A coupled continuum/discrete model of dense granular flow

Chris Rycroft


Collaborators:
Martin Bazant (MIT), Ken Kamrin (MIT),
Arshad Kudrolli (Clark University), Gary Grest (Sandia Nat. Lab.),
Jim Langer (UCSB), Frederic Gibou (UCSB), Jon Wilkening (UC Berkeley)
Problems modeling granular materials

- **Particle discreteness:**
  - Force chains
  - Difficulty defining continuum quantities
  - Inelastic collisions

- **Solid-like and liquid-like behavior**


![Force chains in a 2D shear cell](image)
Smooth flow fields / Stochastic behavior

- Despite force chains, granular materials often exhibit smooth average flows
- Exponential and gaussian velocity profiles – suggests stochastic effects
- Void Model: an approximate description of mean flow

Discrete-Element Simulation (DEM)

- Brute force approach:
  - Model individual particles according to Newton’s Laws
  - Treat particles as spheres with spring interaction
  - Stiff equations, small timestep

- Example: pebble-bed reactor drainage using LAMMPS (Sandia)
  - A single drainage cycle takes one month on 90 processors
  - Interested in microscopic statistics (eg. diffusion and packing structure)

http://lammps.sandia.gov/

(440,000 particles in a cylindrical hopper)
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 *a priori* if this will produce realistic flowing random packings
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 $50d$ by $8d$ by $110d$
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)
Microscopic packing statistics

Microscopic packing statistics

Spot model evaluation

- The spot model successfully predicts velocity profiles, particle diffusion, and microscopic packing structure.
- However, it is only applicable to hopper flow – the notion of diffusing free volume does not easily apply to other flows.
- We need a model with a reasonable physical basis, handling forces and stress.
Mohr–Coulomb Plasticity

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

- Need additional hypotheses:

  H1: M–C incipient yield
      (\(\mu\) constant everywhere)

  H2: Coaxiality
      (stress/strain rate e-vectors aligned)

Direct measurements of a granular “continuum element”

• 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
\[ T = \frac{M^T + M}{2}. \]

C. H. Rycroft et al., Defining and testing a granular continuum element, submitted.
Material quantities in a tall silo

(Simulations periodic in $y$-direction)
Two experiments in a wide silo

**Drainage**

**Pushing**

- **mu**
- **Packing fraction**
- **Strain rate**
Data points from all three experiments collapse: a direct verification of shear dilation.
• 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)
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
Modern granular continuum modeling

**Partial Fluidization**
Aranson & Tsimring (2001,2002)
Separate stress tensor into solid-like part and liquid-like part controlled by order parameter

**Granular elasticity**
Jiang (2003,2007)
Nonlinear elasticity that disallows tension

**A granular flow rule**
Jop, Forterre, Pouliquen (2006)
Plastic deformation controlled by strain rate

**Granular elastoplasticity**
Kamrin (2008)
Combination of Jiang elasticity and Jop plasticity

**Shear Transformation Zones**
Langer et al. (1998)
Elastoplastic model controlled by effective temperature

**Common themes:**
- Elastic stresses
- Plasticity controlled by internal parameter
A coupled continuum / discrete simulation

**Continuum:**
- One grid point per element
- Explicit finite-difference
- Level set free boundary
- Elastic stresses
- Plasticity controlled by packing fraction

**Discrete:**
- Initial packing from DEM
- Advect according to continuum velocity field
- Apply relaxation to enforce packing constraints
- Recompute packing fraction
Comparison to DEM for drainage

Continuum / discrete

DEM simulation

Strain rate

Stress
Comparison to DEM for pushing

• **Current successes:**
  - Fast
  - Applies to a general flow
  - Handles continuum quantities
  - Handles microscopic quantities

• **Problems:**
  - Needs improved physical model
  - Needs better numerics and better coupling
  - Only applicable at high density
Conclusions

The spot model: a simulation of a flowing random packing. Successful for hopper drainage but no general physical basis.

Continuum quantities can be successfully interpreted at the correlation length scale, allowing the rheology to be investigated.

Coupled continuum / discrete model

A rapid simulation technique for engineering problems with granular flow

A more general framework for investigating granular flow and capturing stochastic effects

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