Multiscale Modeling in Granular Flow

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Support:
U. S. Department of Energy,
NEC, Norbert Weiner Research Fund
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

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.

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
  \[ C(r) = \frac{\langle u(0)u(r) \rangle}{\sqrt{\langle u(0)^2 \rangle \langle u(r)^2 \rangle}} \]
- 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

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 \textit{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

http://lammps.sandia.gov/

(55000 particles poured into a container of size 50d by 8d by 110d)
Two very different simulations

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

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

Initial packing of 55000 poured particles 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)

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

![Graph showing bond angles with different simulations including Initial packing, DEM Simulation, and Spot simulation.](image)

- Frequency density on the y-axis.
- Bond angle (degrees) on the x-axis.
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

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

(Spot simulation)  (DEM simulation)  (Spot simulation)  (DEM simulation)

Simulation snapshots  Voronoi density plots
Mohr-Coulomb Plasticity

- Ideal Coulomb Material: fails when
\[
\left(\frac{\tau}{\sigma}\right)_{max} = \mu
\]

- Need additional hypotheses to formulate continuum model

Hypothesis 1: **M-C incipient yield** (\(\mu\) constant everywhere)

Hypothesis 2: **Coaxiality** (strain rate aligned with stress)

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

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?

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 $2.5d \times 8d \times 2.5d$ 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
Direct test of coaxiality

- Eigenvectors of strain rate tensor overlaid in orange
- Good match in flowing regions

Wide drainage simulation

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
  - Ken Kamrin
  - Jaehyuk Choi
  - Kevin Chu
  - Pak Wing Fok

• Collaborators:
  - Arshad Kudrolli
  - Gary Grest
  - James Landry

• Friends
• Family
• Yuhua
Why divide by the square root of P?

- Construct a dimensionless quantity:

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

\[
\Rightarrow \left[ \frac{Dd\sqrt{\rho}}{\sqrt{P}} \right] = 1
\]
Discrete Element Simulation

\[ F_n = f(\delta/d) \left( k_n \delta n - \frac{\gamma_n v_n}{2} \right) \]

\[ F_t = f(\delta/d) \left( -k_t \Delta s_t - \frac{\gamma_t v_t}{2} \right) \]

- \( F_{n,t} \): Normal/tangential forces
- \( v_{n,t} \): Normal/tangential velocities
- \( d \): Particle diameter
- \( \delta \): Particle overlap
- \( n \): Outward-pointing normal vector
- \( k_{n,t} \): Normal/tangential elastic constants
- \( \gamma_{n,t} \): Normal/tangential viscoelastic constants
- \( \Delta s_t \): Elastic tangential displacement

Coulomb: \( |F_t| \leq \mu |F_n| \)

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

An exact solution:

\[ p_{m,n}^p = \frac{p_{m,n}^v}{2} \left( \frac{p_{m+1,n+1}^p}{p_{m+1,n+1}^v} + \frac{p_{m-1,n+1}^p}{p_{m-1,n+1}^v} \right) \]

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

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

\[ x_p = \frac{x_0 z}{z_0} \]

\[ \sigma_p = \sqrt{2bz \left(1 - \frac{z}{z_0}\right)} \]

- \( P_p \) = conditional probability of being at \( x \) after falling to \( z \)

- The particle diffuses at the same rate as the voids.
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