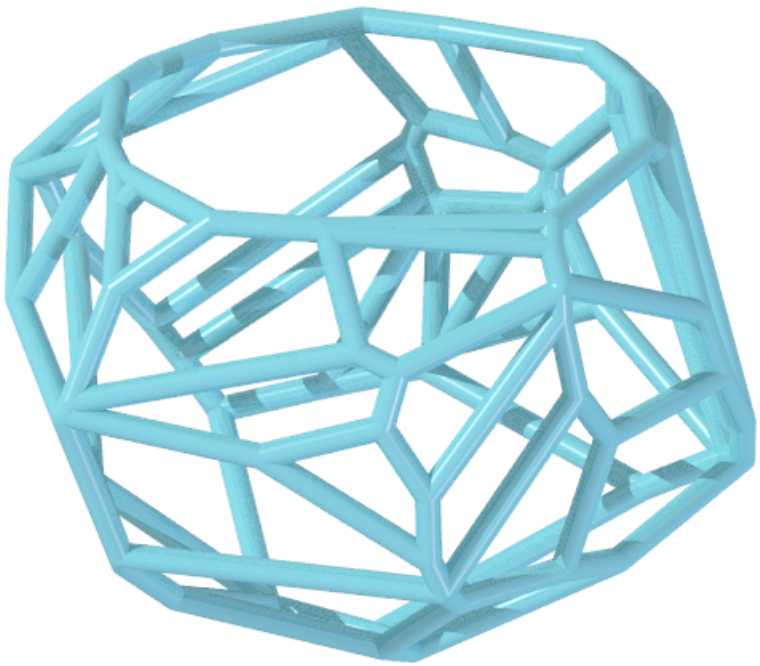
J. Palacci, *Computer simulations of granular materials with periodic boundary conditions using the Spot Model*, MIT, 2005.

Measuring packing fraction using Voronoi volumes

- Investigate changes in packing fraction at the scale of a spot
- Voronoi cell: the region of free space closer to a particle than any other
- Packing fraction defined as the ratio of a particle volume to its Voronoi cell
- Averaged over particles in a small region

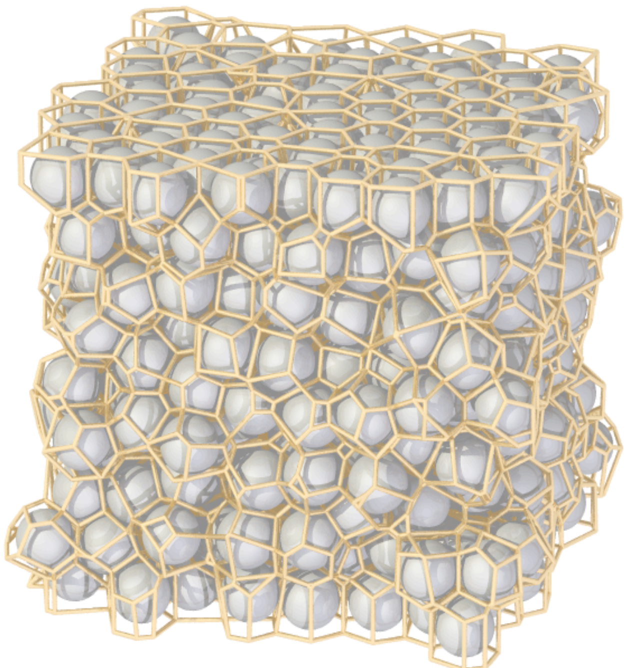


Calculating 3D Voronoi cells

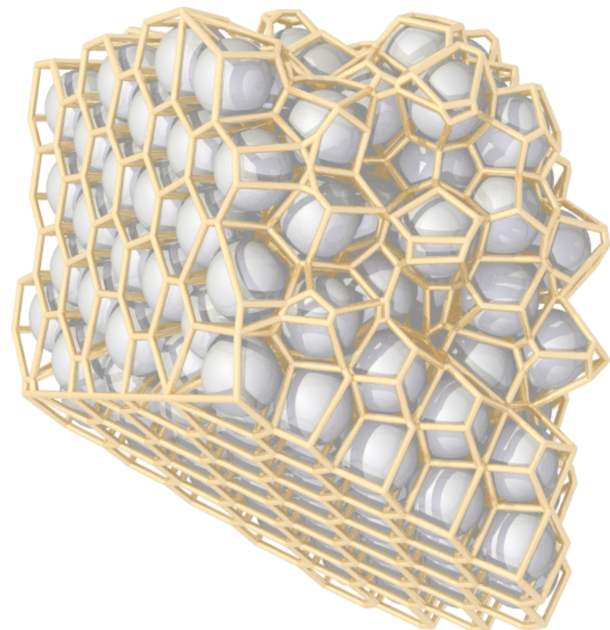


- Routine available in MATLAB using dual Delaunay triangulation
- Made use of our own plane-cutting algorithm:
  - Start from any vertex
  - Move towards plane, exploiting convexity
  - Find intersected edge
  - Trace around new face
  - Remove any deleted vertices

Examples of algorithm results

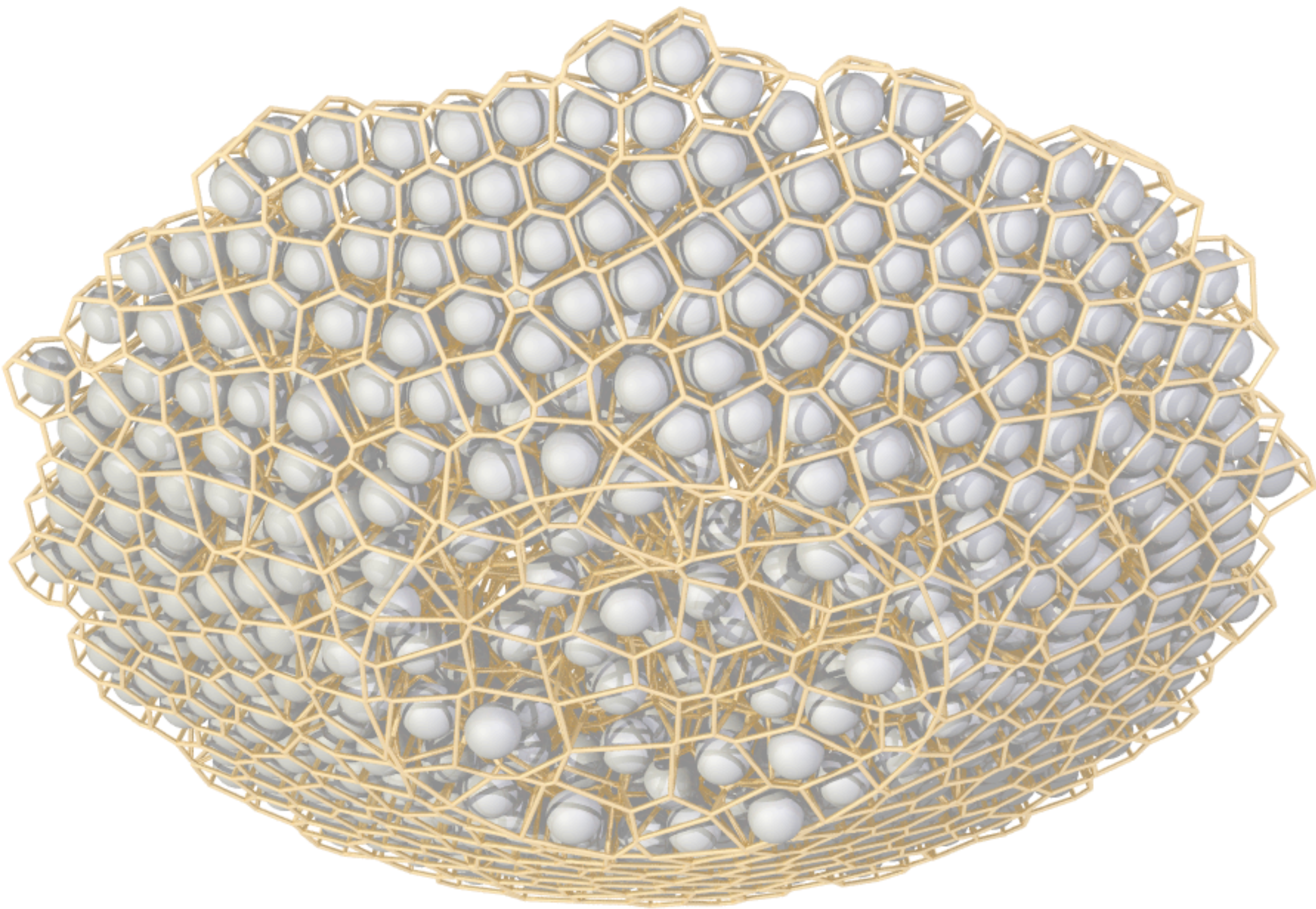


Cross section through
a thin container



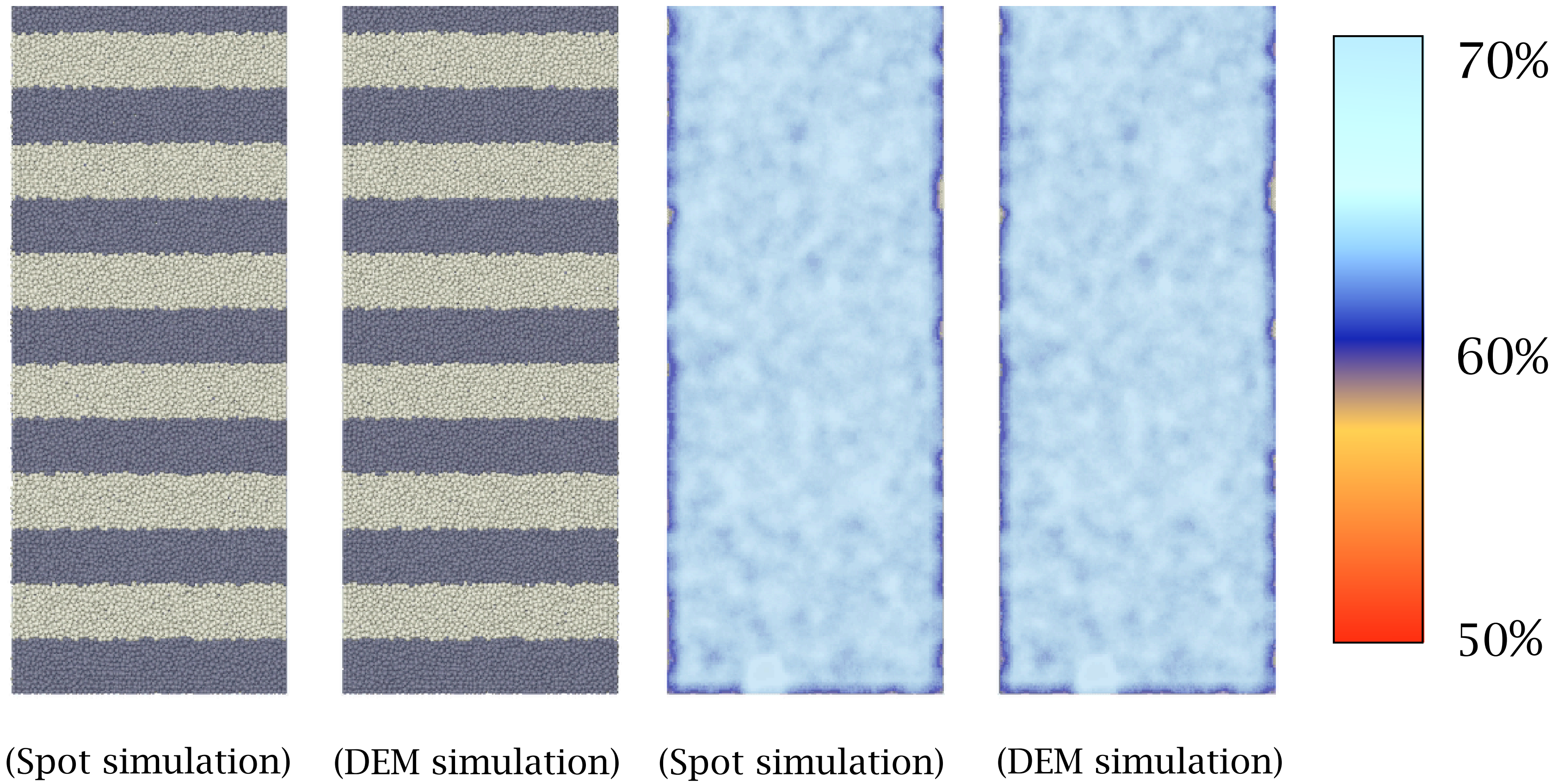
Corner boundary
condition

Complicated boundaries



Looking up from below at a funnel

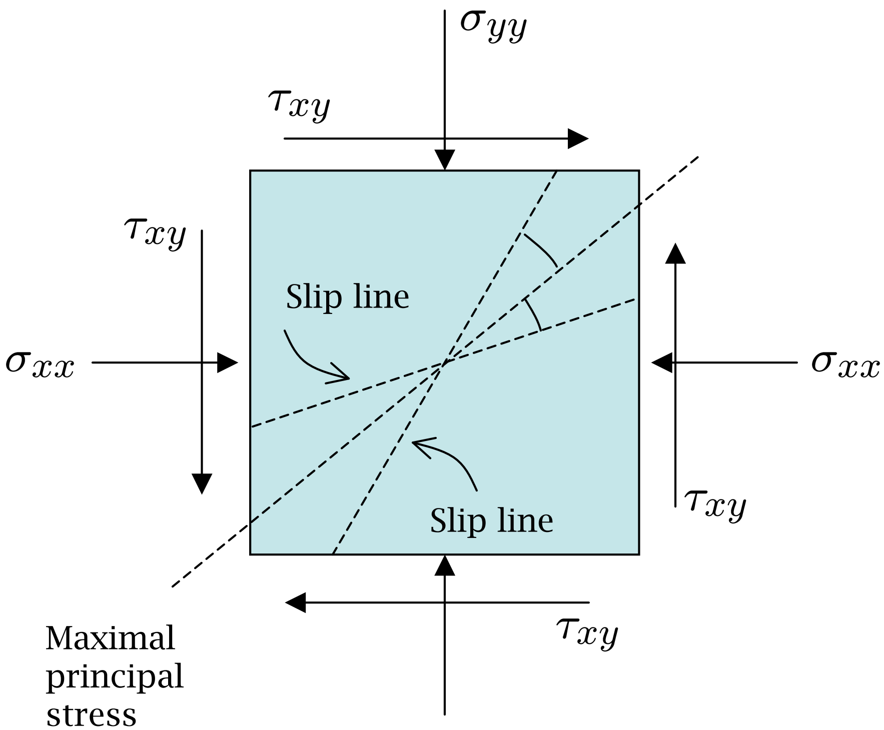
Comparison of density changes



Simulation snapshots

Voronoi density plots

Mohr-Coulomb Plasticity



- Ideal Coulomb Material: fails when

$$(\tau/\sigma)_{max} = \mu$$

- Need additional hypotheses to formulate continuum model

Hypothesis 1: **M-C incipient yield** (mu constant everywhere)
Hypothesis 2: **Coaxiality** (strain rate aligned with stress)

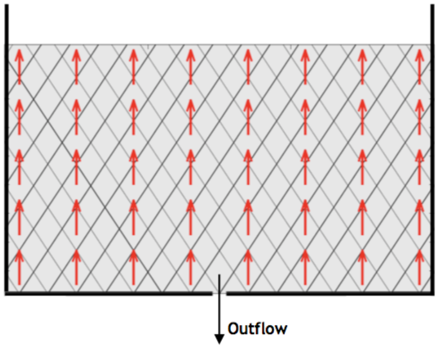
?

R. M. Nedderman, *Statics and Kinematics of Granular Materials*, (Nova Science, 1991).

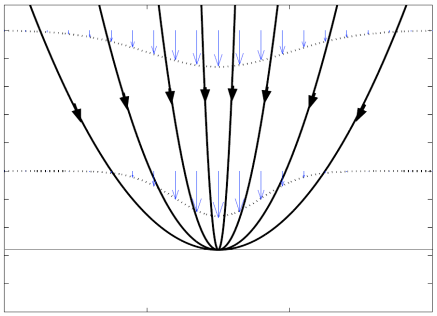
Stochastic Plasticity

- Spots carry out a random walk on the slip lines
- Spot drift vector: average of the two slip lines
- Predicts mean flow in both silo drainage and shear cell

Silo drainage

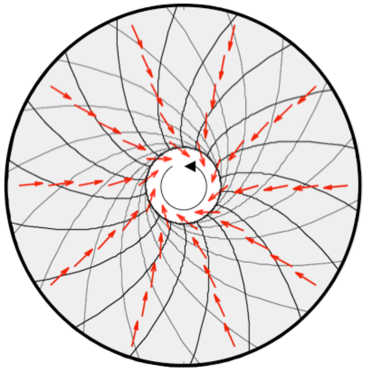


Slip lines and drift vectors

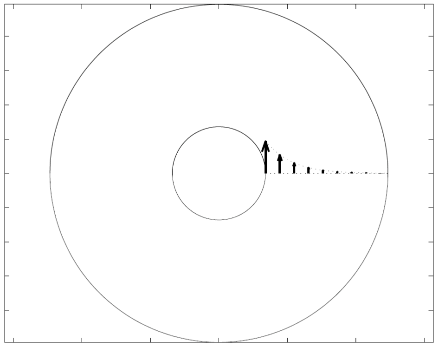


Velocity field

Couette shear cell



Slip lines and drift vectors



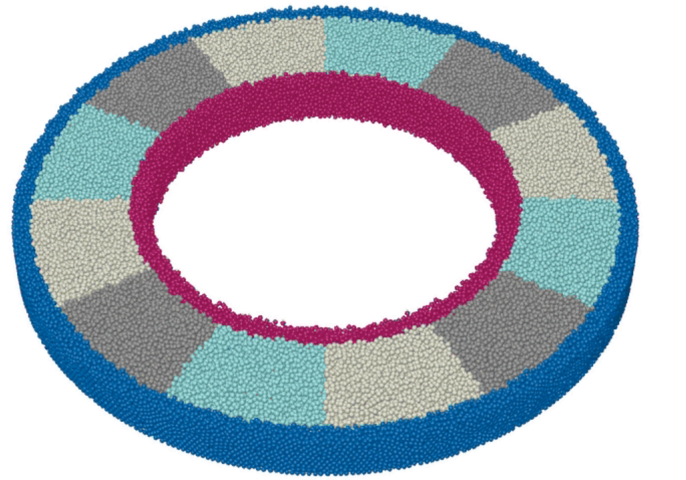
Velocity field

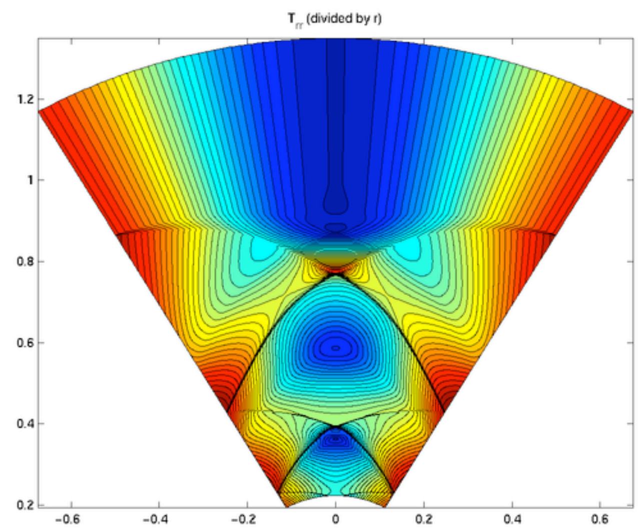
Kamrin and Bazant, *A stochastic flow rule for granular materials*, Phys. Rev. E **75**, 041301 (2007).

Direct test of continuum assumptions

- Matches closely to simulation and experiment for both cases
- Not easily generalized to other geometries
- Underlying equations still predict shocks
- **Can we test the fundamental hypotheses of model?**

Kamrin, Rycroft, and Bazant, *The Stochastic Flow Rule: A Multi-Scale Model for Granular Plasticity*, Mod. Sim. Mat. Sci. Eng. **15**, S449-S464 (2007).

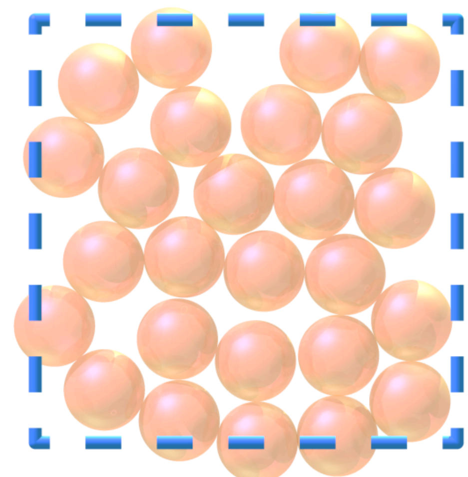




(Gremaud *et al.*)

Direct measurements of material quantities

- Can't accurately define stress and strain rate for a single particle
- But they can be approximately defined at the spot scale
- Carry out DEM simulations:
  - Calculate material parameters for 2.5d x 8d x 2.5d boxes
  - View as ensemble of granular elements
  - Seek statistical signatures



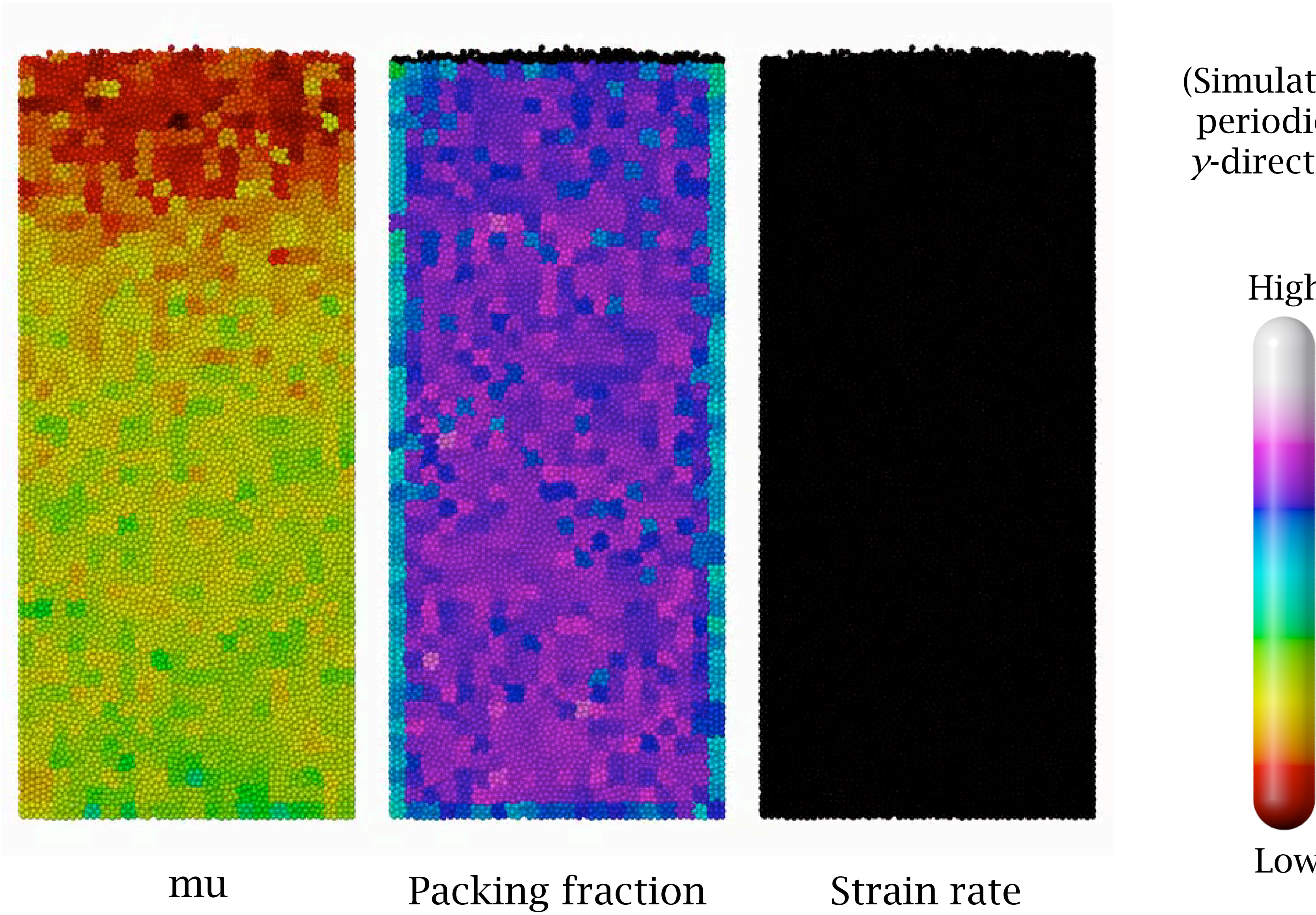
Strain rate calculation:
Use least squares to fit M such that

$$\mathbf{v} = M\mathbf{x} + \mathbf{v_0}.$$

Strain rate tensor defined as

$$T = \frac{M^T + M}{2}.$$

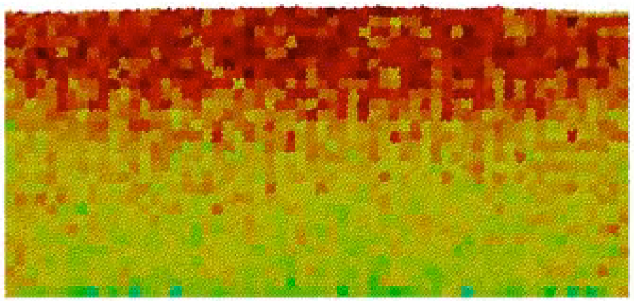
Material quantities in a tall silo



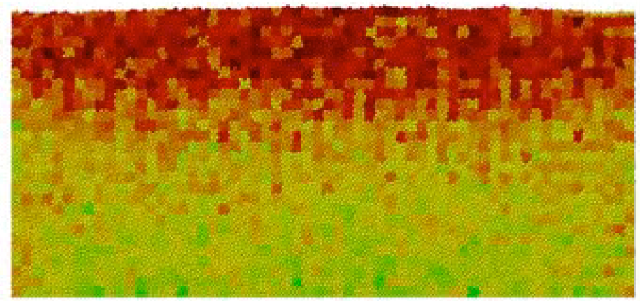
(Simulations periodic in y-direction)

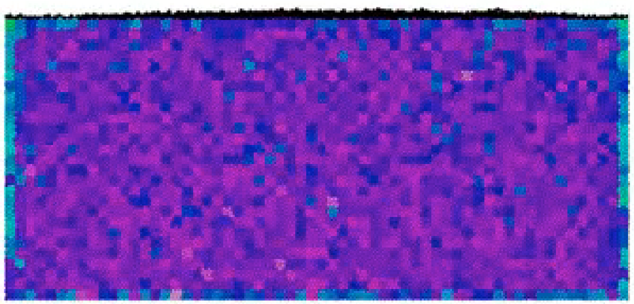
Two experiments in a wide silo

Drainage | **Pushing**

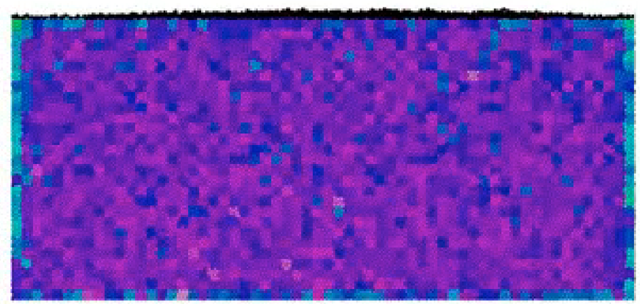


mu



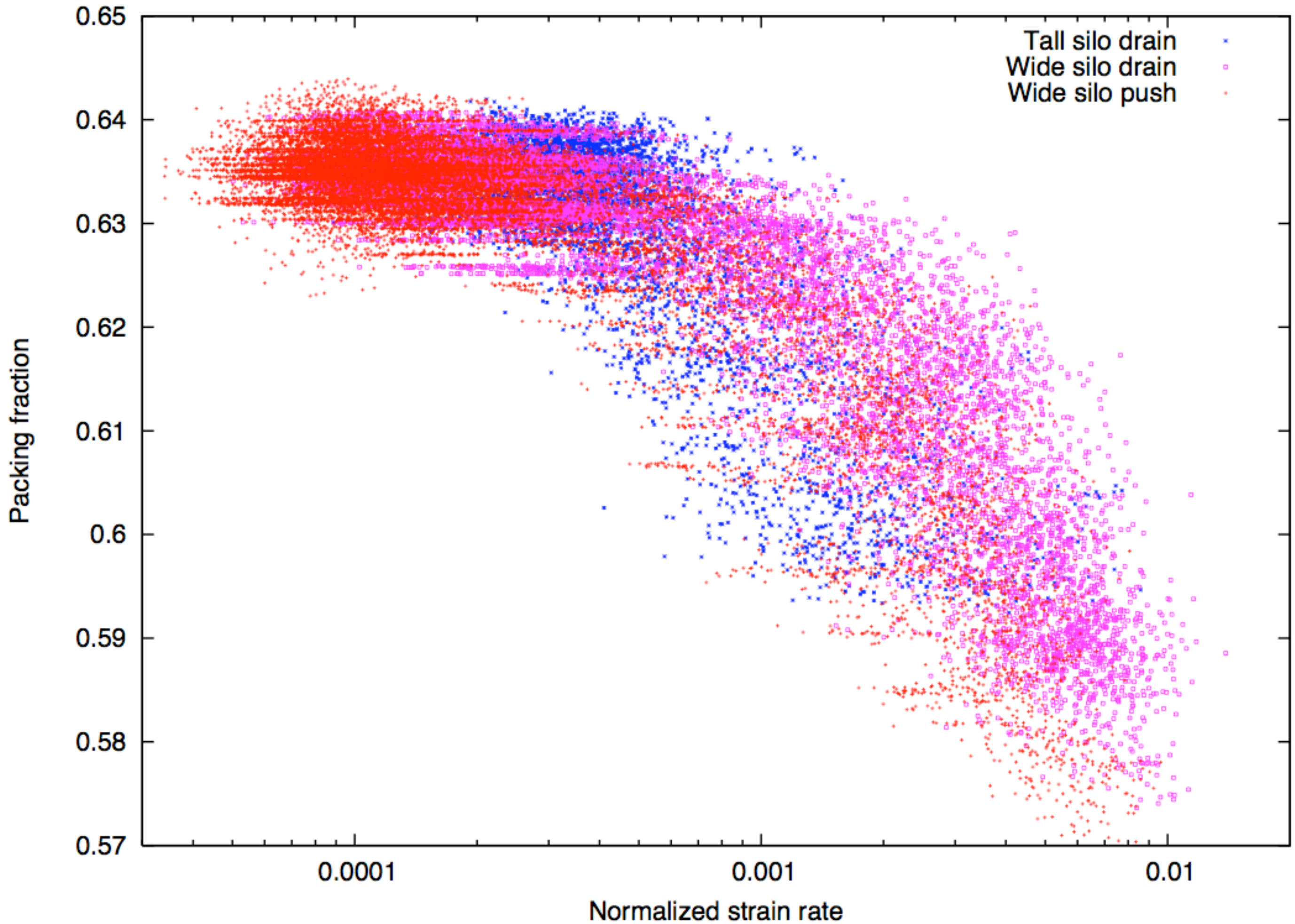


Packing fraction



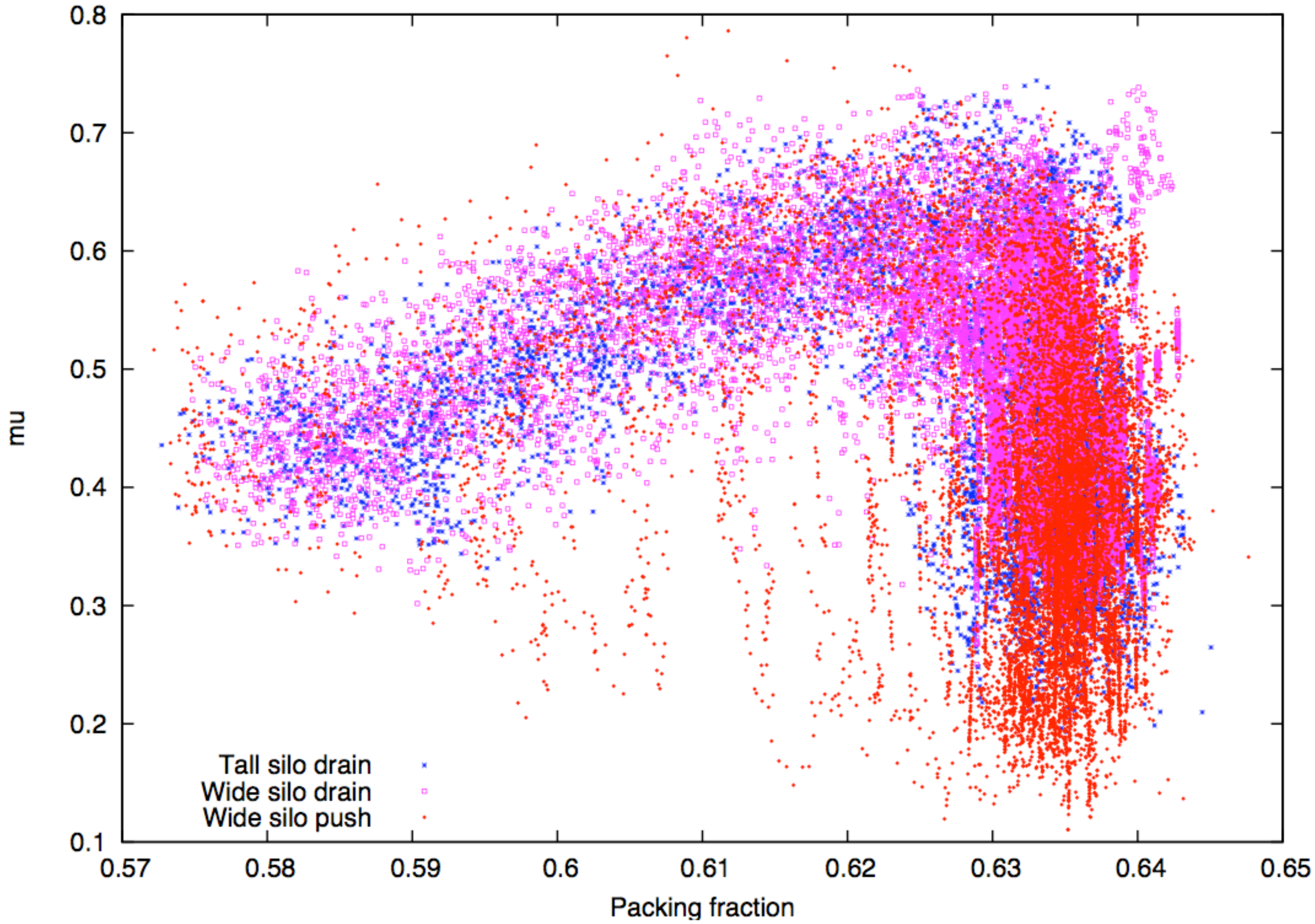
Strain rate

Strain rate v. Packing fraction



Data points from all three experiments collapse:
a direct verification of shear dilation.

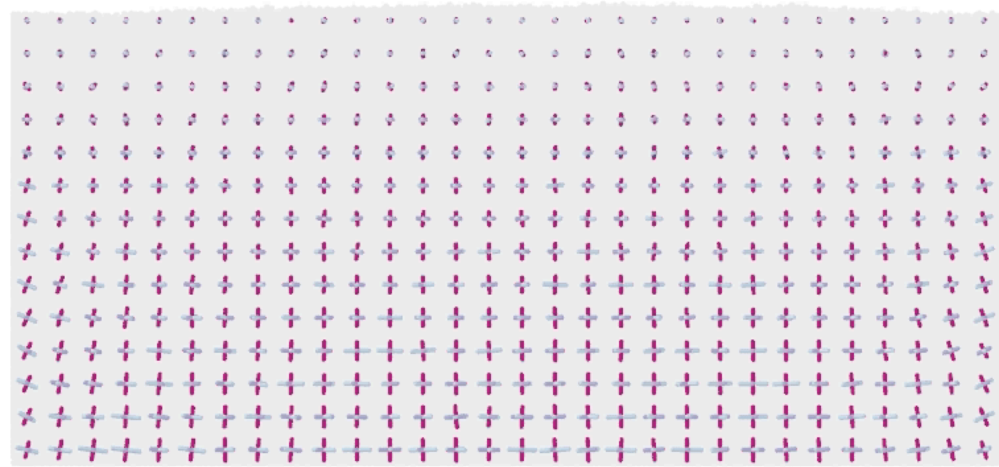
mu v. Packing fraction



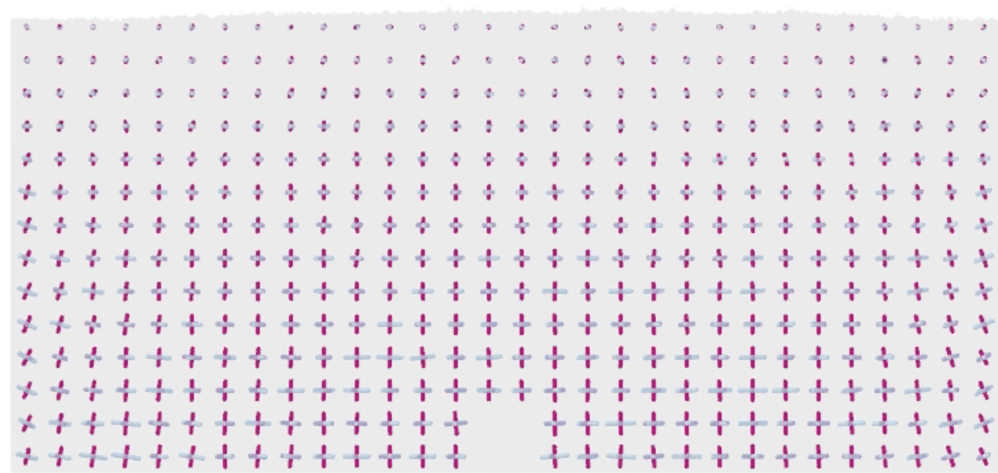
Data does not collapse so well, but it is still clear that the Mohr-Coulomb Incipient Yield Hypothesis is invalid.

Principal stress tensor

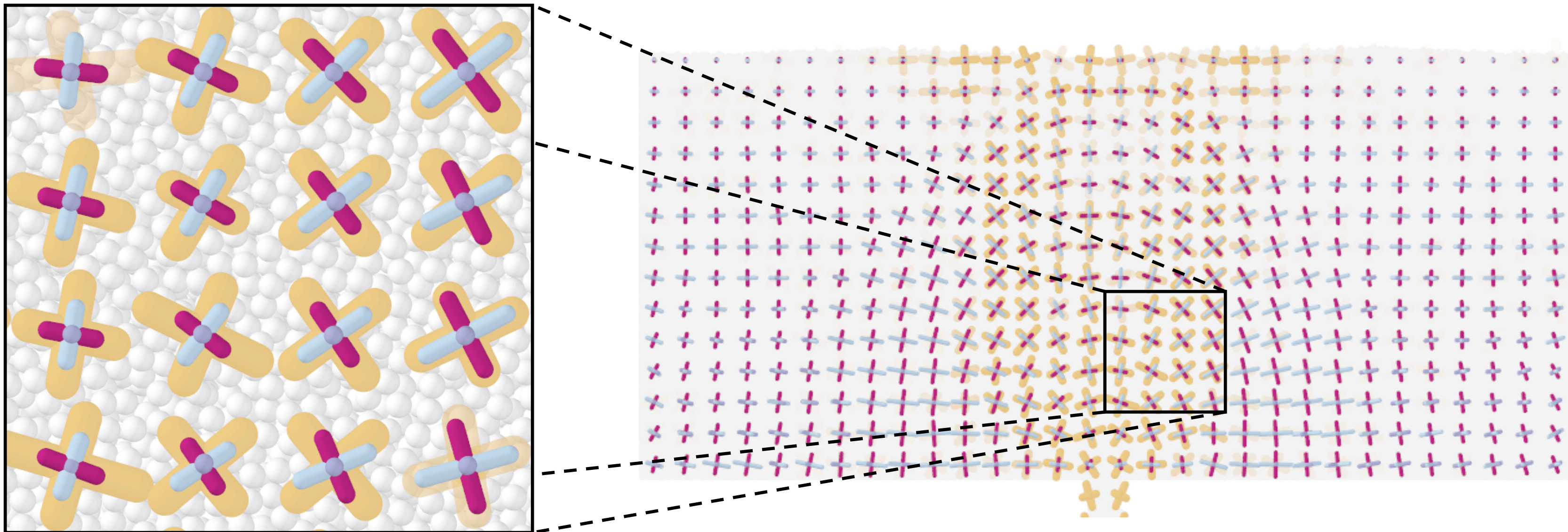
- Compute eigenvectors for stress tensor
- Maximal eigenvector shown in purple
- Background pressure subtracted; only deviatoric part shown



Wide drainage simulation



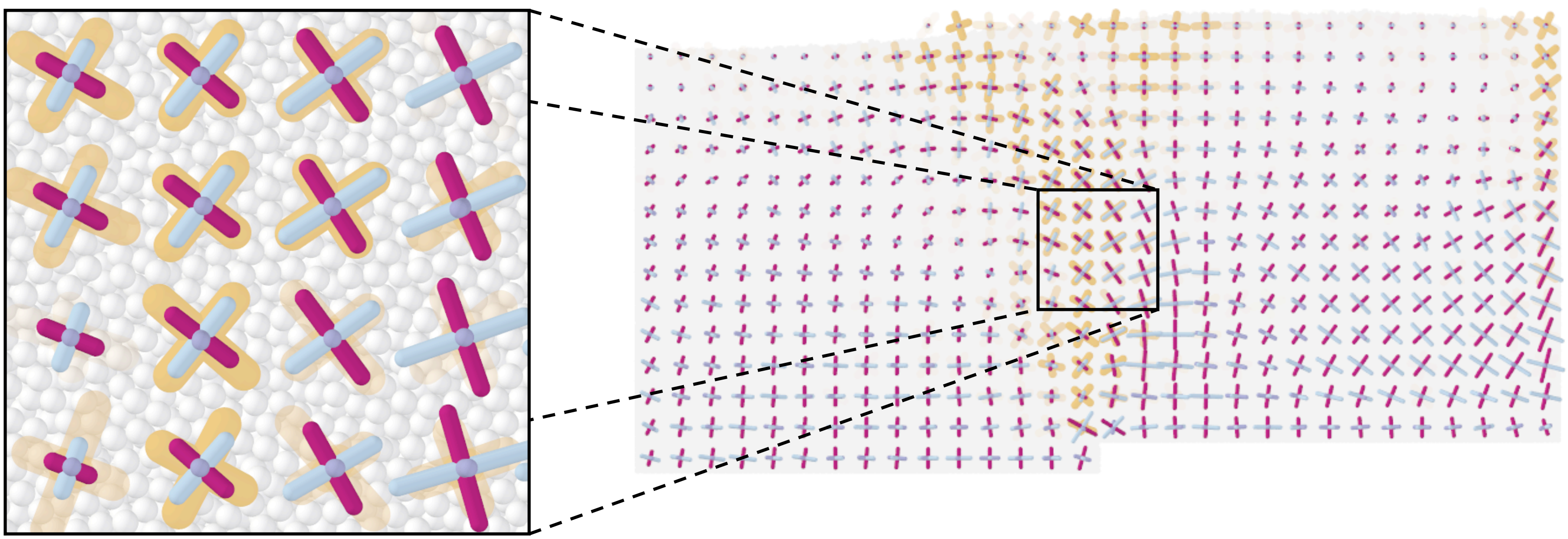
Wide pushing simulation



Wide drainage simulation

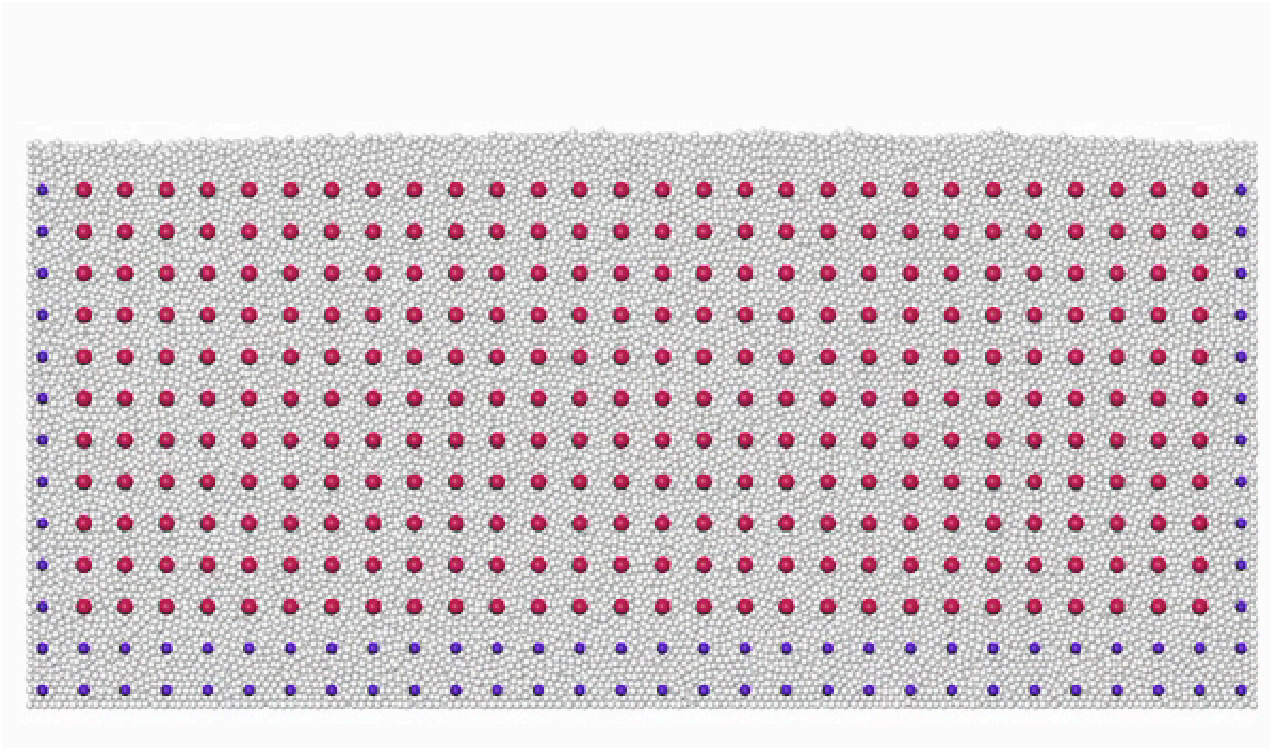
overlaid in orange

- Good match in



Wide pushing simulation

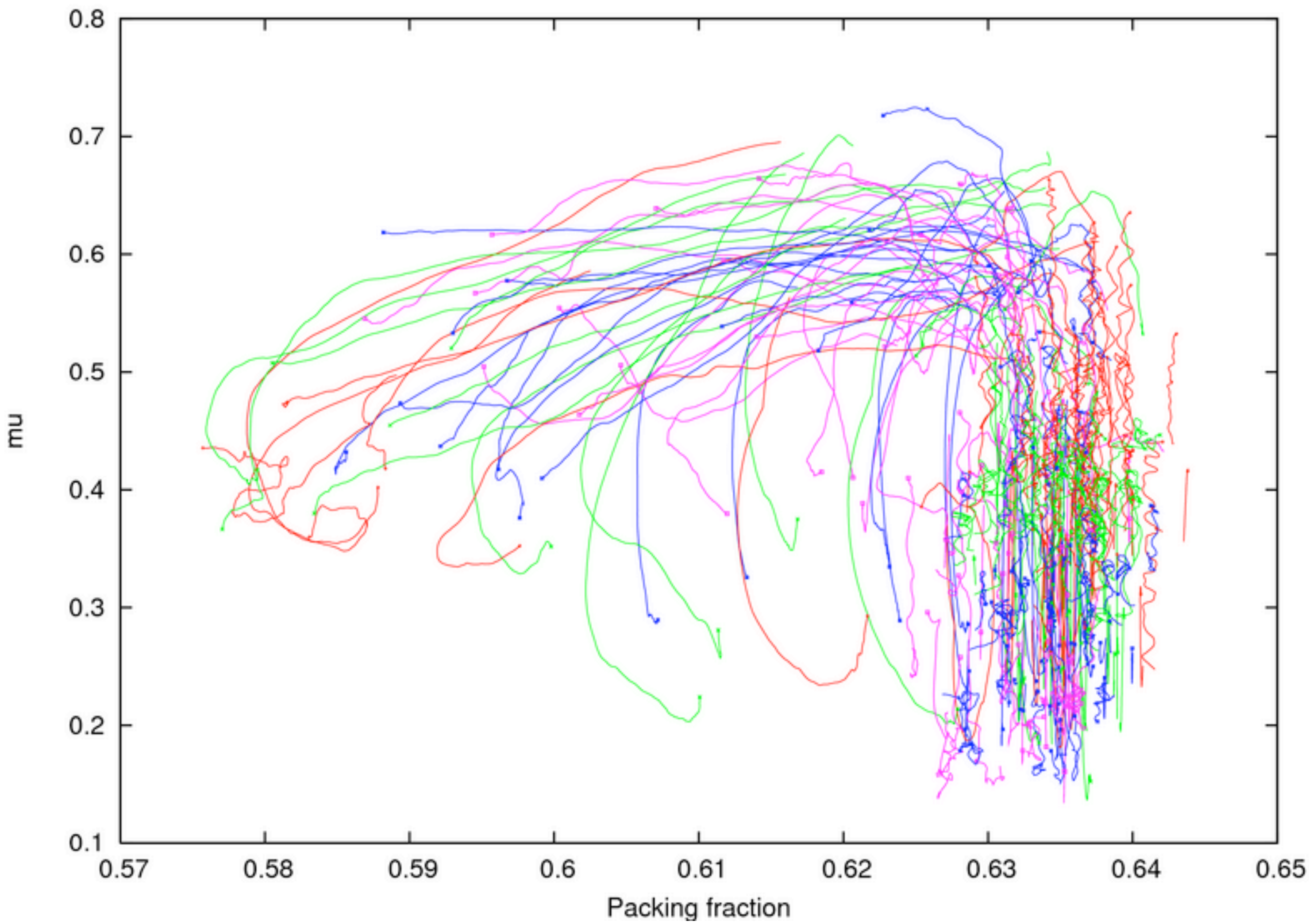
History of a granular element



- Introduce tracers on a 5d by 5d grid
- Move tracers according to velocity field
- Interpolate material quantities from underlying data

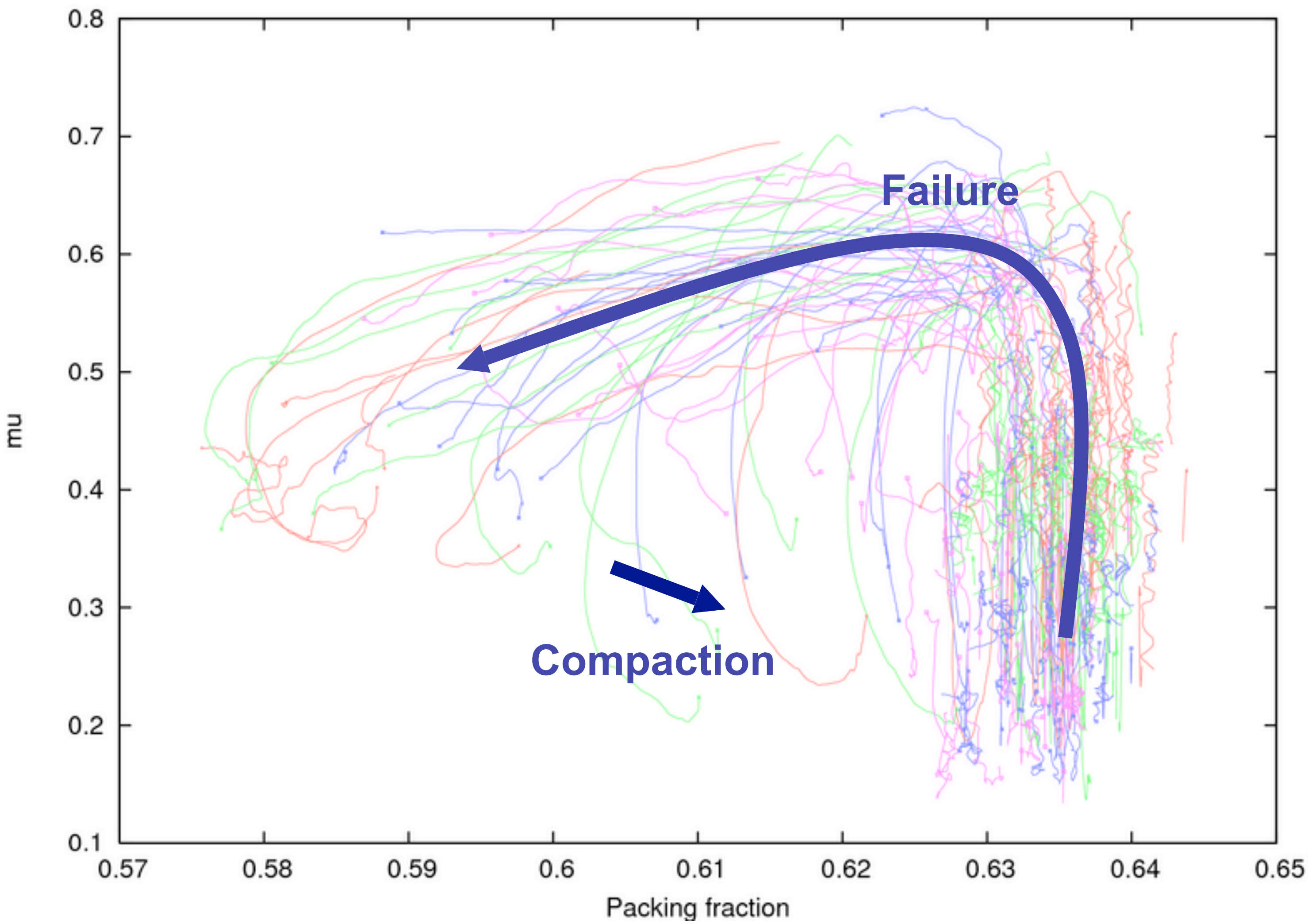
mu v. Packing fraction

(for wide pushing simulation)

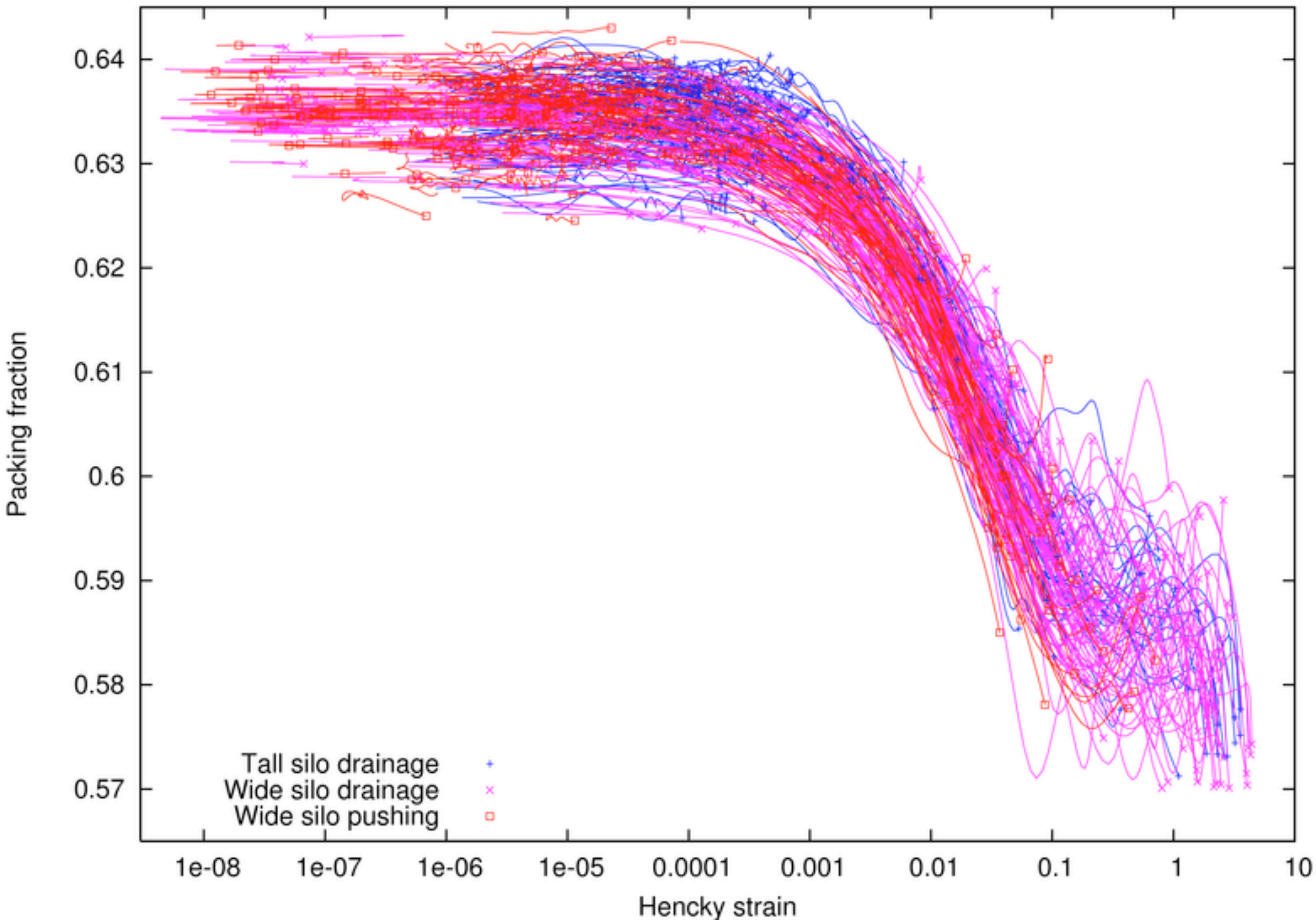


mu v. Packing fraction

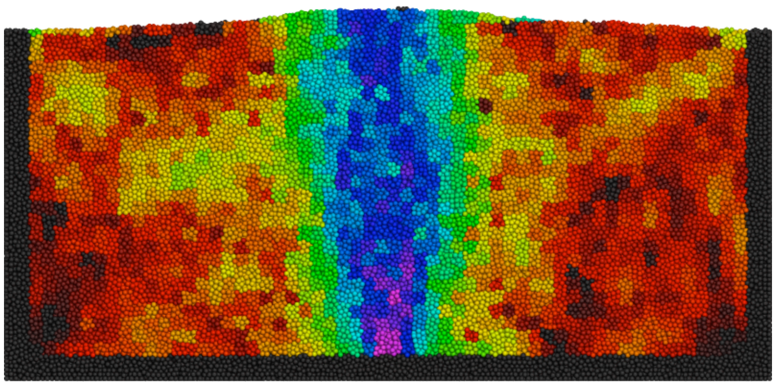
(for wide pushing simulation)

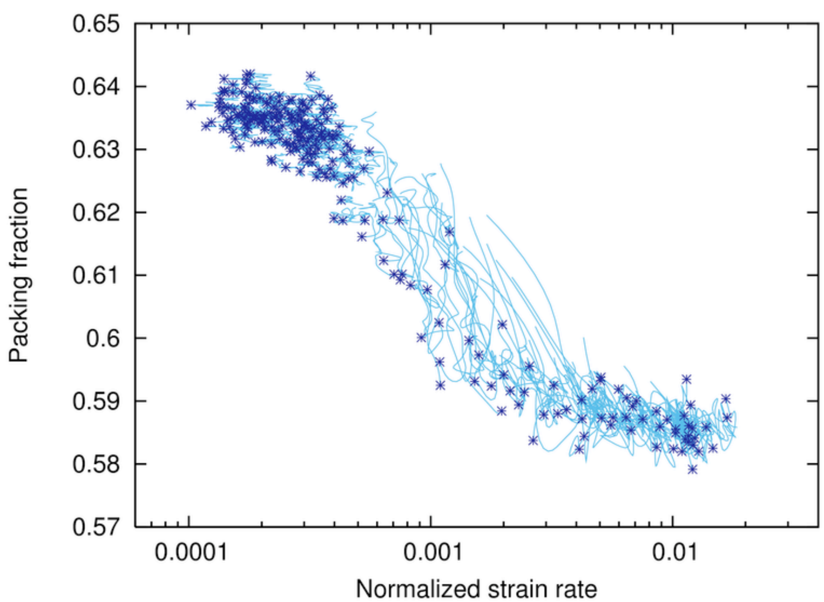


Shear dilation: strain or strain rate?



Shearing experiment





- Strain rate approximately constant for each element
- Strain rate v. packing fraction: end points collapse
- Strain determines dilation process, strain rate determines steady state

Conclusions

- The spot model provides one of the first theoretical models of a flowing dense amorphous packing, and can accurately reproduce packing dynamics from a DEM simulation of granular flow at a fraction of the computational cost.

- Bulk material quantities can be modeled at the scale of a spot, providing new insight into how to construct a continuum theory, or a general multiscale simulation technique.

Papers, images, and movies available at:
http://math.mit.edu/dryfluids/
http://math.mit.edu/~chr/

Acknowledgements

- MIT Applied Math:
  - Martin Bazant
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Why divide by the square root of P?

- Construct a dimensionless quantity:

$$
\begin{aligned}
\text{Pressure} \quad & [P] &=& \quad ML^{-1}T^{-2} \\
\text{Density} \quad & [\rho] &=& \quad ML^{-3} \\
\text{Diameter} \quad & [d] &=& \quad L^{-1} \\
\text{Strain rate} \quad & [\mathbf{D}] &=& \quad T^{-1}
\end{aligned}
$$

$$
\Longrightarrow \left[\frac{\mathbf{D}d\sqrt{\rho}}{\sqrt{P}}\right] = 1
$$

Discrete Element Simulation

$$\mathbf{F}_n = f(\delta/d)\left(k_n\delta\mathbf{n} - \frac{\gamma_n\mathbf{v}_n}{2}\right)$$

$$\mathbf{F}_t = f(\delta/d)\left(-k_t\Delta\mathbf{s}_t - \frac{\gamma_t\mathbf{v}_t}{2}\right)$$

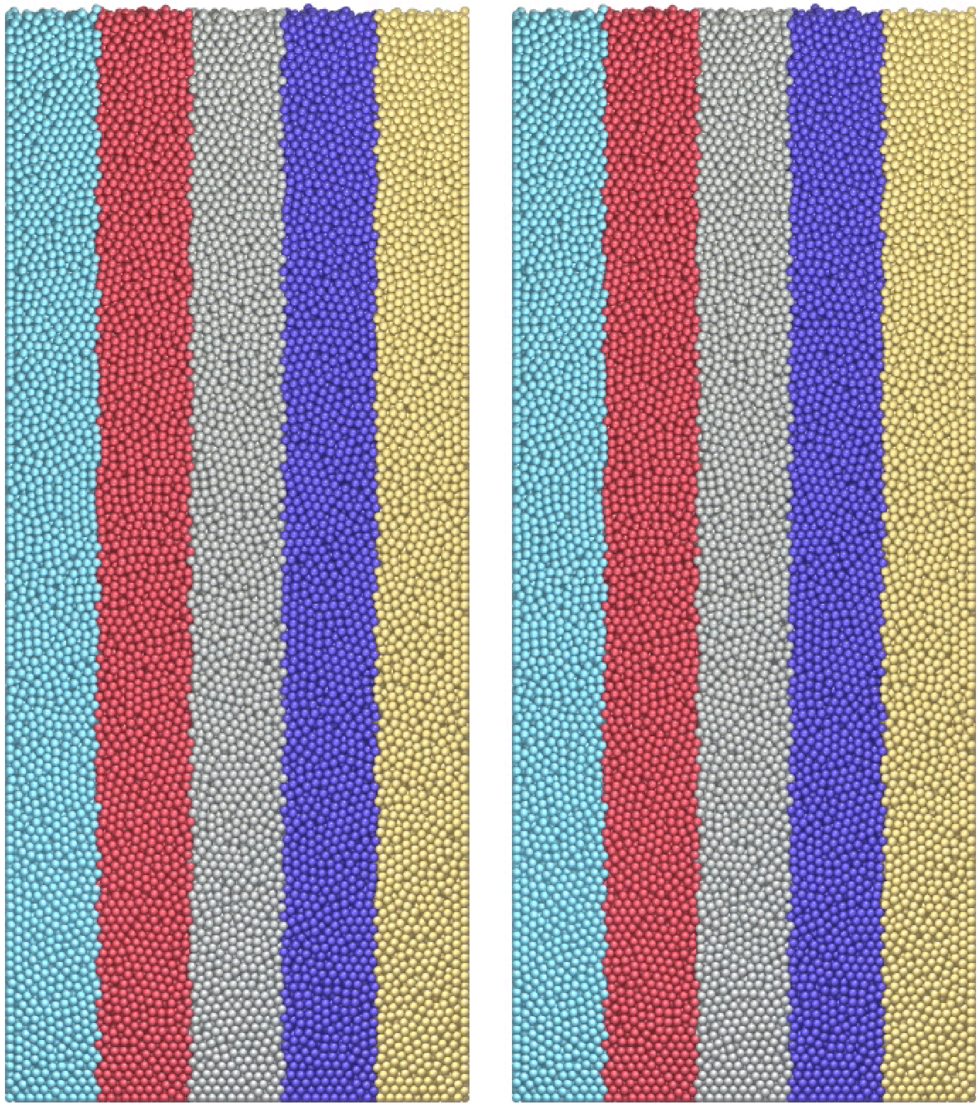
$\mathbf{F}_{n,t}$	:	Normal/tangential forces	$\mathbf{n}$	:	Outward-pointing normal vector
$\mathbf{v}_{n,t}$	:	Normal/tangential velocities	$k_{n,t}$	:	Normal/tangential elastic constants
d	:	Particle diameter	$\gamma_{n,t}$	:	Normal/tangential viscoelastic constants
δ	:	Particle overlap	$\Delta\mathbf{s}_t$	:	Elastic tangential displacement

$$\text{Coulomb: } |\mathbf{F}_t| \le \mu|\mathbf{F}_n|$$

$$f(z) = \begin{cases} \sqrt{z} & \text{for Hertzian contacts} \\ 1 & \text{for Hookean contacts} \end{cases}$$

Avalanching free surface

- Basic spot model does not capture free surface behavior
- Bias the spot random walk towards regions with more particles
- Qualitatively captures avalanching free surfaces seen in DEM

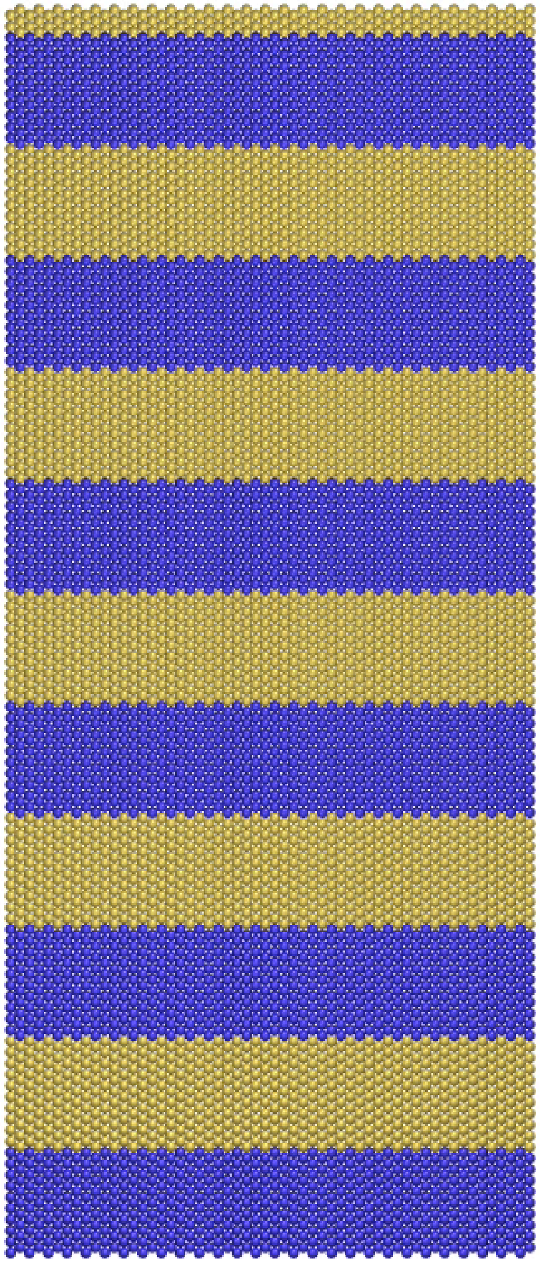


DEM

Biased spot

A two dimensional spot model

- Start particles on a 2D hexagonal lattice
- Dislocations and voids can be seen
- Extended features larger than the spot scale are visible
- Spot model never breaks down



Diffusion in the Void Model

$$p^p_{m,n} = \frac{p^v_{m,n}}{2}\left(\frac{p^p_{m+1,n+1}}{p^v_{m+1,n+1}} + \frac{p^p_{m-1,n+1}}{p^v_{m-1,n+1}}\right)$$

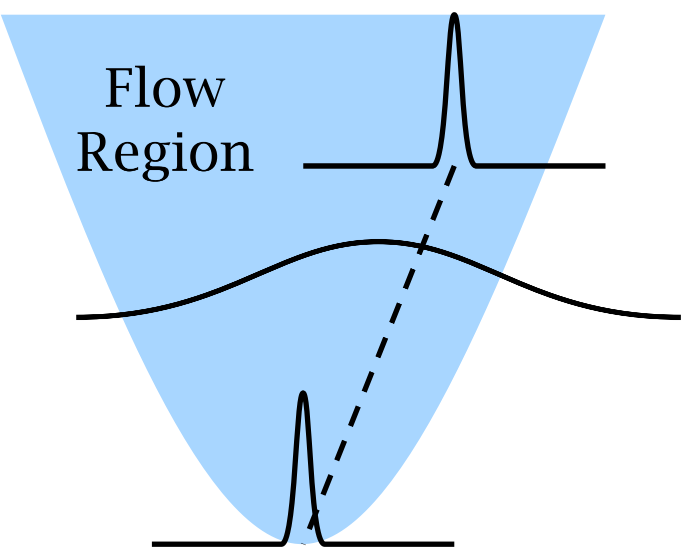
$$-\frac{\partial P_p}{\partial z} = b\frac{\partial}{\partial x}\left(\frac{\partial P_p}{\partial x} + P_p\frac{\partial \log\,\rho_v}{\partial x}\right)$$

- P_p = conditional probability of being at x after falling to z
- The particle diffuses at the same rate as the voids

An exact solution:

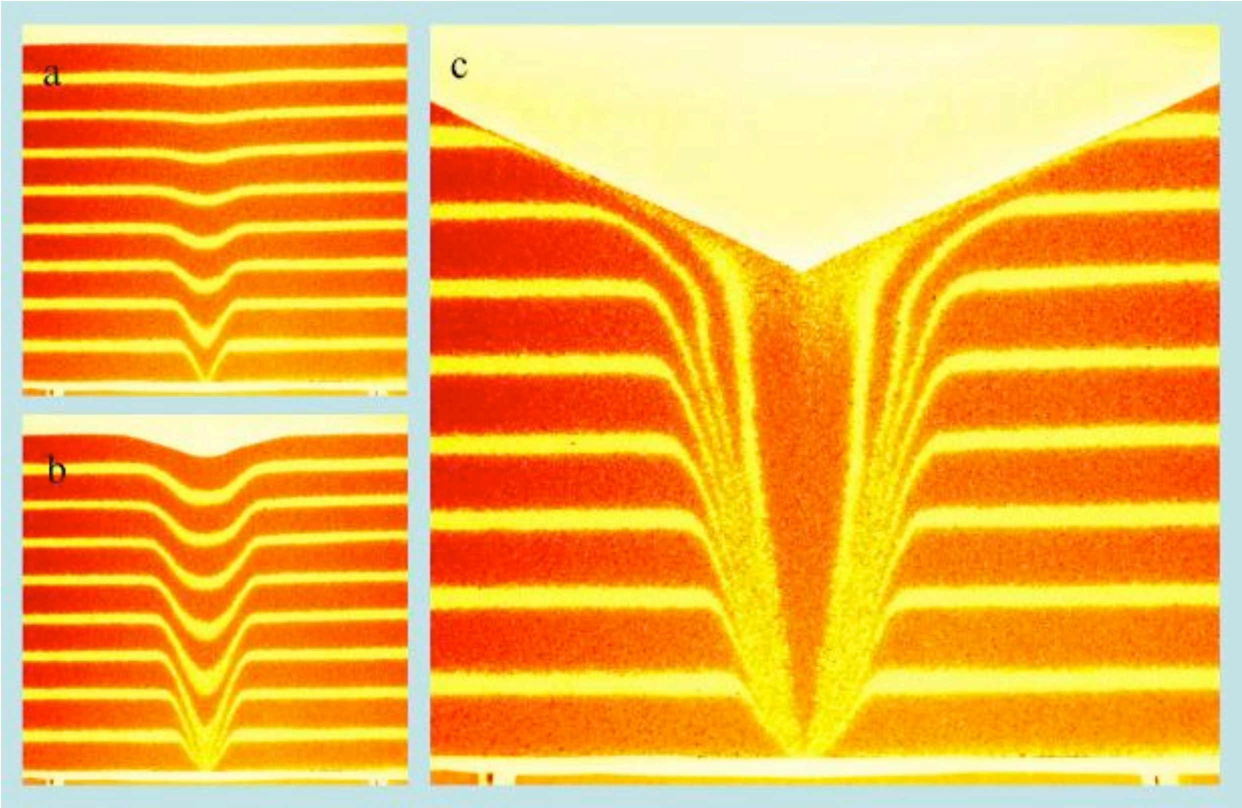
$$P_p(x|z, x_0, z_0) = \frac{e^{-(x-x_p)^2/2\sigma_p^2}}{\sqrt{2\pi}\sigma_p}$$

$$x_p = \frac{x_0 z}{z_0} \quad \sigma_p = \sqrt{2bz\left(1 - \frac{z}{z_0}\right)}$$

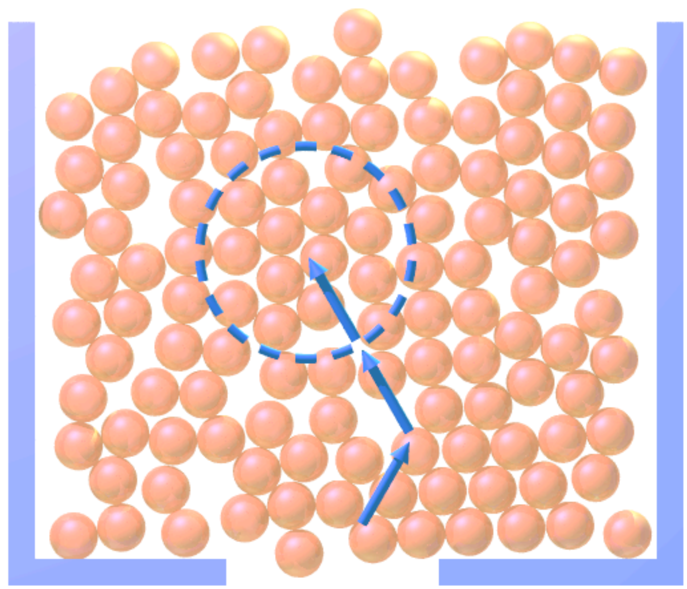


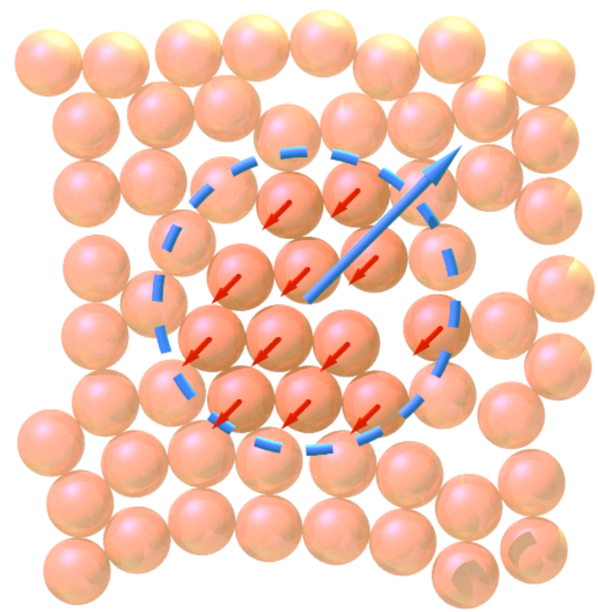
Paradox of granular diffusion:

Particles diffuse much more slowly than free volume.



Spot Model





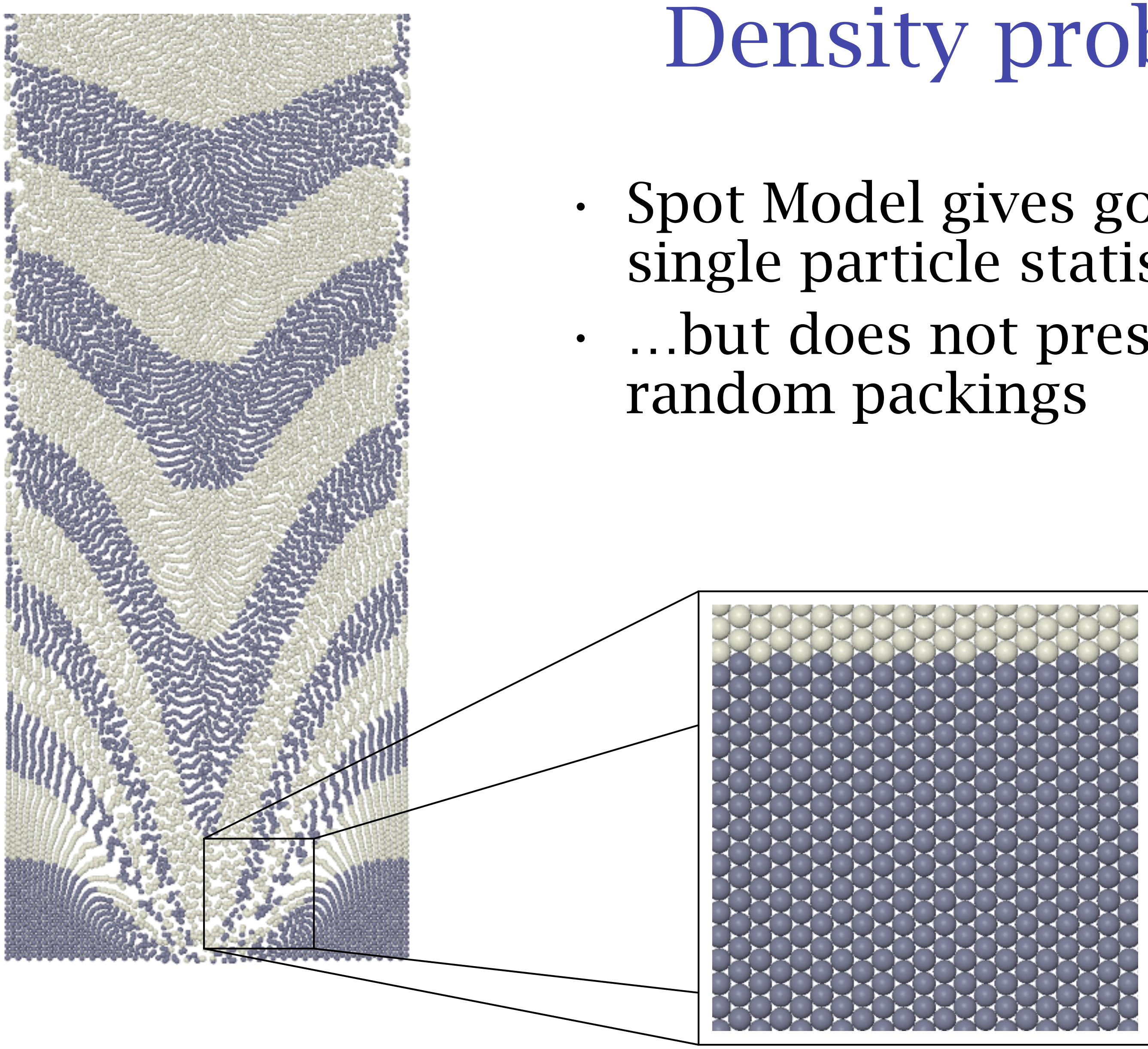
- Extended spots of slightly enhanced interstitial volume diffuse upwards from the orifice
- Spots cause correlation downward displacements of passive, off-lattice particles within range

MD, Spot, Void comparison

(Molecular Dynamics)

(Spot Model)

(Void Model)

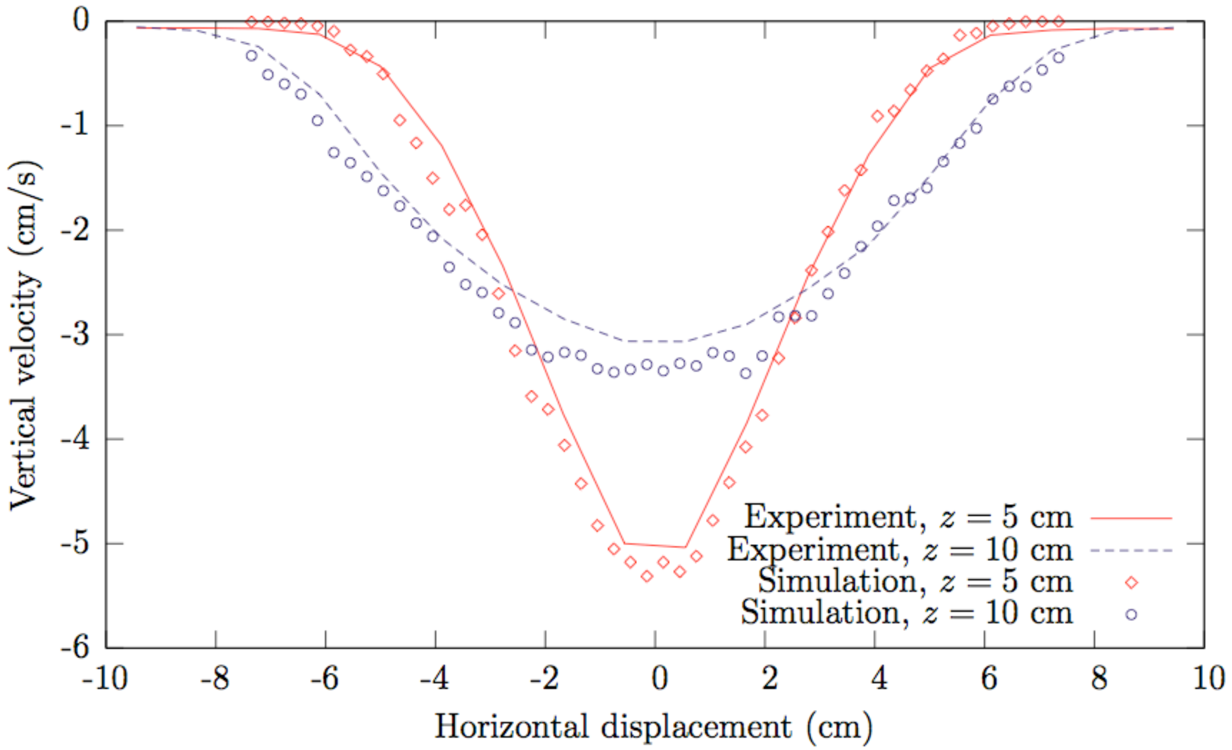


Density problem

- Spot Model gives good single particle statistics
- …but does not preserve random packings

Comparison to Choi's experiment

- Glass beads in a 20cm by 2.5cm by 1m hopper



Choi, Kudrolli, Rosales, and Bazant, *Diffusion and mixing in gravity driven dense granular flows,* Phys. Rev. Lett. **92**, 174301 (2004).