Cooperative Diffusion and Stochastic Plasticity in Dense Granular Flow

Martin Z. Bazant

Department of Mathematics, MIT

Students:

Ken Kamrin, Chris Rycroft, Jaehyuk Choi

Collaborators:

Arshad Kudrolli (Clark University, Physics)

Andrew Kadak (MIT Nuclear Engineering)

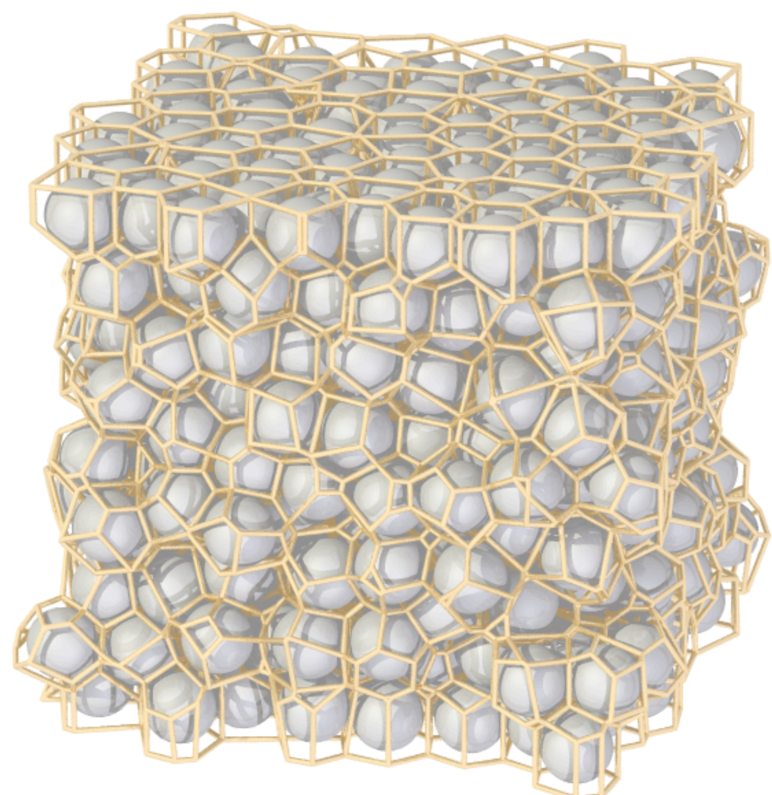
Gary Grest (Sandia National Laboratories)

Ruben Rosales (MIT Applied Math)

Support: U. S. Department of Energy,

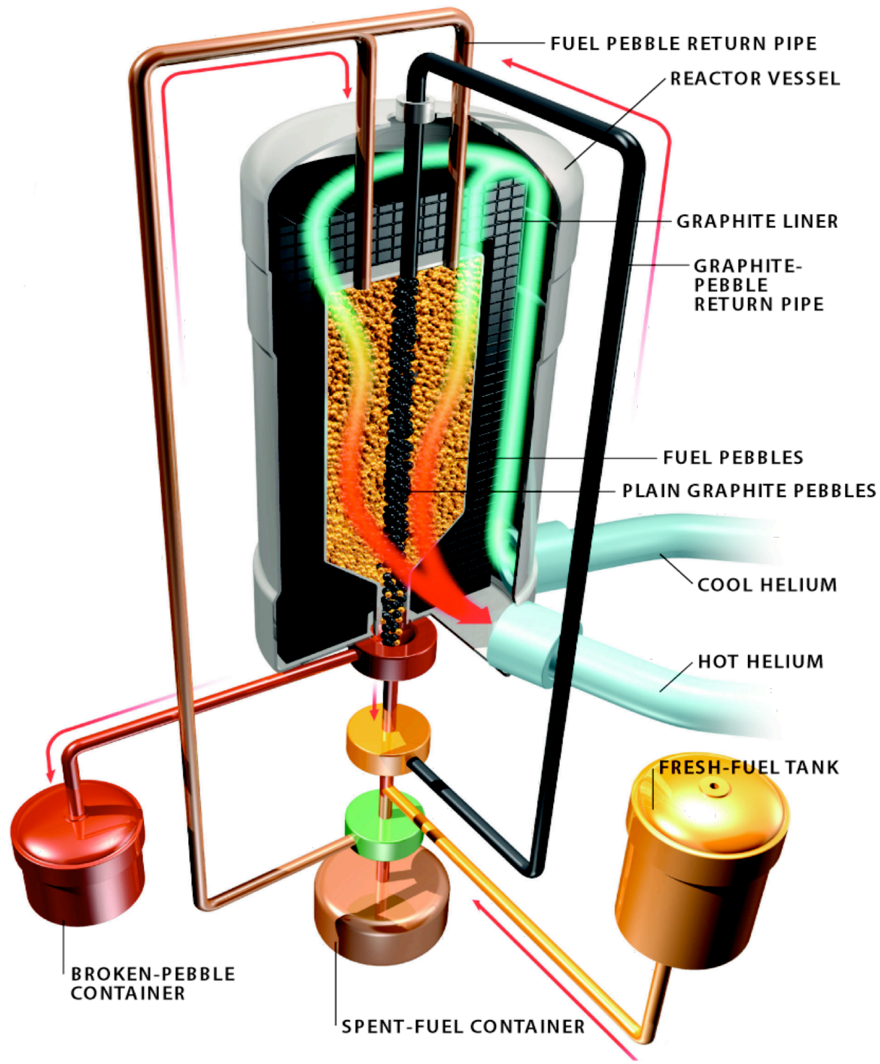
NEC, Norbert Weiner Research Fund (MIT)

http://math.mit.edu/dryfluids



MIT Modular Pebble-Bed Reactor

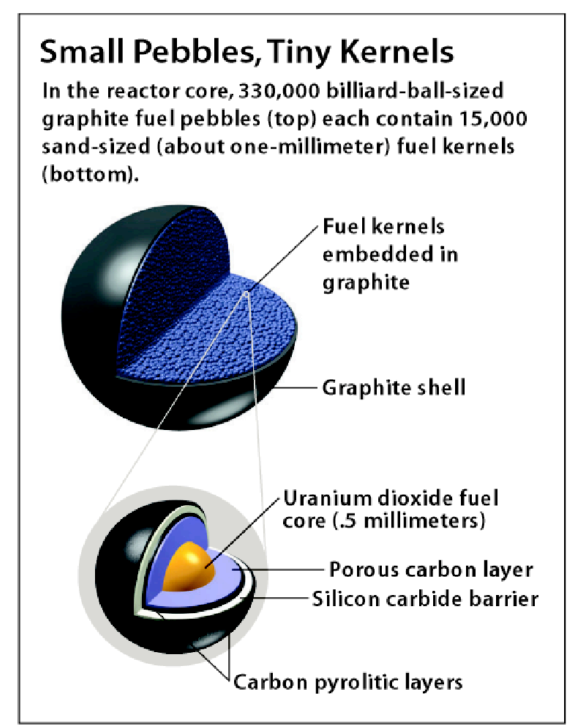
http://web.mit.edu/pebble-bed



MIT Technology Review (2001)

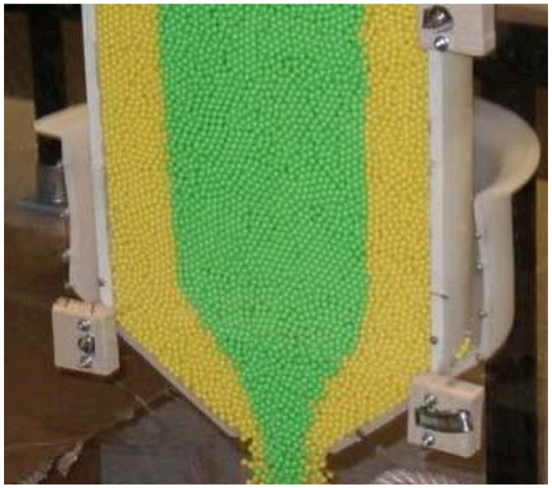
Reactor Core :

- D = 3.5 m
- H = 8-10m
- 100,000 pebbles
- d = 6 cm
- Q =1 pebble/min



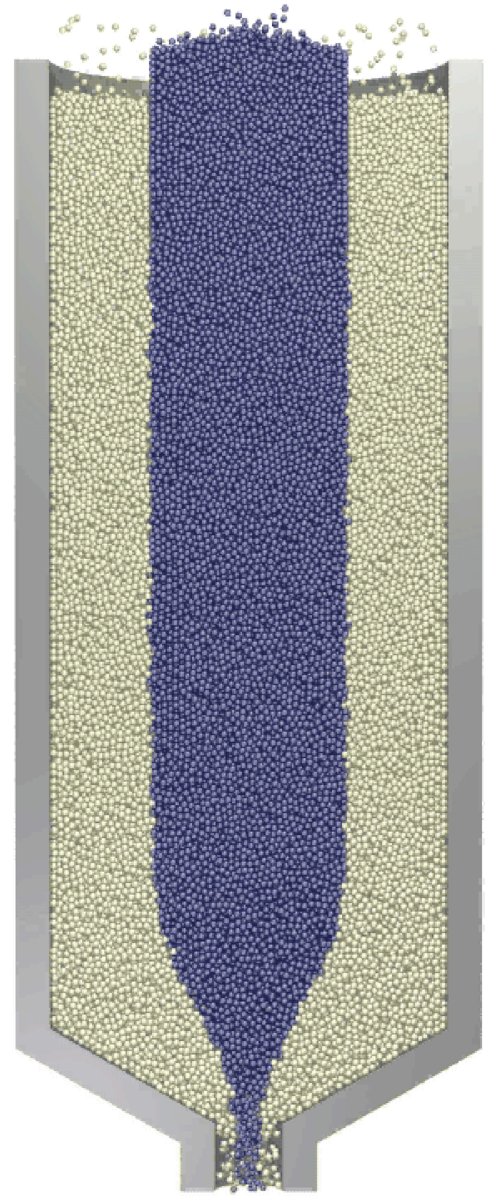
Experiments and Simulations

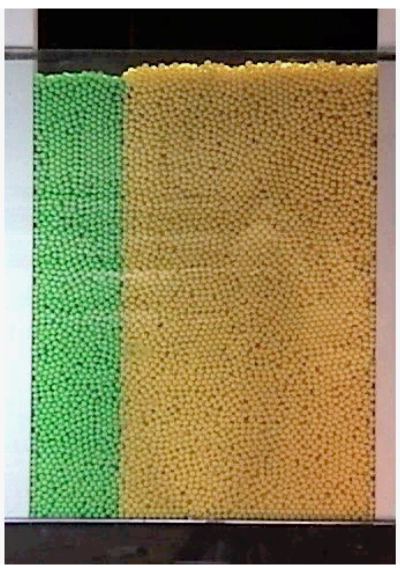
MIT Dry Fluids Lab
http://math.mit.edu/dryfluids



Half-Reactor Model
Kadak & Bazant (2004)
Plastic or glass beads

3d Discrete Elements (“Molecular Dynamics”)
Sandia parallel code from Gary Grest
Rycroft, Bazant, Landry, Grest (2005)
Frictional, viscoelastic spheres
N=400,000



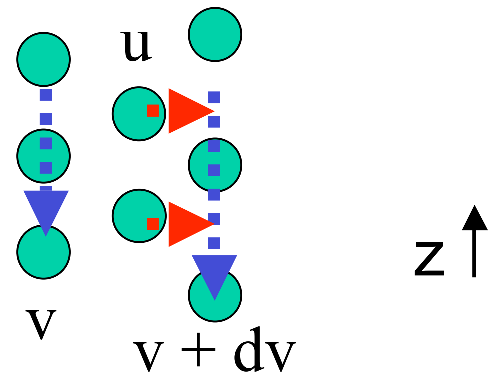


Quasi-2d Silo
Choi et al., Phys. Rev. Lett. (2003)
Choi et al., Granular Matter (2005)
d=3mm glass beads
Digital-video particle tracking near wall

"Kinematic Model" for the *Mean* Velocity in a Silo

Nedderman & Tuzun, *Powder Tech.* (1979)

Choi, Kudrolli & Bazant, *J. Phys. A: Condensed Matter* (2005).



$$u = b\,\frac{\partial v}{\partial x}\ , \quad \frac{\partial v}{\partial z} = b\,\frac{\partial^2 v}{\partial x^2}$$

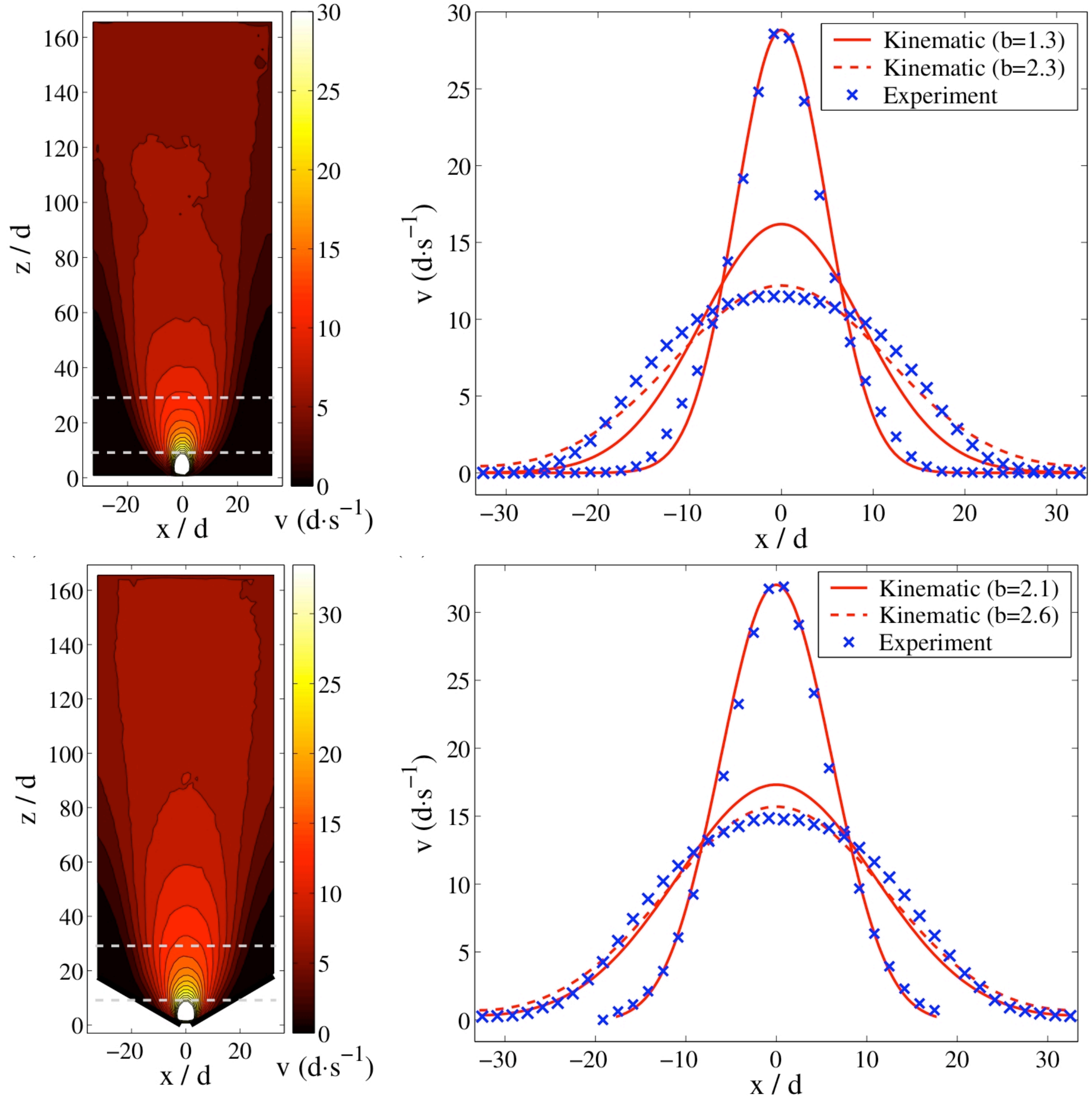
Green function = point opening

Parabolic streamlines

$$v(x, z=0) = Q\delta(x)$$

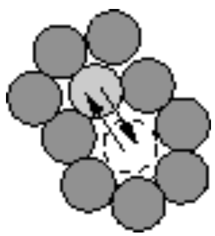
$$v = \frac{Q}{\sqrt{4\pi b z}}\exp\left(-\frac{x^2}{4bz}\right)$$

What is "diffusing"?

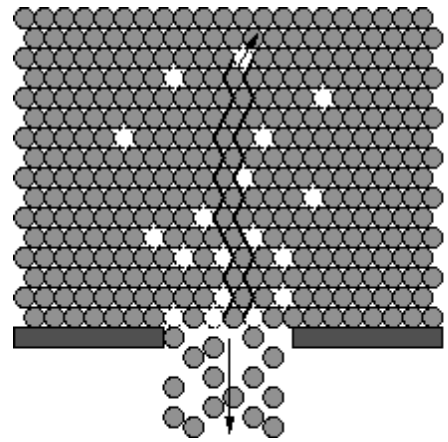


Microscopic Flow Mechanisms for Dense Amorphous Materials

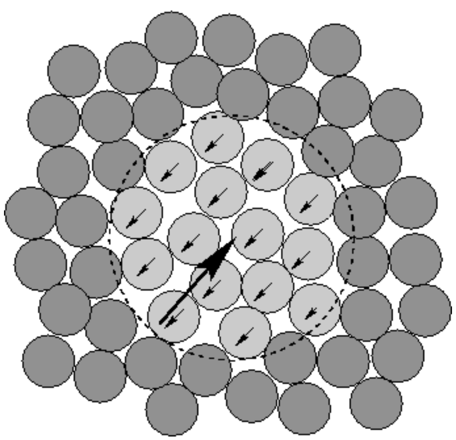
1. "Vacancy" mechanism for flow in viscous liquids (Eyring, 1936);
   Also: "free volume" theories of glasses
   (Turnbull & Cohen 1958, Spaepen 1977,…)

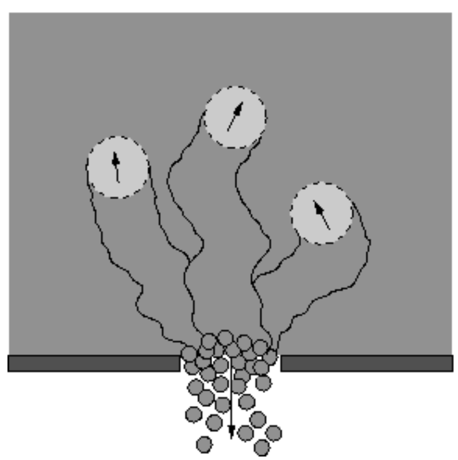


2. "Void" model for granular drainage
   (Litwiniszyn 1963, Mullins 1972)



3. "Spot" model for random-packing dynamics
   (M. Z. Bazant, Mechanics of Materials 2005)

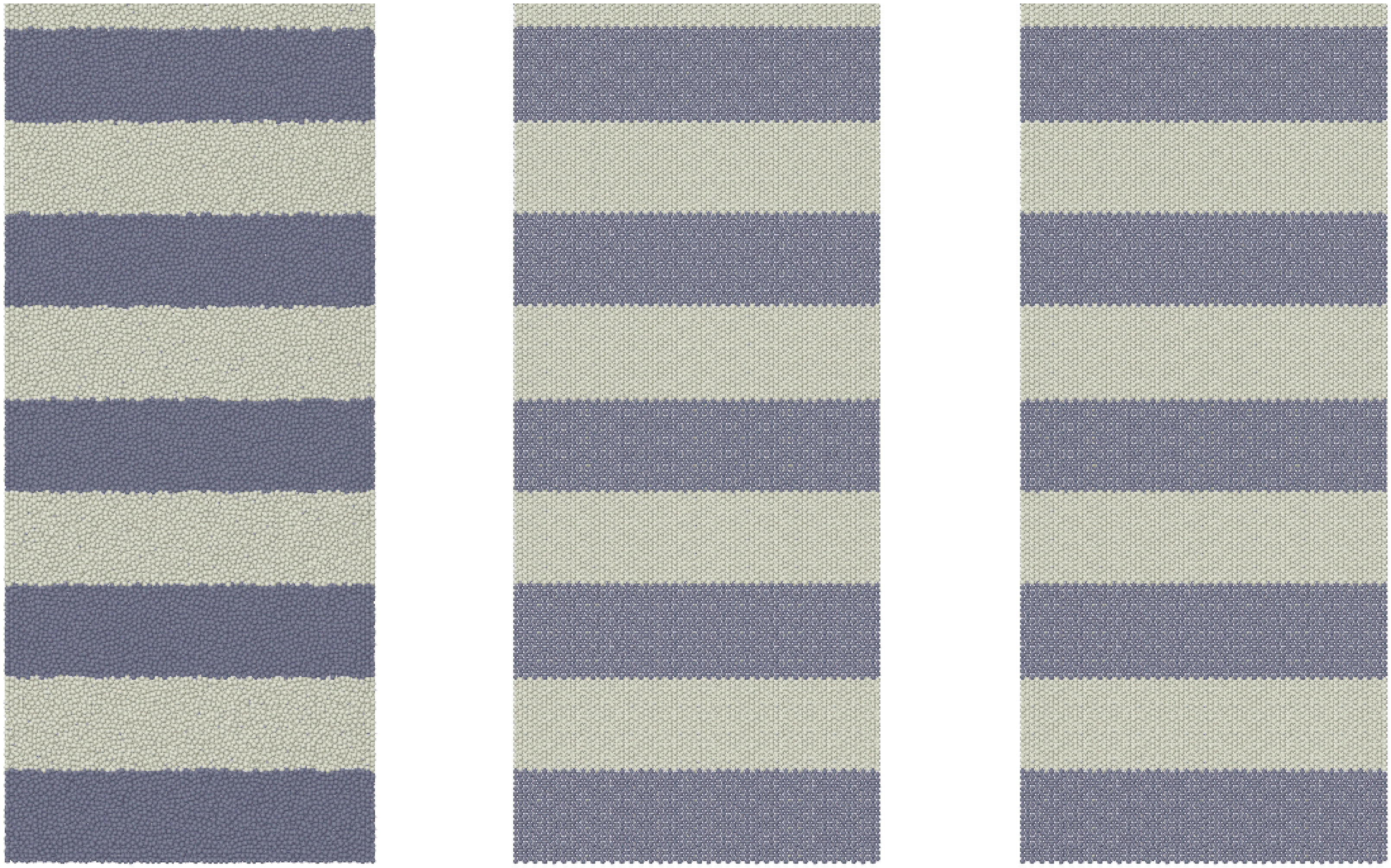




4. "Localized inelastic transformations"
   (Argon 1979, Bulatov & Argon 1994)

   "Shear Transformation Zones"
   (Falk & Langer 1998, Lemaitre 2003)

DEM **Spot Model** **Void Model**

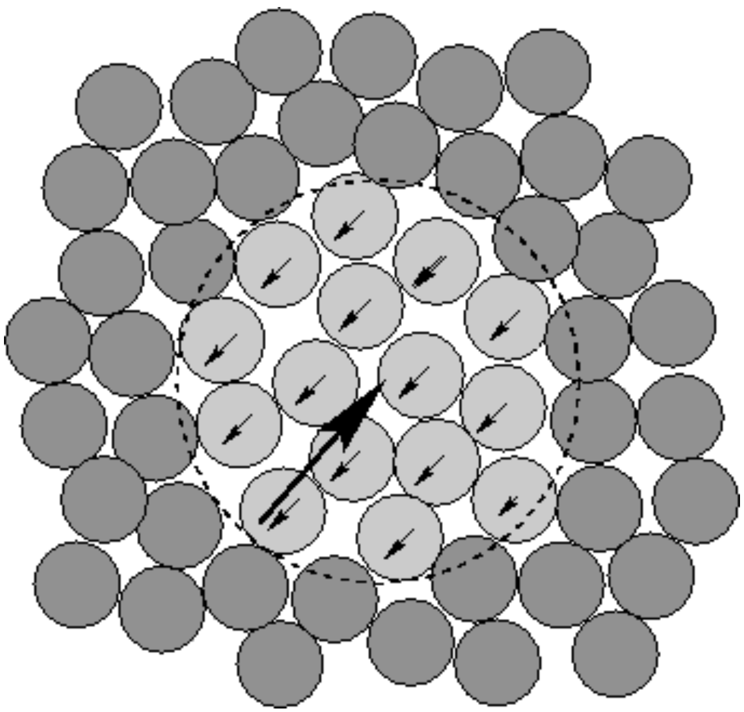


Simple spot model predicts mean flow and tracer diffusion in silo drainage fairly well (with only 3 params), but does not enforce packing constraints.

Simulations by Chris Rycroft

Correlations Reduce Diffusion

Simplest example: A uniform spot affects N particles.



- Volume conservation (approx.)

$$N\,V_p\,(\Delta x_p, \Delta z_p) = -V_s\,(\Delta x_s, \Delta z_s)$$

- Particle diffusion length

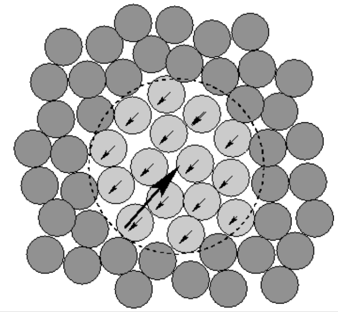
$$b_p = \frac{\mathrm{Var}(\Delta x_p)}{2|\Delta z_p|} = \frac{\alpha^2 \mathrm{Var}(\Delta x_s)}{2\alpha \Delta z_s} = \alpha\, b$$

where

$$\alpha = \frac{V_s}{N V_p} \approx \frac{\Delta\phi}{\phi^2} \approx 10^{-2}$$

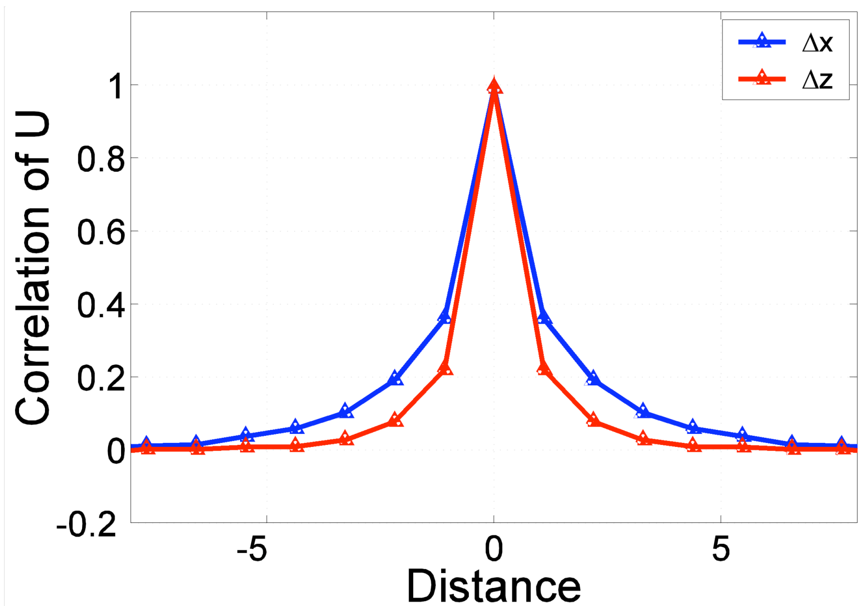
Experiment: 0.0025 DEM Simulation: 0.0024 (some spot overlap)

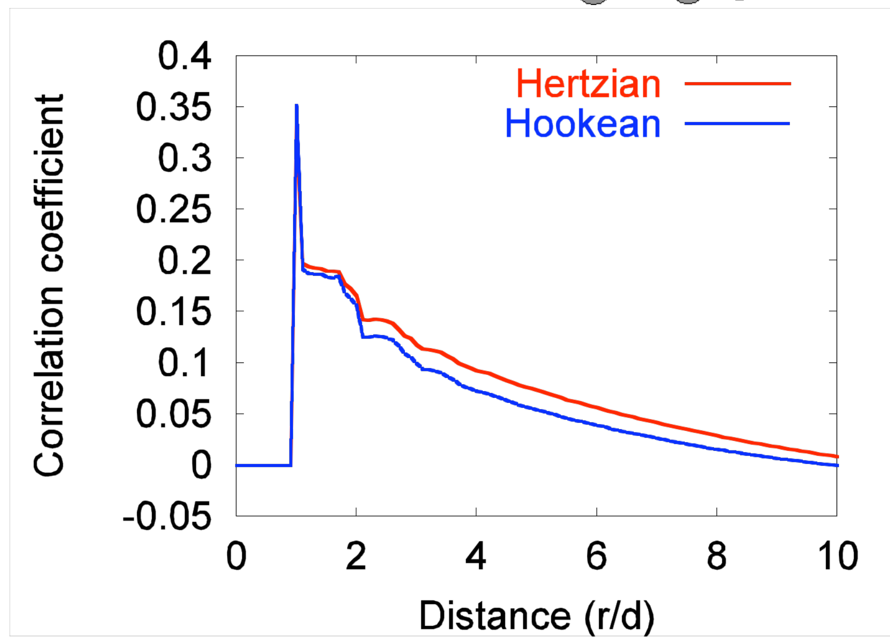
Direct Evidence for Spots



Spatial correlations in velocity fluctuations

(like “dynamic hetrogeneity” in glasses)





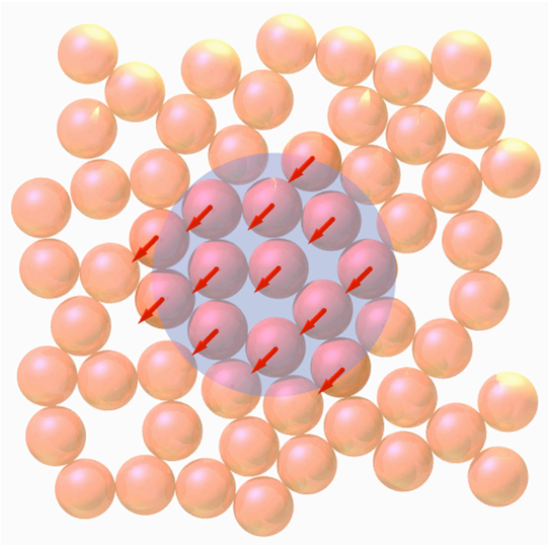
EXPERIMENTS

- MIT Dry Fluids Lab
- 3mm glass beads, slow flow (mm/sec)
- particle tracking by digital video
- 125 frames/sec, 1024-1024 pixels
- 0.01d displacements (near wall)

SIMULATIONS

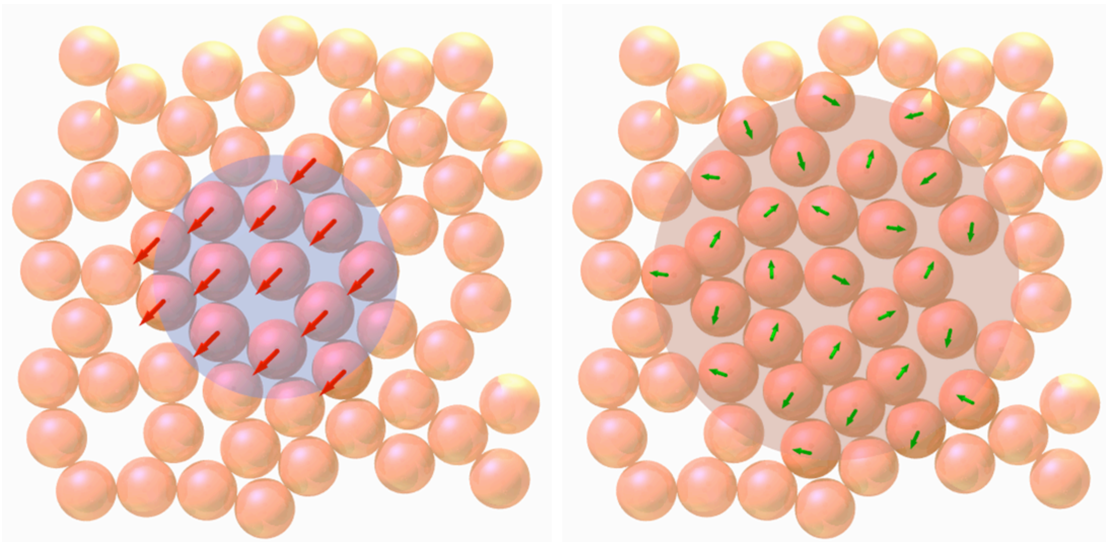
- 3d molecular dynamics (discrete elements)
- Sandia parallel code on 32-96 processors
- Friction, Coulomb yield criterion
- Visco-elastic damping
- Hertzian or Hookean contacts

“Multi-scale” Spot Algorithm
1. Simple spot-induced motion



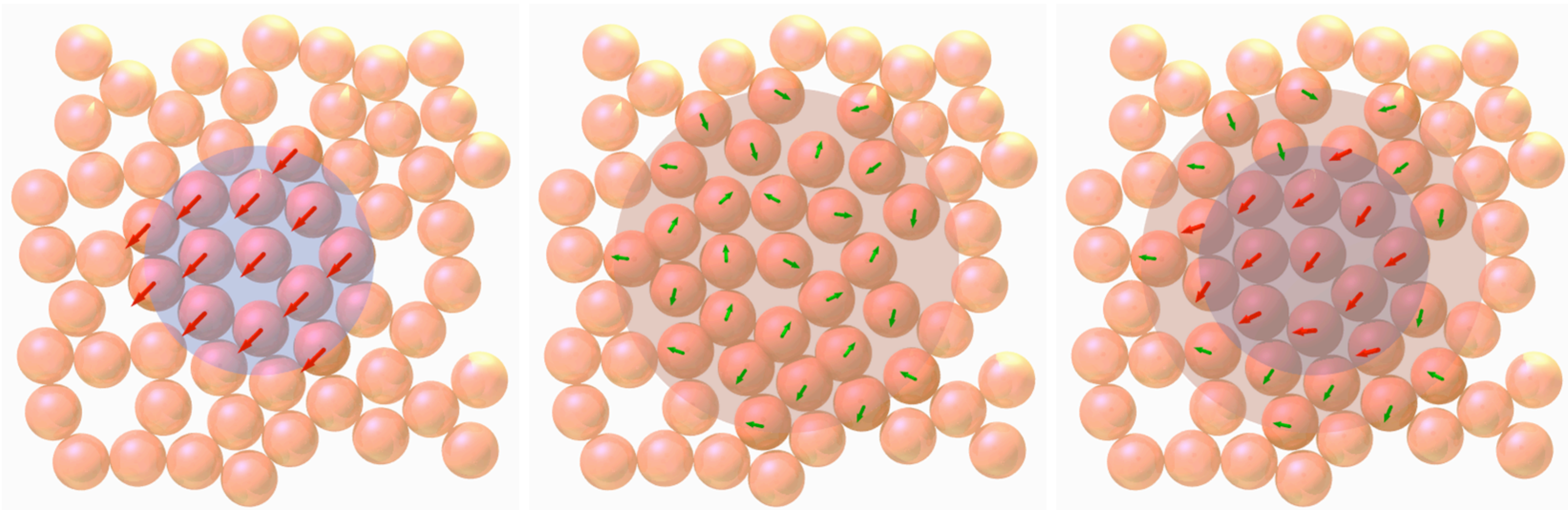
- Apply the usual spot displacement first to all particles within range

“Multi-scale” Spot Algorithm
2. Relaxation by soft-core repulsion



- Apply a relaxation step to all particles within a larger radius
- All overlapping pairs of particles experience a normal repulsive displacement (soft-core elastic repulsion)
- Very simple model - no “physical” parameters, only *geometry*.

"Multi-scale" Spot Algorithm
3. Net cooperative displacement



- Mean displacements are mostly determined by basic spot motion (80%), but packing constraints are also enforced
- *Can this algorithm preserve reasonable random packings?*
- *Will it preserve the simple analytical features of the model?*

3d Multiscale Model

Rycroft, Bazant, Landry, Grest (2005)

- Infer 3 spot parameters from DEM, as from expts:

  * radius = 2.6 d

  * volume = 0.33 v

  * diffusion length = 1.39 d

- Relax particles each step with soft-core repulsion

- "Time" = number of drained particles

- Very similar results as DEM, but >100x faster

- How might spot dynamics follow from

Spot Model

DEM

Classical Mohr-Coulomb Plasticity

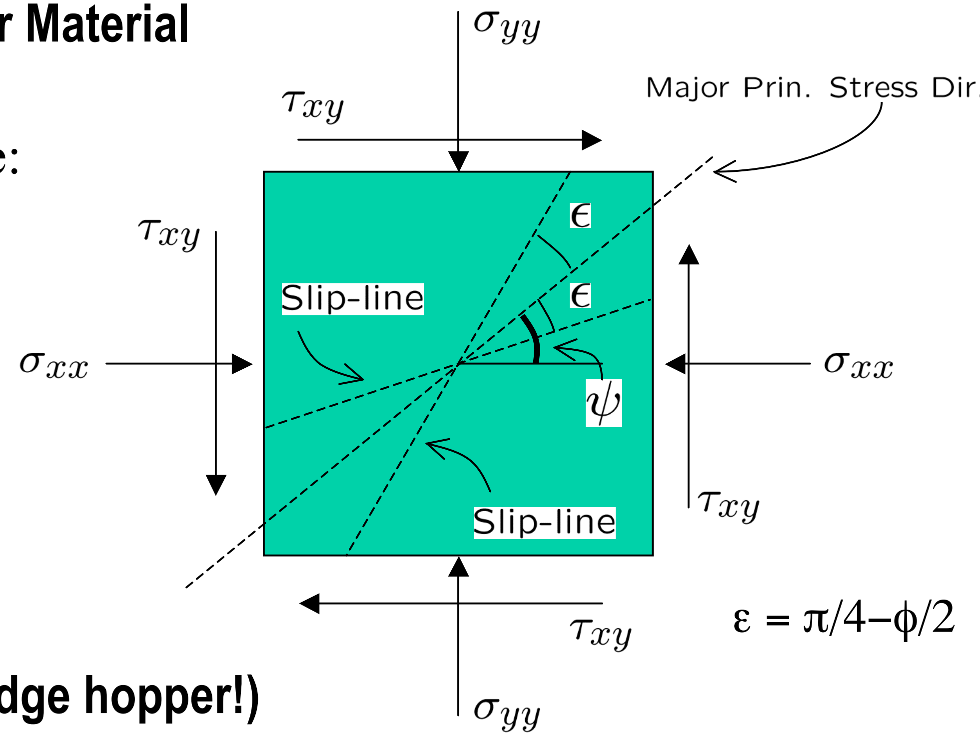
1. Theory of Static Stress in a Granular Material

Assume "incipient yield" everywhere:

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

μ= internal friction coefficient

ϕ= internal failure angle = $\tan^{-1}\mu$



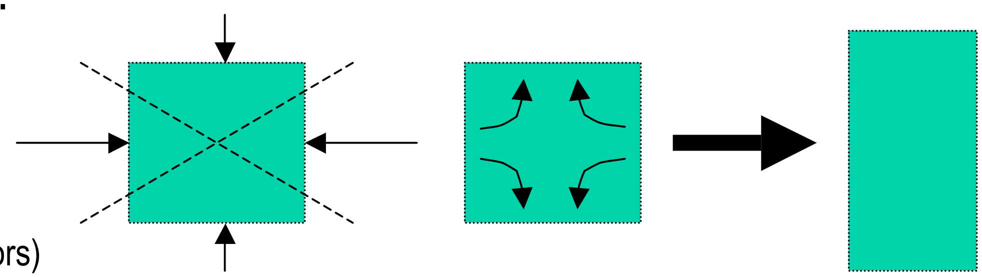
$\varepsilon = \pi/4 - \phi/2$

2. Theory of Plastic Flow (only in a wedge hopper!)

Levy flow rule / Principle of coaxiality:

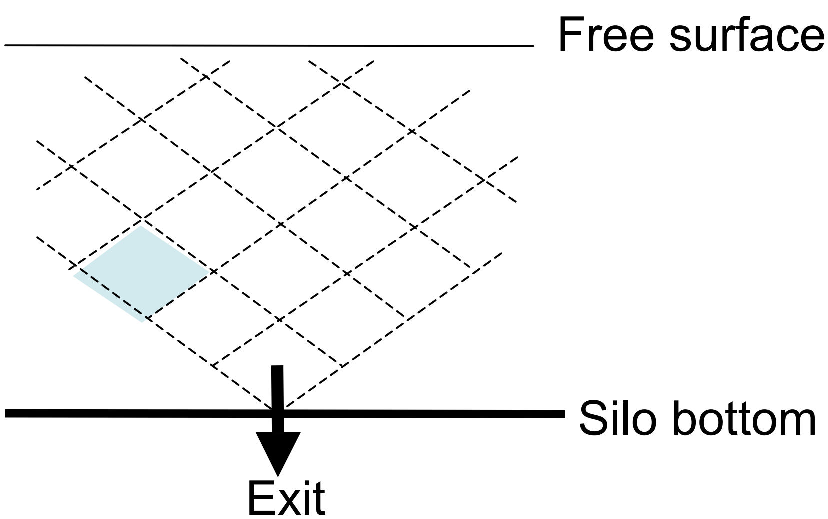
Assume equal, continuous slip along *both* incipient yield planes

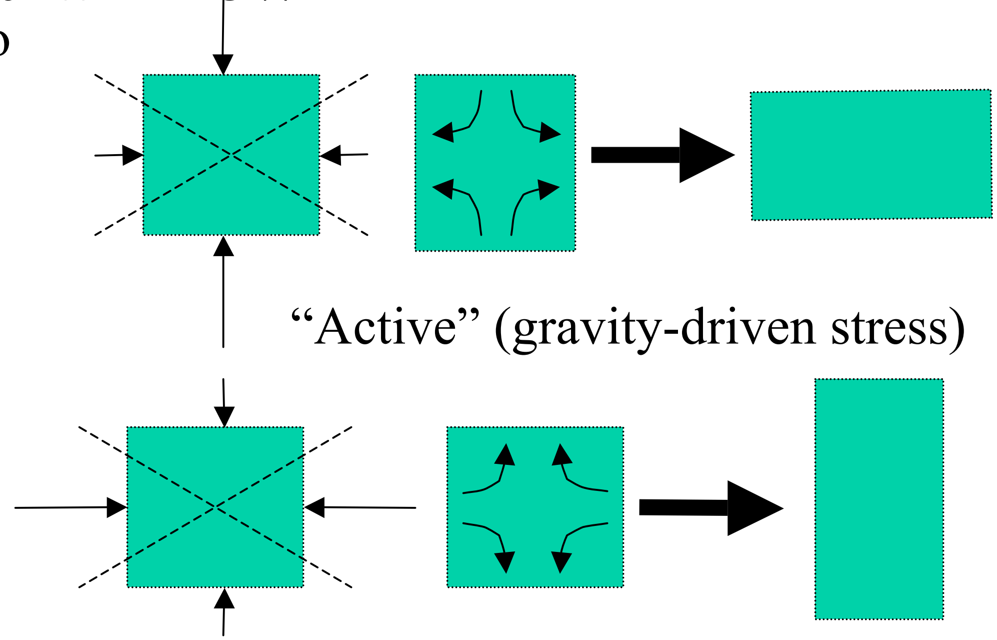
(stress and strain-rate tensors have same eigenvectors)



Failures of Classical Mohr-Coulomb Plasticity to Describe Granular Flow

1. Stresses must change from active to passive at the onset of flow in a silo (to preserve coaxiality).

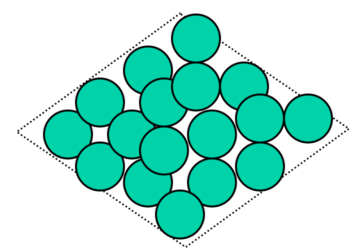




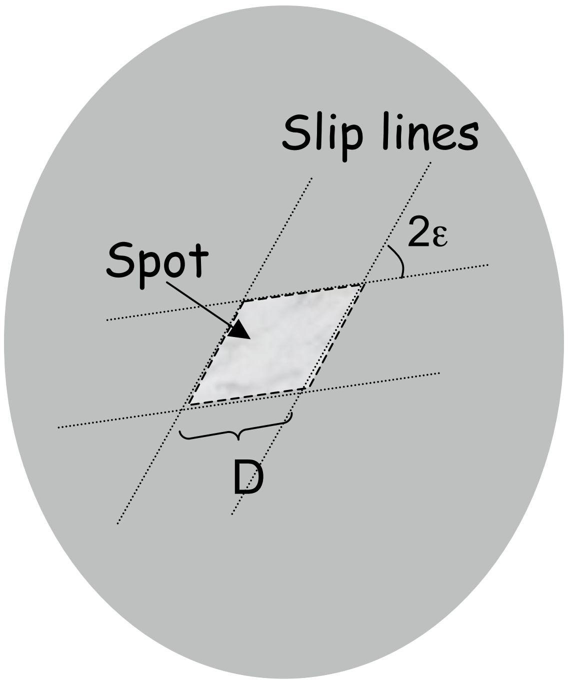
"Active" (gravity-driven stress)

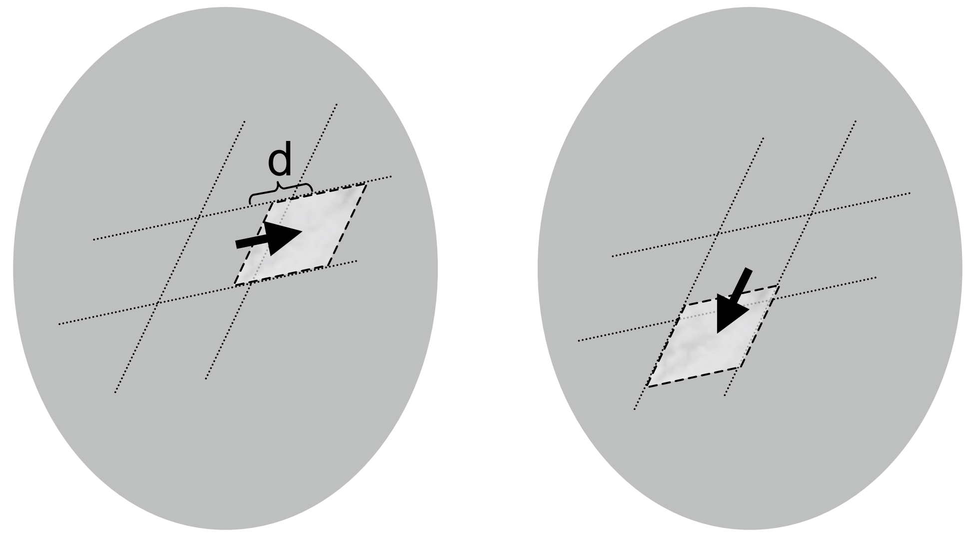
"Passive" (side-wall-driven flow)

2. Walls produce complicated velocity and stress discontinuities ("shocks") not seen in experiments with cohesionless grains.
3. No dynamic friction
4. No discreteness and randomness in a "continuum element"

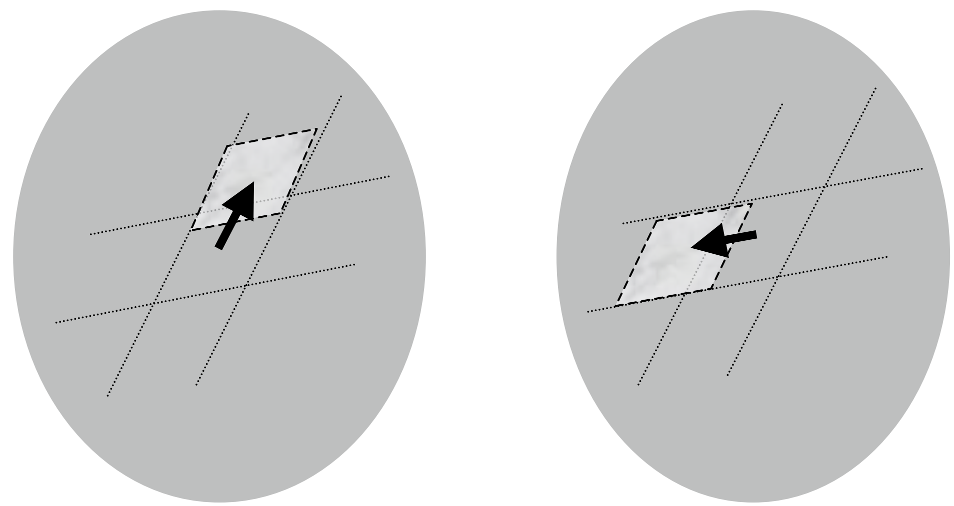


Idea (Ken Kamrin):
Replace coaxiality with an appropriate discrete spot mechanism





Stochastic "Flow Rule"



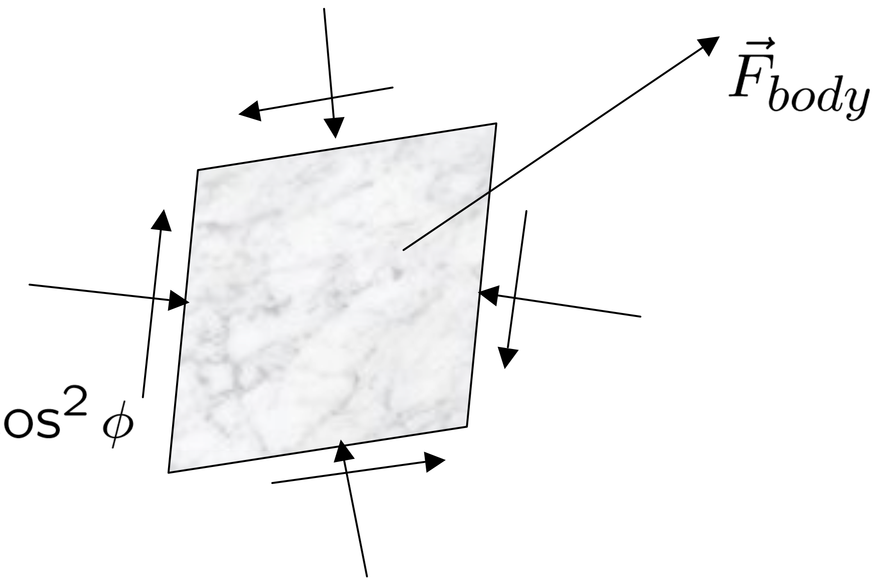
Spots random walk along Mohr-Coloumb slip lines (but not on a lattice)

Similar ideas in lattice models for glasses:
Bulatov and Argon (1993), Garrahan & Chandler (2004)

A Simple Theory of Spot Drift

Spot = localized failure where μ is replaced by μ_k (static to dynamic friction)

(Assume quasi-static global stress distribution is unaffected by spots.)



Net force on the particles affected by a spot

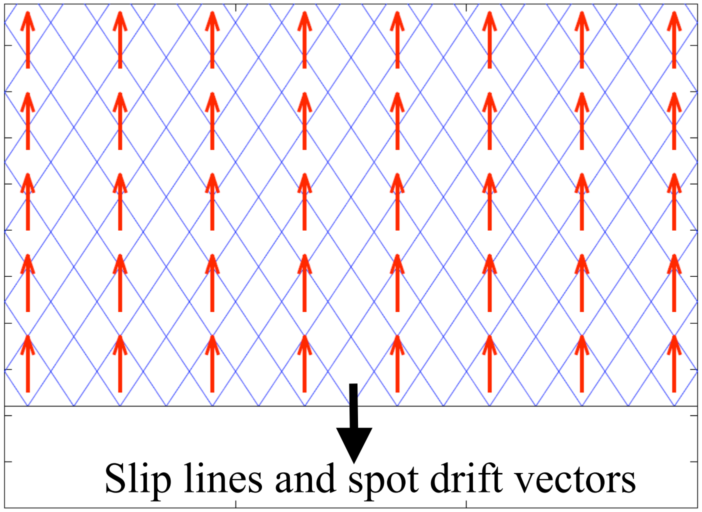
$$\vec{F}_{net} = (1 - \mu_k/\mu)\ (\vec{F}_{body} - \cos^2\phi\ \vec{\nabla} p)$$

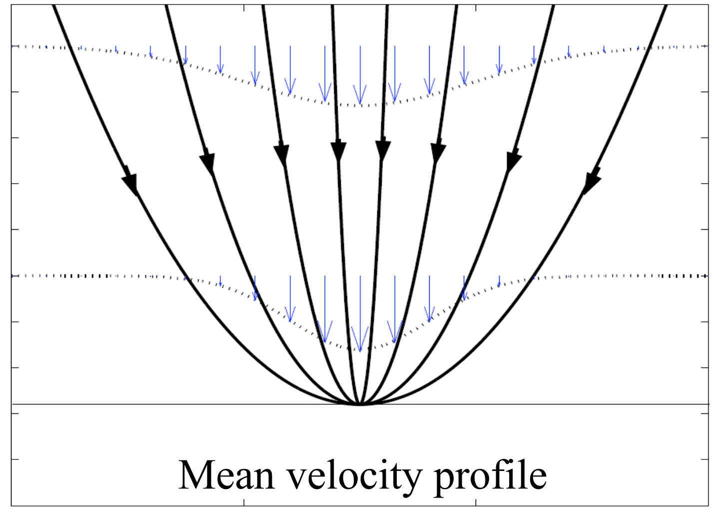
A spot's random walk is biased by this force projected along slip lines.

Next derive a Fokker-Planck equation for particle drift and diffusion which depends non-locally on the spot distribution in space (and time?)…

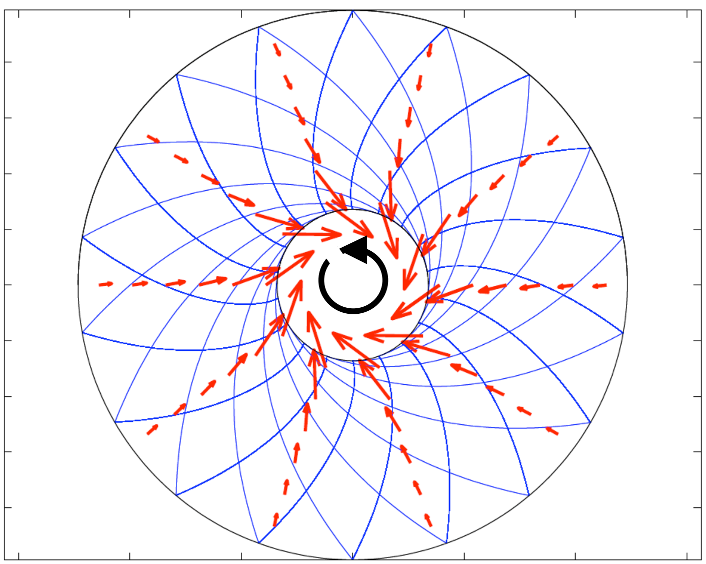
A General Theory of Dense Granular Flow?

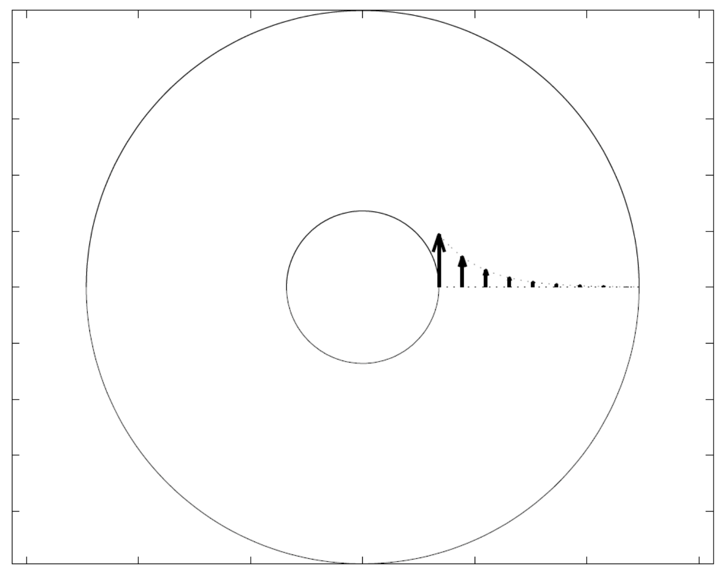
Gravity-driven drainage from a wide quasi-2d silo: Predicts the kinematic model



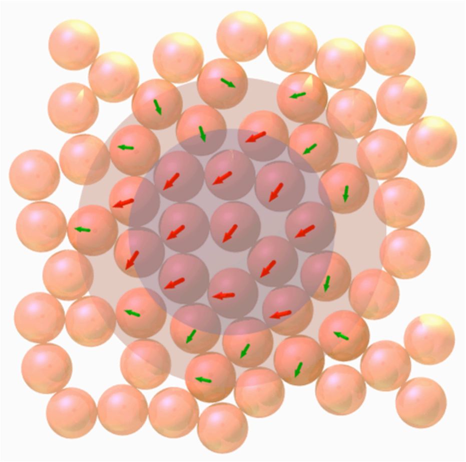


Coette cell with a rotating rough inner wall: Predicts shear localization

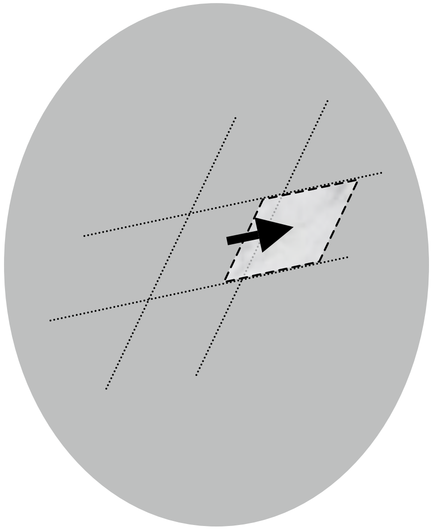




Conclusion



- "Spot model" = precise, simple mechanism for the dynamics of dense random packings
- Random walk of spots along slip lines yields "stochastic flow rules" for continuum plasticity
- Stochastic Mohr-Coulomb plasticity seems capable of predicting *different* granular flows



- Interactions between spots? Extend to 3d, other materials,…?

For papers, movies,… http://math.mit.edu/dryfluids

Mohr-Coulomb Stress Equations (assuming incipient yield everywhere)

$$(1+\sin\phi\cos 2\psi)p_x - 2p\sin\phi\sin 2\psi\ \psi_x + \sin\phi\sin 2\psi\ p_y + 2p\sin\phi\cos 2\psi\ \psi_y = F_x^{body}$$

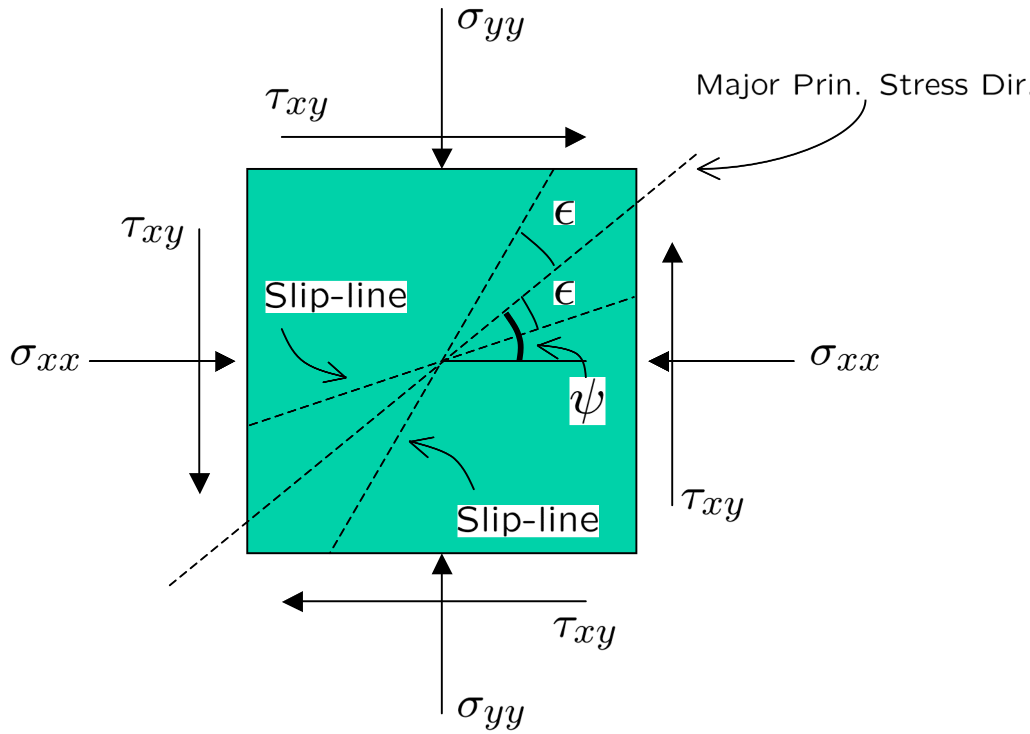
$$\sin\phi\sin 2\psi\ p_x + 2p\sin\phi\cos 2\psi\ \psi_x + (1-\sin\phi\cos 2\psi)p_y + 2p\sin\phi\sin 2\psi\ \psi_y = F_y^{body}$$

Characteristics (the slip-lines)

$$\frac{dy}{dx} = \tan(\psi - \epsilon)$$

$$\frac{dy}{dx} = \tan(\psi + \epsilon)$$

$$\varepsilon = \pi/4 - \phi/2$$



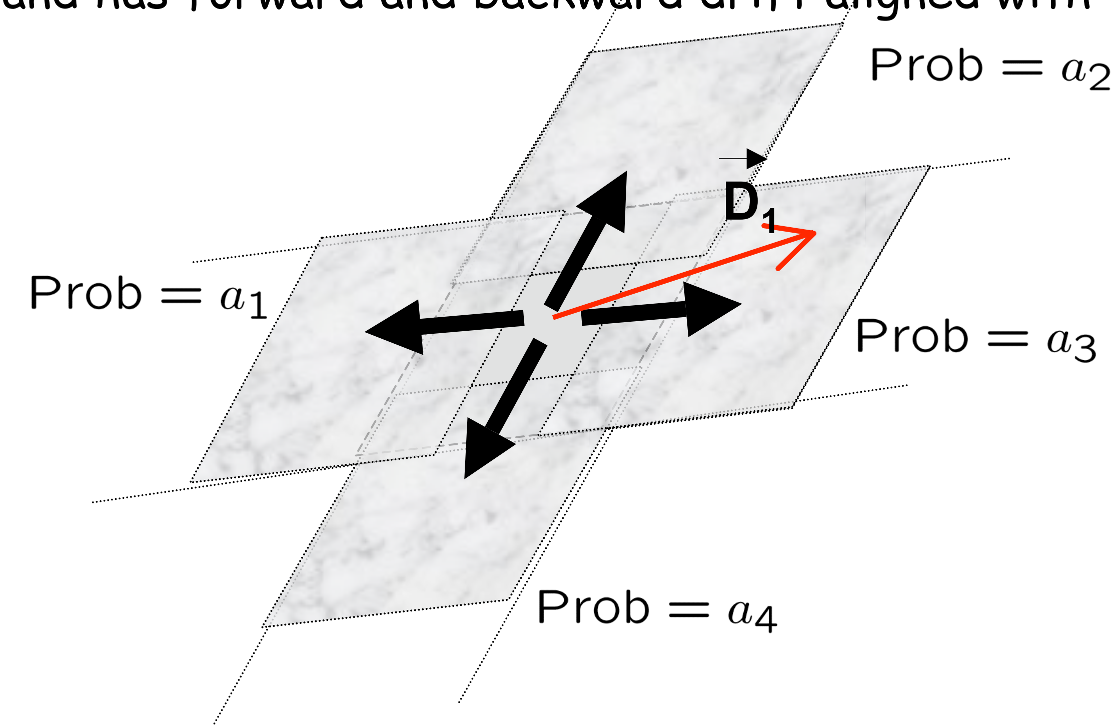
$$p = \frac{\sigma_{xx} + \sigma_{yy}}{2} = \text{Average normal stress}$$

$$\psi = -\frac{1}{2}\arctan\left(\frac{2\tau_{xy}}{\sigma_{xx} - \sigma_{yy}}\right) = \text{Angle anti-clockwise from x-axis to major principal stress direction}$$

- Spot drift opposes the net material force.
- Spots drift through slip-line field constrained only by the geometry of the slip-lines. Probability of motion along a slip-line is proportional to the component of $-F_{net}$ in that direction. Yields drift vector:

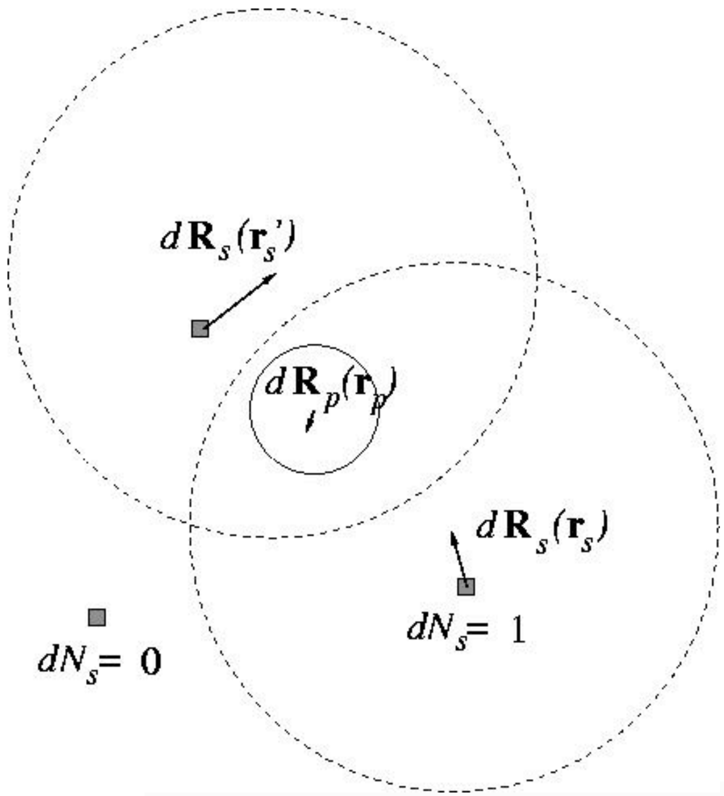
$$\vec{D}_1 = -\gamma\,(1-\mu_k/\mu)\left(\mathbf{I} + \cos 2\epsilon \begin{bmatrix} \cos 2\psi & \sin 2\psi \\ \sin 2\psi & -\cos 2\psi \end{bmatrix}\right)(\vec{F}_{body} - \cos^2\phi\,\vec{\nabla}p)$$

- For diffusion coefficient $\underline{D}_2$, must solve for the unique probability distribution over the four possible steps which generates the drift vector and has forward and backward drift aligned with the drift direction.



$$\frac{a_1}{a_4} = \frac{a_3}{a_2}$$

A *Nonlocal* Stochastic Differential Equation for Tracer Diffusion



w = spot influence function

$$d\mathbf{R}_p(\mathbf{r}_p, t) = -\int dN_s(\mathbf{r}_s, t)\, w(\mathbf{r}_p, \mathbf{r}_s + d\mathbf{R}_s(\mathbf{r}_s, t))\, d\mathbf{R}_s(\mathbf{r}_s, t)$$

Random Riemann sum of random variables:

$$\Delta\mathbf{R}_p(\mathbf{r}_p) = -\sum_n \sum_{j=1}^{\Delta N_s^{(n)}} w\left(\mathbf{r}_p, \mathbf{r}_s^{(n)} + \Delta\mathbf{R}_s^{(j)}(\mathbf{r}_s^n)\right)\, \Delta\mathbf{R}_j^{(n)}(\mathbf{r}_s^n)$$

A Mean-field Fokker-Planck Equation

$$\frac{\partial P_p}{\partial t} + \nabla \cdot (\mathbf{u}_p P_p) = \nabla\nabla : (\mathbf{D}_p P_p)$$

- Poisson process for spot positions
- Independent spot displacements

$$\langle dN_s \rangle = \mathrm{Var}(dN_s) = \rho_s dV$$

Drift velocity

$$\mathbf{u}_p(\mathbf{r}_p, t) = -\int d\mathbf{r}_s\, w(\mathbf{r}_p, \mathbf{r}_s)\, [\rho_s(\mathbf{r}_s, t)\mathbf{u}_s(\mathbf{r}_s, t) - 2\,\mathbf{D}_s(\mathbf{r}_s, t) \cdot \nabla \rho_s(\mathbf{r}_s, t)]$$

Diffusivity tensor

$$\mathbf{D}_p(\mathbf{r}_p, t) = \int d\mathbf{r}_s\, w(\mathbf{r}_p, \mathbf{r}_s)^2 \rho_s(\mathbf{r}_s, t)\, \mathbf{D}_s(\mathbf{r}_s, t)$$