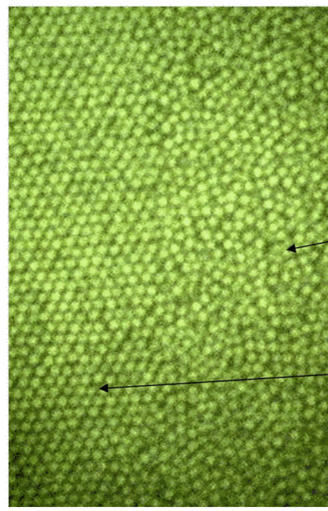
Jammed Ellipsoids beat Jammed Spheres

Experiments with Colloids and Candies

1st Annual Halsey Granular Workshop KITP'05

a) Colloids as Model Systems
Liquids, crystals, glasses

$\longleftarrow \nabla E \quad \otimes E$



Colloids are just like Granular Materials

But:
-Gravity irrelevant
-Inertia irrelevant
-Friction irrelevant
-Nonequilibria irrelevant
-Set "Effective Temperature" = Temperature

What's left?

--***Geometry***

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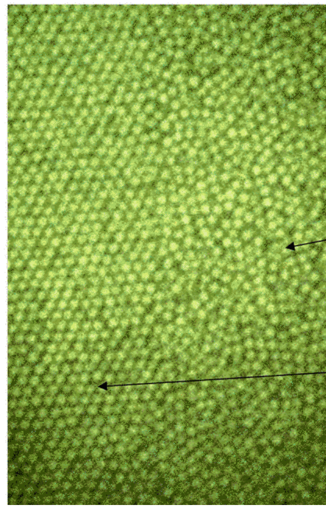

1μ colloidal hard spheres

Liquid

Crystal

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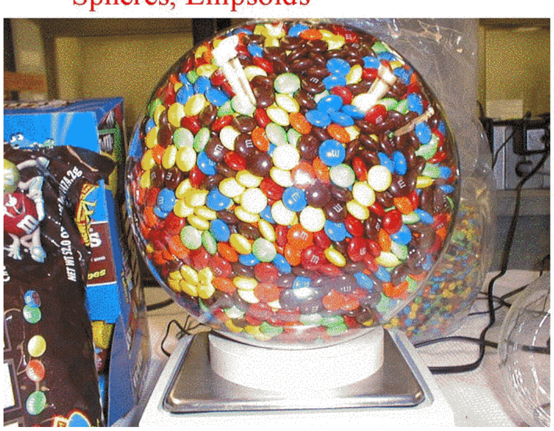
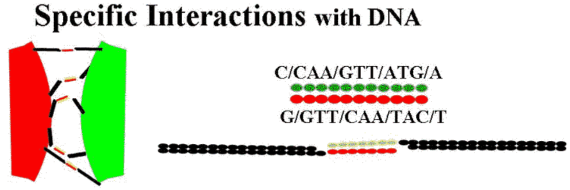
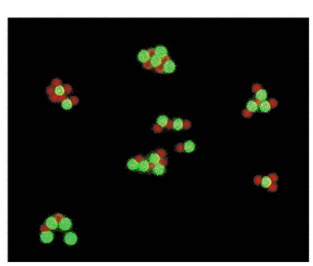
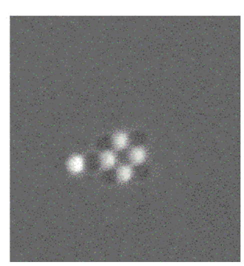


b) **Toward Colloidal Architecture**
Building complex stuff, structures, machines

Specific Interactions with DNA







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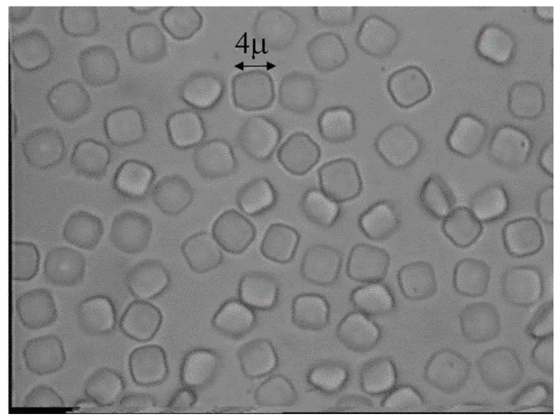
Square Disks in an E field



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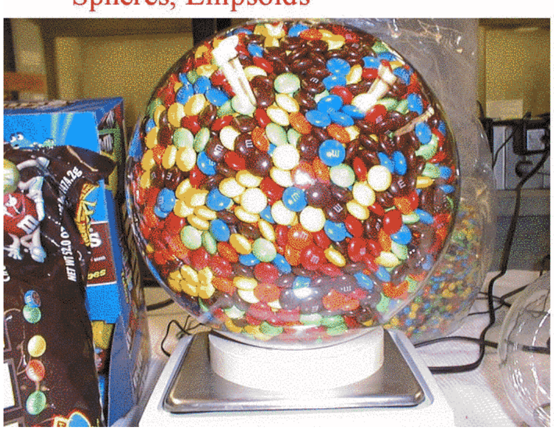
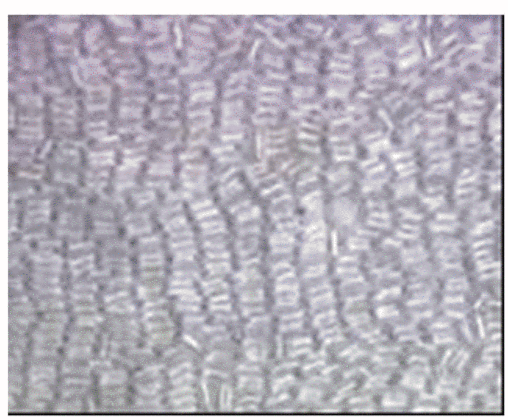


b) Toward Colloidal Architecture
Building complex stuff, structures, machines

2D Smectic - disks on edge, concentrated



Jammed Ellipsoids beat Jammed Spheres

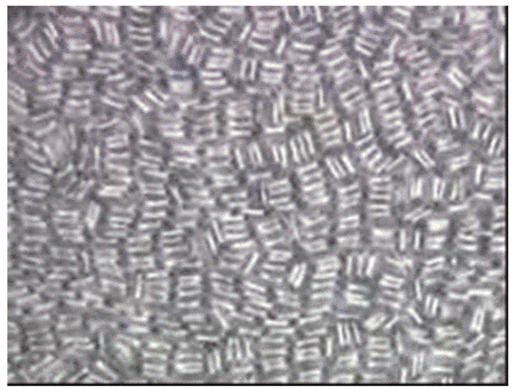
Experiments with Colloids and Candies

1st Annual Halsey Granular Workshop KITP'05

a) Colloids as Model Systems
Liquids, crystals, glasses
Packings: Random, Crystals, Spheres, Ellipsoids

b) **Toward Colloidal Architecture**
Building complex stuff, structures, machines

2D Tetratic - disks on edge, concentrated



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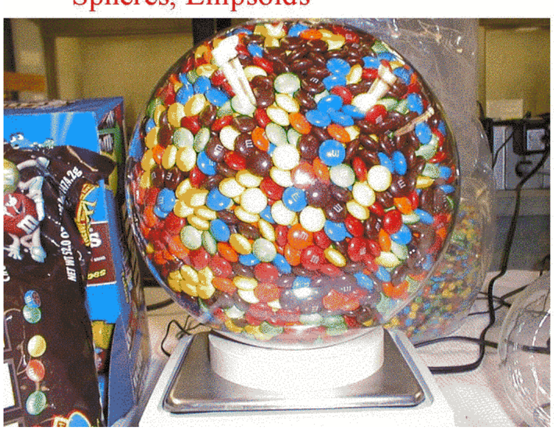


b) **Toward Colloidal Architecture**
Building complex stuff, structures, machines

Disk in circularly polarized light

Who's to Blame

Princeton - Physics

Matt Sullivan Kun Zhao Bob Austin
Chris Harrison Marie-Pierre Valignant
Weining Man ***Ibrahim Cisse***

Princeton - Chem Eng.

Andrew Hollingsworth Bill Russel

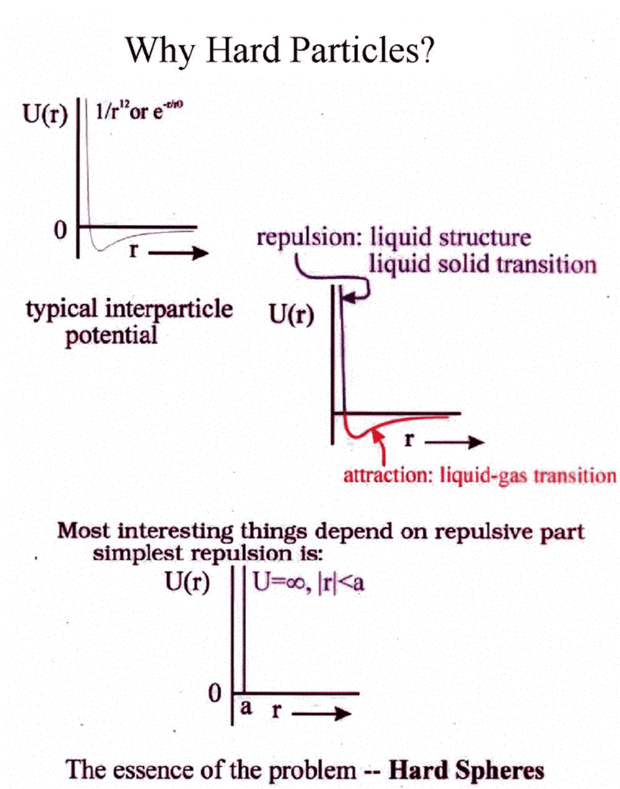
Princeton - Chemistry

Sal Torquato ***Frank Stillinger***
Aleksandar Donev

ExxonMobil

- Zhengdong Cheng (Texas A&M)
- Tom Mason (UCLA)

A presentation from the Russel-Chaikin Colloid Group, PRISM



ala Chandler, Weeks

Bernal Proc. Roy. Soc. A. volume 280, plate 16

Packing Densities for Spheres

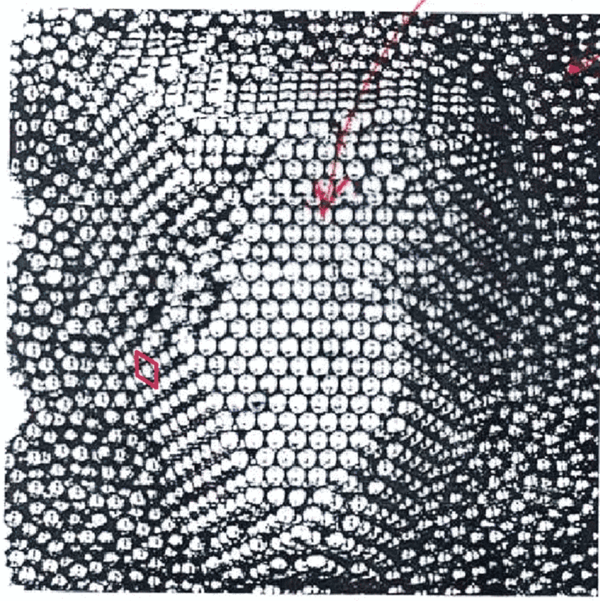
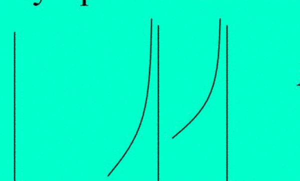


FIGURE 14. Face-centred cubic 'crystal' surrounded by 'liquid' caused by shearing ball-bearing mass. 111 face is shown at the top surface.

van der Waals and excluded volume

$$S = Nk_B \ln(V - Nb) = Nk_B \ln(V(1-\phi/\phi_C)) \qquad P = \frac{Nk_BT}{V-Nb} = \frac{Nk_BT}{V(1-\phi/\phi_C)}$$ Exact in 1D

Exact asymptotic form in any dimension



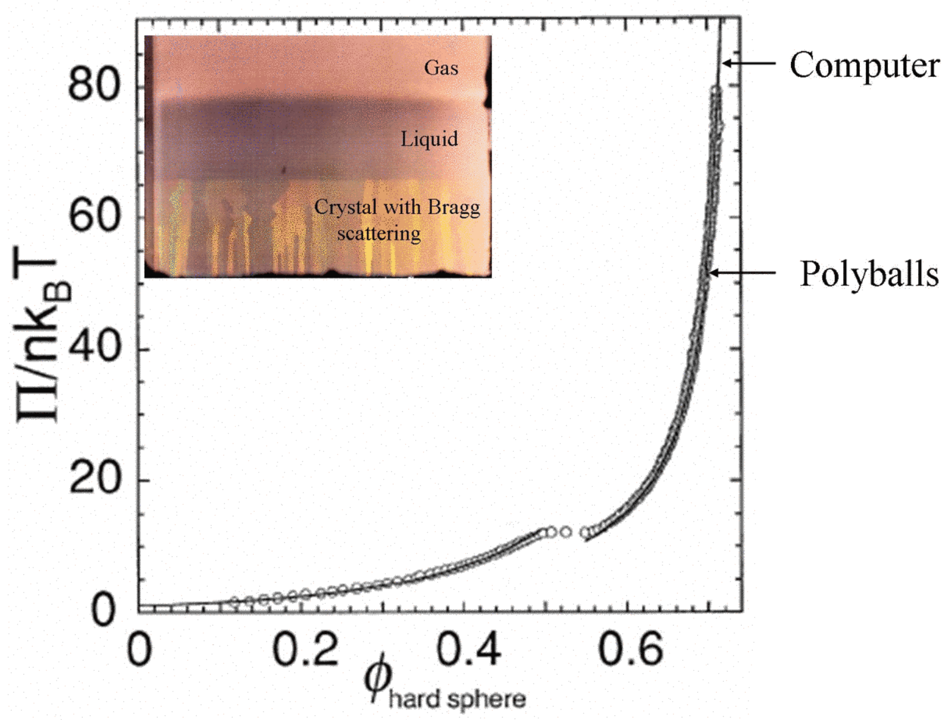
$$P \to \left.\frac{dnk_BT}{(1-\phi/\phi_C)}\right|_{\phi\to\phi_c}$$

$\Rightarrow$ ***Entropy drives liquid to crystal***

$S_{liquid} \to 0$ as $\phi \to .64$ $\qquad S_{crystal} \to 0$ as $\phi \to .74$

Highest Packing Fraction determines Stable High Density Phase

M. Rutgers

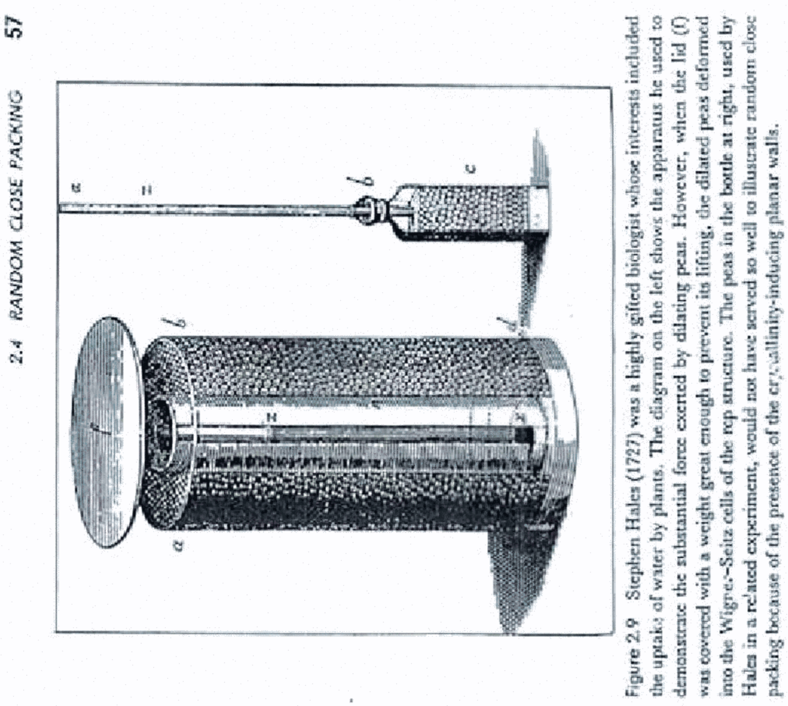


Packing of Hard Particles

Important for:

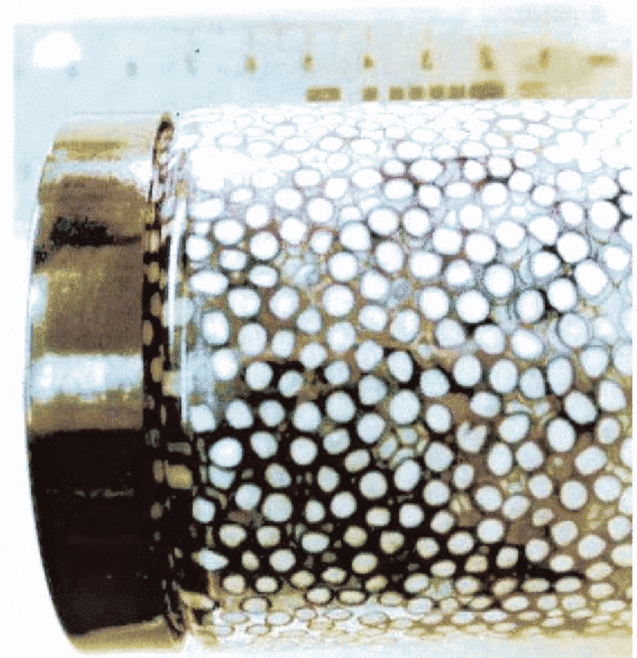
- Grain*
- Structure of Liquids, Solids and Glasses
- Freezing Transition
- Flow and Plasticity of Sand
- Optimization of data storage and transmission in the presence of Noise
- Opto-electronic Materials, Light localization and Photonic Bandgaps

In closing we must not forget the commentary on Random Packing which Saint Luke attributes to Jesus, “Give and it shall be given unto you; good measure, pressed down, and shaken together, and running over, shall men give into your bosom. For with the same measure that ye mote withal shall be measured to you again.” -Bernal

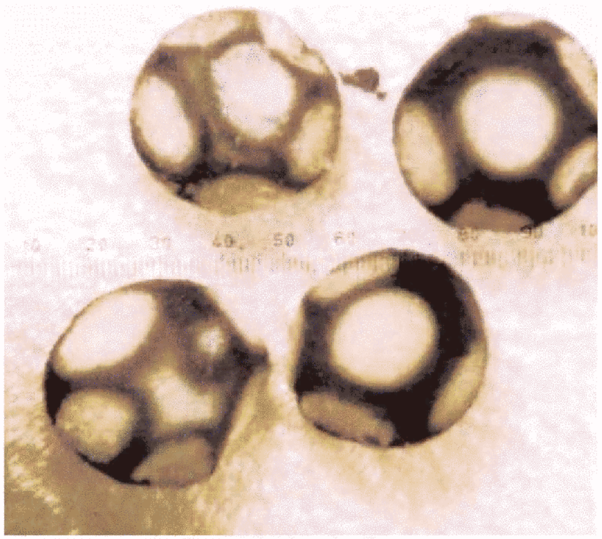


2.4 RANDOM CLOSE PACKING 57

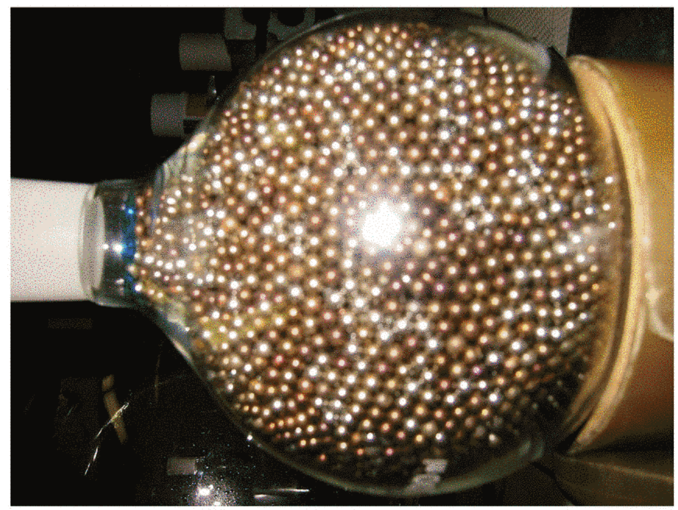
Figure 2.9 Stephen Hales (1727) was a highly gifted biologist whose interests included the uptake of water by plants. The diagram on the left shows the apparatus he used to demonstrate the substantial force exerted by dilating peas. However, when the lid (f) was covered with a weight great enough to prevent its lifting, the dilated peas deformed into the Wigner-Seitz cells of the rcp structure. The peas in the bottle at right, used by Hales in a related experiment, would not have served so well to illustrate random close packing because of the crystallinity-inducing planar walls.

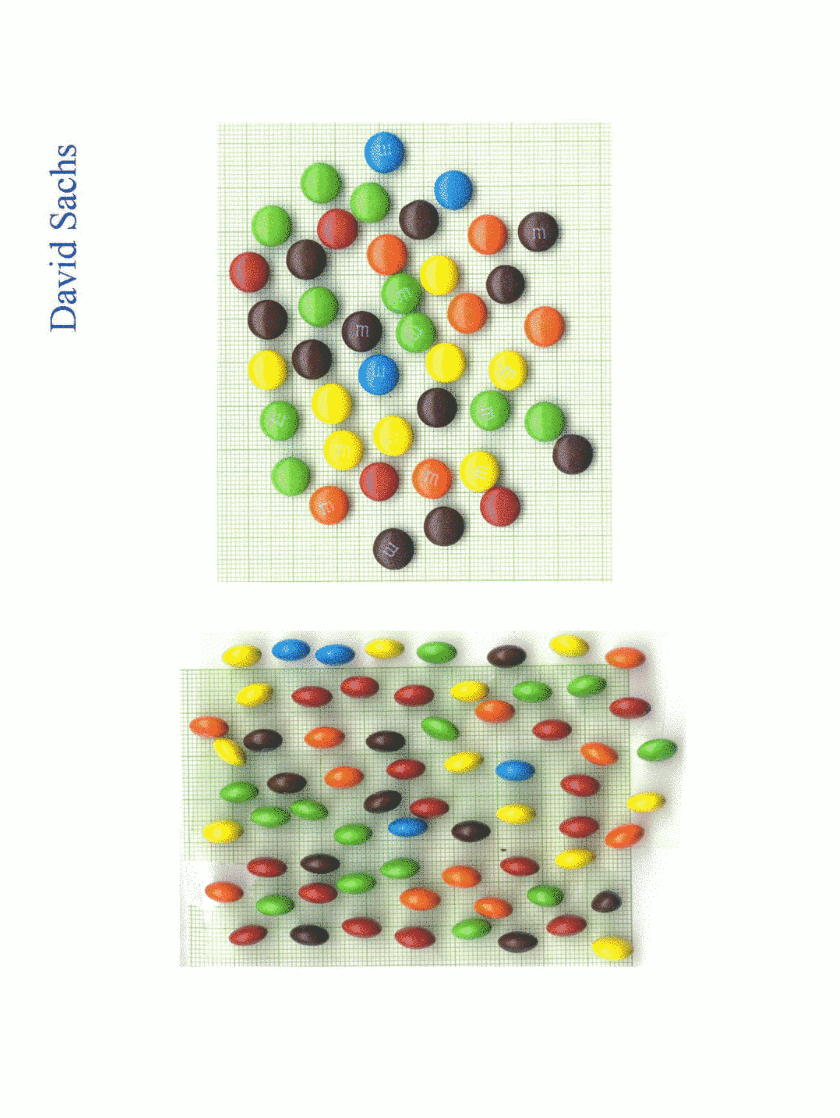


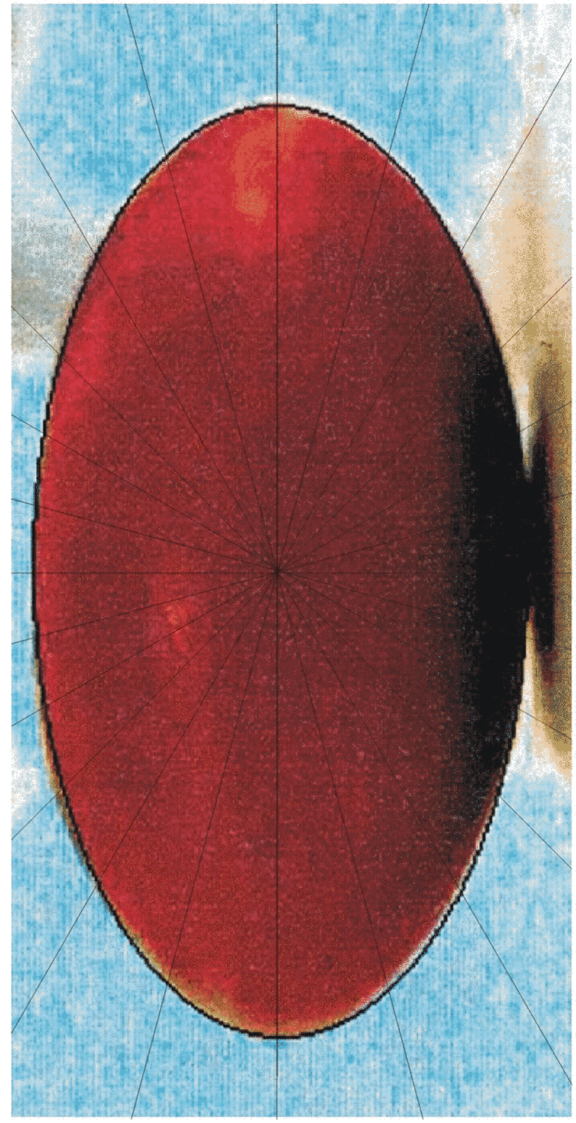
Evan Variano



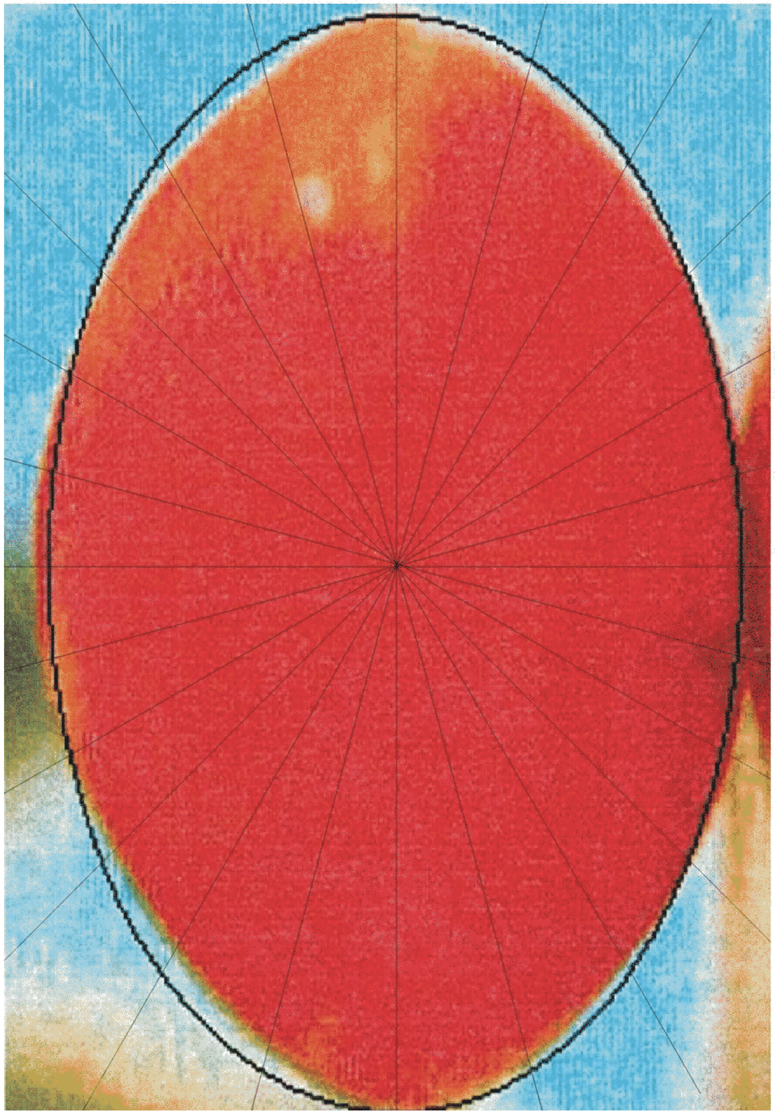
Evan Variano







M&M ® $(\delta r^2/<r>^2)^{1/2} <.01$



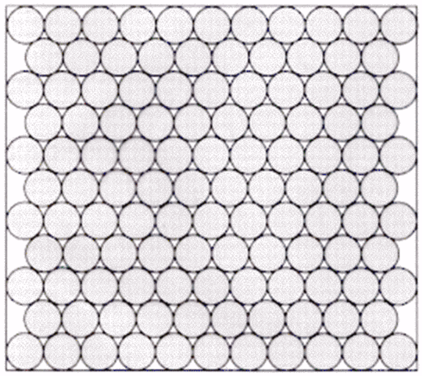
Skittle ® $(\delta r^2/\langle r\rangle^2)^{1/2} \sim .03$

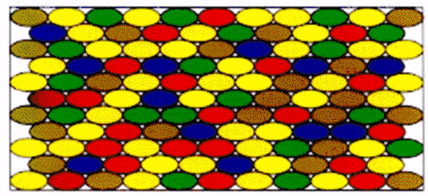
~28,000 m&m's® minis

Crystal Packing of Spheres and Ellipsoids

Affine deformation – coordinate change,
doesn't change packing fraction.

M&M®s aspect ratio 1.91

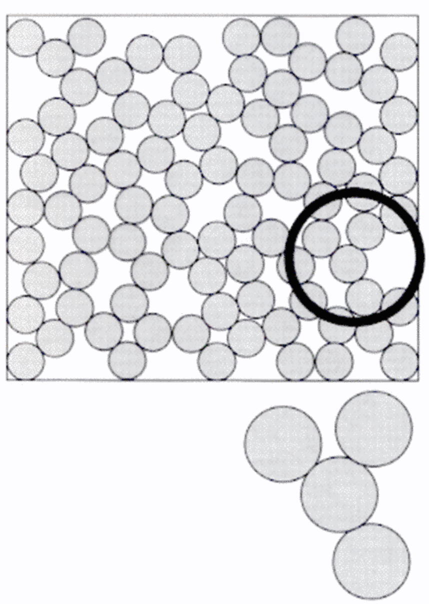


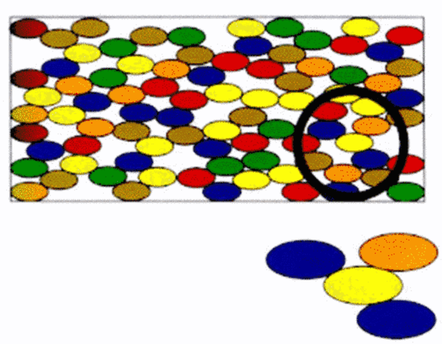


$$\varphi = \frac{N\frac{4}{3}\pi r^3}{L^3}$$

$$\varphi = \frac{N\frac{4}{3}\pi r^2 (r/1.91)}{L^2 (L/1.91)}$$

Volume Fraction 0.7404





Do ellipsoids pack denser than spheres?

	Aspect ratio	5 litre	1 litre	0.5 litre
Regular M&M's ®	1.89+/- .005	.685	.676	.674
M&M minis ®	1.91+/- .005	**.689 ±.01**	.677	.676
Ball bearings	1+/- .001			**.636**

YES!

The *isostatic* conjecture – Shlomo Alexander, Sam Edwards

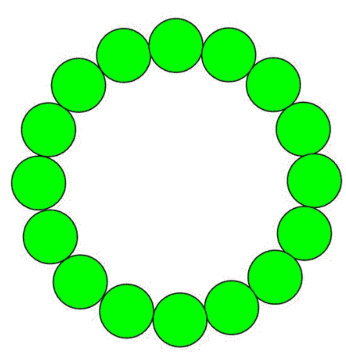
Coordination number Z=2d

Random packings are just barely constrained.

d degrees of freedom per particle
→Nd constraints to define system
→Nd contacts → 2Nd touching neighbors

Spheres 1D, d=1, Z=2
2D, d=2, Z=4
3D, d=3, Z=6

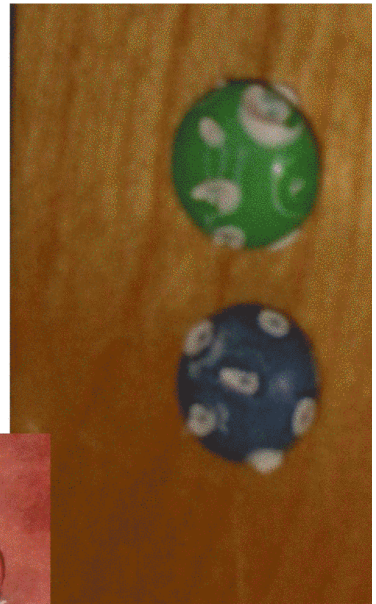
RCP 3D, 6+ε neighbors



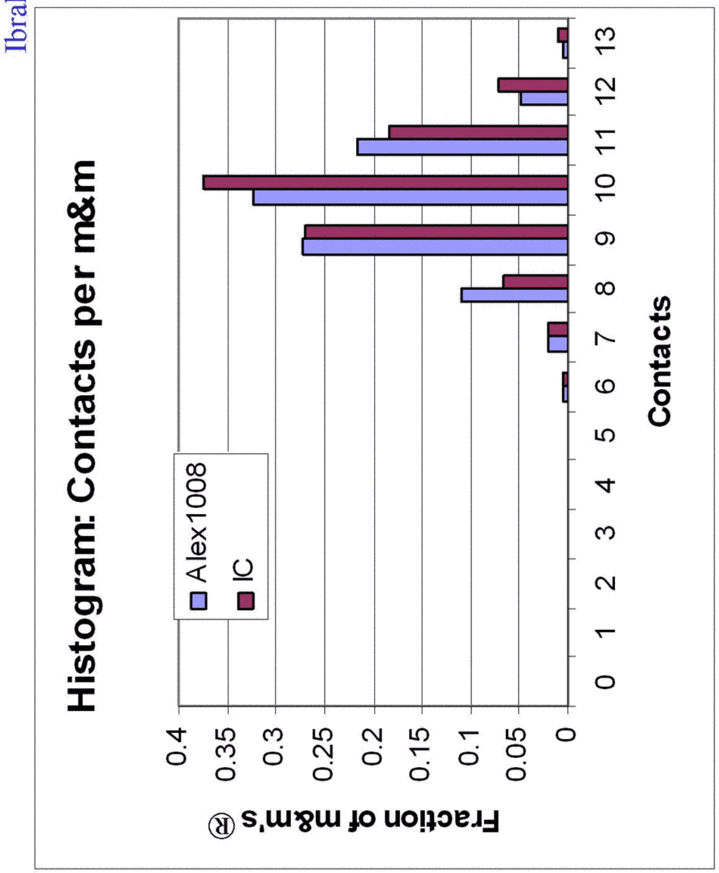
m&m's ® 3D, d=3trans+2rotate=5, Z=10

To get 10 neighbors needs to pack denser

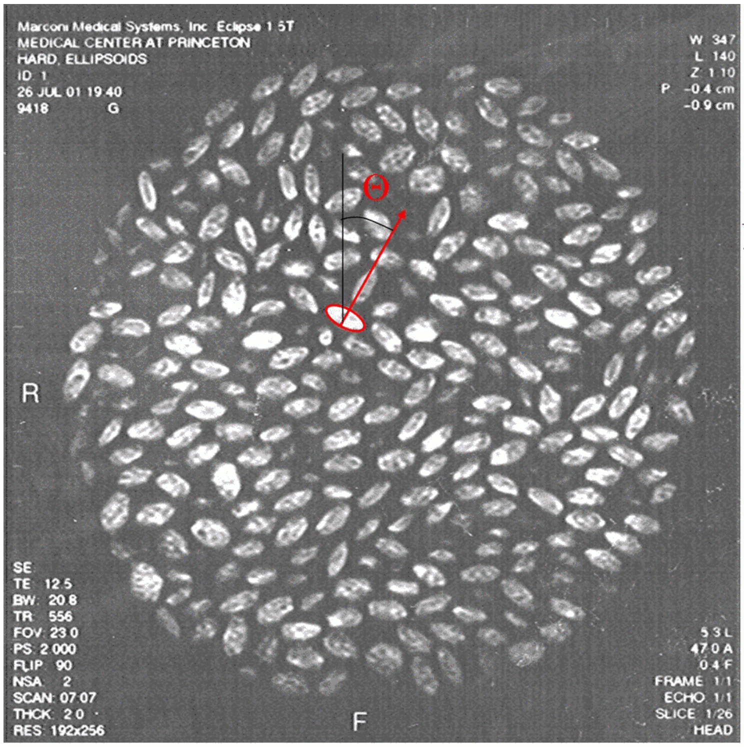
Ibrahim Cisse



Ibrahim Cisse



Average # contacts/m&m =9.87



Full Head Scan MRI – Princeton Hospital

No orientational order

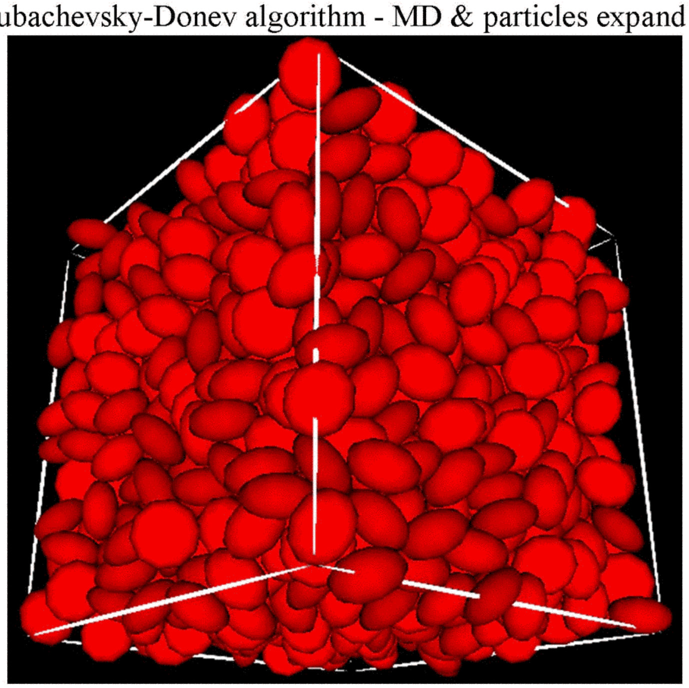
Nematic order parameter
$\eta = 2\cos^2(\Theta) - 1 = .04$

if random
$\eta = 0 \pm .06$

Torquato, Chaikin

Aleksandar Donev, Frank Stillinger, Sal Torquato

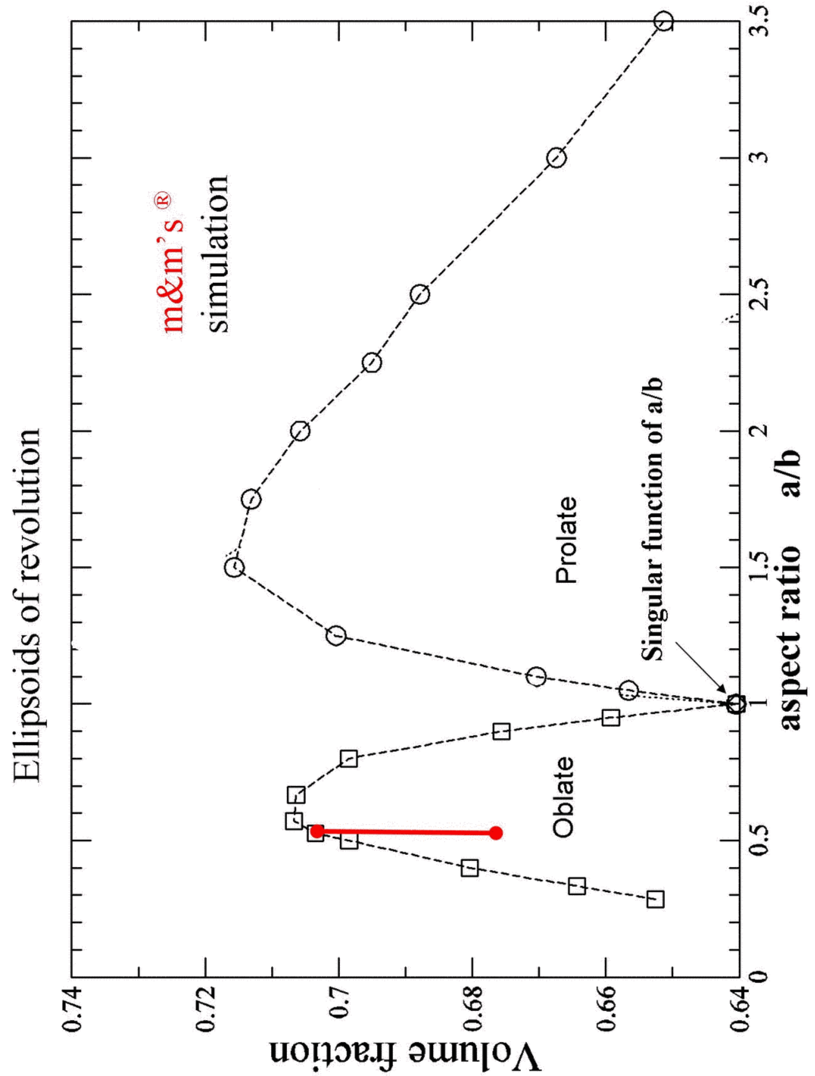
Stillinger-Lubachevsky-Donev algorithm - MD & particles expand

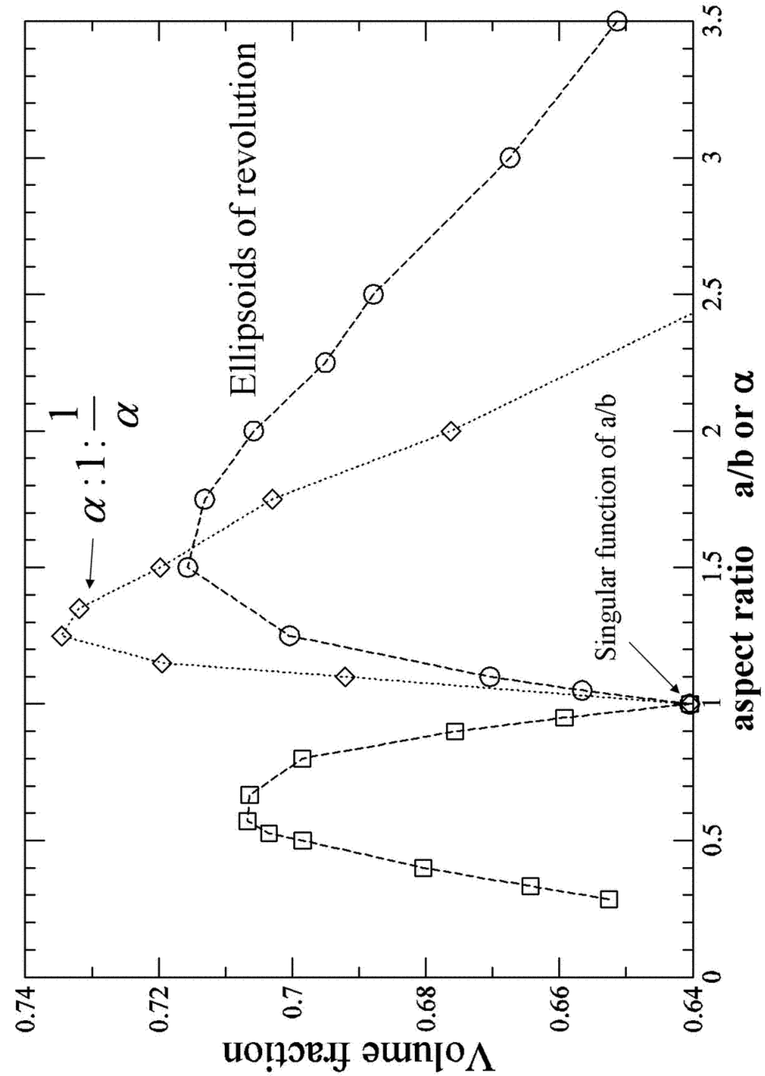


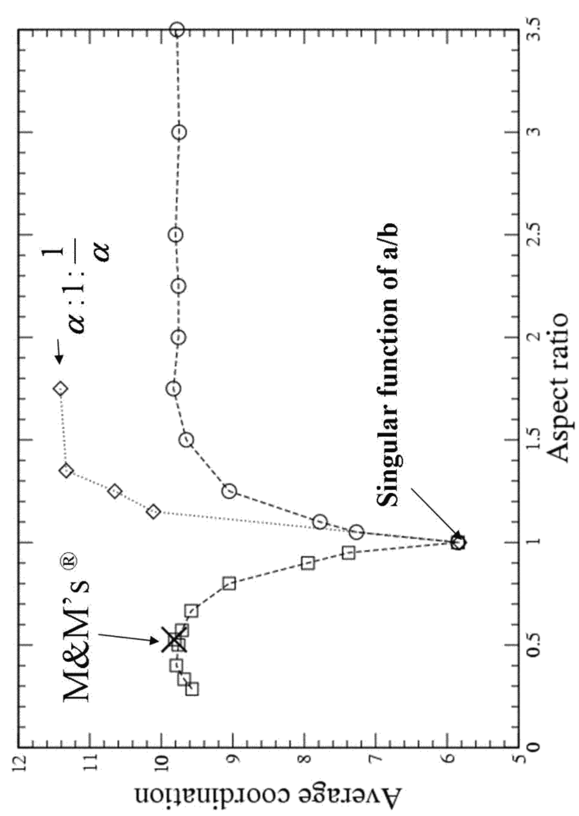
$\eta = (3\cos^2(\Theta) - 1)/2 = .01$

1000
1.91:1
Ellipsoids

$\bar{\eta} = \frac{1}{2}\sqrt{\frac{3}{N}}$

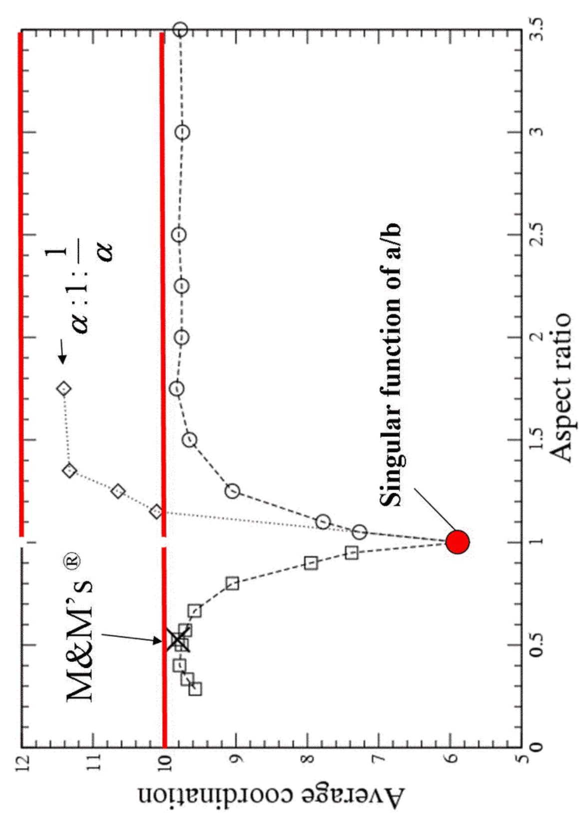

Ellipsoids of revolution
m&m's ®
simulation
Prolate
Oblate
Singular function of a/b
aspect ratio a/b
Volume fraction
0.74
0.72
0.7
0.68
0.66
0.64
0
0.5
1
1.5
2
2.5
3
3.5


Ellipsoids of revolution
$\alpha : 1 : \frac{1}{\alpha}$
Singular function of a/b
aspect ratio a/b or α
Volume fraction
0.74
0.72
0.7
0.68
0.66
0.64
0
0.5
1
1.5
2
2.5
3
3.5



Why is isostatic result only approximately right?

Jammed states don't maximize configurations/entropy?



Isostatic Conjecture

Equations

For each particle

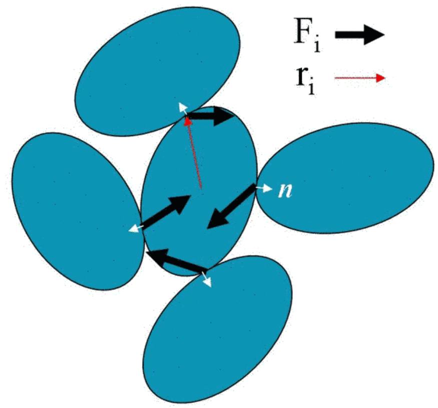
$\sum_{contacts} F_i = 0$ d force eqs.

$\sum_{contacts} (r \times F)_i = 0$ n torque eqs*. 2D n=1 3D n=3

Degrees of freedom f = d+n

Unknowns

F_i's at the N_c contacts $=dN_c$



coordination number $Z = 2 N_c / N$

Frictional Case: $dN_c = fN$ $Z=2f/d$

1D	d=1	n=0	f=1	f/d=1	Z=2
2D	d=2	n=1	f=3	f/d=3/2	Z=3
3D	d=3	n=3	f=6	f/d=2	Z=4

$^*n_{max}=d(d-1)/2$

Frictionless Case $(n \times F)_i = 0$

Additional $(d-1)N_c$ equations

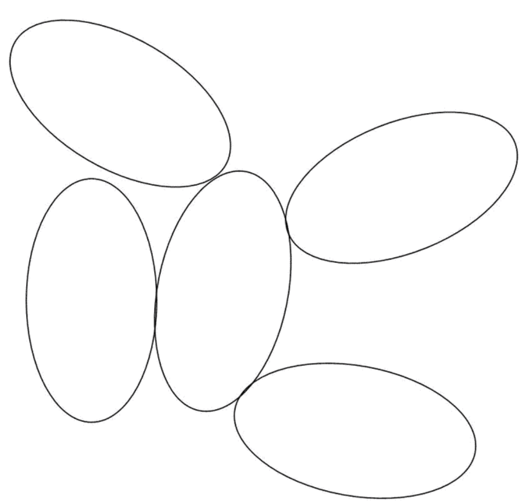
$dN_c = (d-1)N_c + fN : N_c = fN$

Z=2f

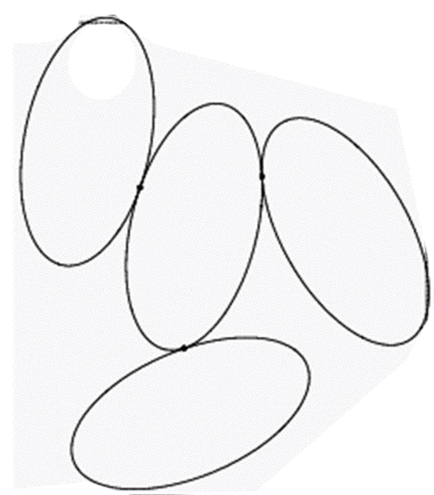
If contacts are random i.e. most likely case?

Local Jamming (hold neighbors fixed)

Donev



4 neighbors always works

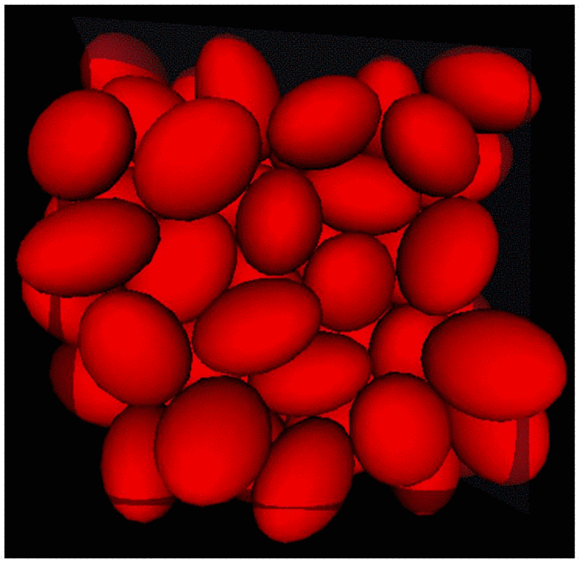


3 neighbors sometimes works
- But less "entropy"

Translationally trap, expand,
-always find Jammed state

Random Ellipsoid Packing Exceeds FCC Spheres

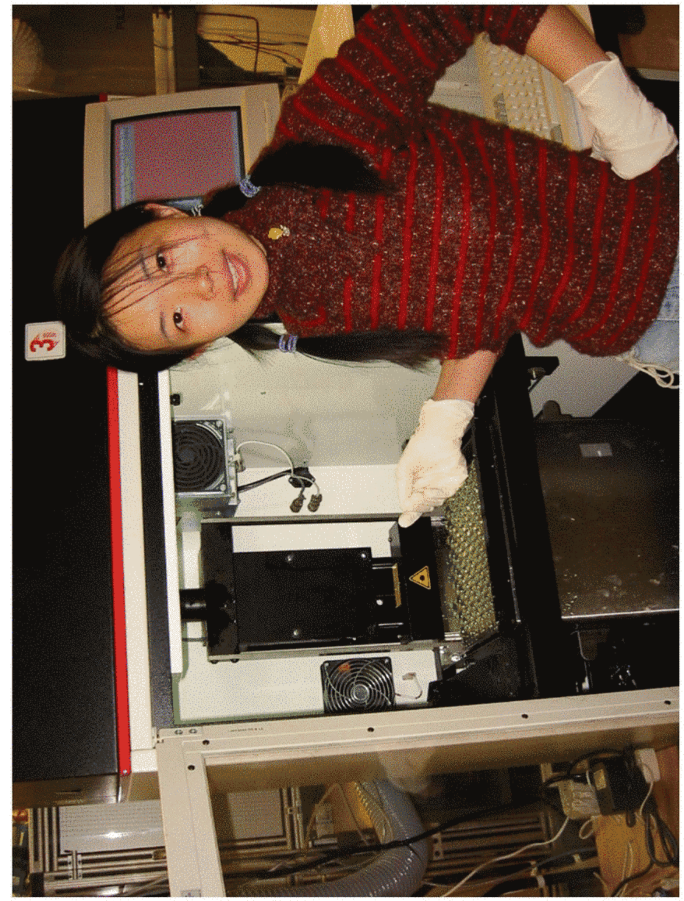
a:b:c =1.25:1:0.8



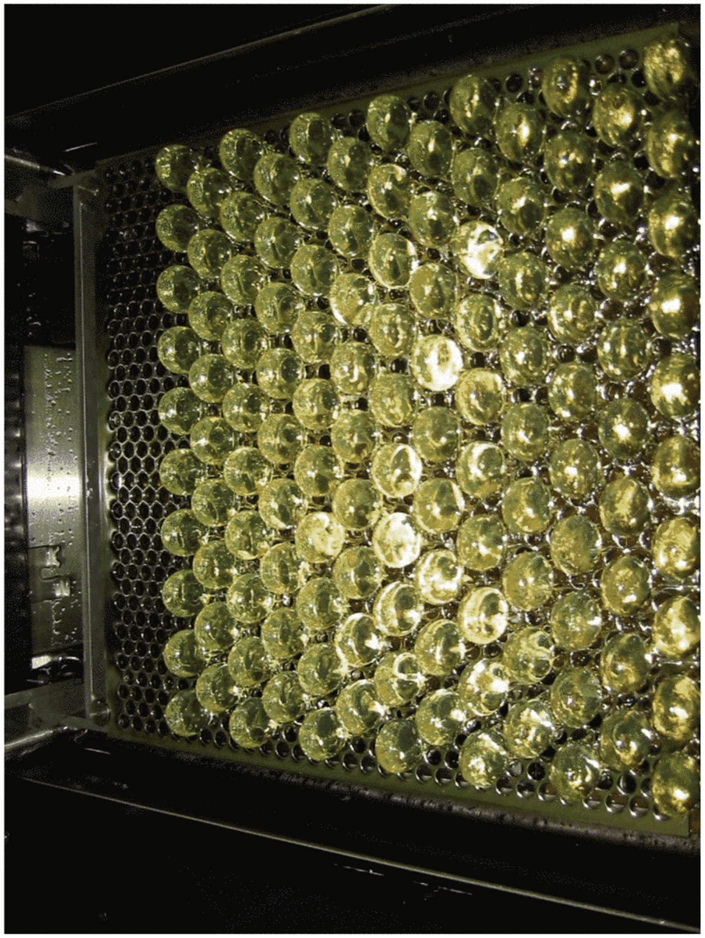
Φ=.7427

32 ellipsoids
Periodic boundaries

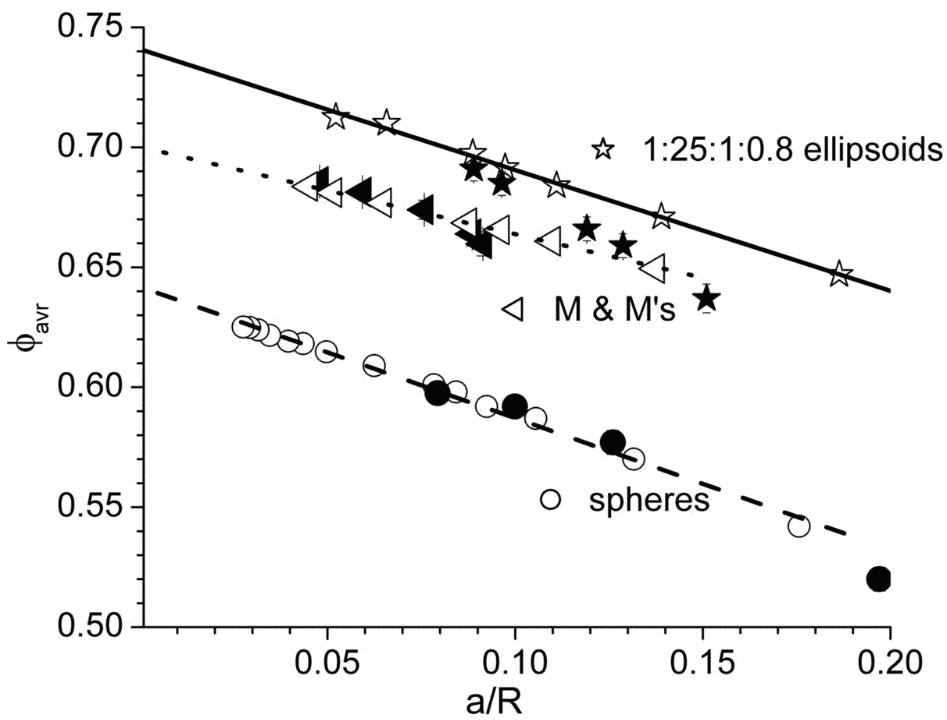
Weining Man



Stereolithography for 1.25:1:0.8 ellipsoids

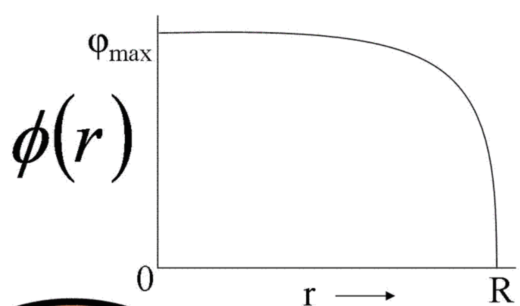


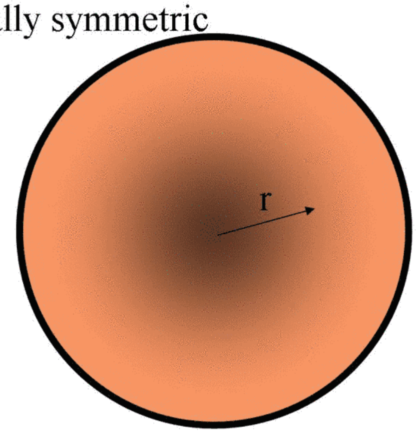
Average Packing in Spherical Container

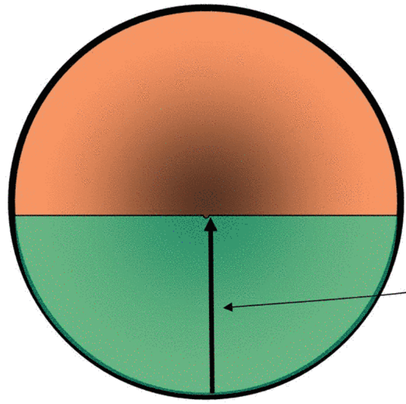


Packing fraction from finite spherical container

Expect packing less dense at walls, spherically symmetric



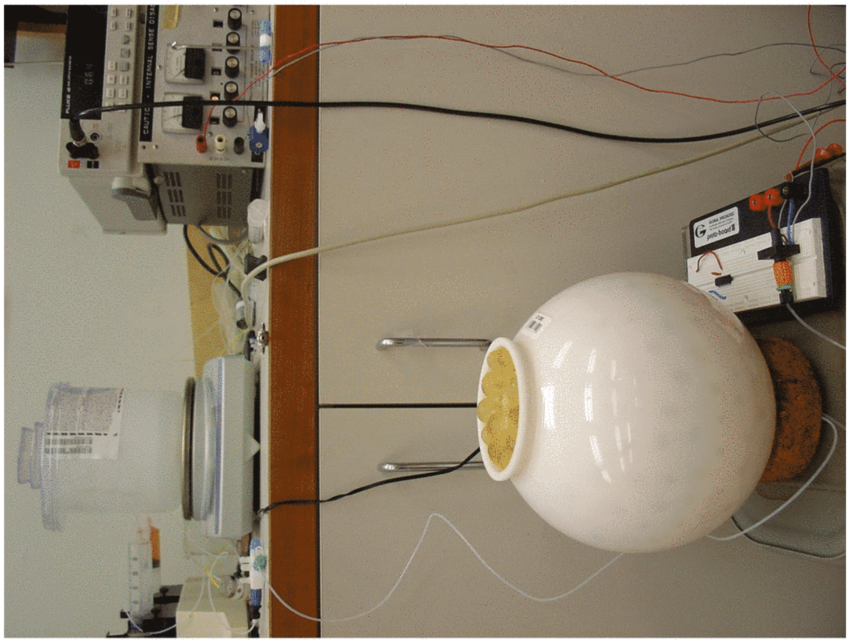


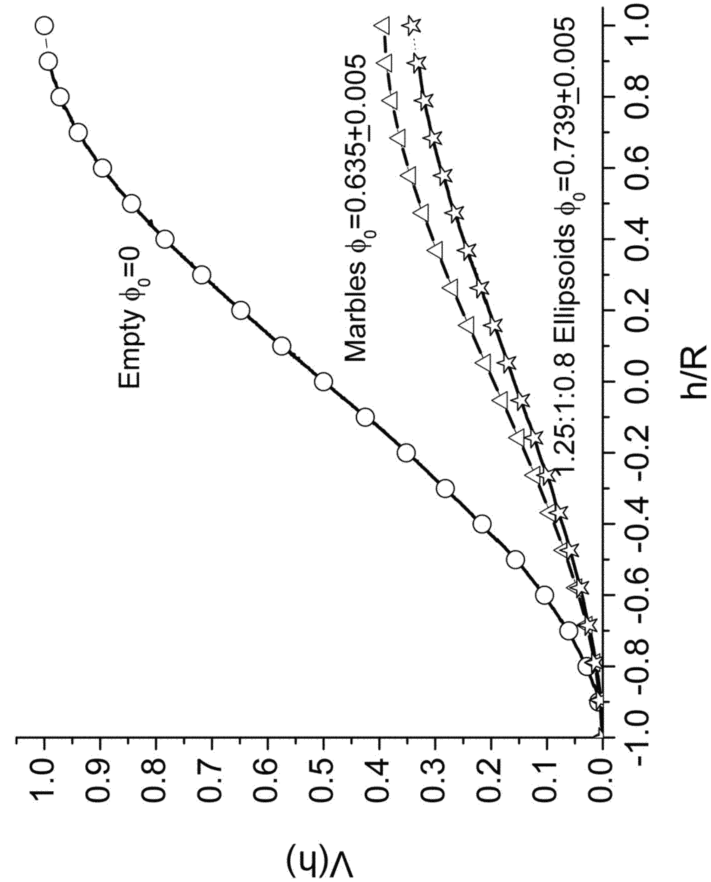


Measure height as a function of added fluid

$$V(h) = \int_h^R (1-\phi(r))\left(1-\frac{h}{r}\right)2\pi r^2 dr$$

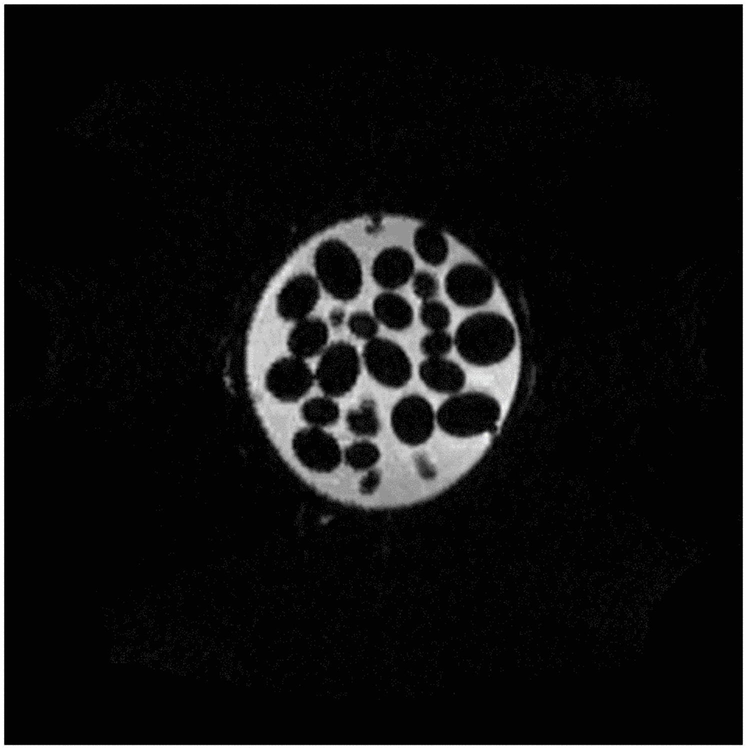
Invert to get $\phi(r) = 1 - \frac{1}{2\pi}\frac{\partial^2 V(h)}{\partial h^2}\Big|_{h=r}$

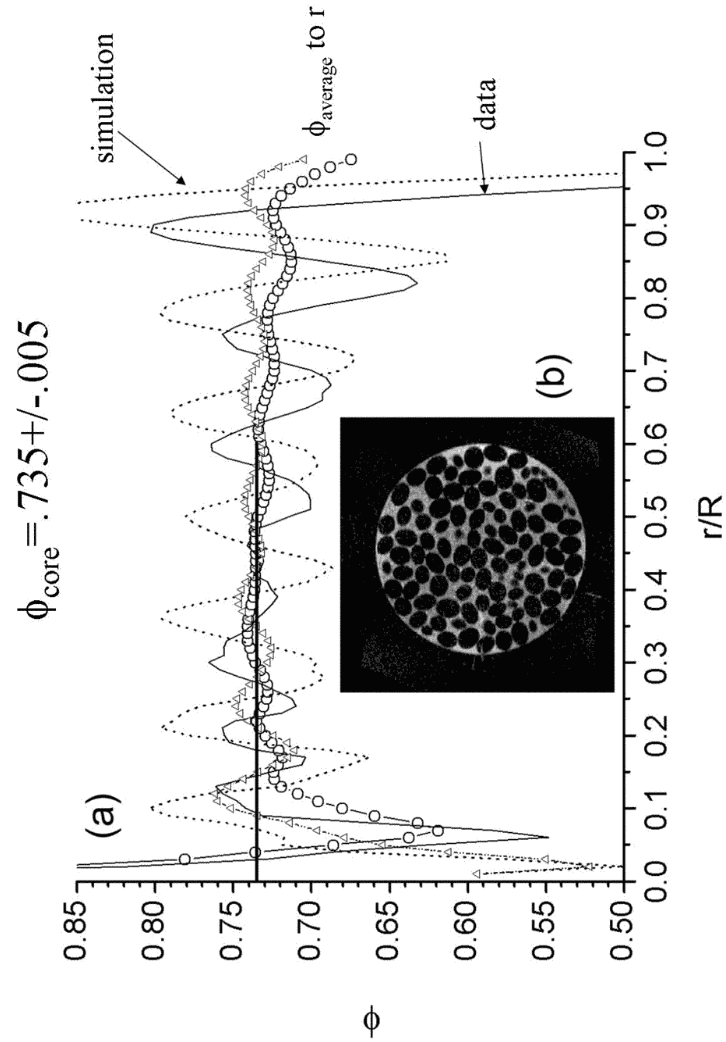




Empty ϕ_0=0
Marbles ϕ_0=0.635±0.005
1.25:1:0.8 Ellipsoids ϕ_0=0.739±0.005
h/R
V(h)
-1.0 -0.8 -0.6 -0.4 -0.2 0.0 0.2 0.4 0.6 0.8 1.0
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

David Heeger, Souhil Inati



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SCIENCE & SPACE

M&M's obsession leads to physics discovery

Monday, February 16, 2004 Posted: 1939 GMT (3:39 AM HKT)

WASHINGTON (Reuters) -- Princeton physicist Paul Chaikin's passion for M&M's candies was so well known that his students played a sweet practical joke on him by leaving a 55-gallon drum of the candies in his office.

Little did they know that their prank would lead to a physics breakthrough.

The barrel full of the oblate little candies made Chaikin think about how well they packed in. A series of studies have shown they pack more tightly than perfect spheres -- something that surprises many physicists and Chaikin himself.

"It is a startling and wonderful result," said Sidney Nagel, a physicist at the University of Chicago. "One doesn't normally stop to think about this. If you did, you might have guessed what would happen, but you'd have guessed wrongly."

The issue of how particles pack together has intrigued scientists for centuries and has implications for fields such as the design of high-density ceramic materials

(DENISE APPLEWHITE/PRINCETON UNIVERSITY)

Professors Paul Chaikin, left, and Salvatore Torquato used M&M candies to reveal fundamental principles governing the random packing of particles.

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News & Views

Princeton profs Paul Chaikin, *left*, and Salvatore Torquato

The physics of M&Ms Who knew candy could solve an ancient physics problem? It all began as a prank on Princeton physics professor Paul Chaikin, whose students left a 55-gallon drum of M&Ms in his office to sweeten him up. Instead, it inspired an "Aha!" moment as Chaikin pondered a centuries-old physics mystery: how objects (in this case, "oblate spheroids" — science-speak for the M&M shape) settle. He and Princeton chemist Salvatore Torquato supervised experiments like pouring paint on a container of the candies to see how it covered them. Their scientific conclusion: Unlike sphere shapes, oblate spheroids act like tiny levers, rotating until they find the most stable packing position, making for better packaging and shipping. In short, Chaikin says: "You can pack more M&Ms than gum balls [of similar size] into the same space."

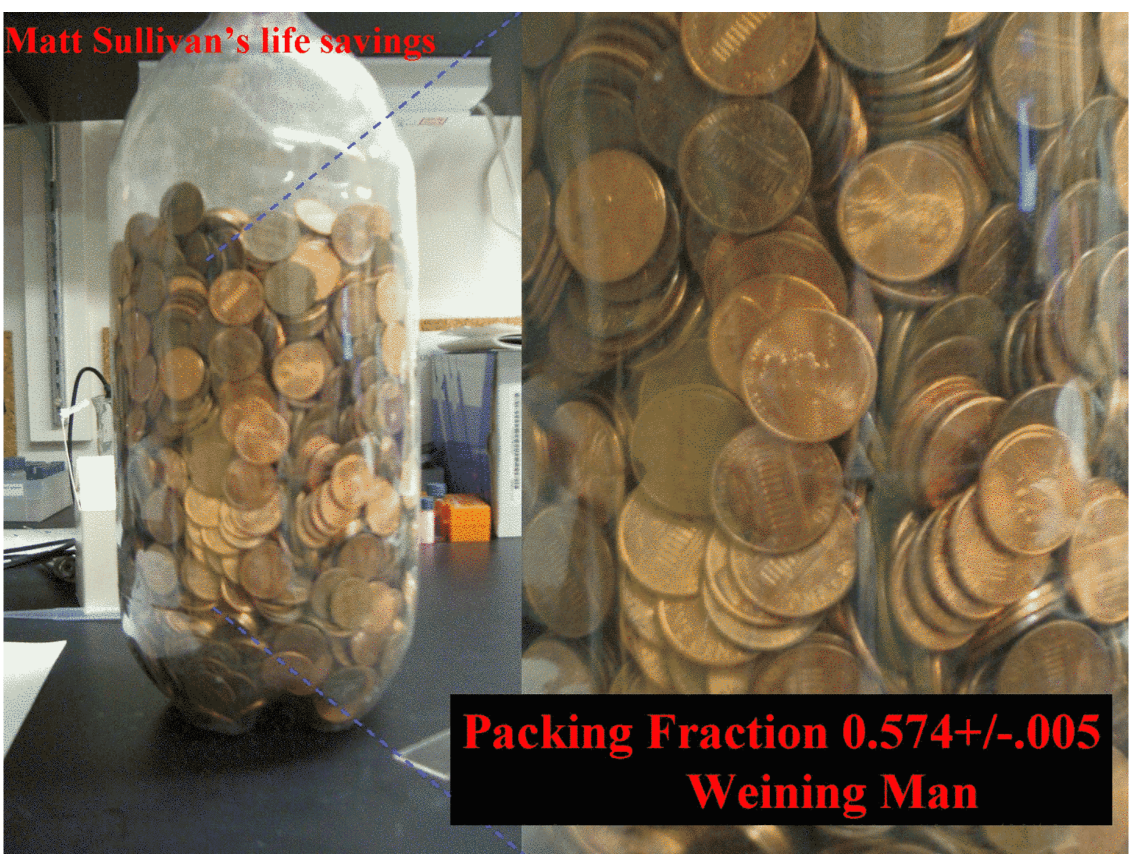
Public opinions as to why M&M's ® pack denser:

They're flatter and tend to orient and order
- Nope: If they oriented it's an affine deformation of spheres, packing is 63.6%. No evidence of order.

If you make them flat they're like pennies and stack better
If you make them long they're like cylinders and pack better.
- Nope: Cylinders and pennies pack to 91%, but an ellipsoid only fills a cylinder to 2/3 => 67%

.67x.91=.604 and that's crystal packing,
random pennies and sticks pack much less dense.

They can rotate to fit into open spaces
- Yep, that's it.



Comparison of Packings

	Degrees of Freedom	Touching Neighbors	Volume Fraction
FCC Crystal	3	12	.7404
MRJ Spheres	3	6	.636
MRJ Ellipsoid of Revolution	5	10	.68-.70
MRJ $a \neq b \neq c$ Ellipsoid	6	>11.4	>.747

We have found a random packing $\geq$ .7405
higher than crystal packing of spheres

Do we have a higher random packing
than crystal packing??????

What is the densest packing of ellipsoids?

Summary

Random Ellipsoid packings :

-Are singular at a/b=1

-***Can be denser than .74 with 12 neighbors***

-Tend toward the isostatic limit: Z=2d

-Are comparable to (and may yet surpass) crystal packings

-Does Random ever beat crystal?

-Why are packings near α=1 not isostatic

125 lbs of Almond M&M's
Polydispersity ~17%

2 liters packs to ϕ~.67

PHYSICAL REVIEW E **67**, 051301 (2003)

Random packings of spheres and spherocylinders simulated by mechanical contraction

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(Received 21 October 2002; published 7 May 2003)

We introduce a simulation technique for creating dense random packings of hard particles. The technique is particularly suited to handle particles of different shapes. Dense amorphous packings of spheres have been formed, which are consistent with the existing work on random sphere packings. Packings of spherocylinders have also been simulated out to the large aspect ratio of $\alpha = 160.0$. Our method packs randomly oriented spherocylinders to densities that reproduce experimental results on anisotropic powders and colloids very well. Interestingly, the highest packing density of $\phi = 0.70$ is achieved for very short spherocylinders rather than
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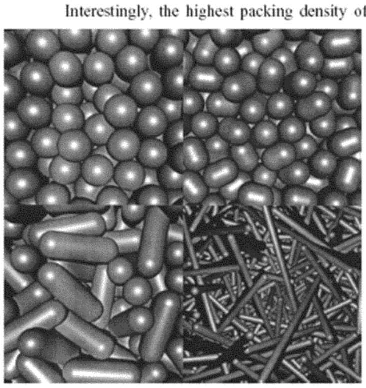


FIG. 1. Images (ray tracings) of tightly packed isotropic spherocylinders for several aspect ratios α. Aspect ratios of (clockwise from top left) $\alpha = 0$ (spheres), $\alpha = 0.4$, $\alpha = 40.0$, and $\alpha = 2.0$. For $\alpha = 0.4$, the highest packing density $\phi = 0.70$ is achieved (see Fig. 2). The packing for $\alpha = 2.0$ is already to the right of the density maximum, and has a density $\phi = 0.616$, which is close to that of the random sphere packings.

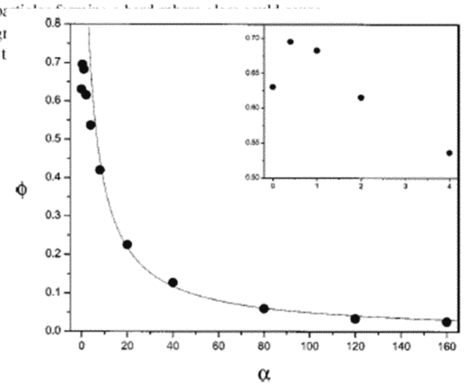
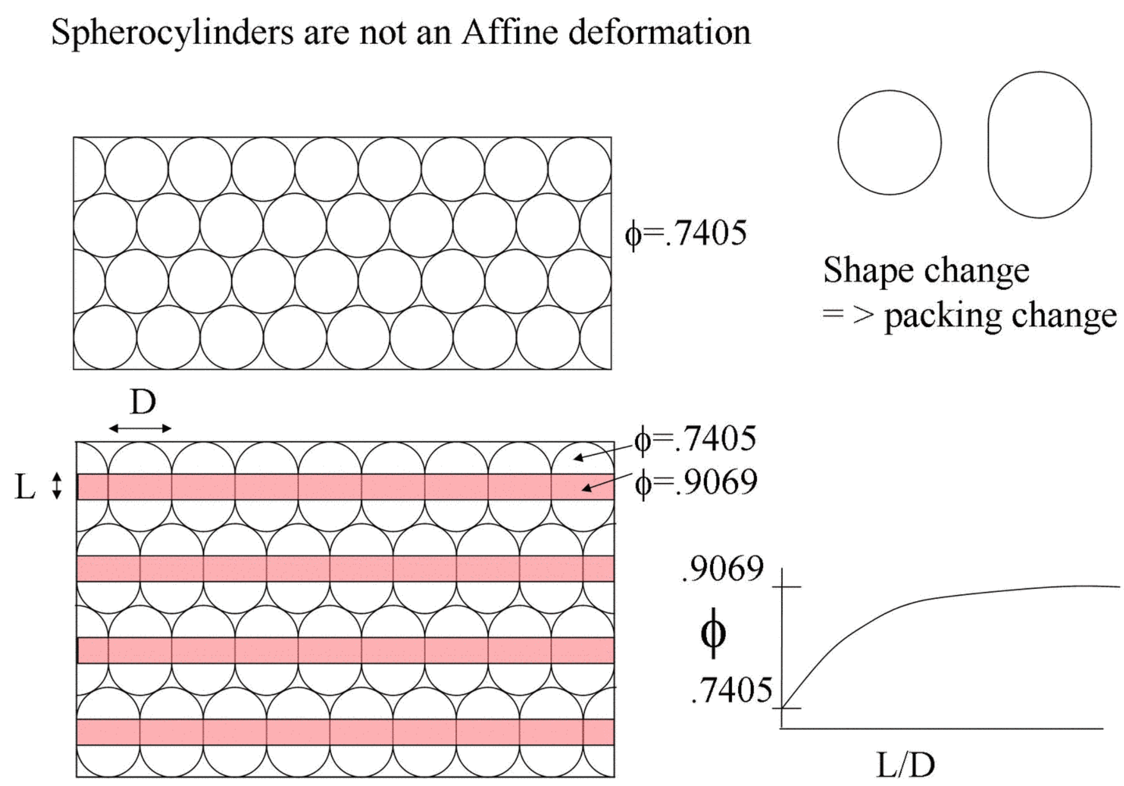
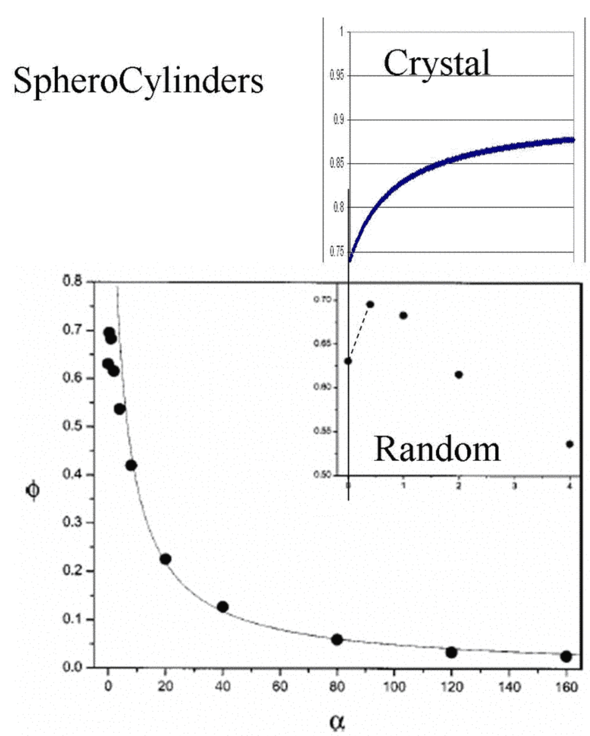


FIG. 2. Final volume fractions ϕ for the amorphous packings as a function of aspect ratio α. The solid line is a theoretical fit from the random contact equation $\phi\alpha = 5.1$ [see Eq. (1)]. The inset shows a magnified view of the same graph at low aspect ratio.





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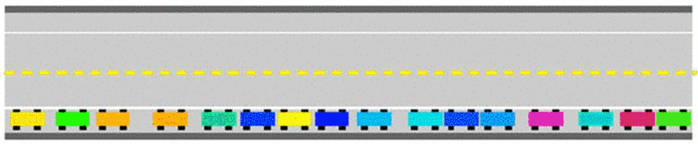
"The Parking Problem"

Random Sequential Addition – a random tiling

Rényi's Parking Constants



Given the closed interval $[0, x]$ with $x > 1$, let one-dimensional "cars" of unit length be parked randomly on the interval. The mean number $M(x)$ of cars which can fit (without overlapping!) satisfies

$$M(x) = \begin{cases} 0 & \text{for } 0 \le x < 1 \\ 1 + \frac{2}{x-1}\int_0^{x-1} M(y)\,dy & \text{for } x \ge 1. \end{cases} \quad (1)$$

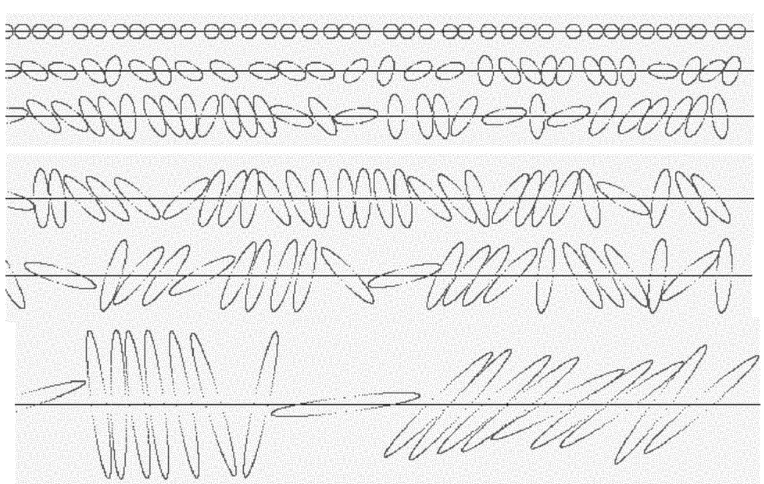
The mean density of the cars for large x is

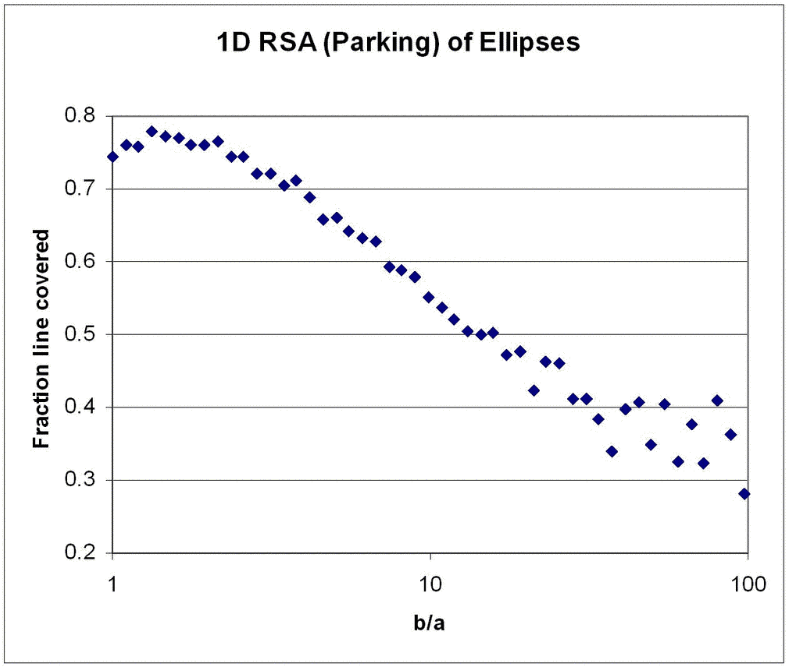
$$m \equiv \lim_{x\to\infty} \frac{M(x)}{x} \quad (2)$$

$$= \int_0^\infty \exp\left(-2\int_0^x \frac{1-e^{-y}}{y}\,dy\right)dx \quad (3)$$

$$= 0.7475979202\ldots \quad (4)$$

Parking Ellipsoids





This is from a simulation randomly adding randomly oriented ellipses to a line.
It seems to capture the basic behavior of the ellipsoid packing?