Dynamics of Dense Granular Materials Dynamics Days, 2008 January 4, 2008

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- Gordon conference on Granular and Granular-Fluid Flow
- Colby College
- June 22-27, 2008
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Roadmap

- What/Why granular materials?
- Where granular materials and molecular matter part company—open questions of relevant scales
- Use experiments to explore:
- Forces, force fluctuations
- Jamming
- Plasticity, diffusion—unjamming from shear
- Granular friction

What are Granular Materials?

- Collections of macroscopic 'hard' particles: interactions are dissipative
 - Classical $h \rightarrow 0$
 - A-thermal T $\rightarrow 0$
 - Draw energy for fluctuations from macroscopic flow
 - Exist in phases: granular gases, fluids and solids
 - Large collective systems, but outside normal statistical physics
 - Analogues to other disordered solids: glasses, colloids..

Examples of Granular Materials

- Earthquake gouge
- Avalanches and mudslides
- Food and other natural grains: wheat, rice,...
- Industrial materials: coal, ores,...
- Soils and sands
- Pharmaceutical powders
- Dust
- Chemical processing—e.g. fluidized beds

Questions

- Fascinating and deep statistical questions
 - What is the nature of granular fluctuations—what is their range?
 - What are the statistical properties of granular matter?
 - Is there a granular temperature?
 - Phase transitions
 - Jamming and connections to other systems: e.g. colloids, foams, glasses,...
 - The continuum limit and 'hydrodynamics—at what scales?
 - What are the relevant macroscopic variables?
 - What is the nature of granular friction?
 - Novel instabilities and pattern formation phenomena

Practical Issues

Massive financial costs Claim:
 ~\$1 Trillion/year in US alone for granular handling

• Failures are frequent, typical facilities operate at only ~65% of design

o Soil stability is difficult to predict/assess

• How is stress/information transmitted in granular materials?

Problems close to home



Photo—Andy Jenike



Assessment of theoretical understanding

- Basic models for dilute granular systems are reasonably successful model as a gas—with dissipation
- For dense granular states, theory is far from settled, and under intensive debate and scrutiny

Are dense granular materials like dense molecular systems?

How does one understand order and disorder, fluctuations, entropy and temperature?

What are the relevant length/time scales, and how does macroscopic (bulk) behavior emerge from the microscopic interactions?

Granular Material Phases-Gases

Molecular Gases:

Collisions are short, velocities satisfy the Maxwell-Boltzmann distribution (speeds) and are in random directions

 $P(v) \sim exp[-(m/2)v^2/(k_BT)]$ —

 $< v^2 > \sim k_B T$ width of distribution

Granular Gases:

Again, collisions are short, velocities can be Maxwell-Boltzmann-like

$$\sim Tg$$

Expect that granular gases flow much like molecular gases with extra dissipation

Granular gases cool spontaneously, show clustering instability

Granular Material Phases-Dense Phases Granular Solids and fluids much less well understood than granular gases

Forces are carried preferentially on force chains→multiscale phenomena

Friction and extra contacts → preparation history matters

Deformation leads to large spatio-temporal fluctuations

In many cases, a statistical approach may be the only reasonable description

When we push, how do dense granular systems move?

• For small pushes, is a granular material elastic, like an ordinary solid, or does it behave differently?

What happens for larger deformations?

Jamming—how a material becomes solid-like as particles are brought into contact, or fluid-like when grains are separated

Plasticity—irreversible deformation when a material is sheared

Is their common behavior in other disordered solids: glasses, foams, colloids,...

Shearing

- What occurs if we 'tilt' a sample—i.e. deform a rectangular sample into a parallelogram?
- Equivalent to compressing in one direction, and expanding (dilating) in a perpendicular direction
- Shear causes irreversible (plastic) deformation. Particles move 'around' each other
- What is the microscopic nature of this process for granular materials?

A look at fluctuations, force chains and history dependence

GM's exhibit novel meso-scopic structures: Force Chains

2d Shear → Experiment

Howell et al. PRL 82, 5241 (1999)

Rearrangement of force chains leads to strong force fluctuations



Video of 2D shear flow



Frictional indeterminacy => history dependence



Note: 5 contacts => 10 unknown force components.

3 particles => 9 constraints

Point of View: To understand granular materials, one should take a statistical approach

What does this mean—what do we need to know?

Point-wise distributions for:

forces between particles, displacements/velocities...

Correlations—to tell us the important sizes for collective behavior

Structural information—e.g. how does packing affect granular properties?

Response to perturbations—How do granular solids respond to external forces/displacements?

Experiments to determine vector contact forces $P_1(F)$ is example of particle-scale statistical measure

Experiments use biaxial tester → and photoelastic particles



(Trush Majmudar and RPB, Nature, June 23, 2005)

Overview of Experiments



~2500 particles, bi-disperse, $d_L=0.9cm$, $d_S=0.8cm$, $N_S/N_L=4$

Measuring forces by photoelasticity



Basic principles of technique

- Process images to obtain particle centers and contacts
- Invoke exact solution of stresses within a disk subject to localized forces at circumference
- Make a nonlinear fit to photoelastic pattern using contact forces as fit parameters
- $I = I_o \sin^2[(\sigma_2 \sigma_1)CT/\lambda]$
- In the previous step, invoke force and torque balance
- Newton's 3d law provides error checking

Examples of Experimental and 'Fitted' Images

Experiment





Current Image Size



Force distributions for shear and compression

Shear





 $\varepsilon_{xx} = -\varepsilon_{yy} = 0.04; \quad Z_{avg} = 3.1$



 $\varepsilon_{xx} = -\varepsilon_{yy} = 0.016; \quad Z_{avg} = 3.7$

Edwards Entropy-Inspired Models for P(f)

- Consider all possible states consistent with applied external forces, or other boundary conditions—assume all possible states occur with equal probability
- Compute Fraction where at least one contact force has value $f \rightarrow P(f)$
- E.g. Snoeier et al. PRL 92, 054302 (2004)
- Tighe et al. Phys. Rev. E, 72, 031306 (2005)

Some Typical Cases—isotropic compression and shear

Snoeijer et al. \downarrow



Tigue et al \downarrow .



Correlation functions determine important scales

- $C(\mathbf{r}) = \langle Q(\mathbf{r} + \mathbf{r'}) Q(\mathbf{r'}) \rangle$
- > \rightarrow average over all vector displacements **r**'
- For isotropic cases, average over all directions in
 r.
- Angular averages should not be done for anisotropic systems

Spatial correlations of forces—angle dependent

Shear

Compression



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Jamming—a 'big' picture

Class of systems that are constrained or jammed



FIG. 2. (a) A jammed colloid (schematic). Black: force chains; gray: Other force-bearing particles; white: Spectators. (b) Idealized rectangular network of force chains.

Bouchaud et al.



Liu and Nagel

The Jamming Transition

• Simple question:

What happens to key properties such as pressure, contact number as a sample is isotropically compressed/dilated through the point of mechanical stability?

Z = *contacts/particle*; Φ = *packing fraction*

Predictions (e.g. O'Hern et al. Torquato et al., Schwarz et al.

 $Z \sim Z_{I} + (\varphi - \varphi_{c})^{\dot{\alpha}} \qquad P \sim (\varphi - \varphi_{c})^{\beta} \qquad \begin{array}{l} \beta \text{ depends on force law} \\ (\text{discontinuity}) \\ \text{Exponent } \dot{\alpha} \approx 1/2 \end{array}$

S. Henkes and B. Chakraborty: entropy-based model gives P and Z in terms of a field conjugate to entropy. Can eliminate to get P(z)

Experiment: Characterizing the Jamming Transition—Isotropic compression



Majmudar et al. PRL 98, 058001 (2007)

LSQ Fits for Z give an exponent of 0.5 to 0.6


LSQ Fits for P give $\beta \approx 1.0$ to 1.1



What is actual force law for our disks?



Comparison to Senkes and Chakrabory prediction



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Irreversible motion: diffusion and plasticity

- What happens when grains slip past each other?
- Irreversible in general—hence plastic
- Occurs under shear
- Example1: pure shear



• Example 2: simple shear



• Example 3: steady shear



Experiments: Plastic failure and diffusion—pure shear and Couette shear

Granular plasticity for pure shear



Use biax and photoelastic particles

Mark particles with UV-sensitive Dye for tracking

Work with A. Tordesillas and coworkers

Apply Pure Shear





Resulting state with polarizer

And without polarizer

Consider cyclic shear



Backward shear--polarizer



Forward shear--polarizer

Particle Displacements and Rotations



Reverse shear—under UV

Forward shear—under UV



Deformation Field—Shear band forms





Statistical Measures: Contact Angle Distributions





Reverse shear

Forward shear

Force Distributions



Couette shear—provides excellent setting to probe shear band



B.Utter and RPB PRE 69, 031308 (2004) Eur. Phys. J. E 14, 373 (2004)

Schematic of apparatus



Photo of Couette apparatus



 $\sim 1 m$

~50,000 particles, some have dark bars for tracking

Motion in the shear band



Characterizing motion in the shear band

- Mean azimuthal flow (θ -direction)
- Fluctuating part—looks diffusive
- Other?

How to characterize diffusion?

Random walker: at times τ, step right or left by L with probability 1/2 Motion from step to step is uncorrelated

Mean displacement: $\langle X \rangle = 0$

Variance: $\langle X^2 \rangle = 2Dt$ $t = n \tau$; $D = L^2/\tau$

Imagine many independent walkers characterized by a density P(x,t)

 $\partial P/\partial t = D \partial^2 P/\partial x^2$ \leftarrow Diffusion equation

Variances vs. time—seem to grow faster/slower then linearly!



Could this be fractional Brownian motion?

 $< X^2 > \sim t^{2H}$ H =1/2 for ordinary case

 $H < \frac{1}{2} + \Rightarrow$ anticorrelation—step to the Right reduces probability of another rightward step

 $H > \frac{1}{2} + \Rightarrow$ correlation—step to the Right increases probability of another rightward step

Suggested in calculations by Radjai and Roux, Phys. Rev. Lett. <u>89</u>, 064302 (2002) But there is something else important—shear gradient → Taylor dispersion

In 2D and in the presence of a velocity field, v $\partial P/\partial t = D \ \partial^2 P/\partial x^2 \Rightarrow$

 $\partial P/\partial t + V.grad(P) = D \Delta P$ (D now a tensor)

Simple shear: $V_x = \gamma y$ $V_y = 0$ $\langle YY \rangle = 2D_{yy}t$ $\langle XY \rangle = 2D_{xy}t + D_{yy}\gamma t^2$ $\langle XX \rangle = 2D_{xx}t + 2D_{xy}\gamma t^2 + (2/3)D_{yy}\gamma t^3$

Diffusivities only appear sub- or super-diffusive due to Taylor-like dispersion and rigid

boundary



Experiment



Simulations of random walk, with velocity profile, etc

Is there more than just diffusion and mean flow? Relating experiments to Falk-Langer picture

- Follow small mesoscopic clusters for short times Δt
- Break up motion into 3 parts:
 - Center of mass (CoM)
 - Smooth deformation (like elasticity)
 - Random, diffusive-like motion
- Punch line: all three parts are comparable in size

Procedure

- Identify small clusters of particles
- Follow change in position over Δt of each particle wrt cluster CoM: $r_i \rightarrow r_i$ '
- LSQ fit to affine transformation: $r_i' = E r_i$
- The non-affine part is $\delta r_i = r_i' E r_i$
- $D_{\min}^2 = \Sigma (\delta r_i)^2$ (sum over cluster)
- Write $E = F R_{\theta}$ F symmetric
- $F = I + \epsilon$ ϵ is the strain tensor

Deformation occurs locally—Disks show local values of D^2_{min} —bright \rightarrow large D^2_{min}



Distributions of affine strain



Distributions of D²_{min} for different distances from shearing wheel

Useful candidate for measure of disorder?



What about distributions of the δr_i ?



Quasi-Gaussians

If $P = \exp(-a(\delta ri)^2)$ then $\log(\log(P)) \sim \log(|\delta ri|)$



Understanding distributions of D^2_{min}

•
$$P(\mathbf{D}_{\min}^2) = \int P_N(\delta r_1, \dots, \delta r_N) *$$

 $\delta(\mathbf{D}_{\min}^2 - \Sigma (\delta r_i)^2) d(\delta r_i)$

Assume $P_N(\delta r_1,...,\delta r_N) = \prod P_1(\delta r_i)$ ($P_1(\delta r_i)$ gaussians)

Then $P(D^2_{min}) \approx (D^2_{min})^{N-1} \exp(-D^2_{min}/C)$

Comparison of various 'width' parameters

All quantities have similar behavior and similar sizes:

 $V_{\theta} \Delta t$ = macroscopic motion Strains from ϵ $(D \Delta t)^{1/2}$ = diffusive motion



Why does granular friction matter?

- Frictional failure is at the base of our understanding of the macroscopic slipping in classical granular models
- We depend on granular friction (traction) for motion on soils...
- Granular friction is important for the stick-slip motion in earthquake faults
- Granular friction controls avalanche behavior

Granular Rheology—a slider experiment



Granular bed = 500 d × 20 d deep, d = 0.41 cm and 0.51 cm bidi sperse photoelastic disks. Typical speeds = 0.1-2 d/s. Slider length = 30-40 d. Dragging force = 0-100 grams (0-1 Newtons).

Experimental apparatus






Non-periodic Stick-slip motion

- Stick-slip motions in our 2D experiment are non-periodic and irregular
- Time duration, initial pulling force and ending pulling force all vary in a rather broad range
- Random effects associated with small number of contacts between the slider surface and the granular disks.

Size of the slider \sim 30-40 d



Definitions of stick and slip events

Stick-slip Events Distributions

- Gutenberg Richter Relation for earthquake events distribution: where b is around -1.
- The change of F² during stick-slip events is a measure of the energy stored or released in these events.
- For lower Δ(F²) events, a power law fit applies quite well.
- For higher Δ(F²) events, we need more data to get a better statistics.

$$\log N = a + bM$$



Observations:

- Force chain structures change significantly in a slip event.
- As a build-up to a big event, force chains tend to be bent by the moving slider, releasing some energy, but not much.
- When bent too much, some force chains can no longer hold, there is rearrangement of these chains, with the significant energy release.
- Build force-chain-spring model with failure thresholds

Video of force chain failure model



Simple comparison—model/experiment distribution of energy loss in pulling spring



Conclusions

- Statistical approach provides an important new way to understand the properties of granular materials
- Use distributions of forces, correlation functions...
- Long-range correlations for forces in sheared systems—thus, force chains can be mesoscopic at least
- Predictions for jamming (mostly) verified
- Z may be key variable for shear failure
- Diffusion in sheared systems: insights into microscopic statistics of driven granular materials
- Granular friction with dynamics—many open and challenging puzzles