

Packings of circles and spheres

Lectures III and IV

Session on Granular Matter

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What model is good for
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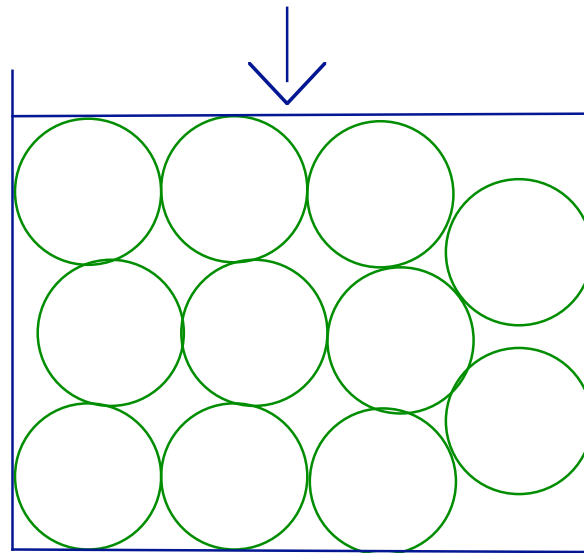
- There must be a container of some sort for the packing elements.
- Is the packing jammed?

What model is good for packings?

- There must be a container of some sort for the packing elements.
- Is the packing jammed?
- If so, what criteria do you want for jamming?

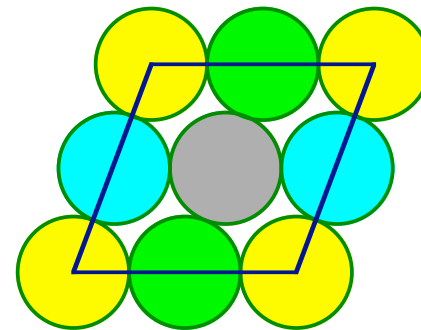
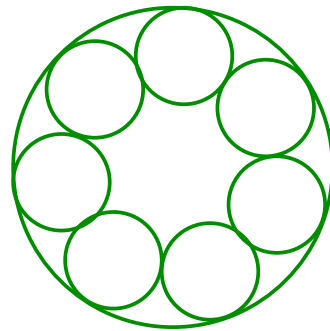
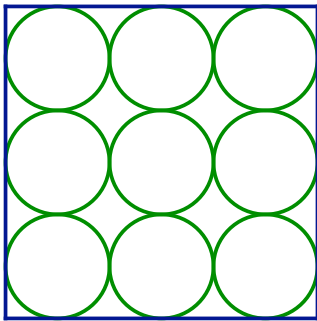
Some containers

Put the packing in a box. Let the box shrink in size or let the packing elements grow in size until you are stuck.



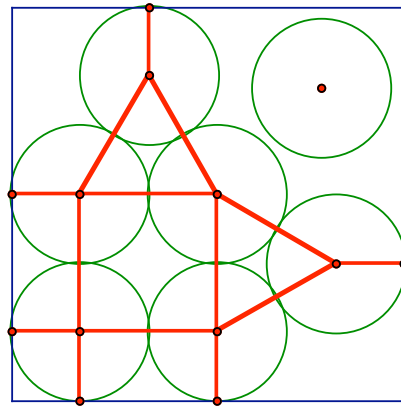
More possible containers

- A rectangular box
- A circle
- A torus



Jammed packings

When the packing is locally most dense, there is a rigid cluster that is jammed, but there could be “rattlers”, non-rigid pieces.



The most dense packing of 7 congruent circles in a square. (Note the "rattler" in the upper right corner.)
(Due to Shaer)

Random close packings

“Is Random Close Packing of Spheres Well Defined?” (Torquato, Truskett and Debenedetti 2000)
Experimentally, if you pour ball bearings into a large container, shake, and calculate the density, you get about 0.636. *But* this depends on the method you use to “densify”. Other methods give 0.642, 0.649, 0.68 ... This paper suggests “order parameters” ...

The following is joint work with A. Donev, F. Stillinger, and S. Torquato. See also my papers in:

<http://www-iri.upc.es/people/ros/StructuralTopology/>

Definitions

If \mathbf{P} is a packing in a container C , call it *locally maximally dense* if every other packing of the same packing elements, sufficiently close to \mathbf{P} in C has a packing density (=packing fraction) no larger than the density of \mathbf{P} in C .

A packing \mathbf{P} is (*collectively*) *jammed* in C if any other packing sufficiently close to \mathbf{P} in C is the same as \mathbf{P} . (I also say \mathbf{P} is *rigid* in C .)

Why jammed?

Theorem: If a packing \mathbf{P} of circles (or spherical balls in 3-space) is locally maximally dense in a polygonal container C , then there is subset \mathbf{P}_0 of \mathbf{P} that is collectively jammed in C .

Theorem (Danzer 1960): A packing \mathbf{P} of circles (or spherical balls in 3-space) is collectively jammed in a polygonal container C , if and only if the underlying strut tensegrity framework is infinitesimally rigid.

Remarks

- If the packing P has no part that is collectively jammed, then the packing can be moved slightly and the container shrunk slightly to improve the overall density.
- Since a necessary condition for being jammed is infinitesimal rigidity, circle packings in polygons can be tested for being jammed with reasonably efficient linear programming (feasibility) algorithms and the nearby improved packing calculated as well.

Proofs

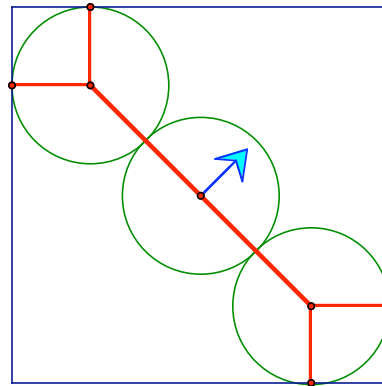
Let the configuration $\mathbf{p} = (p_1, p_2, \dots, p_n)$ be the centers of the packing circles, including the pinned points on the boundary. If the associated strut framework $G(\mathbf{p})$ is infinitesimally rigid, even for a subset of the packing centers, then there is no nearby configuration satisfying the packing constraints for that subset that increases density.

If $G(\mathbf{p})$ is not infinitesimally rigid, let $\mathbf{p} \boxplus (p_1 \boxminus, p_2 \boxminus, \dots, p_n \boxminus)$ be the (non-zero) infinitesimal flex of $G(\mathbf{p})$. Then for each i define $p_i(t) = p_i + t p_i \boxminus, 0 \leq t$.

The crucial calculation

$$|p_i(t) - p_j(t)|^2 = |p_i - p_j|^2 + 2t(p_i - p_j) \cdot (p_i - p_j) + t^2 |p_i - p_j|^2.$$

So $|p_i(t) - p_j(t)| \geq |p_i - p_j|$ for each pair of disks that touch, and there is strict inequality unless $p_i = p_j$.
For example, the following shows this at work.

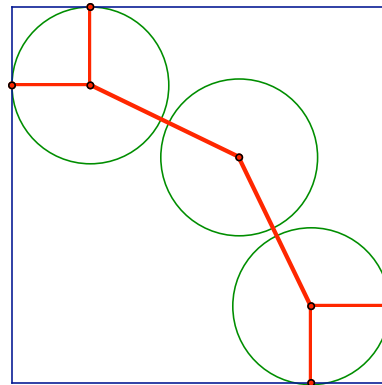


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I call this motion, the *canonical push*. For example, the following shows this at work.



Remarks

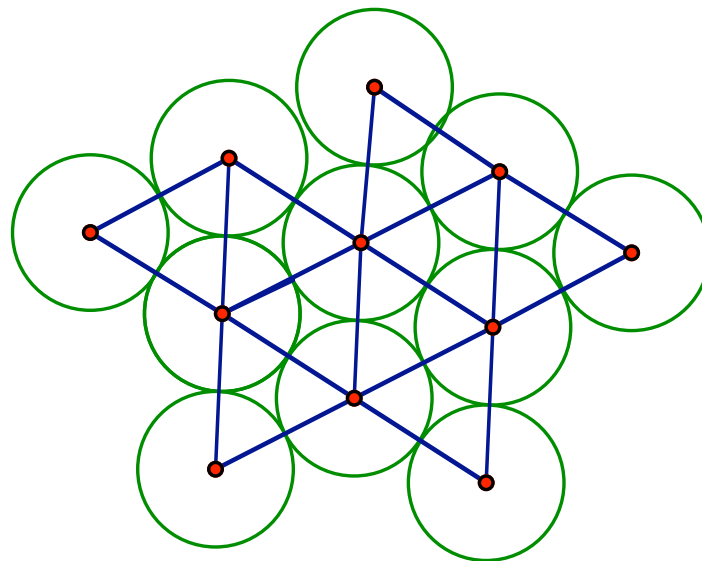
- The motion provided by the linear programming algorithm (LP) can be quite complicated, and it seems best to use it to clear up log jams, rather than ongoing “densification”.
- For example, the Lubachevsky-Stillinger algorithm of slow densification (bump-and-slow down) is more efficient in converging to a jammed state than LP.
- The (LP) motion does not continue forever. Some non-incident packing disks will get closer together and collide, sometimes quite soon.

Statics

When the packing is collectively jammed, it must be statically rigid, which means it must be able to resolve arbitrary loads. But such tensegrity frameworks are never statically determinant, since by the Roth-Whiteley Theorem, there is always a non-zero proper self stress. On the other hand, a physical system must resolve loads in some way... Later more about this. The final resolution of an external load is a function of the relative elasticity in the packing elements. Geometry, alone, cannot “resolve” this.

The fundamental conundrum

Do numerical simulations make sense for large numbers of packing elements? For example, for monodispersed (i.e. congruent) disks in the plane, the following configuration often appears in some simulations, which is impossible.



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Some ideas...

1. Insist that each packing element be fixed by its neighbors. (*Locally jammed.*)
2. Pin all but a finite number. (*Finite stability = collectively jammed*)
3. Enforce periodicity. This amounts to putting the packing on a torus. (*Periodic stability*)

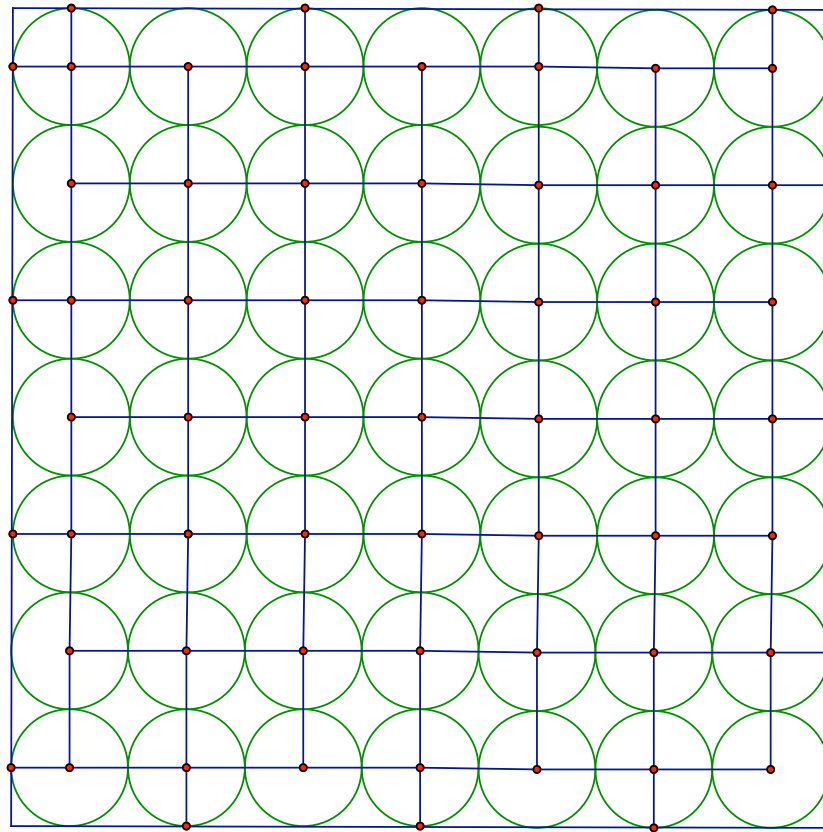
Difficulties

The locally jammed property is very weak. K. Böröczky (1964) showed that there is a packing of congruent disks in the plane with 0 density that is locally jammed. If you move 8 disks at a time, the packing falls apart.

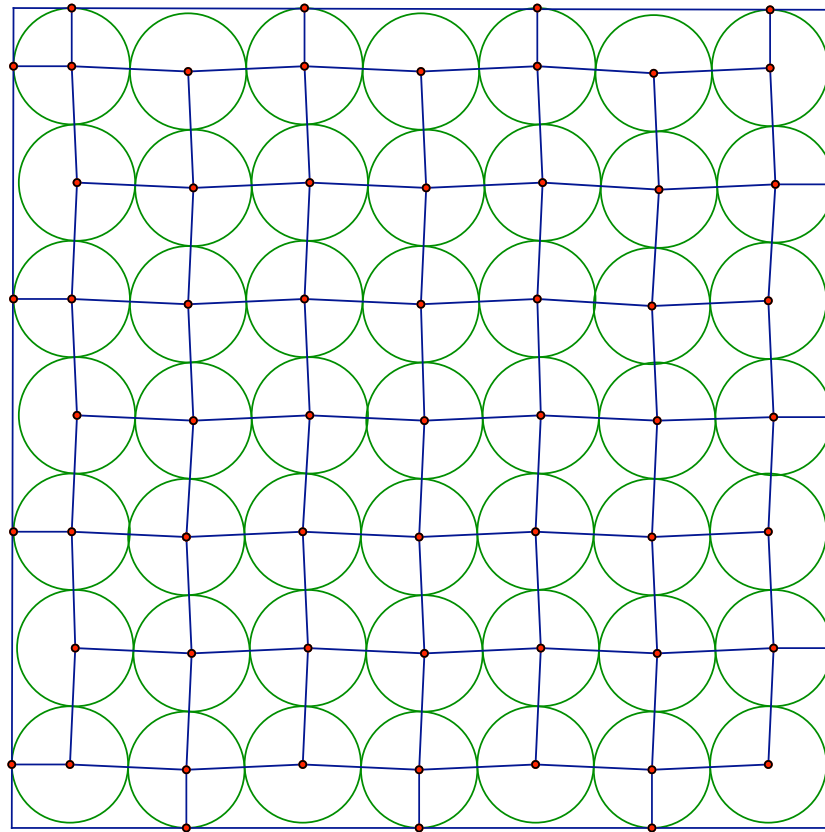
Difficulties

The collectively jammed property is better, but as the number of packing elements that are allowed to move gets large, the packing can be very fragile. For example, the following square lattice packing in a square seems to be not collectively jammed ... (A. Bezdek, K. Bezdek, R. Connelly 1998)

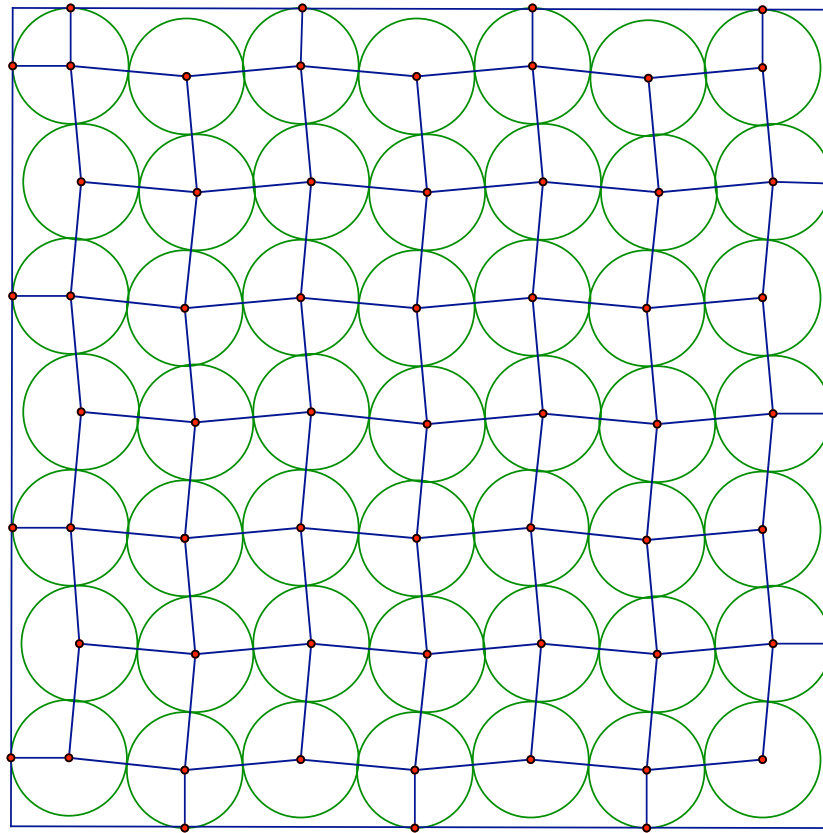
A near unjamming



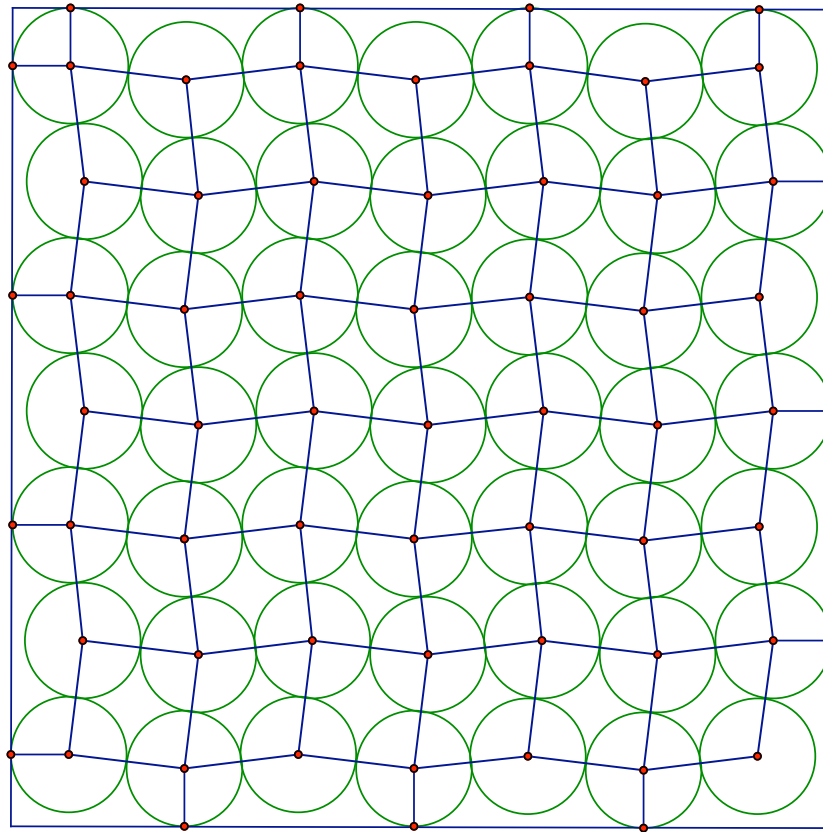
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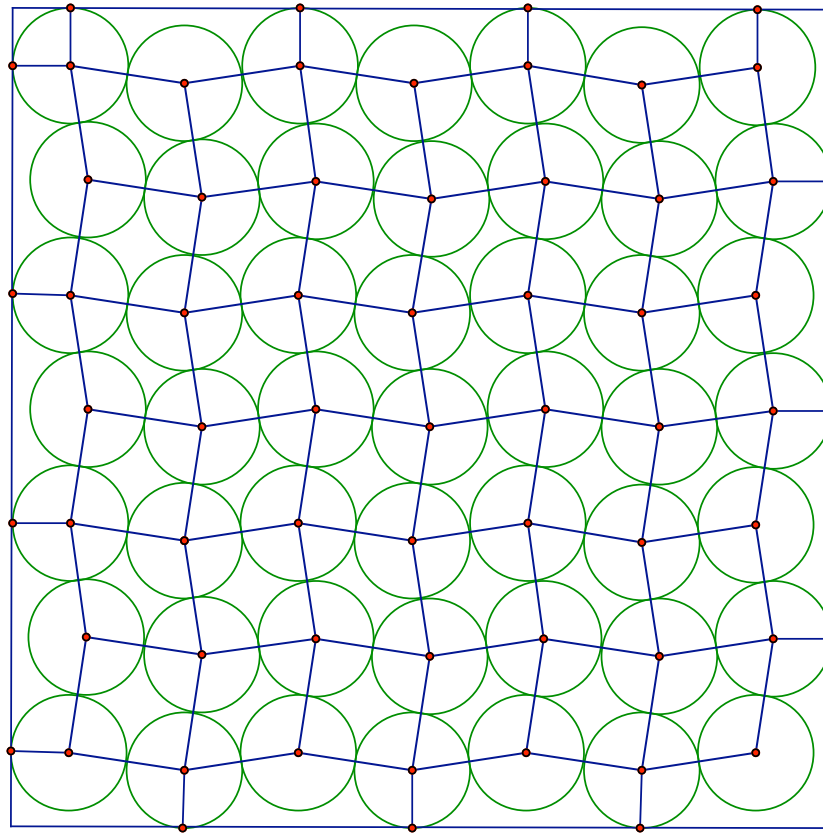
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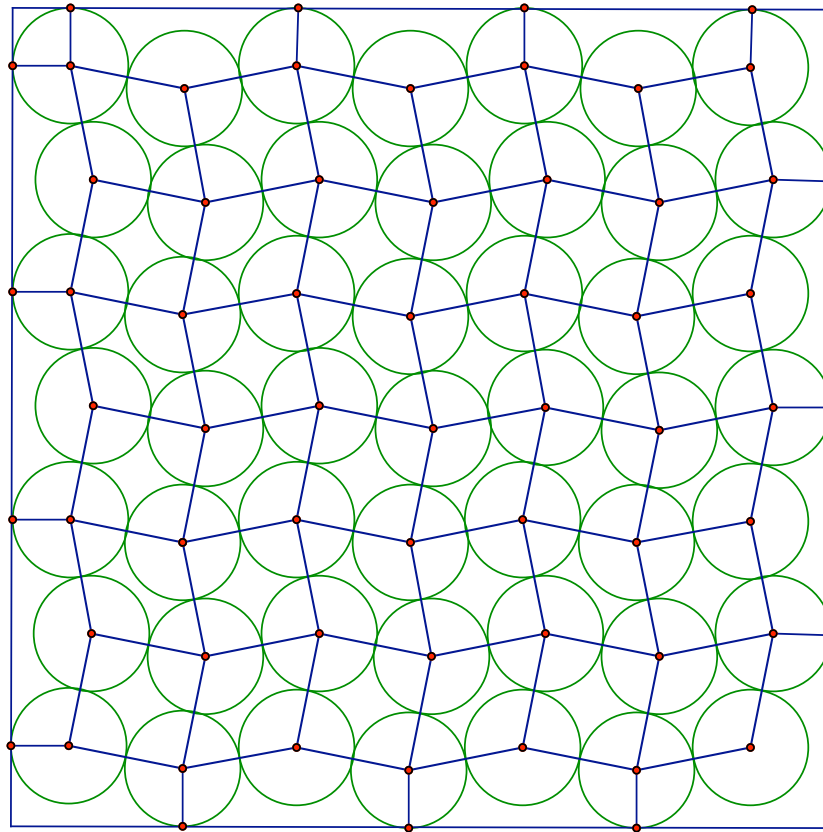
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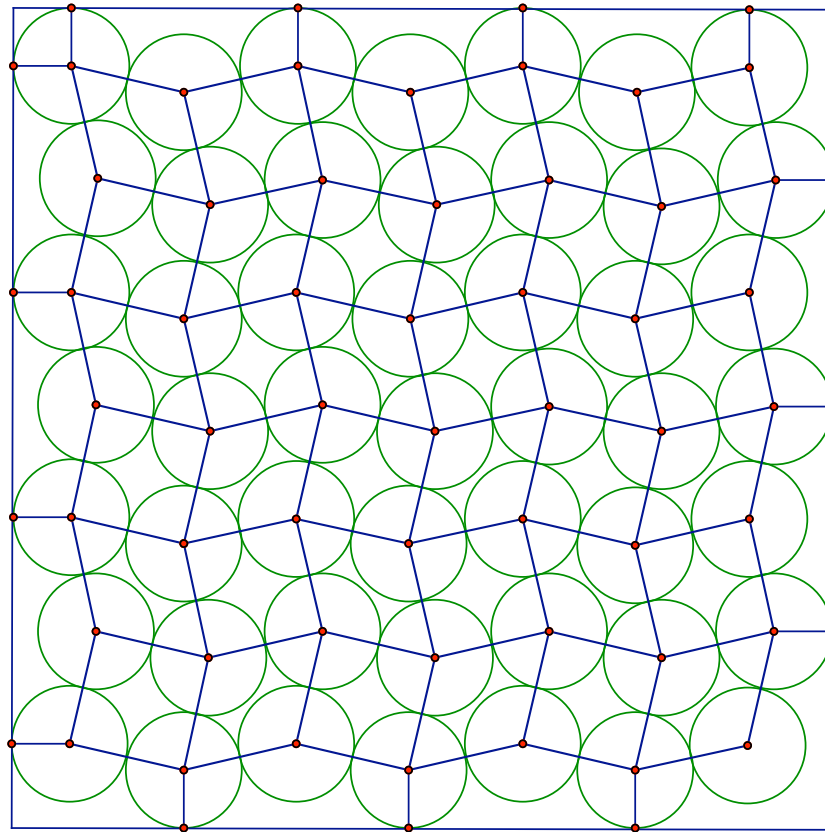
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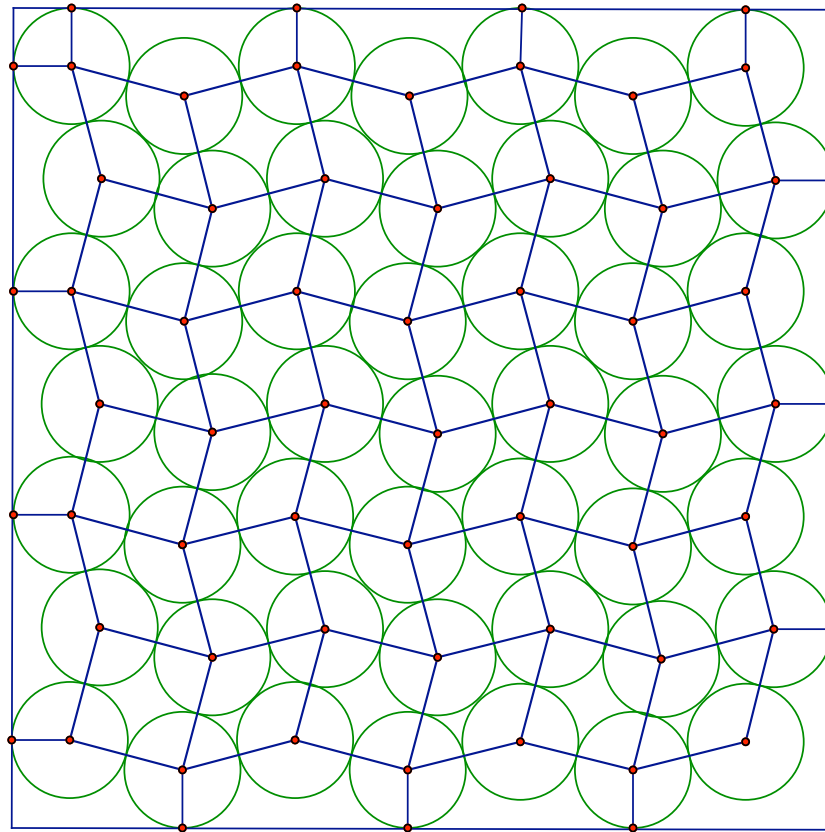
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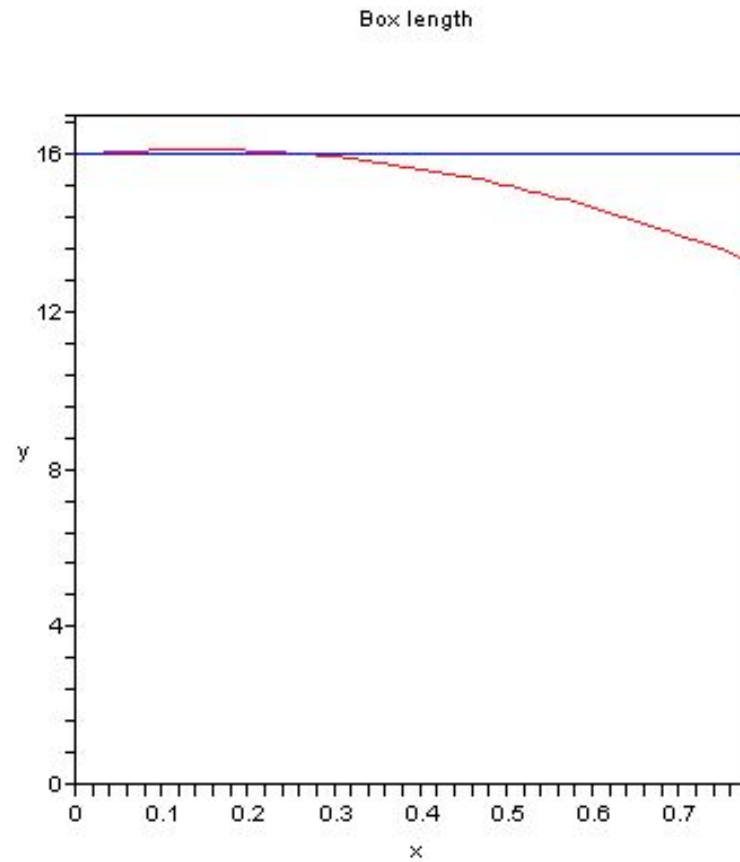
A near unjamming



A near unjamming



The size of the square



Discrete rigidity

Theorem: Suppose that $G(\mathbf{p})$ is a finite (tensegrity) framework, with pinned vertices, that is rigid in \mathbf{E}^d . Then there is an $\epsilon > 0$ such that when $|p_i - q_i| < \epsilon$ for all i , and the same member constraints hold for $G(\mathbf{q})$, then $\mathbf{p} = \mathbf{q}$.

Even when the member constraints are relaxed by $\epsilon > 0$, say, then the configuration can jiggle about, but not too far.

The ϵ for the square lattice packing in a square seems quite small.

Calculations for the square lattice packing in a square

Let s be the length of the side of the bounding square during the deformation shown. Then when the first pair of circles are rotated by θ , then s is calculated as

$$s = 4n \cos \theta + 2 \sin \theta + 2,$$

where the radius of the circles are 1, and there are $n+1$ circles on a side, hence $(n+1)^2$ circles in all.

So the square expands less than $1/(2n)$, and $s < 4n + 2$, the side length of the square, for $\theta > 2/n$.

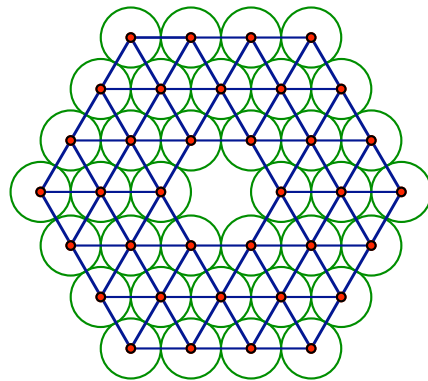
The point

The ϵ needed to insure rigidity converges to 0 as $n \rightarrow \infty$ for the square lattice packing. In other words, you have to decrease the tolerances to 0 as you release more and more of the packing elements and allow them to move.

A suggestion to address this problem ...

Uniform stability

An infinite packing of circles in the plane is *uniformly stable* if there is an $\epsilon > 0$ such that the only finite rearrangement of the disks as a packing, where each center is displaced less than ϵ , is the identity. (This is related to a different, but similar, definition of L. Fejes Toth.)



Examples

1. The square lattice packing (or the cubic lattice packing in higher dimensions) is NOT uniformly stable.
2. The triangular lattice packing in the plane IS uniformly stable, even with the removal of one packing element. (I. Bárány and N.P. Dolbilin (1988) as well as A. Bezdek, K. Bezdek, R.C. (1998))
3. Most of the candidates for the most dense packings of congruent spheres in higher dimensions are uniformly stable. (A. Bezdek, K. Bezdek, R. Connelly 1998)

Another suggestion for this problem:

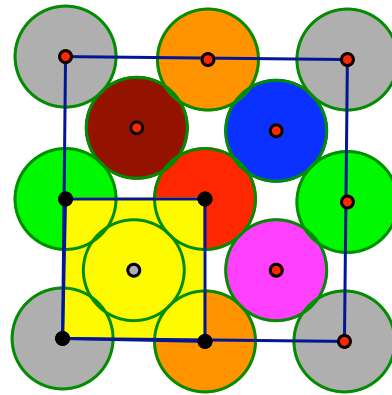
How do you handle infinite packings?

- Only allow a finite number of packings to move. . . . or
- Consider periodic packings with a fixed lattice defining the periodicity . . . or
- Consider periodic packings with a variable lattice as well as a variable configuration, but such that the density is locally maximal.

Periodic Packings

A packing is *periodic with lattice* Λ if for every packing element X , $\Lambda + X$ is a packing element for every λ in Λ . Regard this as a packing of a finite number of packing elements in the torus \mathbb{R}^2/Λ . So such a packing can be regarded as stable if there is no perturbation of the configuration except trivial perturbations.

The problem with fixing the lattice defining the torus



The packing (with only 2 disks) defined on a torus, whose fundamental region is the small yellow square, is jammed.

The packing (with 8 disks) defined on a torus, whose fundamental region is the larger square, is NOT jammed.

Counting in Coverings

Let k be the order of the covering, so there are exactly kn disks in the covering and k_e contacts. If there are the minimal number of contacts $e = 2n-1$ in the original rigid configuration, there will be

$$k_e = k(2n-1) = 2kn-k < 2kn-1$$

contacts in the cover, and so the cover will NOT be rigid.

Strictly Jammed

So we define a packing on a (flat) torus to be *strictly jammed* if there is no non-trivial infinitesimal motion of the packing, as well as the lattice defining the torus, subject to the condition that the total area of the torus does not increase during the infinitesimal motion.

Counting for Strictly Jammed Packings

- **Variables:**
 - Coordinates: $2n$ - Lattice vectors: $2 + 2 = 4$
- **Constraints:**
 - Packing contacts: e - Area constraint: 1
- **Trivial motions:**
 - Translations: 2 - Rotations: 1

The final count is then

$$e + 1 \geq 2n + 4 - 3 + 1 \text{ or } e \geq 2n + 1.$$

So the packing covers have a *chance* to be strictly jammed, although it is not guaranteed. The number of constraints in a cover is *more* than is needed for stability.

The Crystallization Conjecture

If a periodic packing is strictly jammed, what does it look like?

Conjecture: The only strictly jammed periodic packing in the plane is the triangular lattice packing, possibly with some disks missing.

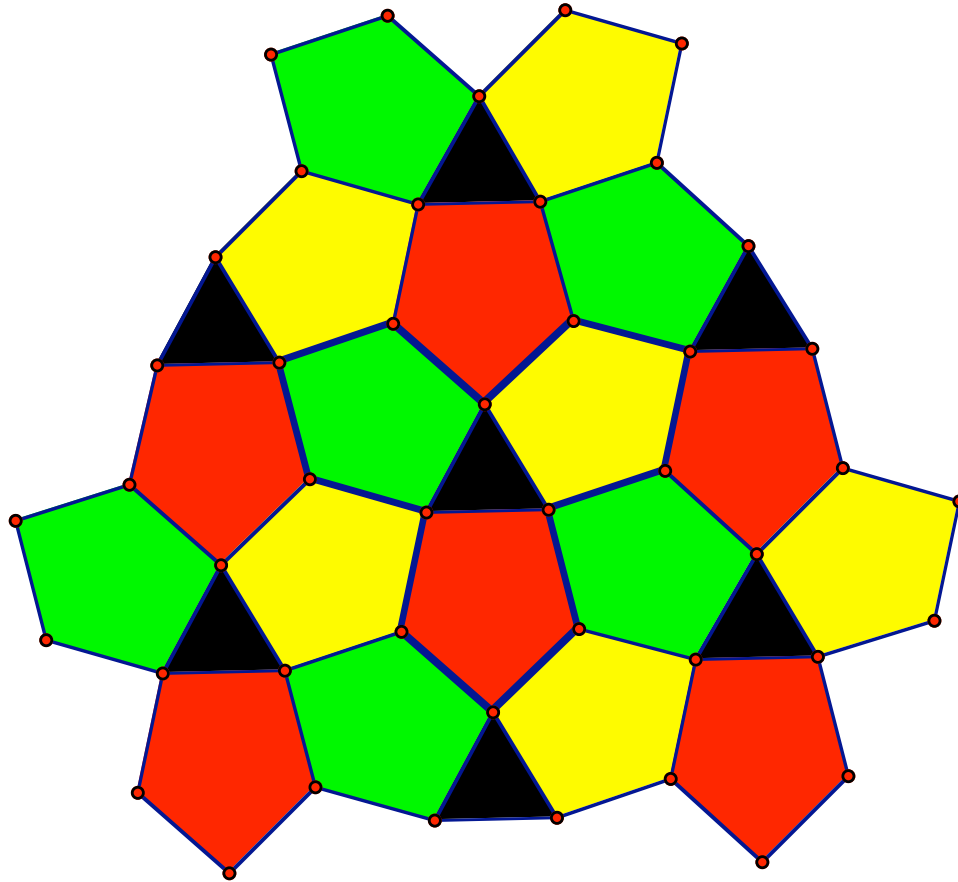
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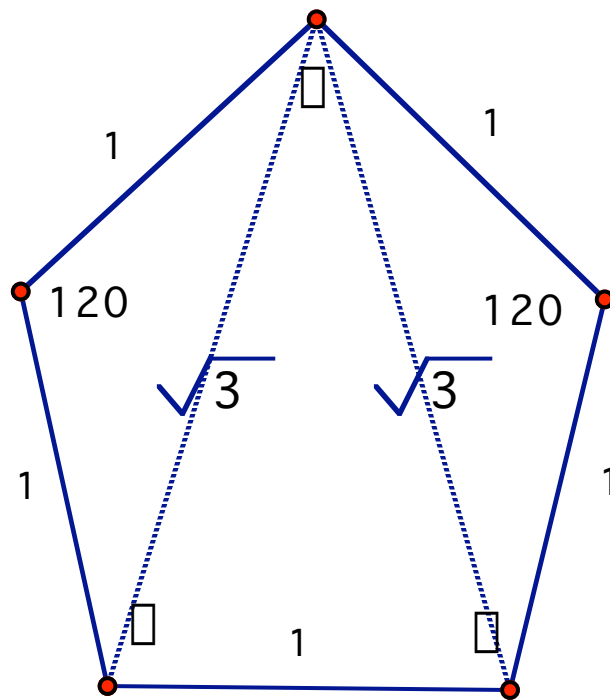
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Sadly this is false.

Start with this tiling

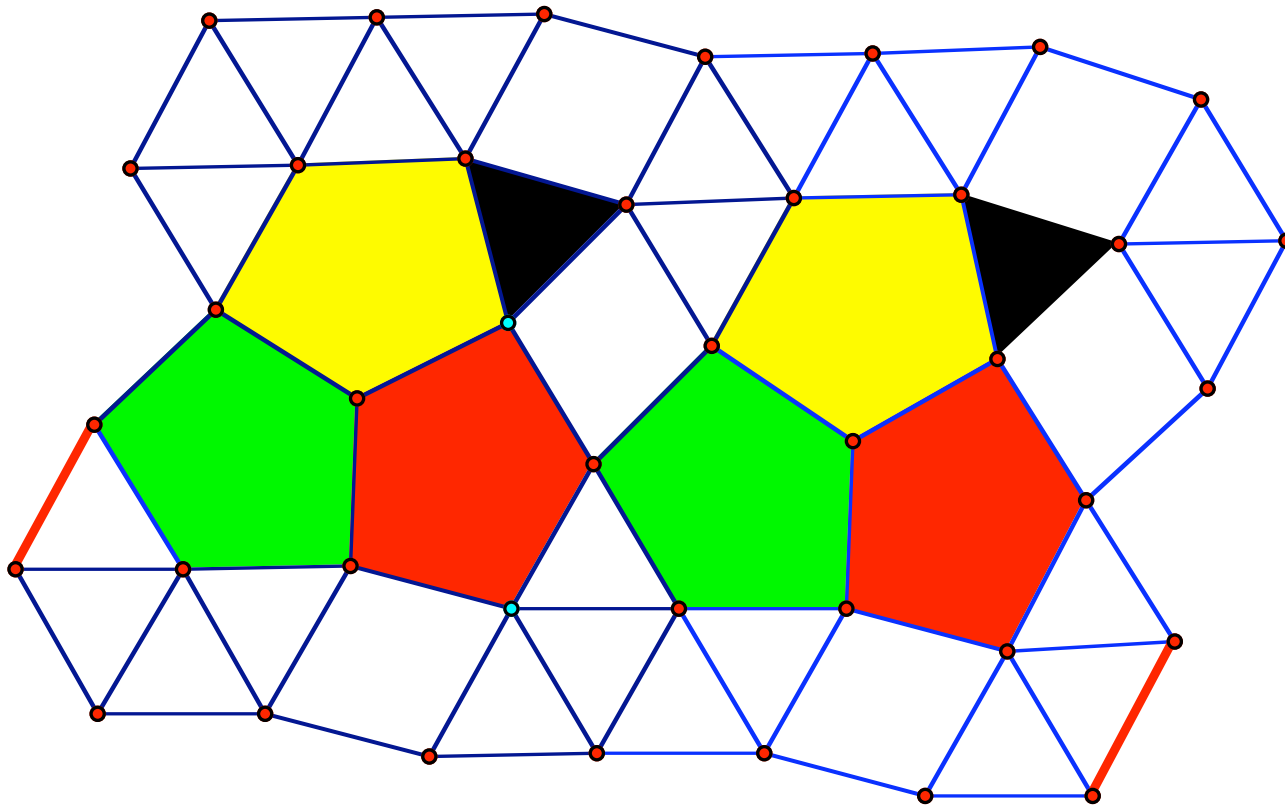


The construction of the pentagon in the tiling

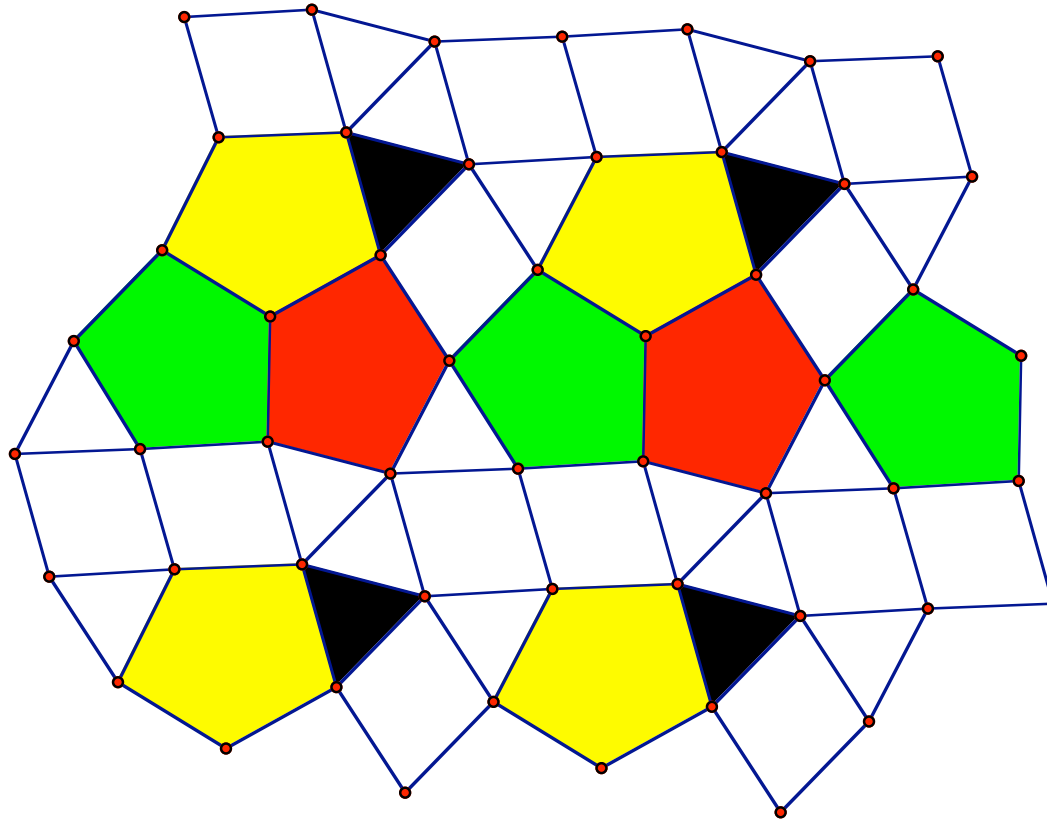


$$2\pi + \pi + 60 = 360$$

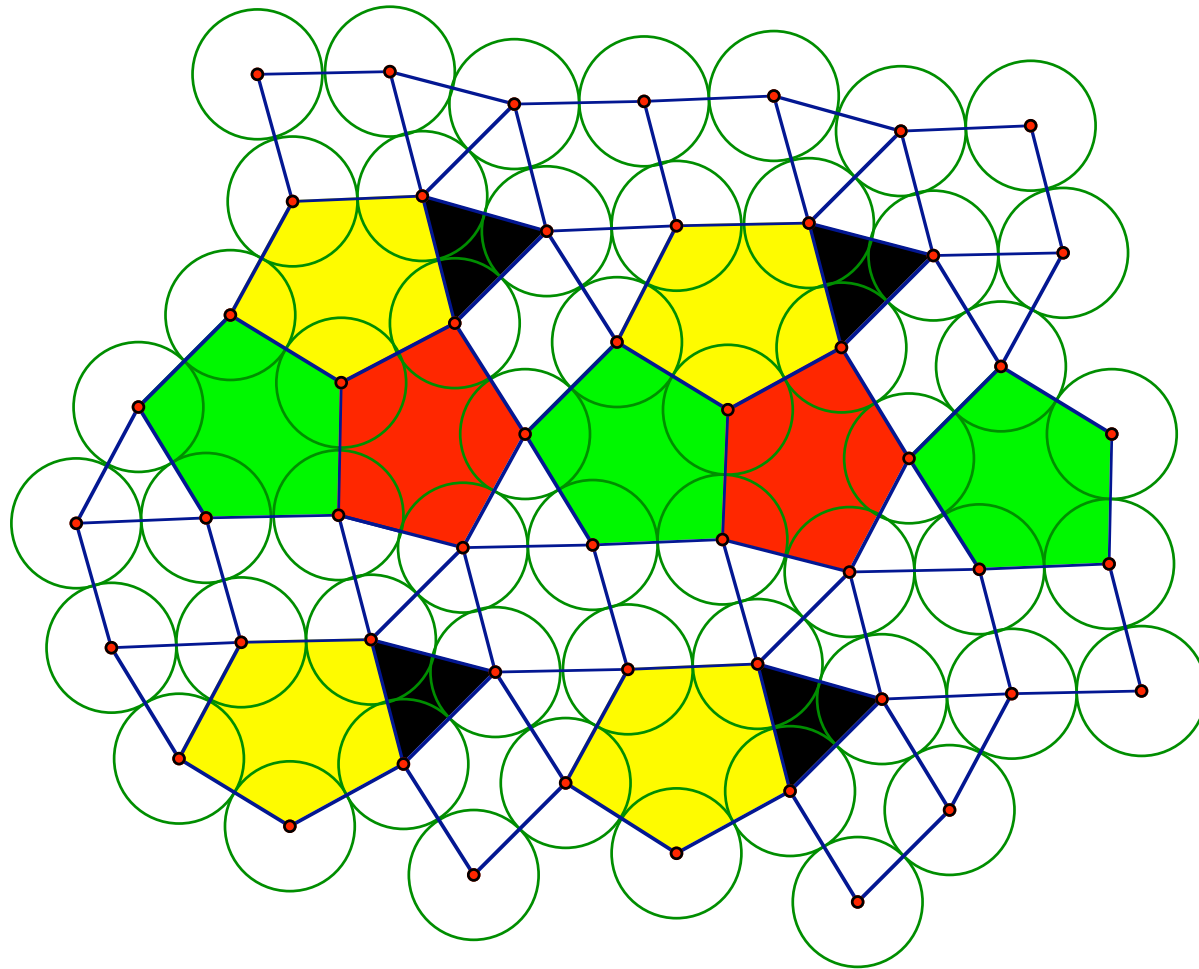
Split it apart and add some
“bracing triangles” as well as
some connecting rhombuses.



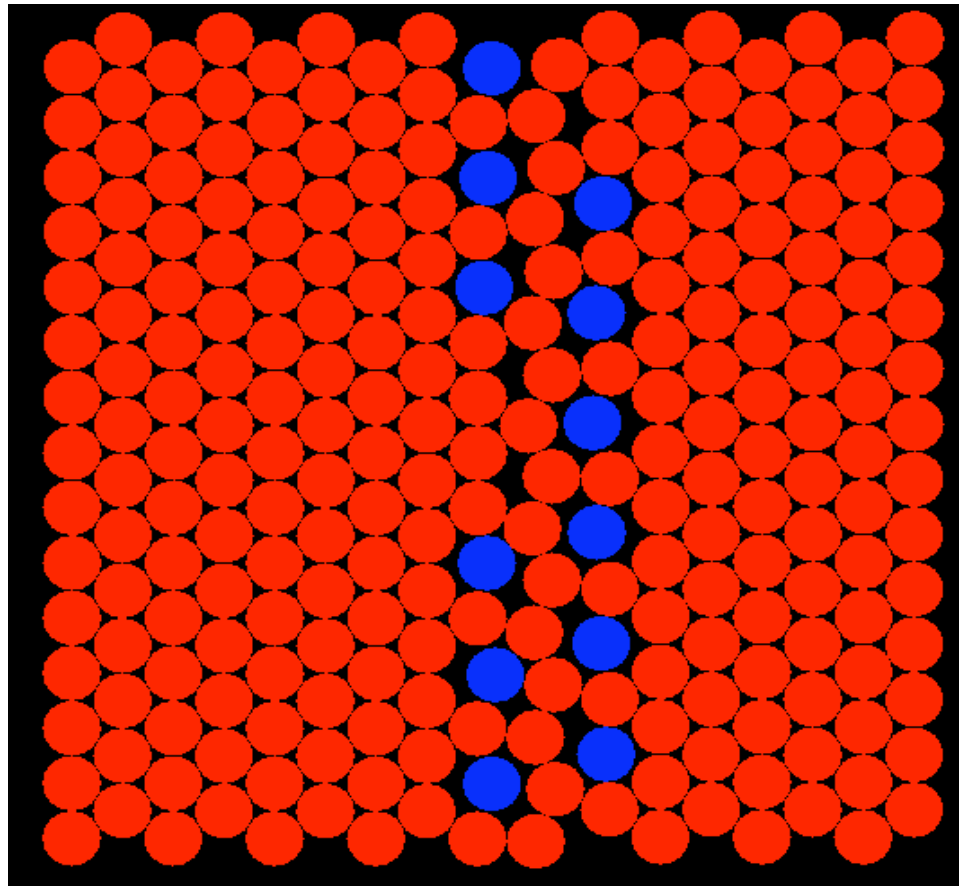
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This what the packing looks like.

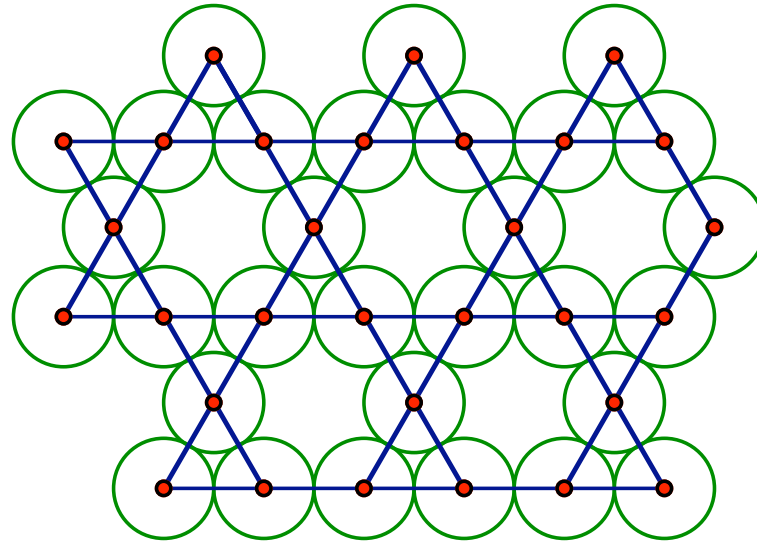


Another possible example of a
strictly jammed packing



Low density strictly jammed packings

Conjecture: The density of a strictly jammed periodic packing is greater than $(3/4)\pi/\sqrt{12}$, the density of the Kagome packing.



“In fact, in a flat two-dimensional space it is believed that only the triangular lattice configuration ... is stable in the alter case.” (Einar L. Hinrichsen, Jens Feder, and Torstein Jossnag, Random packing of disks in two-dimensions, Phys. Rev. A, Vol 41, No. 8, 15 April 1990, p.4200.)

