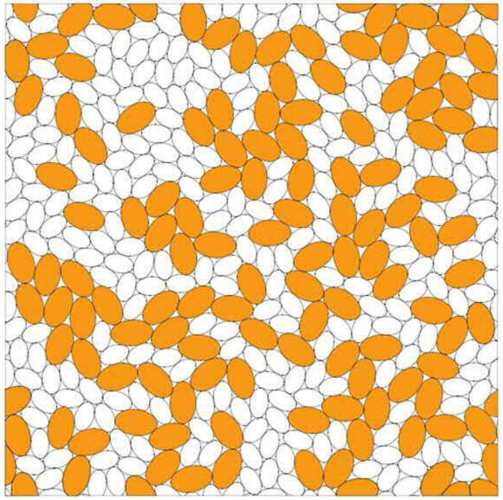
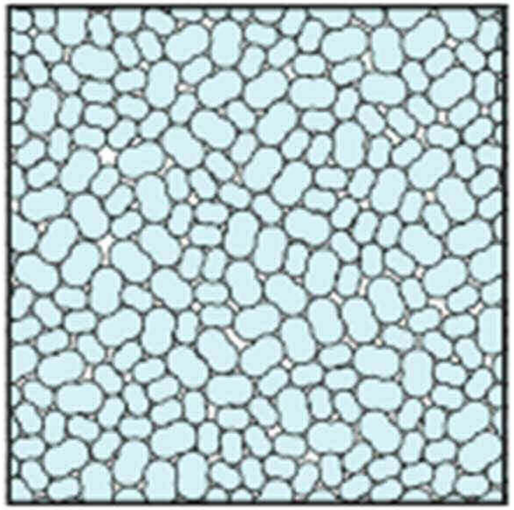
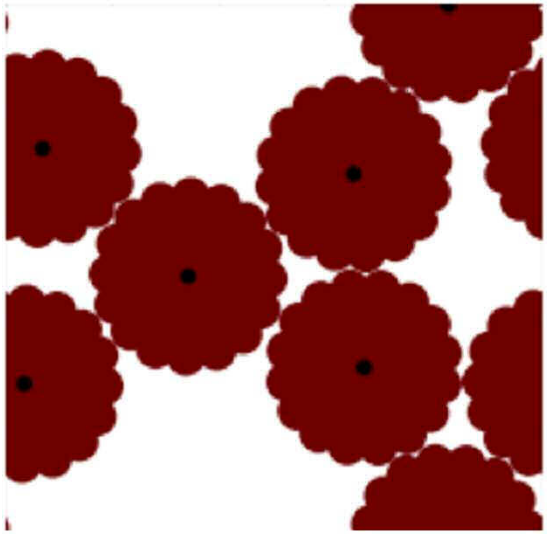
The influence of particle shape on jamming: From ellipsoids to dimers to bumpy particles to friction

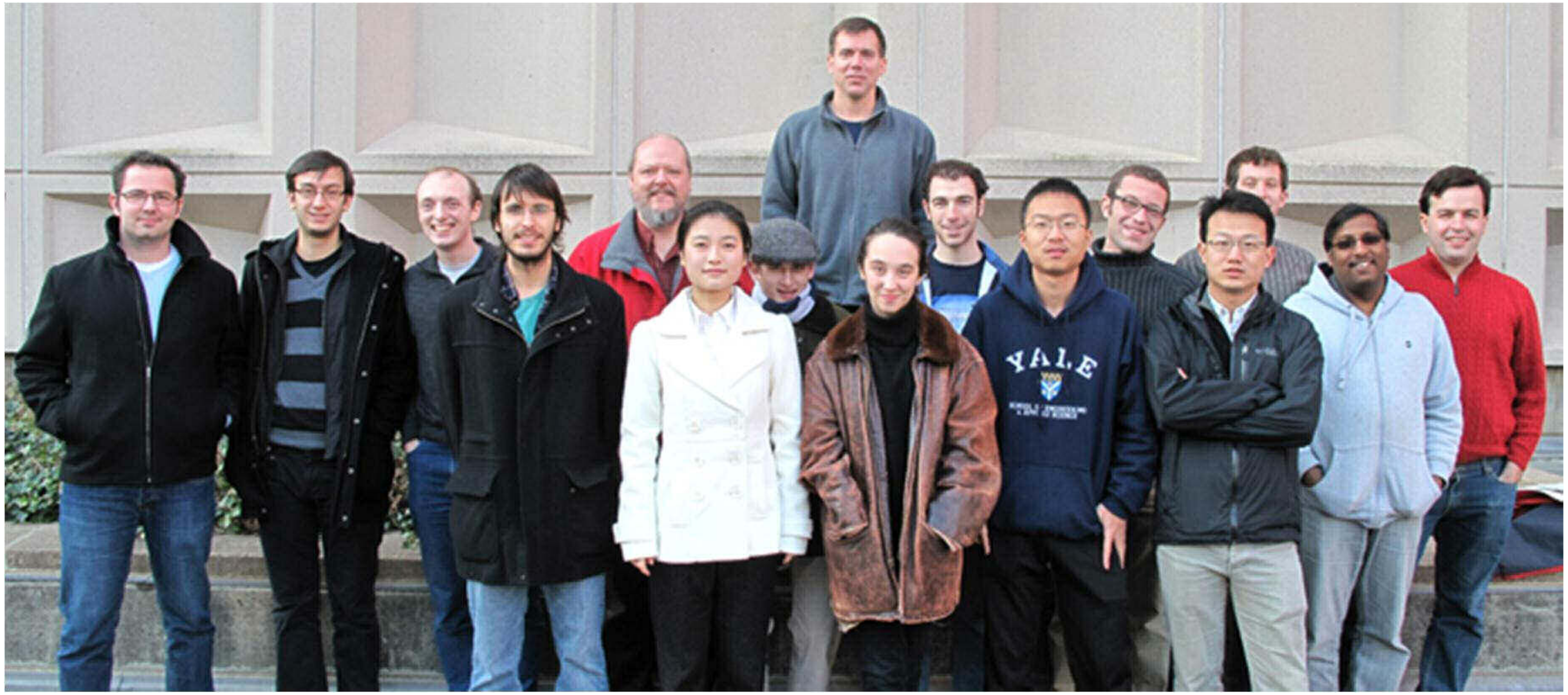


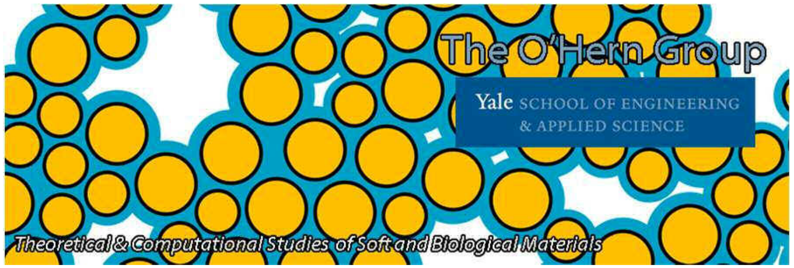




Prof. Corey S. O Hern
Department of Mechanical Engineering & Materials Science
Department of Physics
Yale University

The O Hern Group

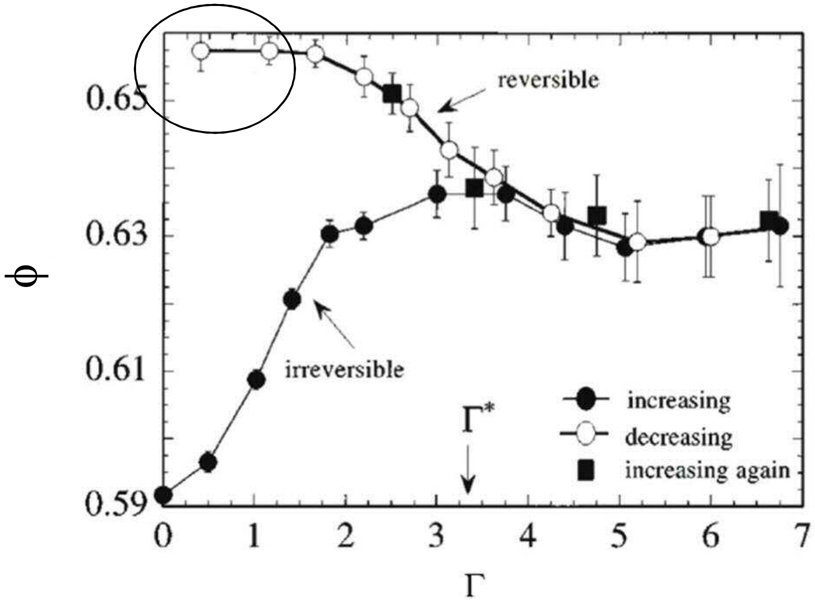




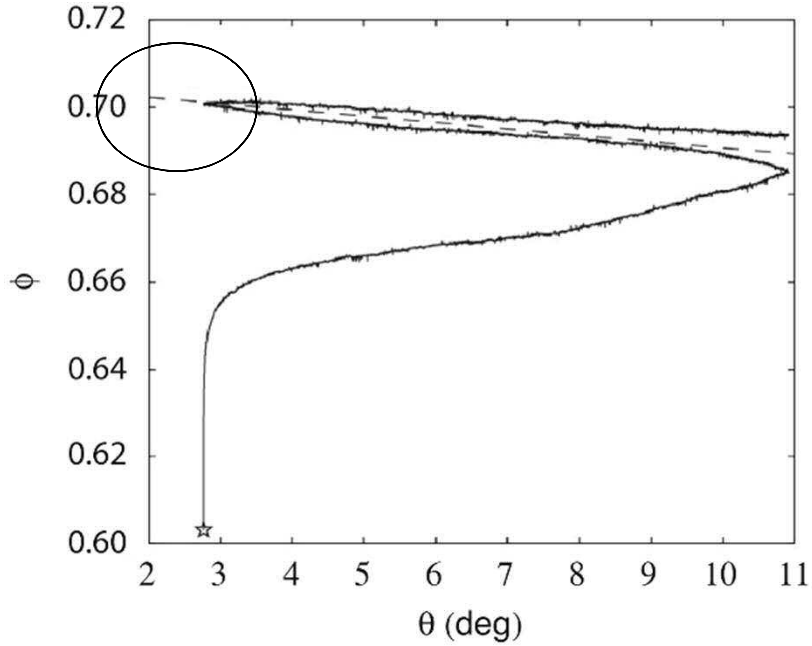
http://jamming.research.yale.edu/

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

Statistical Mechanics of Granular Media



PRE 57 (1998) 1971



EPJE 3 (2000) 309

Apply driving to attain reversible set of states
Different driving mechanisms lead to different sets of states!
What are the microstates of granular packings and what determines their probabilities?

Attributes of Simple Granular Materials

1. Finite number of macroscopic spherical grains

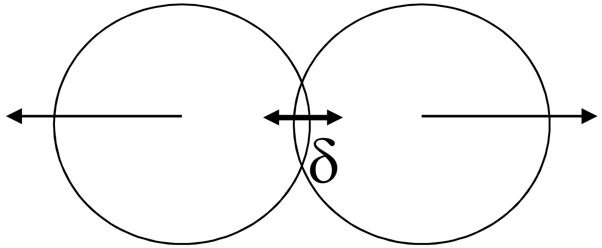
2. Dissipative and repulsive contact interactions; exist at `zero temperature unless driven by external forces

---

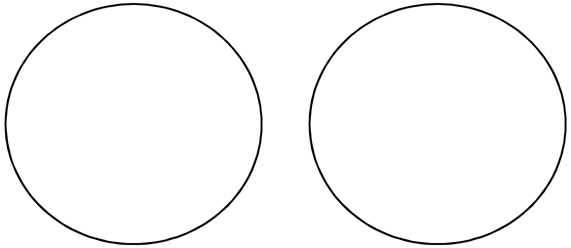
3. Non-spherical particle shapes

4. Static frictional and `history-dependent interactions

Simple Granular Model: Frictionless Disks



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



zero force, $F_{ij} = 0$

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

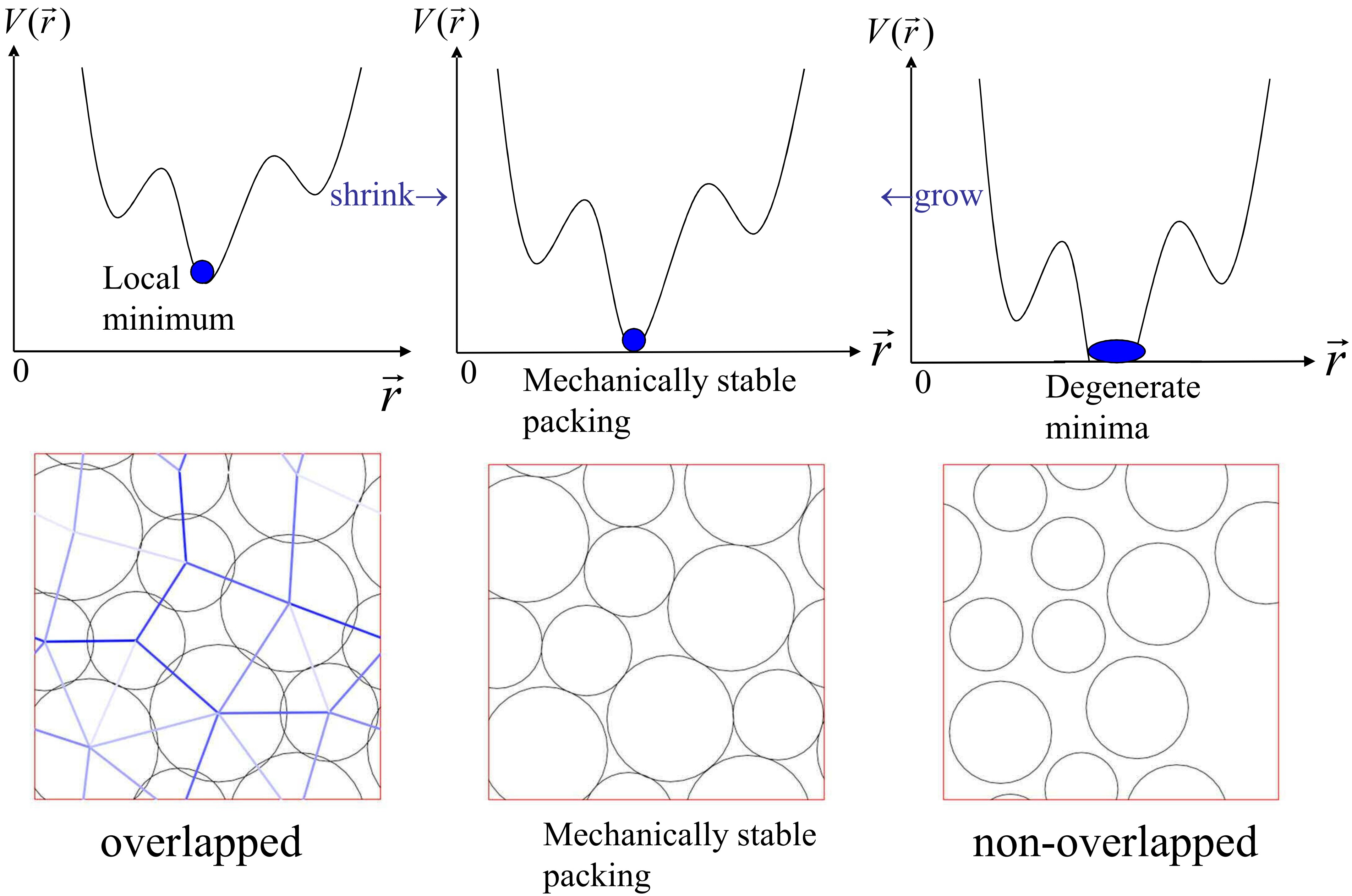
Minimize energy V(r)
to reach T=0 at each ϕ

$$V(\vec{r}) = \sum_{i>j} V(r_{ij})$$

$$V(r_{ij}) = \frac{\varepsilon}{\alpha}\left(1 - \frac{r_{ij}}{\sigma_{ij}}\right)^{\alpha}$$

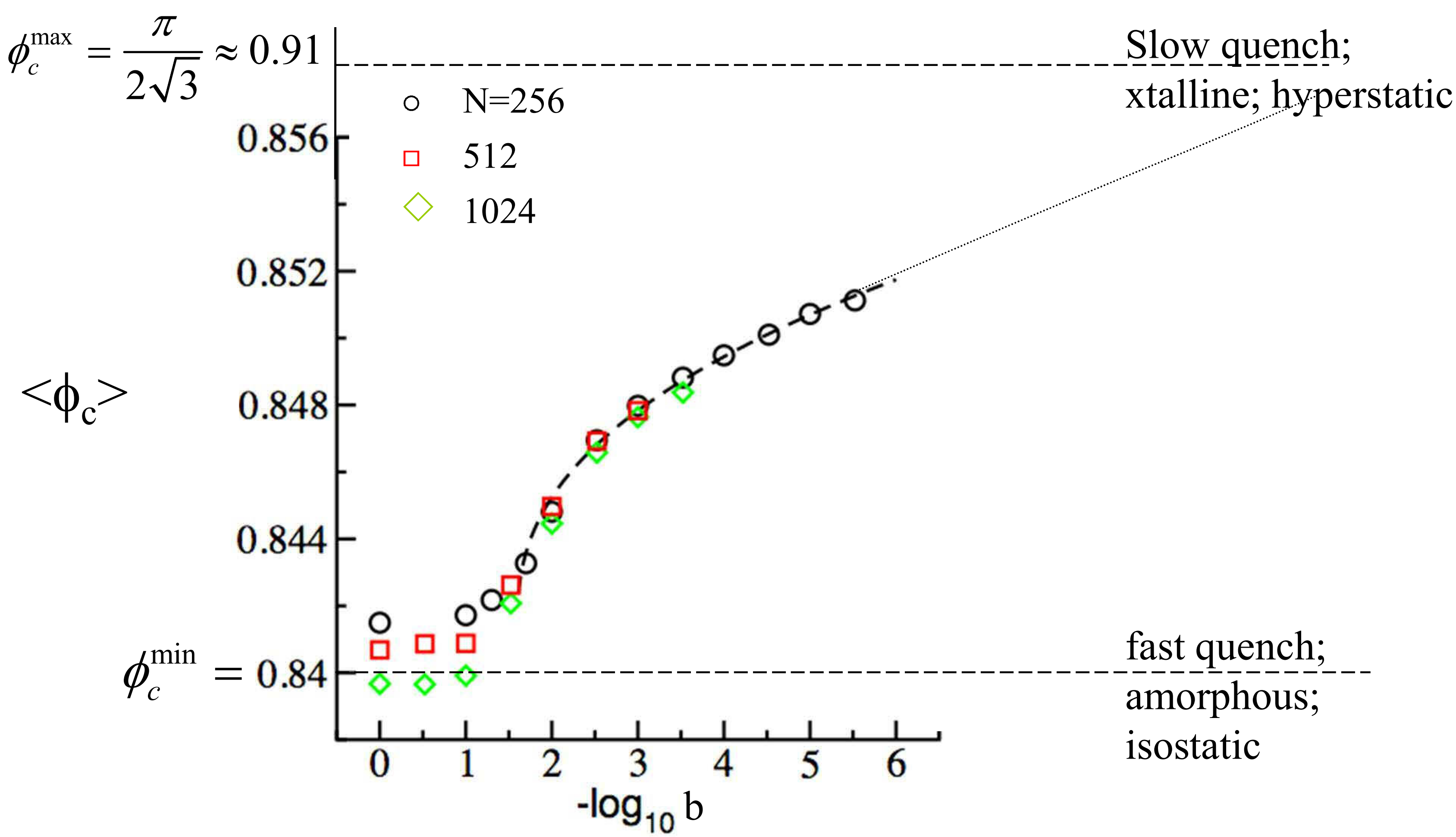
for overlapping particles

MS Packing-Generation Algorithm



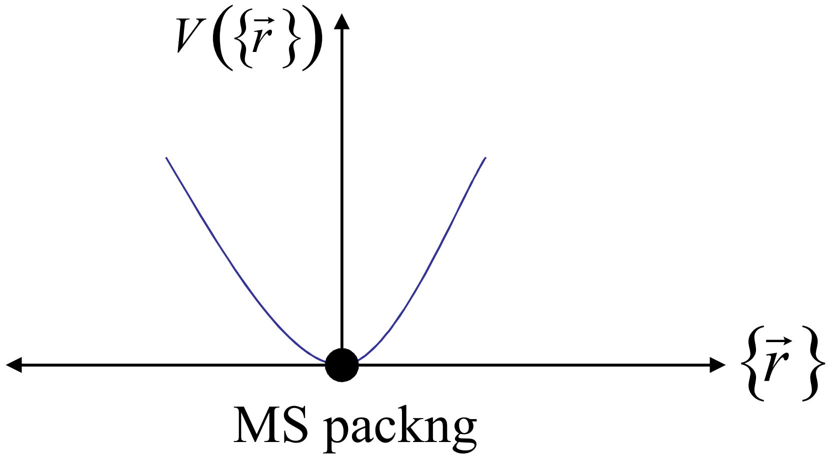
QuickTime and a
TGA decompressor
are needed to see this picture.

Jamming of spherical particles via isotropic compression



P. Chaudhuri, L.Berthier, & S. Sastry, Phys. Rev. Lett, 104, 165701 (2010).
C. F. Schreck, C. S. O Hern, & L. E. Silber, Phys. Rev. E 84, 011305 (2011).

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



Isostaticity

$$N_c = N_c^{iso} = Nd_f - d + 1$$

$$z = z_{iso} = 2d_f; \qquad z = \frac{2N_c}{N}$$

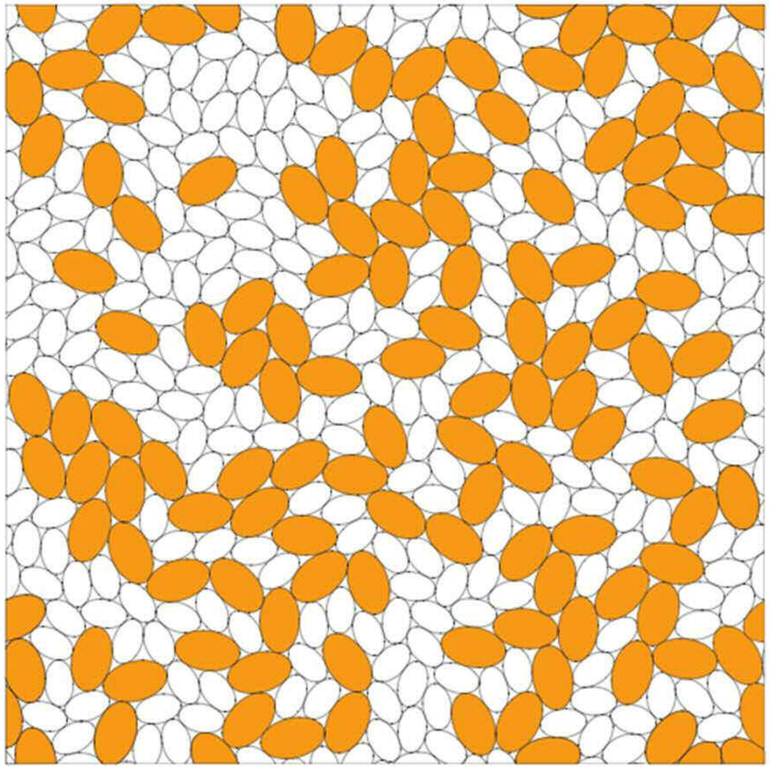
Configuration is mechanically stable if dynamical matrix contains $d_f N$-d eigenvalues $\omega^2 > 0$ (periodic b.c.s)

$$M_{\alpha,\beta} = \left. \frac{\partial^2 V(\vec{r})}{\partial r_\alpha \partial r_\beta} \right|_{\vec{r}=\vec{r}_0}$$

α,β=x, y, z, particle index

$\vec{r}_0$ = positions of MS packing

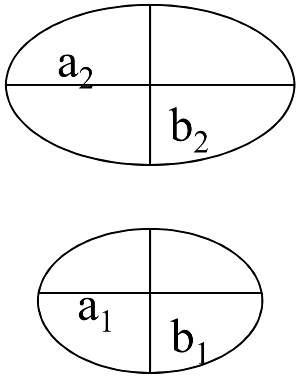
Shape Matters: Packings of Frictionless Ellipsoidal Particles Are Stabilized by Quartic Modes



C. F. Schreck, M. Mailman, B. Chakraborty, & C. S. O Hern, Constraints and vibrations in static packings of ellipsoidal particles, submitted to PRE (2012).
A. Donev, S. Torquato, & F. H. Stillinger, Phys. Rev. E 71 (2005) 011105.
Z. Zeravic, N. Xu, A. J. Liu, S. R. Nagel, & W. van Saarloos, EPL 87 (2009) 26001.

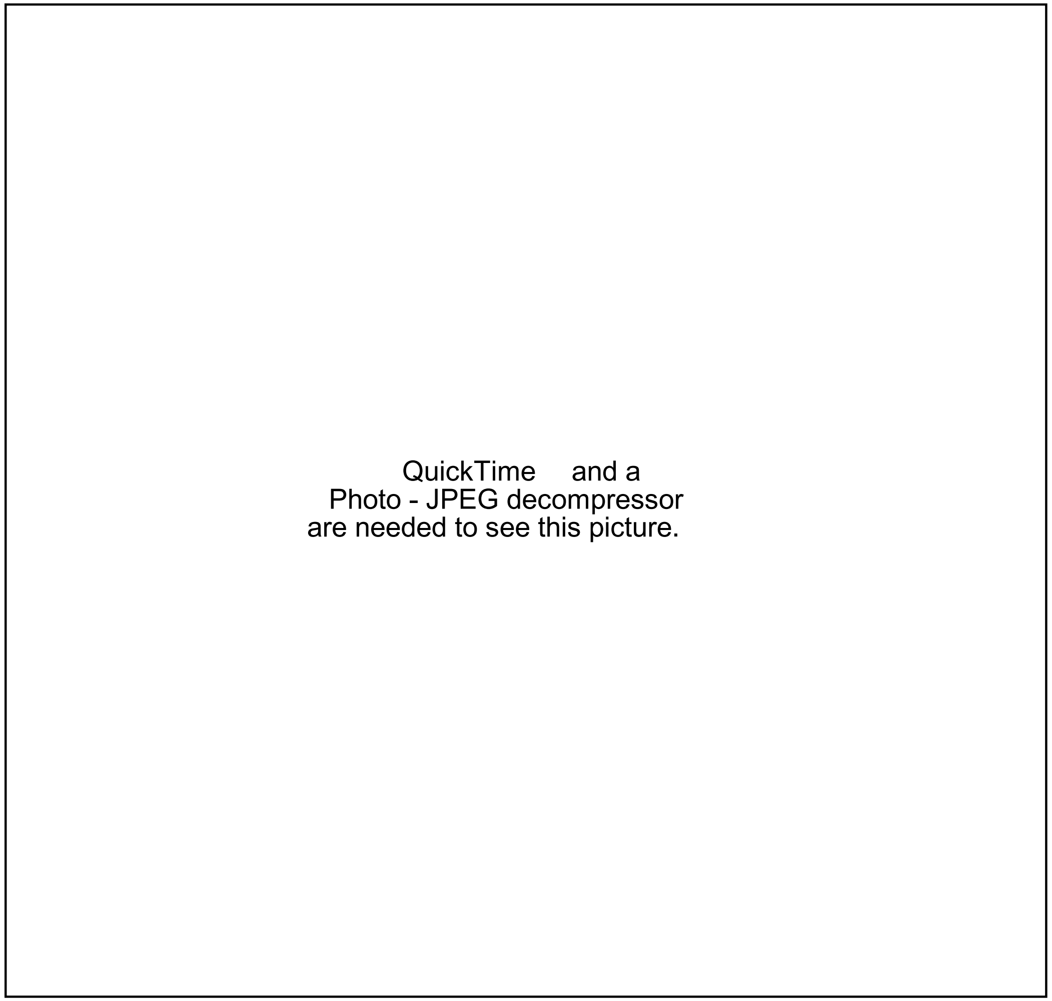
Packings of ellipse-shaped particles

bidisperse



$$\frac{a_1}{b_1} = \frac{a_2}{b_2} = \alpha$$

$$\frac{a_1}{a_2} = 1.4$$



compression method-fixed aspect ratio α

Pairwise Repulsive Interactions: True Contact Distance

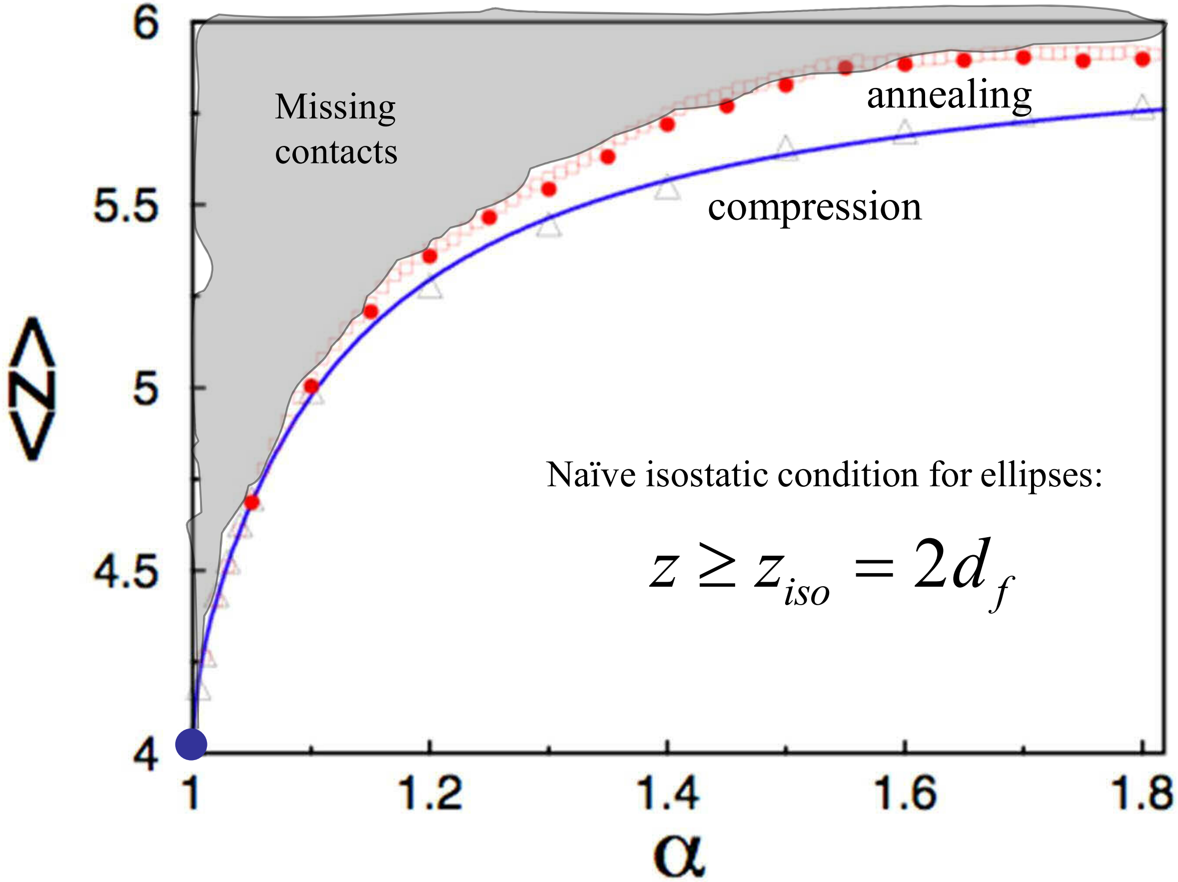
$V(r_{ij}) = 0$

$V(r_{ij}) > 0$

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

α=2; linear springs

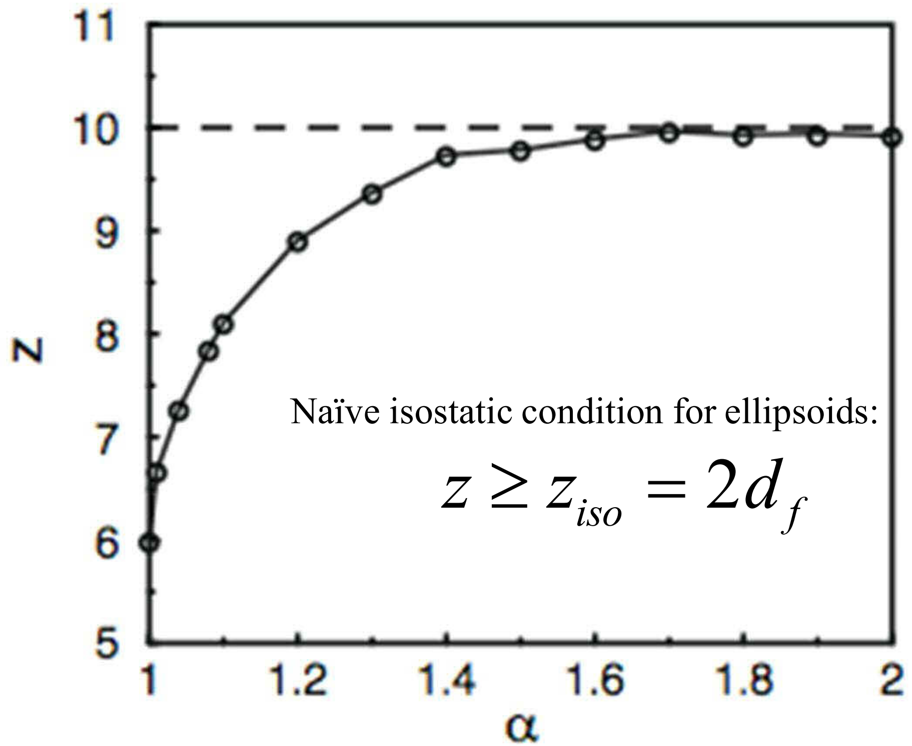
Average Contact Number for Ellipse Packings



$$z \geq z_{iso} = 2d_f$$

Not a discontinuous jump from <z> = 4 to 6.

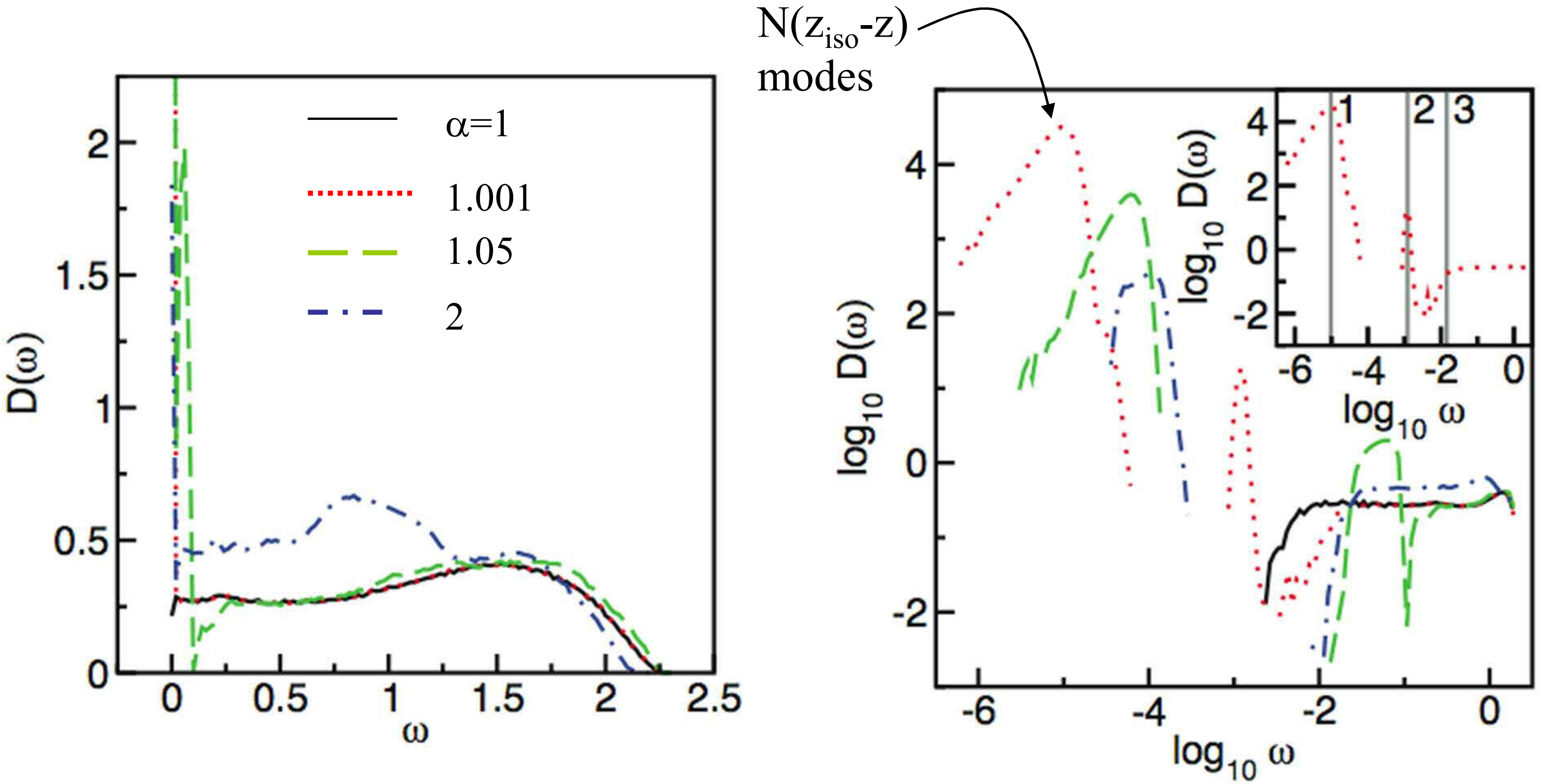
Average Contact Number for Ellipsoid Packings



Not a discontinuous jump from <z> = 6 to 10.

If $z < z_{iso}$, are ellipsoid packings mechanically stable?

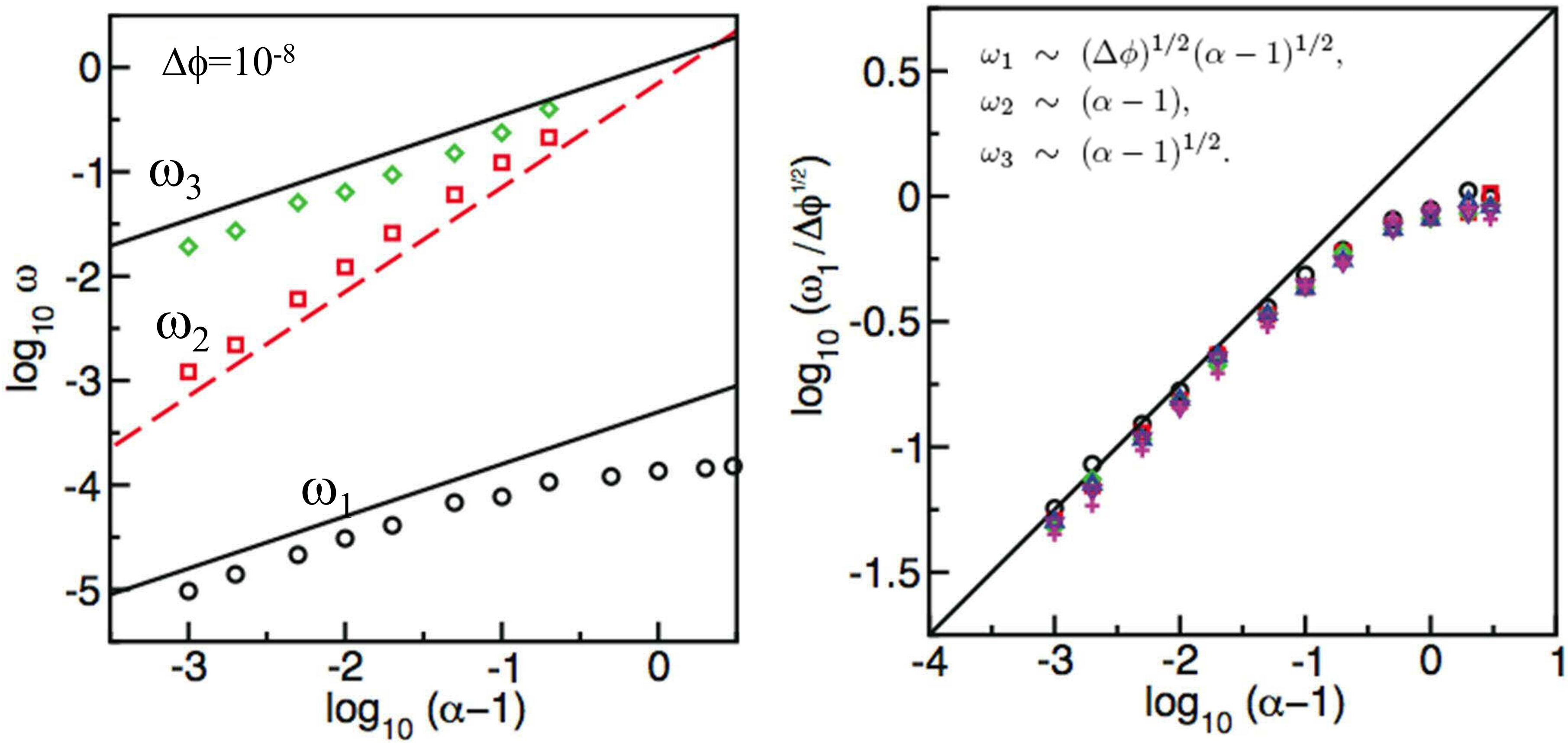
Density of Vibrational Modes from Dynamical Matrix



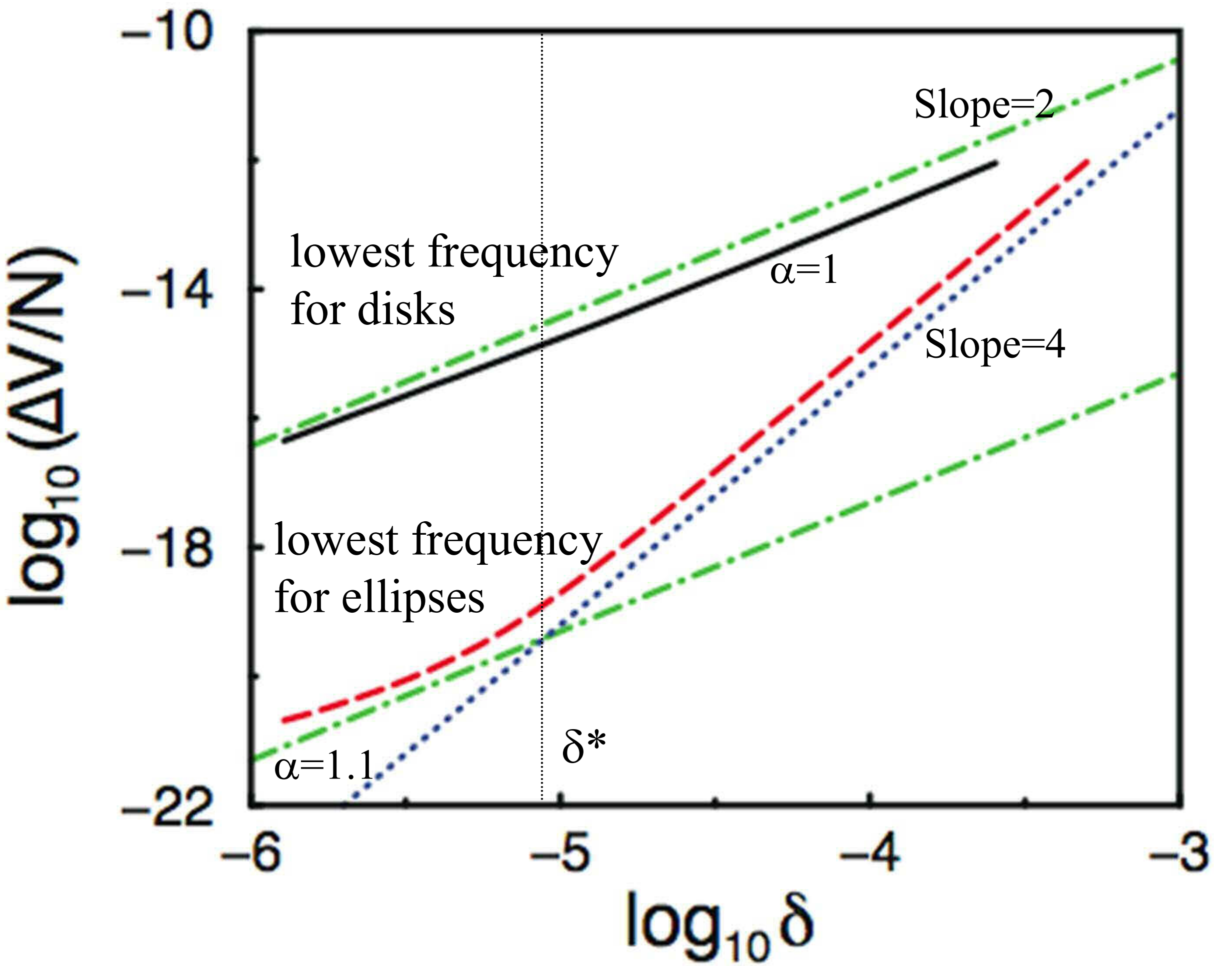
Dynamical matrix eigenvalues $\omega^2 > 0$ for all $d_f N - d$ modes

C. F. Schreck, M. Mailman, B. Chakraborty, & C. S. O Hern, Constraints and vibrations in static packings of ellipsoidal particles, submitted to PRE (2012).

Scaling of Characteristic Frequencies

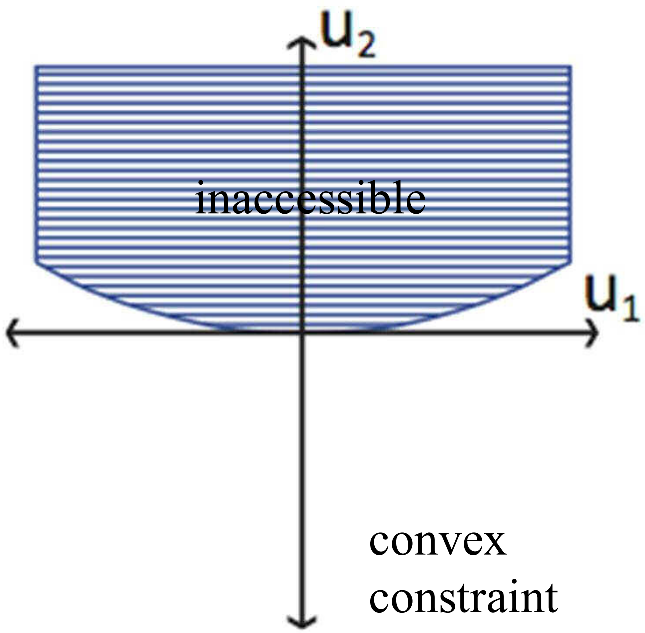


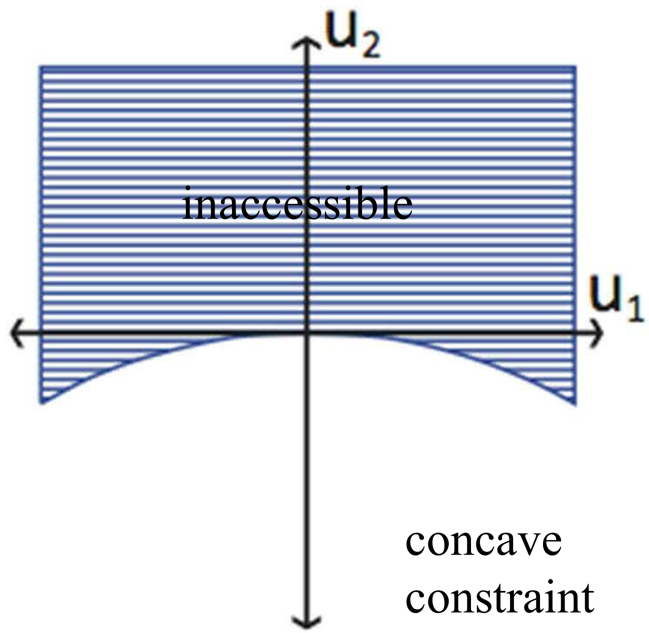
Perturbations along lowest frequency eigenmodes



Crossover frequency scales as $\delta^* \sim \frac{(\Delta\phi)^{1/2}}{(\alpha-1)^{1/4}}$

Ellipsoid packings are quartically stabilized at $\Delta\phi=0$; *i.e.* For $N(z_{iso}-z)$ modes, $\Delta V\sim\delta^4$; for Nz modes, $\Delta V\sim\delta^2$

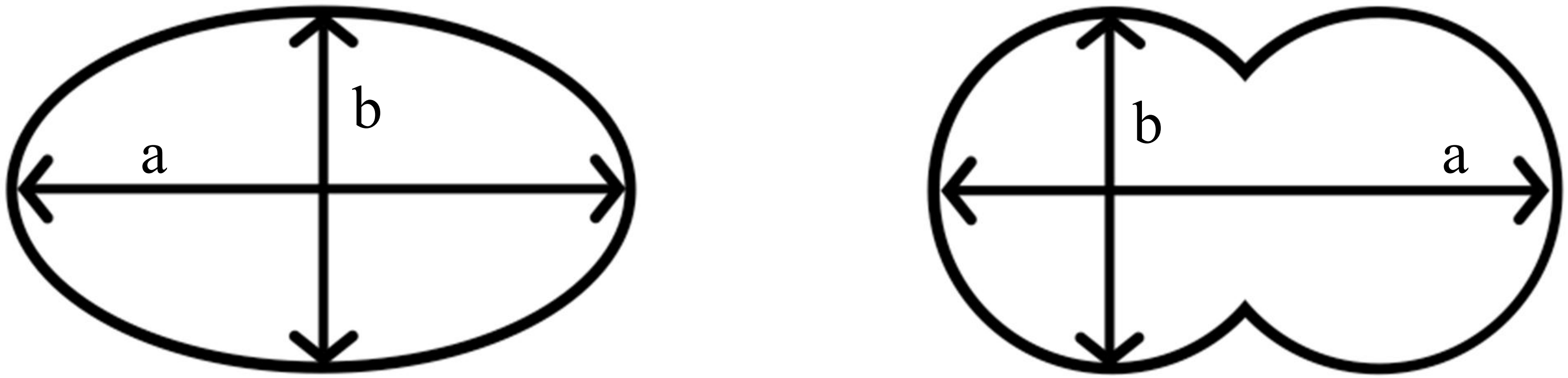




Spherical, ellipsoidal particles

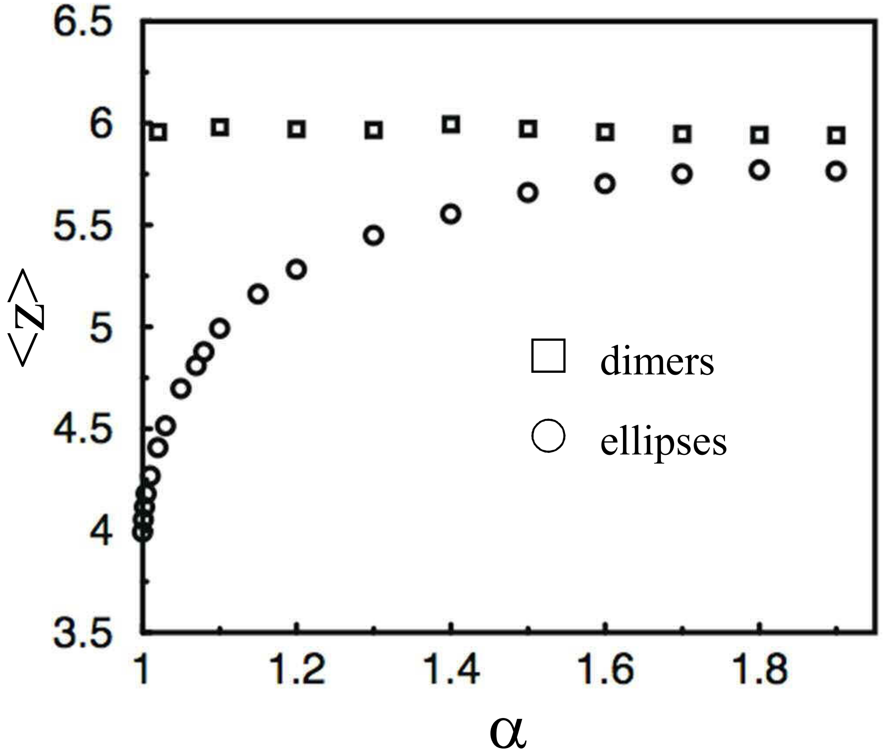
Only ellipsoidal particles

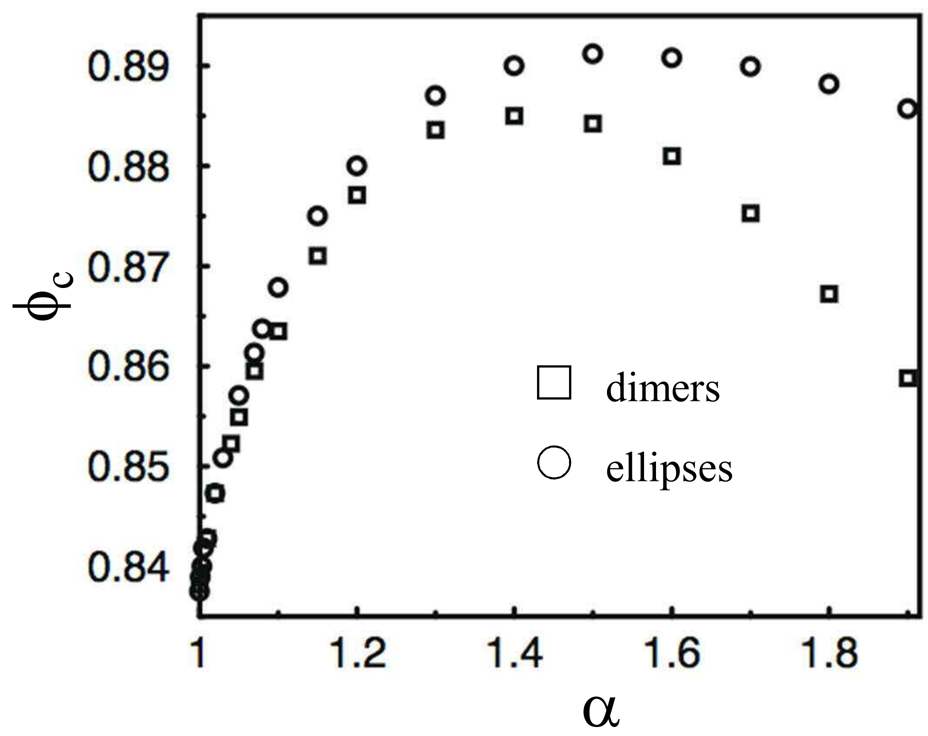
What is the difference between between a dimer and an ellipse?



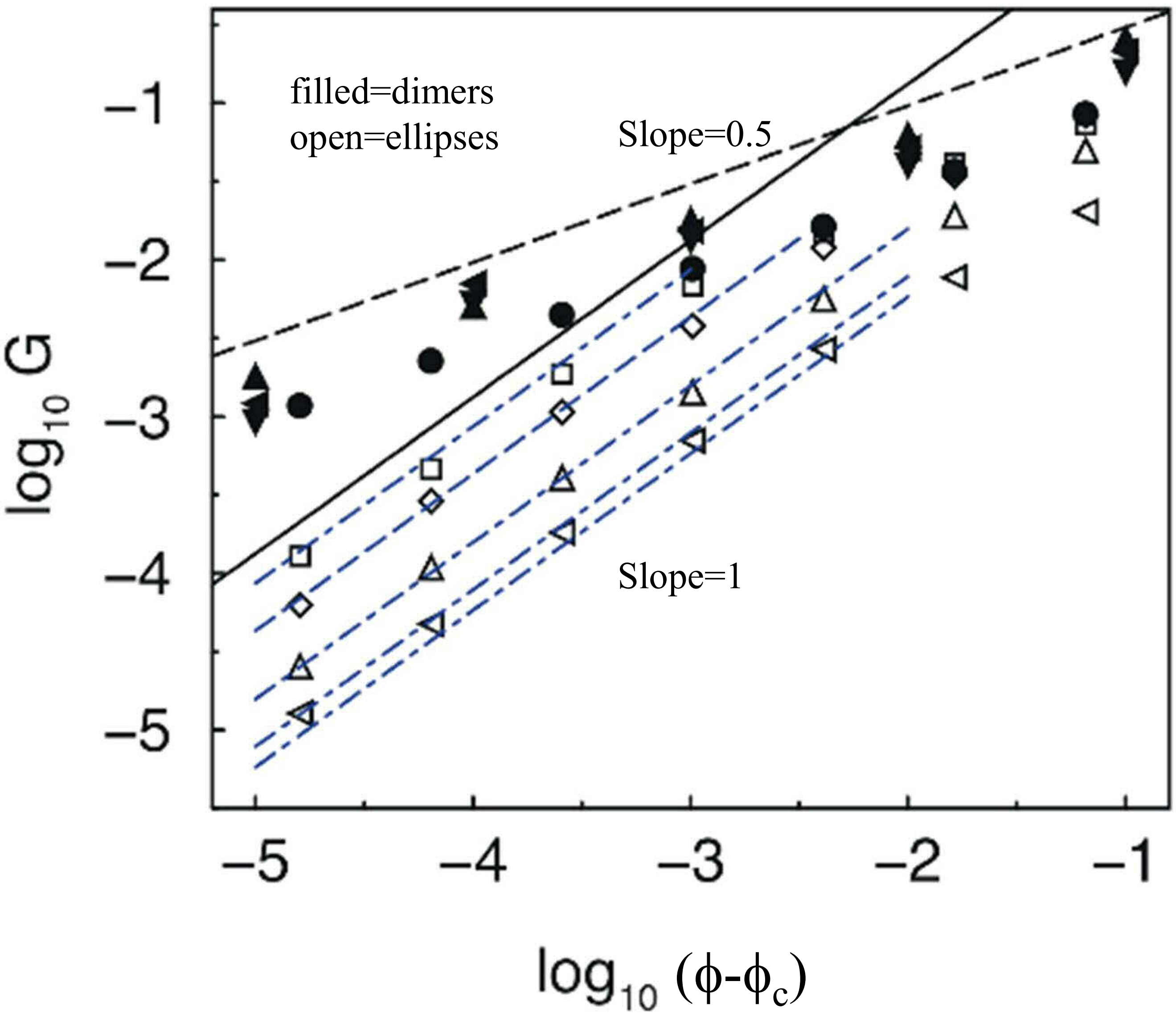
$\alpha = a/b$

Dimer packings are isostatic with no quartic modes

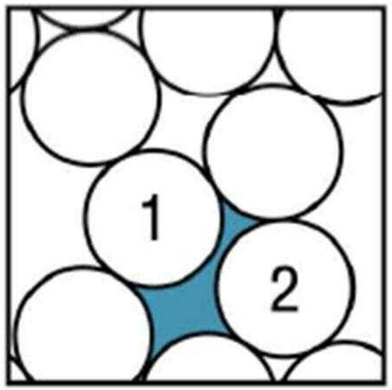




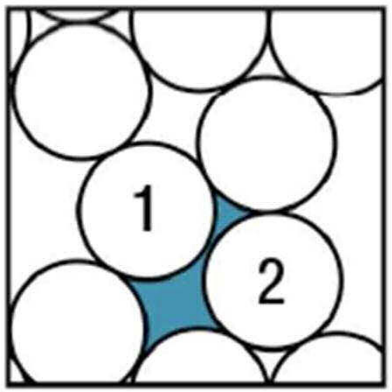
Weaker linear response to shear



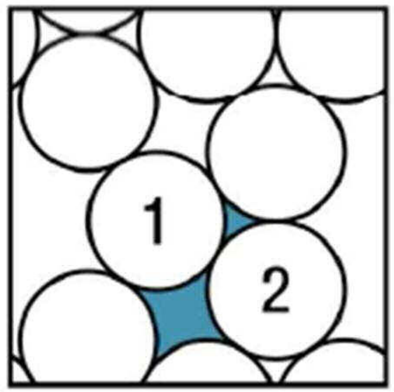
Microstates of Frictional Packings: Geometrical Families



$\phi_7 = 0.7290$



$\phi_7 = 0.7320$

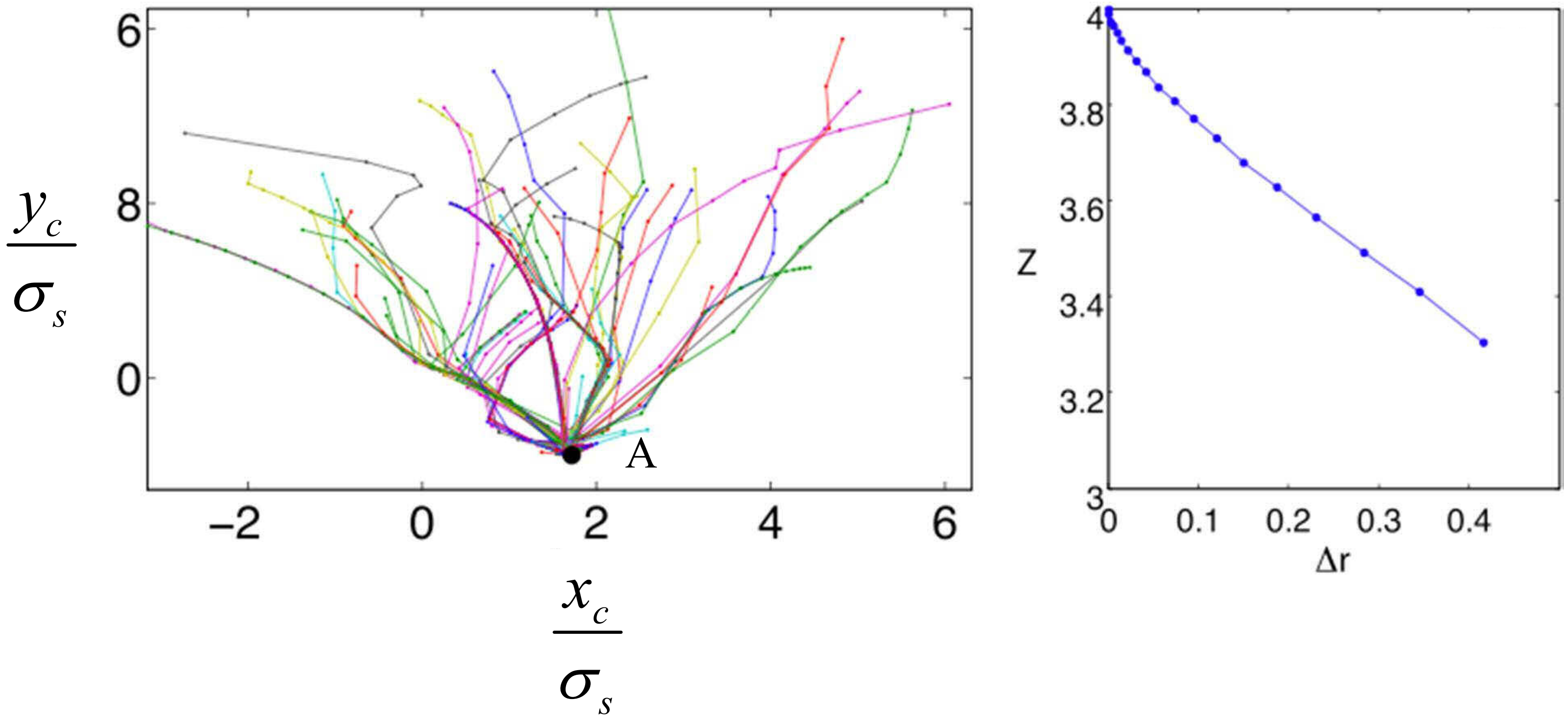


$\phi_7 = 0.7365$

Frictional Geometrical Families

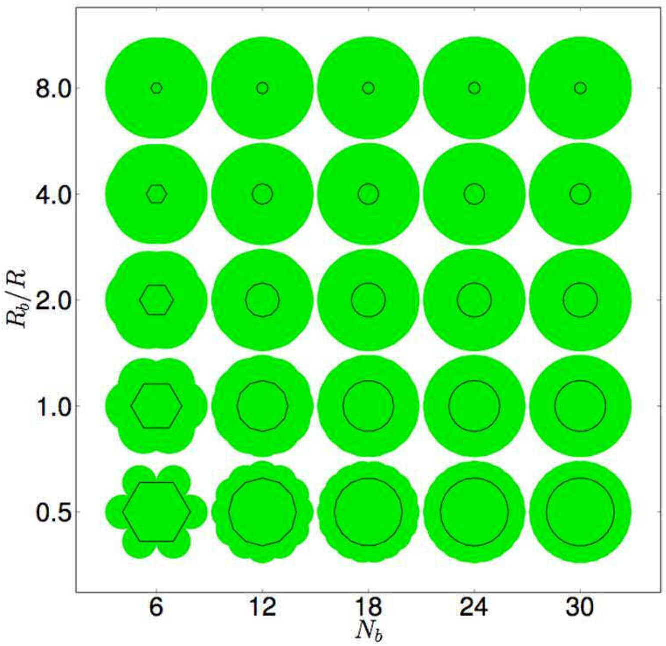
QuickTime™ and a
Cinepak decompressor
are needed to see this picture.

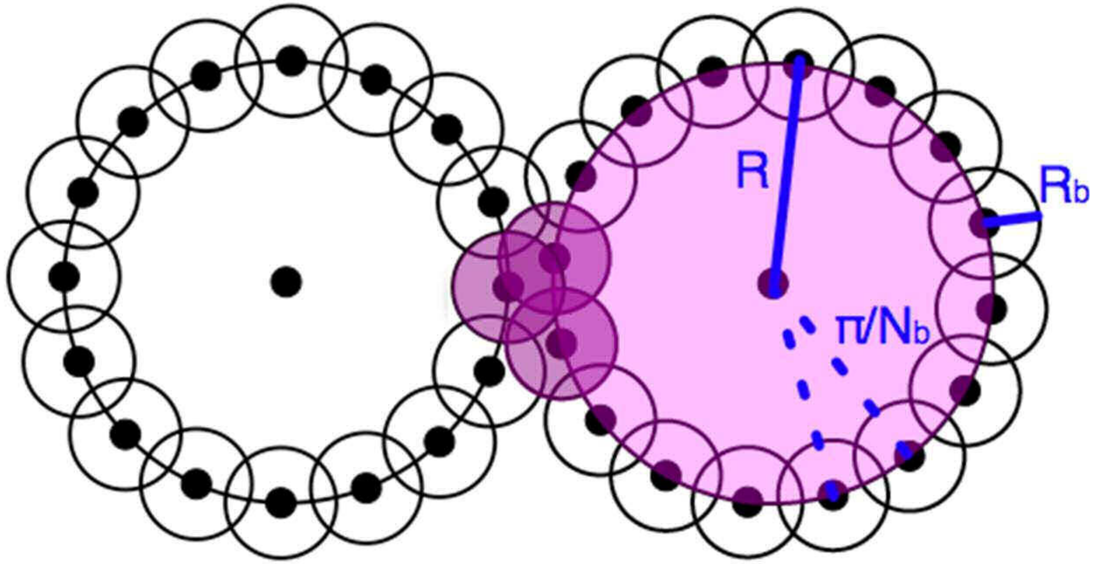
Frictional Geometric Families



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

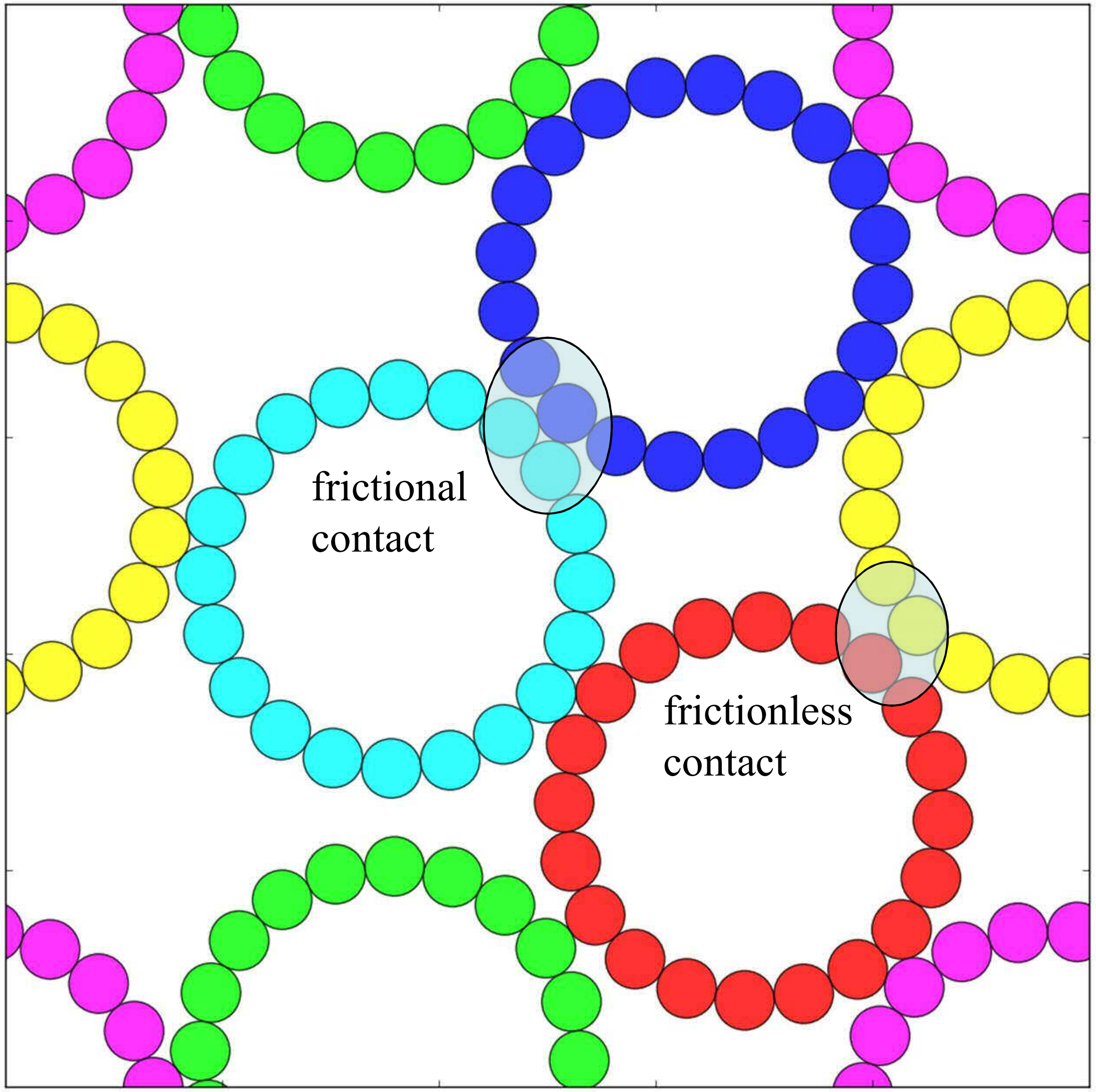
Bumpy Particle Model for Friction





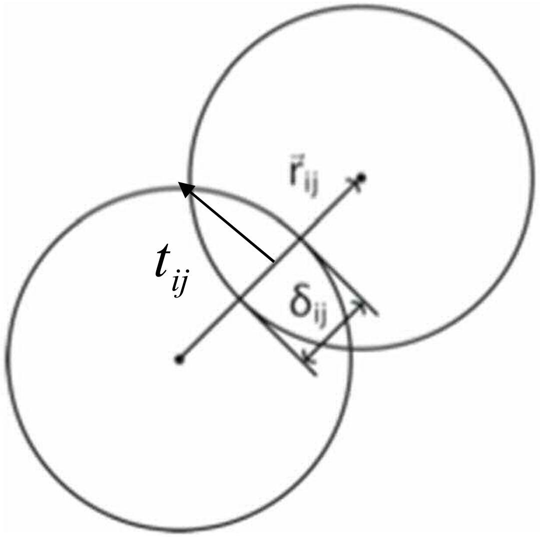
$$\mu_{\max} \cong \frac{\pi R}{2 N_b R_b}$$

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


frictional
contact
frictionless
contact

Hertz-Mindlin Friction Model

Elastic force law



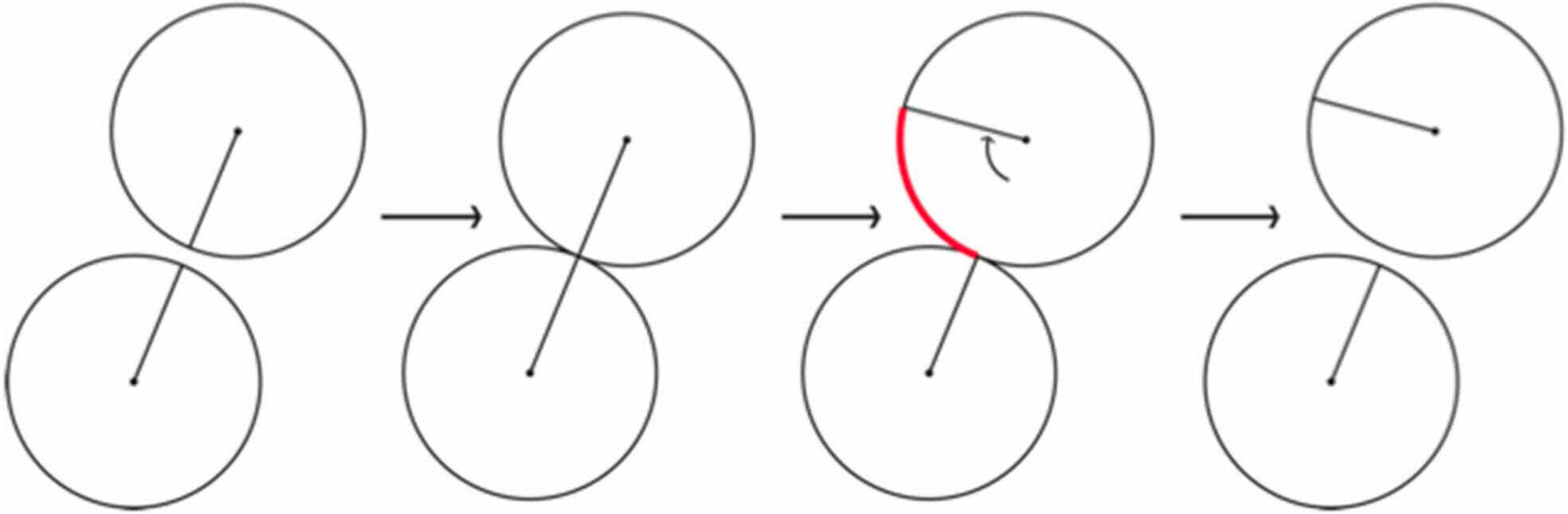
$$\vec{F}_{n_{ij}} = k_n \delta_{ij} \hat{r}_{ij}$$

$$\vec{F}_{t_{ij}} = k_t \vec{u}_{t_{ij}}$$

$$\frac{d\vec{u}_{t_{ij}}}{dt} = \vec{v}_{t_{ij}} - \frac{(\vec{u}_{t_{ij}} \cdot \vec{v}_{ij})\hat{r}_{ij}}{r_{ij}}$$

$$|F_t| \leq \mu |F_n|$$

Tangential displacement resets after contact breaks



Provides energy sink when contacts break

Advantages of Bumpy-Particle Model over Hertz-Mindlin

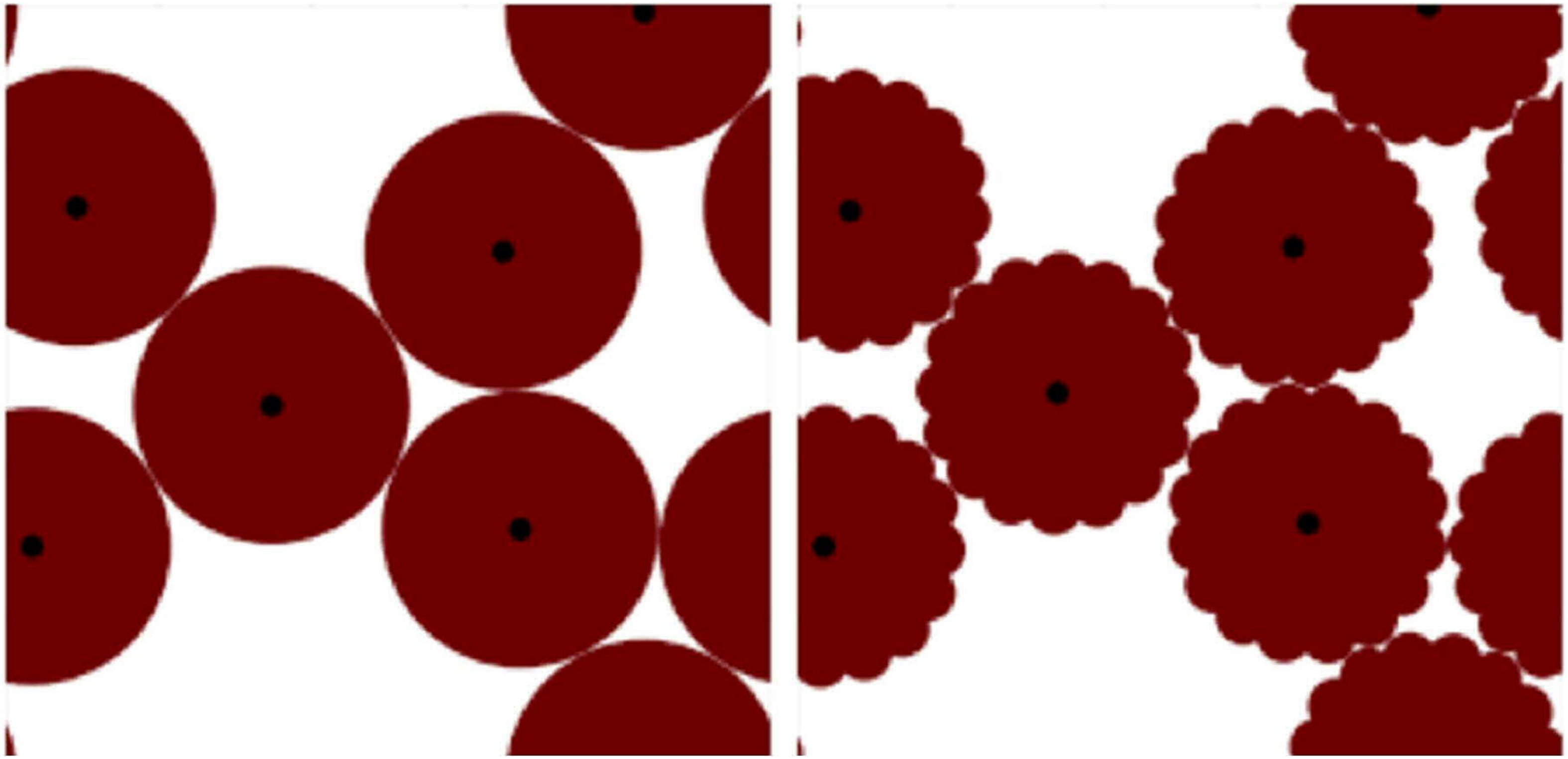
No *ad hoc* sliding, history dependence

Forces depend only on particle positions and orientations;
Use dynamical matrix to calculate vibrational response

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

QuickTime and a
GIF decompressor
are needed to see this picture.

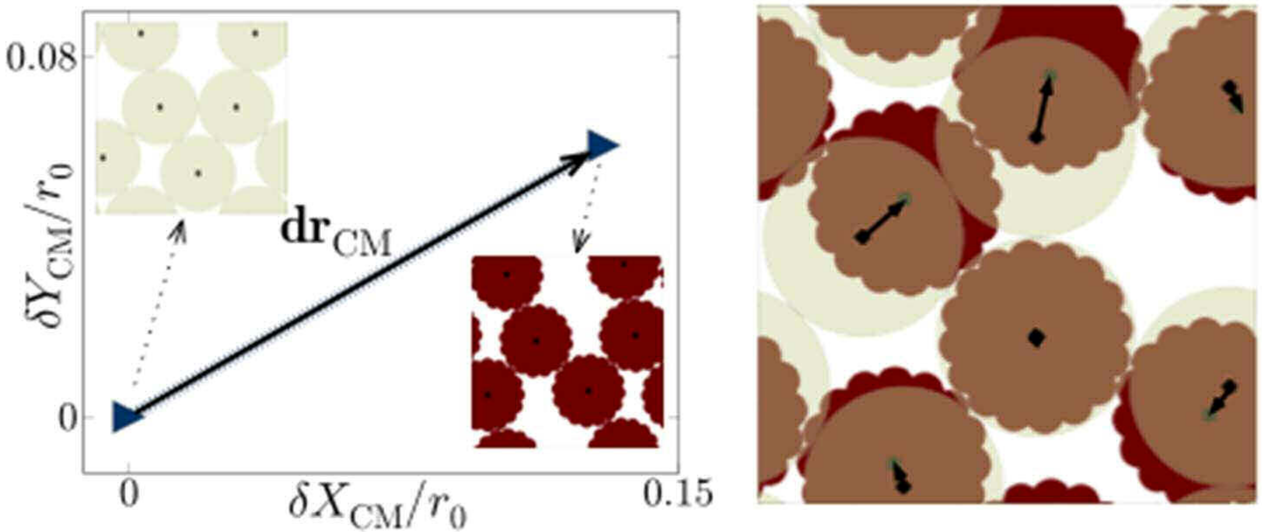
ϕ_c=0.6131, N_c=10, $N_c^{bb} = 17$



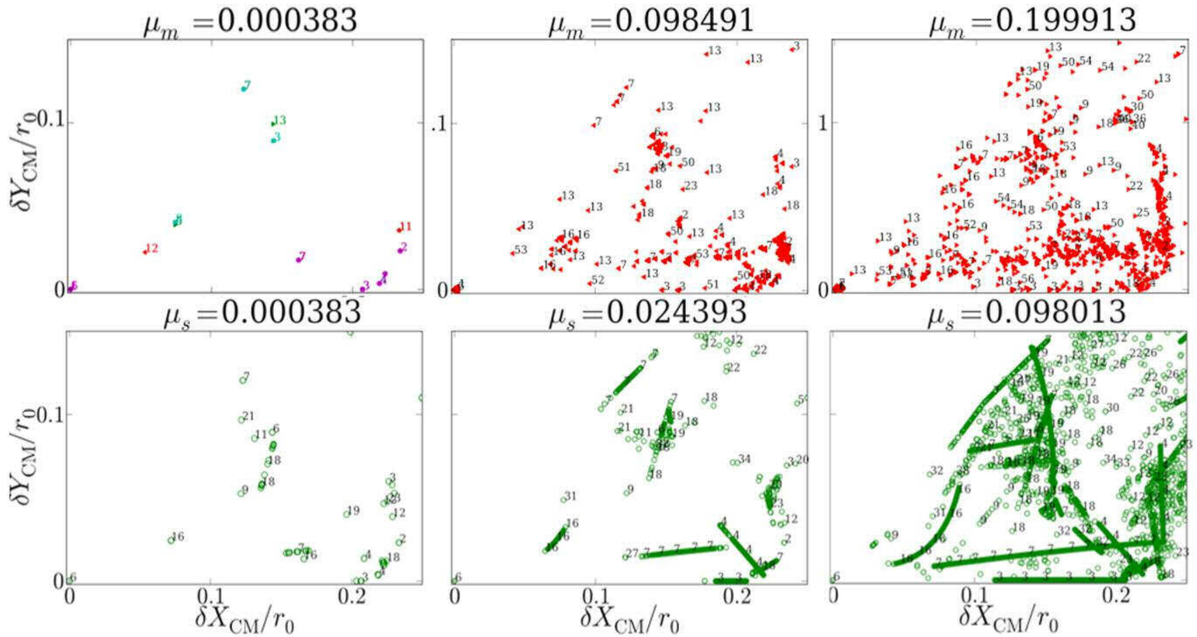
Hertz-Mindlin

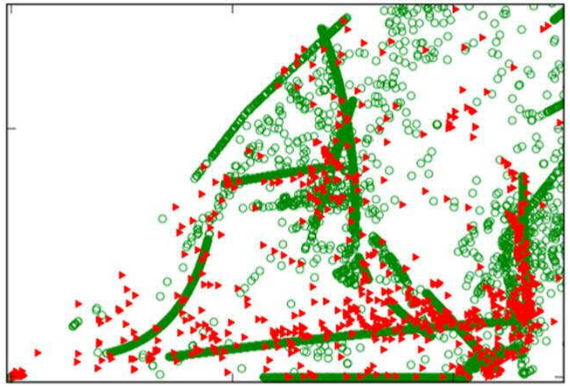
Bumpy-particle model

`Minimum Distance from Reference MS Packing



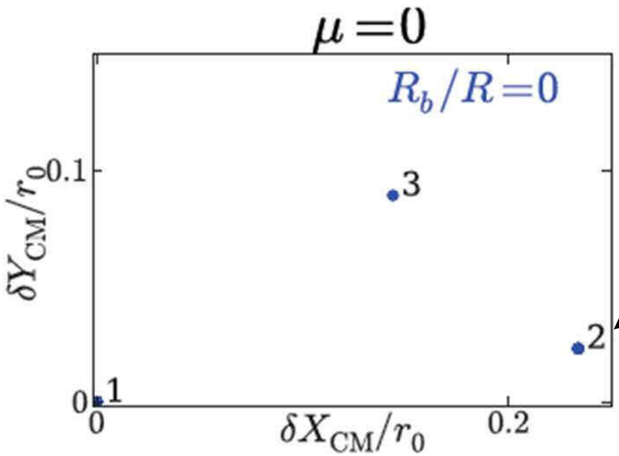
Comparison of Hertz-Mindlin and Bumpy-Particle Minimum-Distance Maps



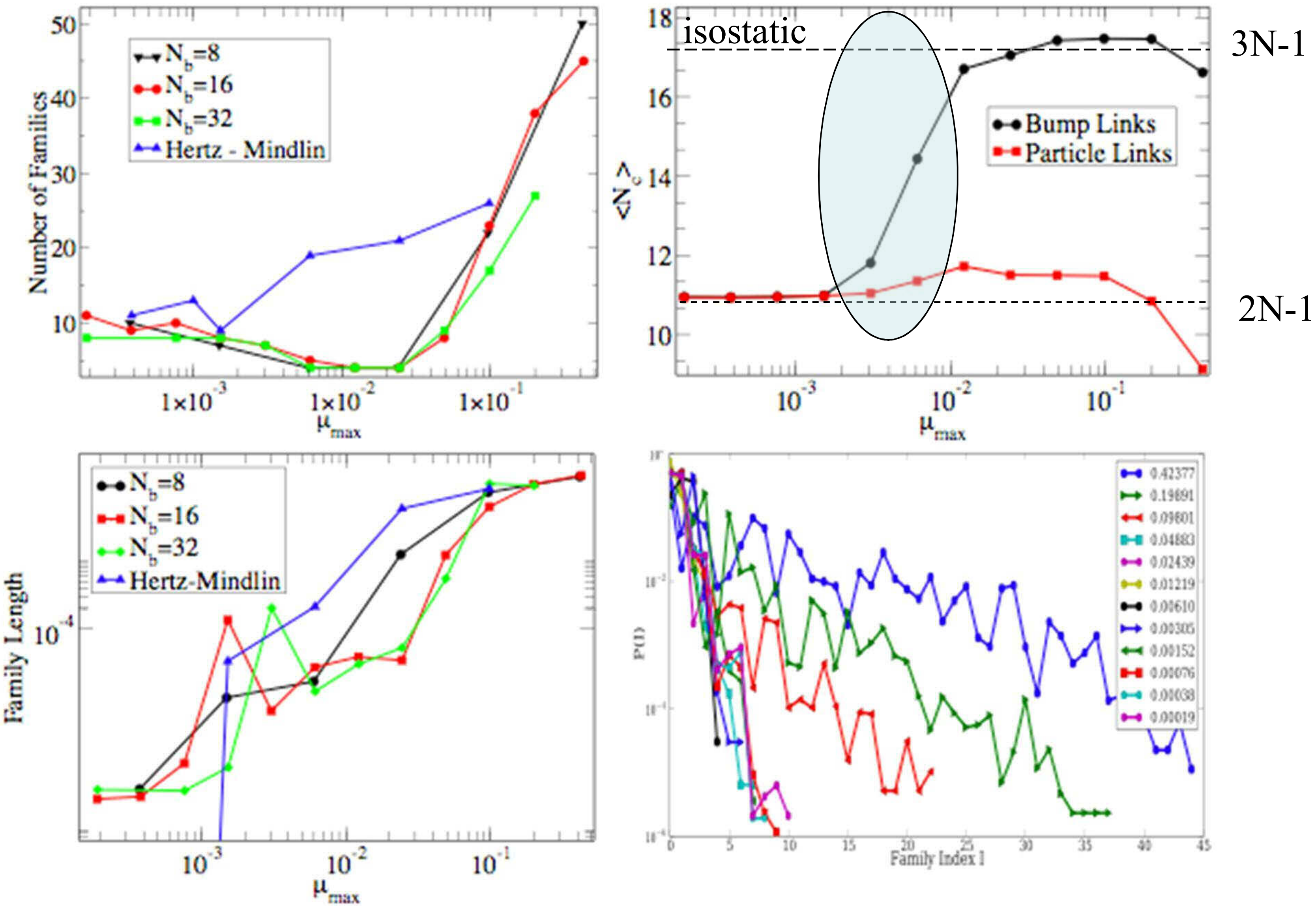


► bumpy particles

○ Hertz-Mindlin

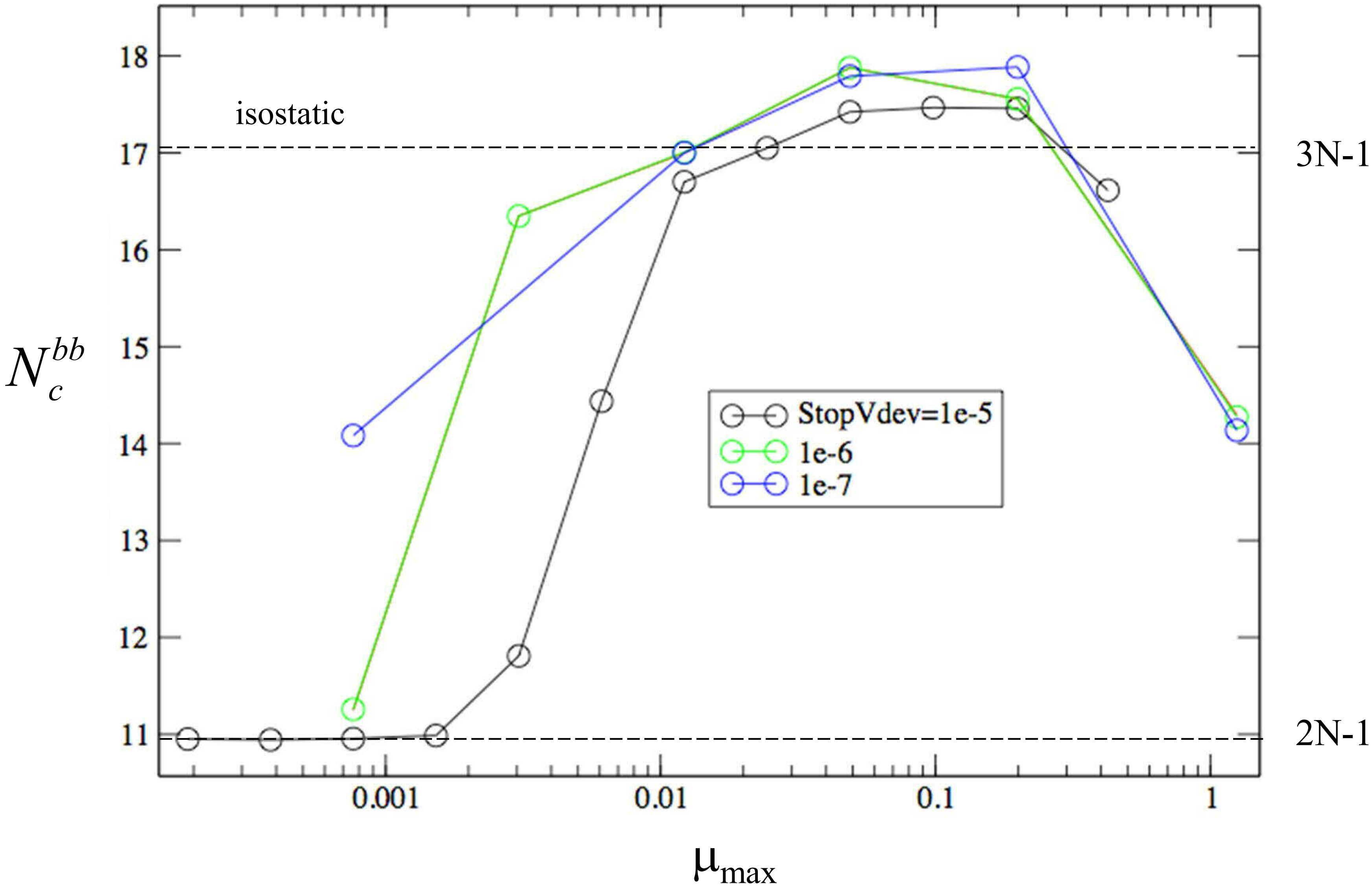


family index



Number of Families
N_b=8
N_b=16
N_b=32
Hertz - Mindlin
μ_{max}
isostatic
3N-1
2N-1
$<N_c>$
Bump Links
Particle Links
μ_{max}
Family Length
N_b=8
N_b=16
N_b=32
Hertz-Mindlin
μ_{max}
P(I)
Family Index I
0.42377
0.19891
0.09801
0.04883
0.02439
0.01219
0.00610
0.00305
0.00152
0.00076
0.00038
0.00019

Energy Minimization Tolerance



Hertz-Mindlin Results

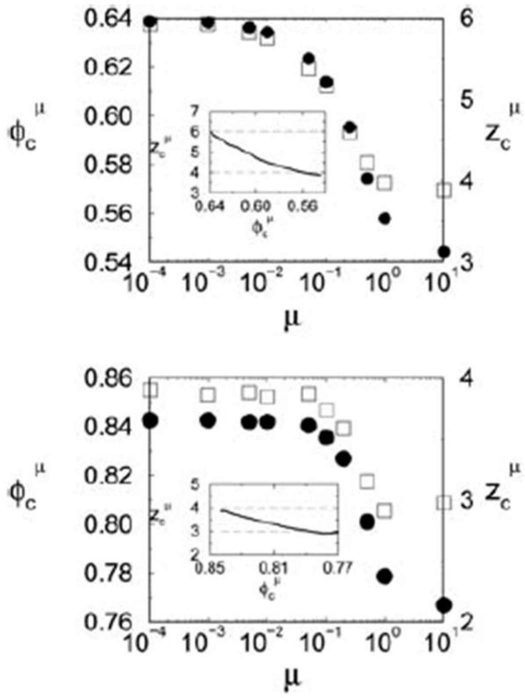


Fig. 1 Dependence of the critical values of the packing fraction $\phi^{\mu}{}_c$ (filled circles), and coordination number $z^{\mu}{}_c$ (open squares), on the particle friction coefficient μ, for monodisperse spheres in 3*D* (upper panel) and bidisperse discs in 2*D* (lower panel). The insets are parametric 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.

Conclusions

Nonspherical particle shapes changes simple `jamming scenario for spherical grains

1. Quartic modes lead to linear softening, perhaps nonlinear strengthening

2. For bumpy particles, microstates occur as geometrical families, instead of random points in configuration space