## **Granular Materials III**



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#### The O'Hern Group





http://jamming.research.yale.edu/

The O'Hern group in the Fall 2011: (from left to right) Thibault Bertrand, Diego Caballero, Wendell Smith, Mate Nagy, Mark Shattuck, Alice Zhou, Jared Harwayne-Gidansky, Corey O'Hern, Georgia Lill, Maxwell Micali, Minglei Wang, Robert Hoy, Tianqi Shen, Carl Schreck, S. S. Ashwin, and Stefanos Papanikolaou

## The O'Hern Group

 Dr. S. S. Ashwin, Ph.D. in Physics, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India (protocol dependence in granular media)
 Dr. Robert Hoy, Ph.D. in Physics, The Johns Hopkins University (polymer collapse, colloidal clusters)

3. Dr. Stefanos Papanikolau, Ph.D. in Physics, University of Illinois, Urbana-Champaign (frictional granular packings)

4. Minglei Wang, 1st year Ph.D. student in Mechanical Engineering & Materials Science (frictional granular packings)

5. Thibault Bertrand, 1st year Ph.D. student in Mechanical Engineering & Materials Science (vibrations in granular packings)

6. Wendell Smith, 2nd year Ph.D. student in Physics (intrinsically disorder proteins)

7. Diego Caballero, 2nd year Ph.D. student in Physics (modeling of chromatin)

8. Jared Harwayne-Gidansky, 3rd year Ph.D. student in Electrical Engineering (polymer collapse and packing)

9. Alice Zhou, 3rd year Ph.D. student in Molecular Biophysics & Biochemistry (protein-protein interactions)

10. Tianqi Shen, 4th year Ph.D. student in Physics (contact percolation)

11. Carl Schreck, 6th year Ph.D. student in Physics (granular packings)

## Static Granular Packings





Stress-induced birefringence

T. S. Majmudar and R. P. Behringer, "Contact force measurements and stress induced anisotropy in granular materials", Nature 43 (2005) 1079.

## Birds' Nests?

Despite the fact that granular materials are the second-most human-manipulated material (behind water), we waste billions of dollars in processing, conveying, and separating granular materials in the pharmaceutical, oil, agriculture, and other industries. Further, we are not able to effectively and efficiently design and make granular composite materials with precisely targeted structural and mechanical properties. For example, granular media with novel acoustic properties, such as band pass and filter capabilities would have many commercial and military applications.

We propose a multi-pronged effort to identify and understand the strategies that many bird species employ to make robust, mechanically stable nests. We will then mimic these design strategies so that we can reliably produce mechanically stable structures from component materials that possess a wide variation of structural and material properties, yet possess robust mechanical properties on the large scale of the structure. These studies will dramatically improve our ability to build composite granular metamaterials with precisely tuned structural and mechanical properties, yet using inexpensive and interchangeable components.

#### Statistical Mechanics of Granular Media



Apply driving to attain reversible set of statesDifferent driving mechanisms lead to different sets of states!

"One must understand static packings of frictionless particles to understand frictional granular packings."

C. S. O'Hern

# Outline

1. What are the microstates for mechanically stable (MS) packings? Are MS packings points or continuous geometrical families in configuration space?

2. Are MS packings equally probable? If not, what determines their probabilities? How do the probabilities depend on the packing-generation protocol?

3. How do particle shape and friction affect the microstate statistics?

4. Can the vibrational response (or heat flow) be determined from *static* MS packings?

## Attributes of Simple Granular Materials

1. Finite number of macroscopic grains with dissipative interactions; exist at `zero temperature' unless driven by external forces

- 2. Contact interactions; no harmonic approximation?
- 3. Non-spherical particle shapes
- 4. Frictional or `history-dependent' interactions

## Granular Model I: Frictionless Disks



repulsive central forces,  $F_{ii} \sim \delta^{\alpha} \sim (1 - r_{ii} / \sigma_{ii})^{\alpha}, \alpha = 1$ 

zero force,  $F_{ii} = 0$ 

 $m\vec{a}_i = \sum_i \vec{F}_{ij} - \underbrace{b\vec{v}_i}_i$  Minimize energy V(r) to reach T=0 at each  $\phi$  $V(\vec{r}) = \sum_{i>i} V(r_{ij}) \qquad V(r_{ij}) = \frac{\varepsilon}{\alpha} \left(1 - \frac{r_{ij}}{\sigma_{ii}}\right)^{\alpha} \quad \text{for overlapping particles}$ 

## Conservation of Total Energy; NVE

$$E = K + V \qquad K = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m} \qquad V = \sum V(r_{ij})$$

$$\frac{dE}{dt} = \sum_{i} \left( \frac{\partial K}{\partial \vec{p}_{i}} \frac{\partial \vec{p}_{i}}{\partial t} + \frac{\partial V}{\partial \vec{r}_{i}} \frac{\partial \vec{r}_{i}}{\partial t} \right) \qquad \dot{\vec{r}_{i}} = \frac{\vec{p}_{i}}{m} \qquad \text{Newton's equations}$$
$$\frac{dE}{dt} = \sum_{i} \frac{\vec{p}_{i}}{m} \left( \frac{d\vec{p}_{i}}{dt} - \vec{F}_{i} \right) = 0 \qquad \dot{\vec{p}}_{i} = \vec{F}_{i}$$

•Newton's equations of motion conserve energy, not T

#### Integration of Equations of Motion

$$\begin{aligned} x_i(t + \Delta t) &= x_i(t) + v_i(t)\Delta t + \frac{1}{2}a_i(t)(\Delta t)^2 & \text{velocity} \\ v_i(t + \Delta t) &= v_i(t) + \frac{a_i(t) + a_i(t + \Delta t)}{2}\Delta t & \text{algorithm} \end{aligned}$$

Leapfrog Verlet Algorithm; calculate unconstrained v(t+ $\Delta t/2$ ), Correct v(t+ $\Delta t$ ); or Gear Predictor-corrector steps

# `Two' Types of Energy Minimization

- 1. Conjugate Gradient (CG)
- Numerical method to find local minima of total potential energy
- Overdamped, infinite quench rate
  b→∞
  - 2. Molecular Dynamics (MD)
  - Solve Newton's eqns. of motion

$$m\vec{a}_i = \vec{F}_i = \vec{F}_{spring} - b\vec{v}_i$$

• Finite damping, quench rate b=0.5



What is the packing fraction  $\phi$ ?



# What are the allowed static packings for a given N with vanishing particle overlaps?



Mechanically stable packing with fixed boundaries

Overlapped soft disks; disallowed hard-disk configs

## Distinct Mechanically Stable Macrostates and Microstates



polarizations/permutations



8 microstates

Jammed = mechanically stable (MS) configuration with extremely small particle overlaps; net forces (and torques) are zero on each particle; quadratically stable to small perturbations



Gold Standard:

# Configuration is mechanically stable if dynamical matrix contains dN-d eigenvalues $\omega^2 > 0$ (periodic b.c.s)

http://gibbs.engr.ccny.cuny.edu/technical/DisorderedSolids/DOSvPcorr.php

#### Exponential Growth of MS macrostates



•What about placement of rattler particles; does this increase scaling of N<sub>s</sub>, *i.e.*  $\binom{N_{cav}}{N_r}$ ?

•What about scaling of  $N_c^{min}$ -1, $N_c^{min}$ -2,... and  $N_c^{min}$ +1, $N_c^{iso}$ +2,... with N?

## MS Packing-Generation Algorithm







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Collectively Jammed Hard Spheres = Mechanically Stable Soft Sphere Packings



A. Donev, S. Torquato, F. H. Stillinger, and R. Connelly, Jamming in Hard Sphere and Disk Packings, Journal of Applied Physics, 95 (2004) 989.

## Are MS packings points in configuration space? Can we show this experimentally?

G.-J. Gao, J. Blawzdziewicz, C. S. O'Hern, and M. Shattuck, ``Experimental demonstration of nonuniform frequency distributions of mechanically stable granular packings", Phys. Rev. E 80 (2009) 061304.



#### **Deposition Algorithm in Simulations**



- •All geometric parameters identical to those for experiments •Terminate algorithm when  $F_{tot} < F_{max} = 10^{-14}$
- •Vary random initial positions and conduct  $N_{trials} = 10^8$  to find 'all' mechanically stable packings for small systems N=3 to 10.

## Mechanically Stable Frictionless Packings



•Distinct MS packings distinguished by particle positions  $\{\vec{r}_i\}$ •# of constraints  $\geq$  # of degrees of freedom **Configuration Space of Mechanically Stable Packings** 

$$R = \left\{ \vec{r}_1, \vec{r}_2, \dots, \vec{r}_N \right\}$$



• $\Delta R_D$  = distance in configuration space between distinct MS packings • $\Delta R_C$  = error in measuring distinct MS packings

## Separation in Configuration Space



• MS frictionless packings are discrete points in configuration space

# **Discrete MS Packings**



How is the quantitative agreement between sims and exps?



•95% of distinct MS packing match; others are unstable in sims

## Are MS packings equally probable?

#### "for a given volume all [jammed] configurations are equally probable"

S. F. Edwards and R. B. S. Oakeshott, "Theory of Powders", Physica A 157 (1989) 1080

G.-J. Gao, J. Blawzdziewicz, C. S. O'Hern, and M. Shattuck, ``Experimental demonstration of nonuniform frequency distributions of mechanically stable granular packings", Phys. Rev. E 80 (2009) 061304.

## Sorted Probabilities



•7 (4) orders of magnitude variation in probabilities in simulations (experiments)

## MS Packing Probabilities Are Robust



• Rare MS packings in exps are rare in sims; frequent MS packings in exps are frequent in sims

## What determines MS packing probabilities?



• What are the important packing fractions?

#### MS packings occur over a range of packing fractions



P. Chaudhuri, L.Berthier, & S. Sastry, Phys. Rev. Lett., 104, 165701 (2010)
# **Contact Percolation Transition**



•Onset of cooperative and non-affine motion, irreversibility and weak protocol-dependence for  $\phi > \phi_P << \phi_c^{\min}$ 

T. Shen, C. S. O'Hern, & M. D. Shattuck, "The contact percolation transition in athermal particulate systems," Phys. Rev. E 85 (2012) 011308.

"Unjammed frictionless packings with  $\phi_P < \phi < \phi_J$  can be made mechanically stable by adding static friction"

# 'Random' Continuum Percolation



 $X_p = N\pi R_p^2/L^2$ 

# **Critical Scaling Exponents**







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## Finite-size scaling analysis for contact percolation



# Percolation Exponents

	continuum percolation	athermal repulsive	athermal attractive
D	1.91	1.89	1.88
τ	2.02	2.01	2.04
ν	1.33	1.68	1.92
φ <sub>P</sub>		0.549	0.558

...but percolation is purely geometrical, so what?

## Non-floppy Modes of Dynamical Matrix

$$M_{\alpha,\beta} = \frac{\partial^2 V(\vec{r})}{\partial r_{\alpha} \partial r_{\beta}} \bigg|_{\substack{\alpha,\beta=x, y \text{ particle} \\ \text{index} \\ \vec{r_0} = \text{positions of} \\ MS \text{ packing}}} \|_{\vec{r}=\vec{r_0}}$$

Calculate 2 N-2 eigenvalues,  $\omega$ 

Number of nonfloppy modes with ω>0

$$F(\phi) = \frac{N(\omega > 0)}{2N - 2} \qquad F(\phi_{\rm J}) = 1 \qquad F(\phi < \phi_{\rm J}) < 0$$

1

# Fraction of Non-Floppy Modes of Dynamical Matrix



How similar are the contact networks at  $\phi$  and  $\phi_J$ ?

$$\begin{array}{c} 1 \\ 2 \\ \end{array} \qquad \qquad A_{ij} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

$$O(\phi) = \frac{1}{N_c} \sum_{i>j} A_{ij}(\phi) A_{ij}(\phi_J) \qquad O(\phi_J) = 1$$

## Adjacency Matrix Overlap



#### **Cooperative Motion**



## Incremental Contour Length of Trajectory



### What determines MS packing probabilities?



fast rate;  $\phi_f = 0.622$ 

slow rate;  $\phi_f = 0.730$ 

• Protocol-dependent basin volume...

#### Density landscape for hard spheres



•Granular media are out-of-equilibrium at all  $\phi$  during packing-generation procedure

S. S. Ashwin, C. S. O'Hern, & M. D. Shattuck, submitted to Phys. Rev. E (2011).



N. Xu, D. Frenkel, and A. J. Liu, Phys. Rev. Lett. 106 (2011) 245502.

#### Method 1 (small l): Probability to return to a given MS packing



# Method 2 (large l): Random initial conditions



# **Basin Volumes**

$$P_{i} = \frac{V_{i}}{L^{dN}} \qquad \qquad V_{i} = \int_{0}^{\sqrt{dN}} S_{i}(l) dl$$

$$S_i(l) = A_{dN} f_i(l) l^{dN-1} \mathbf{P}_i N_s ! N_l! \qquad f_i(l) = \frac{M_i}{M}$$

#### Unweighted and Weighted Basin Profile Functions



• Probability is determined by large  $1 > l_c$ 



•Volumes of hyperspherical cores are much smaller than basin volumes!

#### Form of weighted basin profile functions



#### Protocol dependence of average weighted basin profile function

20

18

14

12└── 10<sup>−2</sup>

**10**<sup>-1</sup>

 $\widetilde{b}$ 

10<sup>0</sup>

10

ີ 16





# Floaters



Particle 2 can exist in two locations with fewer than 3 contacts



•Probability for MS packings determined by large l, not nearby regions of configuration space

- •Universal form for  $S_n(1)$
- •At what  $\phi_i$  do basin volumes become hyperspherical?

## New Directions: Reversibility/Irreversibility



Displacements from strain=0 from previous cycle



'Phase Digram' for Irreversible Flow



Do static granular packings possess a harmonic vibrational response?

## Harmonic Solids



- •Atomic and molecular systems
- •Pair potentials have `double-sided' minimum and are long-ranged
- •Equilibrium positions are well-defined
- •Vibrations at low T captured using harmonic approximation

# Causes of nonharmonicity in granular solids

• Nonlinear Hertzian interaction potential  $\mathbf{X}$ 

- Dissipation from normal contacts  $\chi$
- Sliding and rolling friction

• Breaking existing contacts and forming new contacts

X

# Model Particulate Media



Total potential energy 
$$V = \sum_{\langle i,j \rangle} V(r_{ij})$$

# Harmonic approximation: Normal Modes from Dynamical Matrix

$$M_{\alpha,\beta} = \frac{\partial^2 V(\vec{r})}{\partial r_{\alpha} \partial r_{\beta}} \bigg|_{\vec{r} = \vec{r}_0}^{\alpha,\beta=x, y, z, \text{ particle}} \vec{r}_0 = positions of MS packing}$$

Calculate d N- d eigenvalues;  $m_i = \omega_i^2 > 0$ .

#### Density of Vibrational Modes via Dynamical Matrix



$$D(\omega)d\omega = N(\omega + d\omega) - N(\omega)$$

•Why D( $\omega$ ) ? •Formation of plateau in D( $\omega$ ) (excess of low-frequency modes) as  $\Delta \phi = \phi - \phi_J \rightarrow 0$ 

A. J. Liu, S. R. Nagel, W. van Saarloos, and M. Wyart, "The jamming scenario--an introduction and outlook," Soft Matter (2010).

# Are jammed particulate systems harmonic?

$$\vec{r}_i' = \vec{r}_i + \delta \hat{e}_6$$



- Deform system along each 'eigenmode'  $\omega_i$
- Run at constant NVE, measure power spectrum of grain displacements
- Does system oscillate at frequency  $\omega_i$  from dynamical matrix?
# Power-spectrum of particle displacements



- System becomes strongly nonharmonic at extremely small  $\delta$
- First spreads to `harmonic' set of  $\omega$  (NH1); then continuum of  $\omega$  (NH2)





# Strongly Anharmonic Behavior



## **Geometrical Families**



• How can this happen? Boundary conditions, tangential forces

# How do slow, dense shear flows sample MS packings...with equal probability?



#### Quasi-static Couette Shear Flow $\dot{\gamma} \rightarrow 0$

B. Utter and R. P. Behringer Phys. Rev. Lett. 100 (2008) 203302H. A. Makse and J. Kurchan Nature 415 (2001) 614

#### Quasi-static shear flow at zero pressure



- 1. Initialize MS packing at zero shear strain
- 2. Take small step shear strain  $x_i = x_i + \Delta \gamma y_i$
- 3. Minimize energy
- 4. Find nearest MS packing at P=0 using growth/shrink procedure
- 5. Repeat steps 2, 3, 4



# Quasistatic Shear Flow at Zero Pressure



## Geometric Families Exist over Continuous Range of $\gamma$



•Rearrangement events cause system to switch geometric families

# **Complete Family Tree**



— complete family tree

— deterministic evolution of all  $\gamma$ =0 packings

Small systems sample only negligible fraction of available geometric families!



γ

## Noise-generation Mechanism: Collinear Particles

(a)







(c)

 $\gamma = \gamma_0 - \Delta \gamma$ 

$$\gamma = \gamma_0$$

## Frictional Geometrical Families



## **Frictional Geometric Families**



• Plot of all centers of mass that evolve to MS packing A

#### **Bumpy Particle Model for Friction**



• Linear repulsive spring bump-bump, bump-particle, and particleparticle interactions

## Hertz-Mindlin Friction Model

## Elastic force law



$$\begin{aligned} \vec{F}_{n_{ij}} &= k_n \delta_{ij} \hat{r}_{ij} \\ \vec{F}_{t_{ij}} &= k_t \vec{u}_{t_{ij}} \\ \frac{d \vec{u}_{t_{ij}}}{dt} &= \vec{v}_{t_{ij}} - \frac{(\vec{u}_{t_{ij}} \cdot \vec{v}_{ij}) \hat{r}_{ij}}{r_{ij}} \\ \left| F_t \right| \leq \mu \left| F_n \right| \end{aligned}$$

# Tangential displacement resets after contact breaks



Advantages of Bumpy-Particle Model over Hertz-Mindlin

- No *ad hoc* sliding, history dependence
- Forces depend only on particle positions and orientations; Use dynamical matrix to calculate vibrational response

•Test Hertz-Mindlin mobility distribution, P(m)  $m = \frac{F_t}{\mu F_n}$ 



Hertz-Mindlin

 $\phi_c = 0.6131, N_c = 10, N_c^{bb} = 17$ 

Bumpy-particle model

### `Minimum Distance' from Reference MS Packing



#### Comparison of Hertz-Mindlin and Bumpy-Particle Minimum-Distance Maps





### Hertz-Mindlin Results



**Fig. 1** Dependence of the critical values of the packing fraction  $\phi^{\mu}_{c}$  (filled circles), and coordination number  $z^{\mu}_{c}$  (open squares), on the particle friction coefficient  $\mu$ , for monodisperse spheres in 3D (upper panel) and bidisperse discs in 2D (lower panel). The insets are parametric plots of  $\phi_{c}^{\mu}$  against  $z_{c}^{\mu}$ . Symbol size is representative of sample-to-sample fluctuations and error bars.

L. Silbert, Soft Matter, 6 (2010) 2918.

## Shape Matters: Packings of Frictionless Ellipsoidal Particles Are Stabilized by Quartic Modes



### Packings of ellipse-shaped particles



compression method-fixed aspect ratio  $\alpha$ 

#### Pairwise Repulsive Interactions: True Contact Distance





$$V(r_{ij}) = \begin{cases} \frac{\varepsilon}{\alpha} \left(1 - \frac{r_{ij}}{\sigma_{ij}}\right)^{\alpha} & r < \sigma_{ij} \\ 0 & r \ge \sigma_{ij} \end{cases}$$

 $\alpha$ =2; linear springs

# Average Contact Number



- Not a discontinuous jump from  $\langle z \rangle = 4$  to 6.
- Quartic modes to the rescue!

#### Density of Vibrational Modes from Dynamical Matrix



#### Scaling of Characteristic Frequencies



#### Perturbations along lowest frequency eigenmodes



## Rotational/Translational Character of Eigenmodes



α=1.01

# What is the difference between between a dimer and an ellipse?



 $\alpha = a/b$ 

## **Structural Properties**

