Dynamics of Random Packings in Granular Flow

Chris Rycroft

APS March Meeting, 2005

MIT Dry Fluids Group:
Martin Bazant, Jaehyuk Choi, Ruben Rosales,
Ken Kamrin, Arshad Kudrolli (Clark University)

Collaborators:
Andrew Kadak (MIT Nuclear Engineering)
James Landry, Gary Grest (Sandia Nat. Lab.)

Support:  U. S. Department of Energy,
NEC, Norbert Weiner Research Fund
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 given by
  \[ C'(r) = \frac{\langle u(0)u(r) \rangle}{\langle u(0)^2 \rangle \langle u(r)^2 \rangle} \]

- 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

- Combined motion is bulk spot motion, while preserving packings
- Not clear *a priori* if this will produce realistic flowing random packings
DEM Simulation (Sandia)

- Parallel code on 24 processors
- $50d \times 8d \times 110d$ container
- Drained from circular orifice $8d$ across

L. E. Silbert et al., Phys Rev E, 64, 051302 (2001)
Spot simulation

- Initial packing taken from DEM
- Spots introduced at orifice
- Spots move upwards and do random walk horizontally
- 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)
Spot / DEM comparison

- Calibrated parameters:
  - $R_s = 2.6d$
  - $V_s = 0.2V_p$
  - $b = 1.14d$

- Factor of 100 speedup
- No mechanics, only geometry

DEM simulation (3 days, 24 processors)
Spot simulation (8 hours, single processor)
Microscopic packing statistics
Bond angles

Frequency density vs Bond angle (degrees) with different simulations.
Summary

• The Spot Model shows nearly identical flowing structure to DEM, different from the initial condition

• Publications and image gallery at http://math.mit.edu/dryfluids
Velocity profile comparison

![Graph showing velocity profile comparison for different depths (z = 10d, 30d, 50d) and two models: DEM and Spot Model. The graph plots velocity (v_z) against horizontal displacement (x/d).]