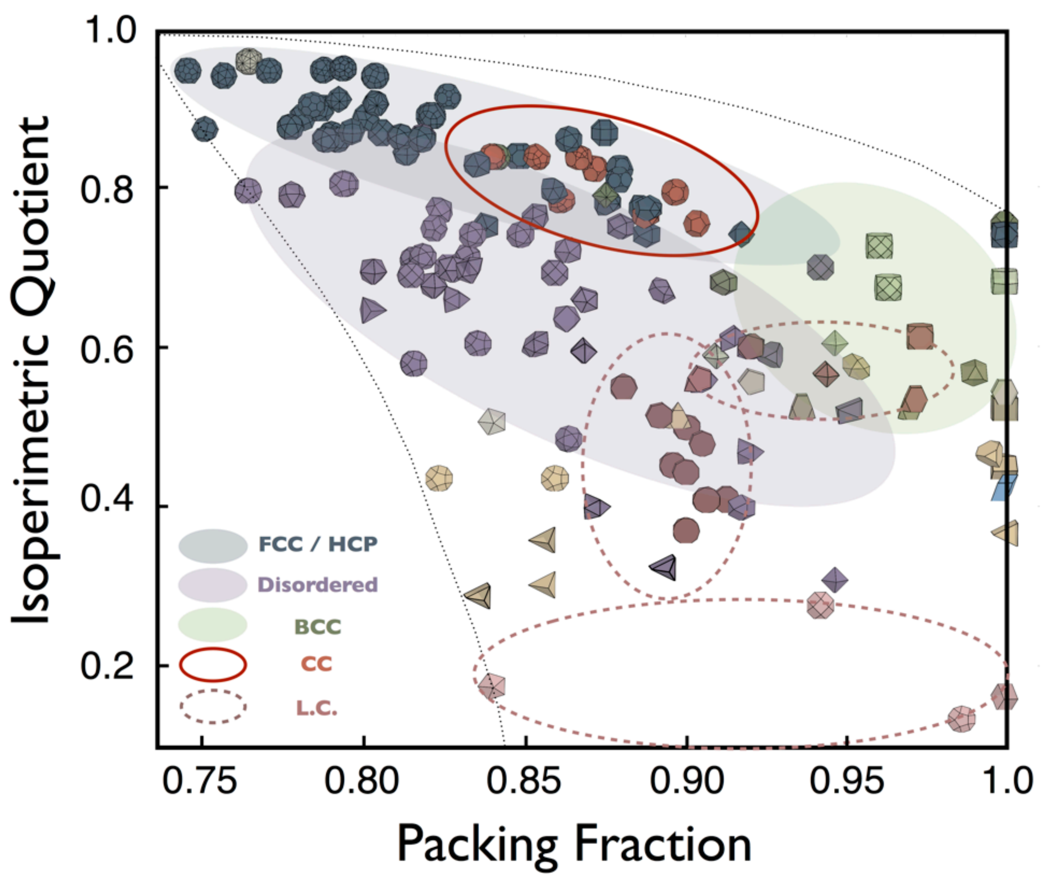
Pessimal Shapes for Packing and Covering

Yoav Kallus
Santa Fe Institute

Background

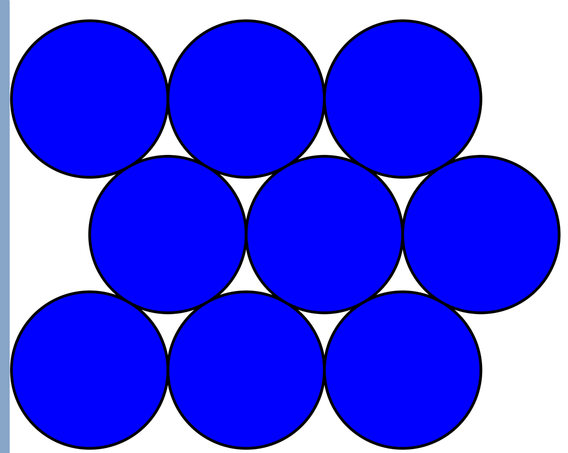
Ulam's Last Conjecture



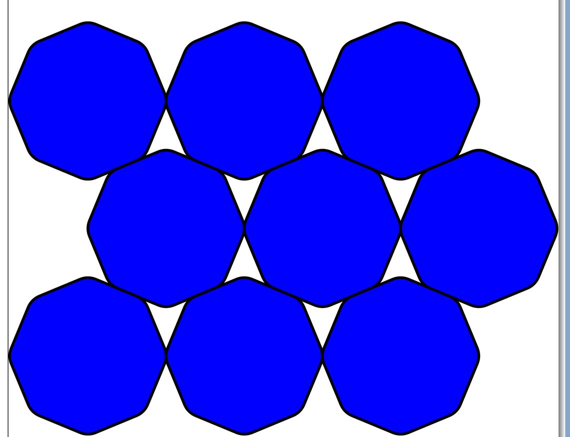
Putative optimal packing densities [1]

"Stanislaw Ulam told me in 1972 that he suspected the sphere was the worst case of dense packing of identical convex solids, but that this would be difficult to prove" [2].

Analogous conjecture fails in 2D

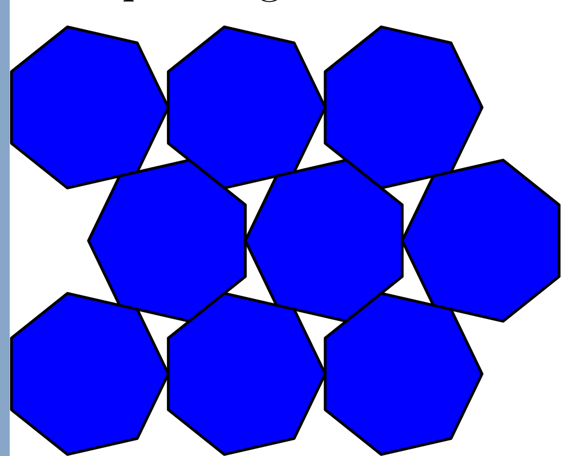


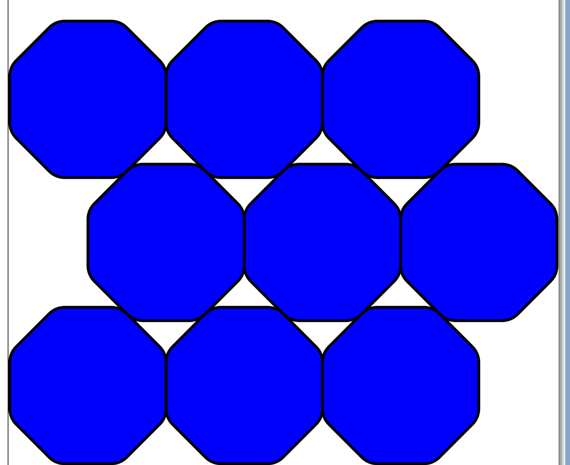
Optimal packing fraction: 0.9069



Optimal packing fraction: 0.9024

Conjectured optimal packing: 0.8926

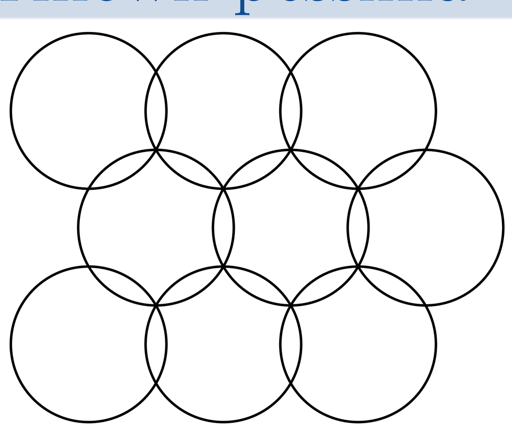




Reinhardt's Conjecture (1934)

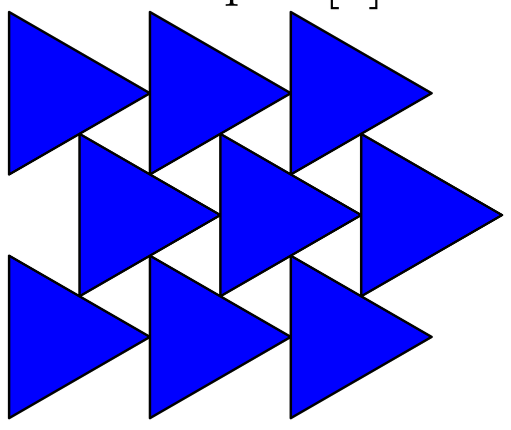
The rounded octagon is the pessimal shape for packing among 2D centrally symmetric convex shapes [3]. (Shown to be locally pessimal [4].)

Known pessima



Circular disks are known to be worst for covering among 2D centrally symmetric convex shapes [5].

Triangles are known to be worst for packing using only translations among 2D convex shapes [6].



Random packing

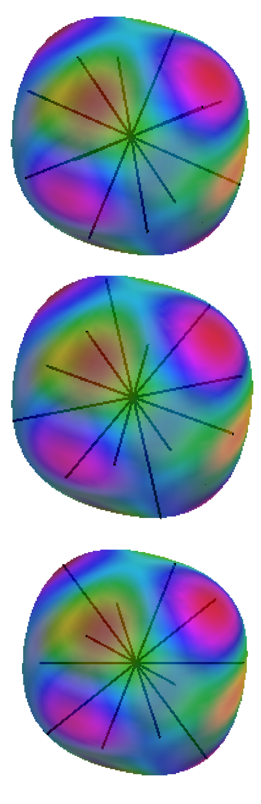
- Most nonspherical particles are observed to jam at higher density than spheres.
- Long rods have lower jamming density than spheres, so spheres are not globally pessimal, but are conjectured to be locally pessimal [7].

Optimal packing & covering

Particle deformation in isostatic packing

- In an isostatic packing, normal contact forces $\mathbf{f}_{ij}$ are uniquely defined up to overall scale (p =pressure).
- When particle shape is deformed, $p\Delta V$ is given to 1st order by the sum over contacts of $\mathbf{f}_{ij} \cdot (\Delta\mathbf{x}_i - \Delta\mathbf{x}_j)$.
- Mean coordination for isostatic nonlattice packing $= 2d$; for lattice packing $= d(d+1)$.

The main lemma



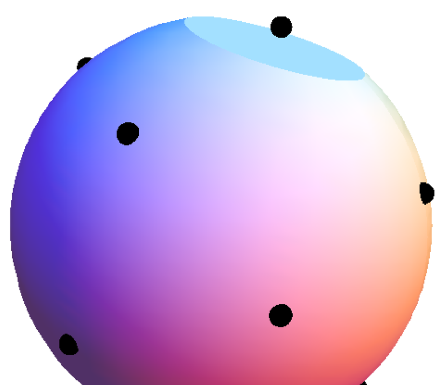
- Consider $\mathbf{u}_1, \ldots, \mathbf{u}_n$, points on the sphere S^2, such that $\sum_{i,j=1}^n P_l(\langle \mathbf{u}_i, \mathbf{u}_j \rangle) = 0$ for $l = 2$, but not for any other even l
- Example: contact points in f.c.c.
- Let f be an even function $S^2 \to \mathbb{R}$, $R \in SO(3)$ a rotation matrix. $\sum_{i=1}^n f(R\mathbf{u}_i)$ is indep. of R if and only if the expansion of $f(\mathbf{u})$ in spherical harmonics terminates at $l = 2$.

Dimension $d = 3$: ball locally pessimal

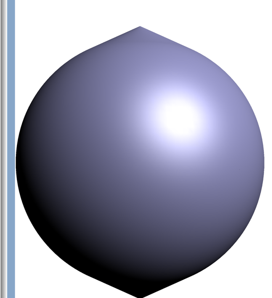
- The 3-ball is a local pessimum for lattice packing among centrally symmetric convex shapes [8].
- Given Kepler's conjecture, the 3-ball is also a local pessimum for general packing among centrally symmetric convex shapes.
- Also, the 3-ball is a local pessimum for lattice covering among centrally symmetric convex shapes [9].

$d \geq 4$: ball not pessimal, even locally

For packing in $d = 6, 7, 8$, and 24, the optimal lattice is hyperstatic and cannot be condensed even if the nonoverlap constraint is relaxed along one contact direction. So, a slightly truncated ball is worse than the ball for lattice packing [8].



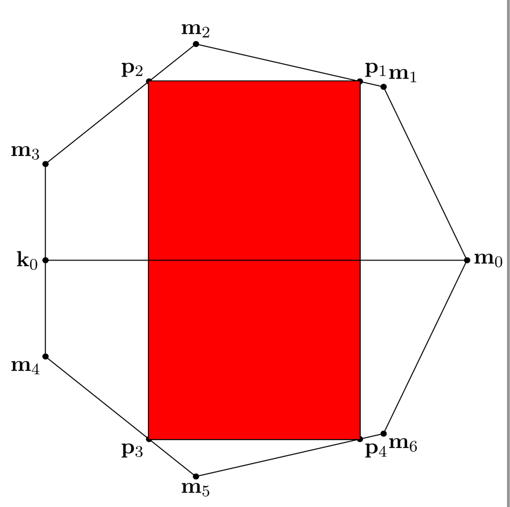
Situation in $d = 4$ and 5 is more delicate, but the ball is still not locally pessimal [8].



For covering in $d = 4$ and 5, the optimal lattice cannot be expanded even if the covering constraint is relaxed around one hole direction. So, a slightly pointed ball is worse than the ball for lattice covering [9].

The regular heptagon

- The regular heptagon is a local pessimum with respect to "double lattice" (DL) packings [10].
- The DL packing is locally optimal among packings of regular heptagons [11].
- If the optimal packing of the regular heptagon is the DL packing, then the heptagon is a local pessimum for general packing.



Random Packing

Jamming of nearly spherical particles

- We assume that subject to same compression protocol, nearly spherical particles will achieve configurations near those achieved by spheres.
- So, we assume we are given a random packing of spheres and seek volume-minimizing nearby configuration after deformation [12].

$$p\Delta V = \sum_i \min_{R_i} \sum_{j \in \partial i} f_{ij} \Delta r(R_i \mathbf{n}_{ij}) + O(\Delta r^{3/2}),$$

$$\Delta r(\mathbf{u}) = \text{ deformation in direction } \mathbf{u}.$$

Spheres are locally pessimal in any d

Under our assumptions, the jamming density of nearly-spherical particles satisfies

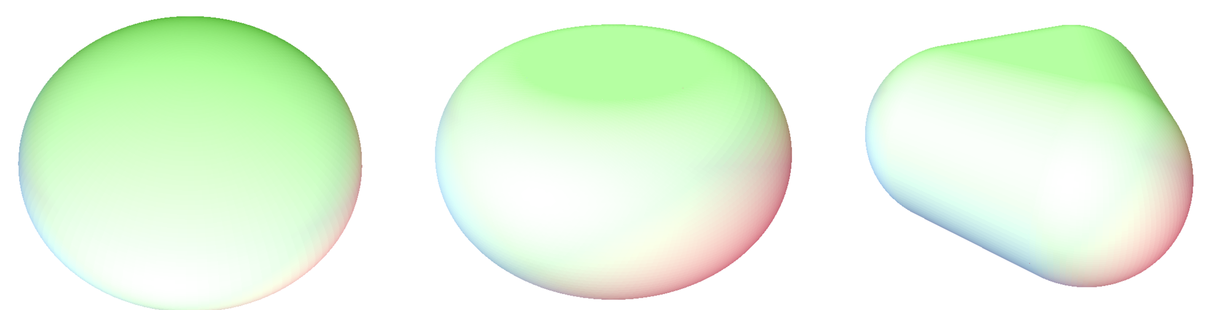
$$\phi - \phi_{\text{spheres}} > c\overline{|\Delta r(\mathbf{u}) - \overline{\Delta r(\mathbf{u})}|} + O(\overline{|\Delta r(\mathbf{u})|}^{3/2}).$$

for any fixed protocol [12].

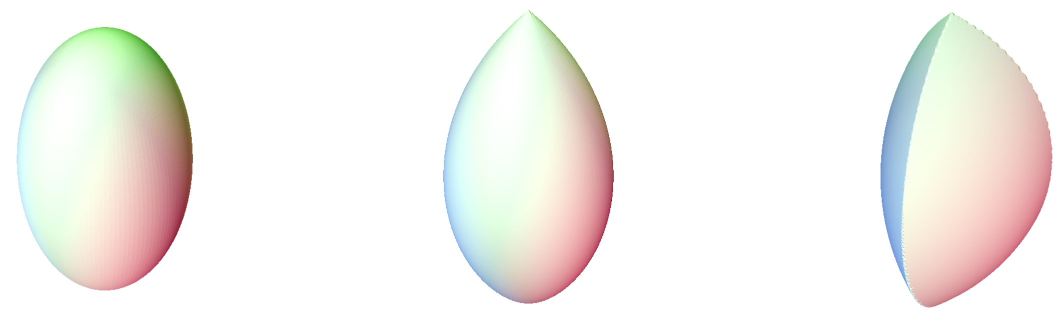
One-parameter shape families

Taking a sample jammed configuration of spheres under a specific protocol, and a specific family of shapes parameterized by $\rho = \overline{|\Delta r(\mathbf{u}) - \overline{\Delta r(\mathbf{u})}|}$, we can calculate $\eta = \frac{1}{3} d\phi/d\rho|_{\rho=0^+}$:

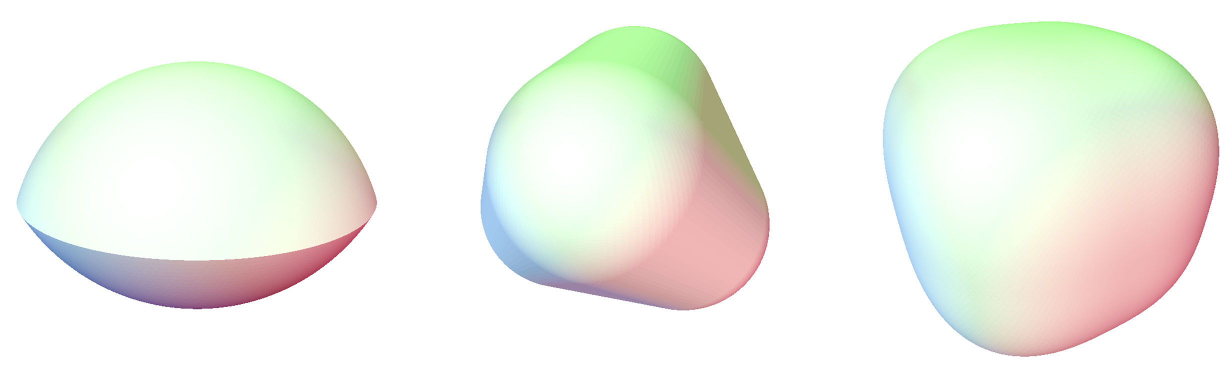
$\eta = 0.94$ $\eta = 1.36$ $\eta = 1.31$



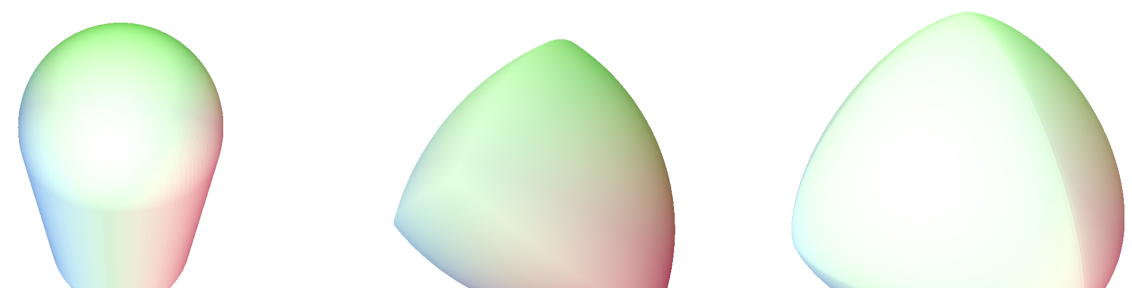
$\eta = 0.79$ $\eta = 0.77$ $\eta = 1.01$



$\eta = 0.86$ $\eta = 1.45$ $\eta = 1.32$



$\eta = 1.08$ $\eta = 1.06$ $\eta = 1.20$



References

[1] P. F. Damasceno, M. Engel, and S. C. Glotzer (2012).
[2] M. Gardner, *New Mathematical Diversions (Revised Edition)* (Math. Assoc. Amer., Washington, 1995).
[3] K. Reinhardt, Abh. Math. Sem., Hamburg, Hansischer Universität, Hamburg **10**, 216 (1934).
[4] F. L. Nazarov, J. Soviet Math. **43**, 2687 (1988).
[5] L. F. Tóth, *Lagerungen in der Ebene, auf der Kugel und im Raum* (Springer, Berlin, 1972).
[6] I. Fáry, Bull. Soc. Math. France **78**, 152 (1950).
[7] Y. Jiao and S. Torquato, Phys. Rev. E **84**, 041309 (2011).
[8] Y. Kallus, Adv. Math. **264**, 355 (2014).
[9] Y. Kallus, Disc. Compu. Geom. **54**, 232 (2015).
[10] Y. Kallus, Geom. Topol. **19**, 343 (2015).
[11] Y. Kallus and W. Kusner, Disc. Compu. Geom. (2016), to appear.
[12] Y. Kallus, Soft Matter **12**, 4123 (2016).