Density of Sphere Packings

The Problem

A **packing** is a set of interior-disjoint spheres in $\mathbb{R}^n$.
Its **density** is

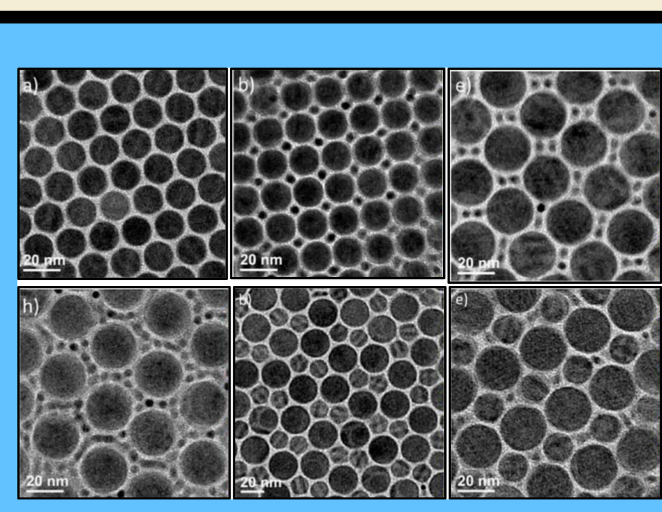
$$\limsup_{k\to\infty} \frac{\text{volume of } [-k,k]^n \text{ inside the spheres}}{\text{volume of } [-k,k]^n}.$$

What is the maximal density?
What are the densest packings?

Motivations

Error correction codes. Information is divided into packets encoded by well-chosen points in $\mathbb{Z}^n$. Each point of $\mathbb{Z}^n$ will then be considered as an alteration (transmission errors) of the coding point it is closest to. Maximizing the number of correctable packets at a given packet size therefore comes down to maximizing the density of a packing of equal spheres in R^n.

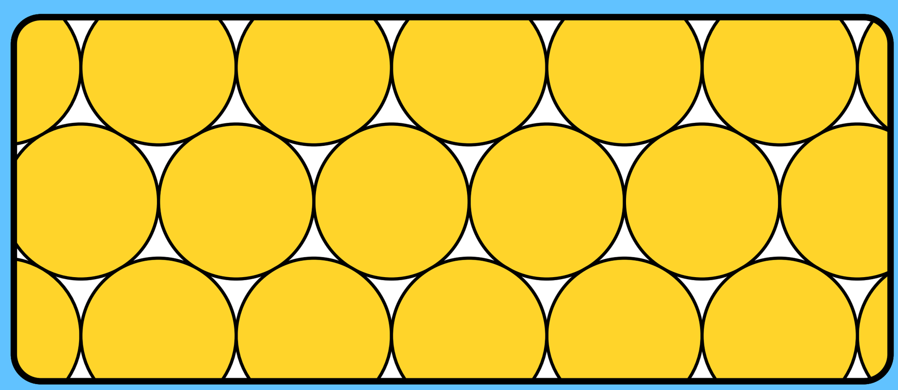
Material sciences. Elementary particles (atoms, nanoparticles...) assemble under the effect of attractive forces. Experimentally, the densest assemblies often seem to be favored. Can we predict how spherical particles of a given size will assemble? Can we design sizes so as to obtain new materials?



Experimental assembly of (cylindrical) nanoparticles.

One Disk

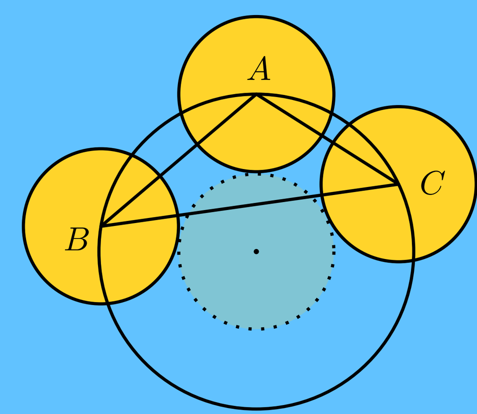
Theorem (Fejes Tóth, 1943)
The maximal density of a packing of equal disks in $\mathbb{R}^2$ is $\frac{\pi}{2\sqrt{3}} \approx 0.91$.



The hexagonal packing reaches the maximal density.

Proof:

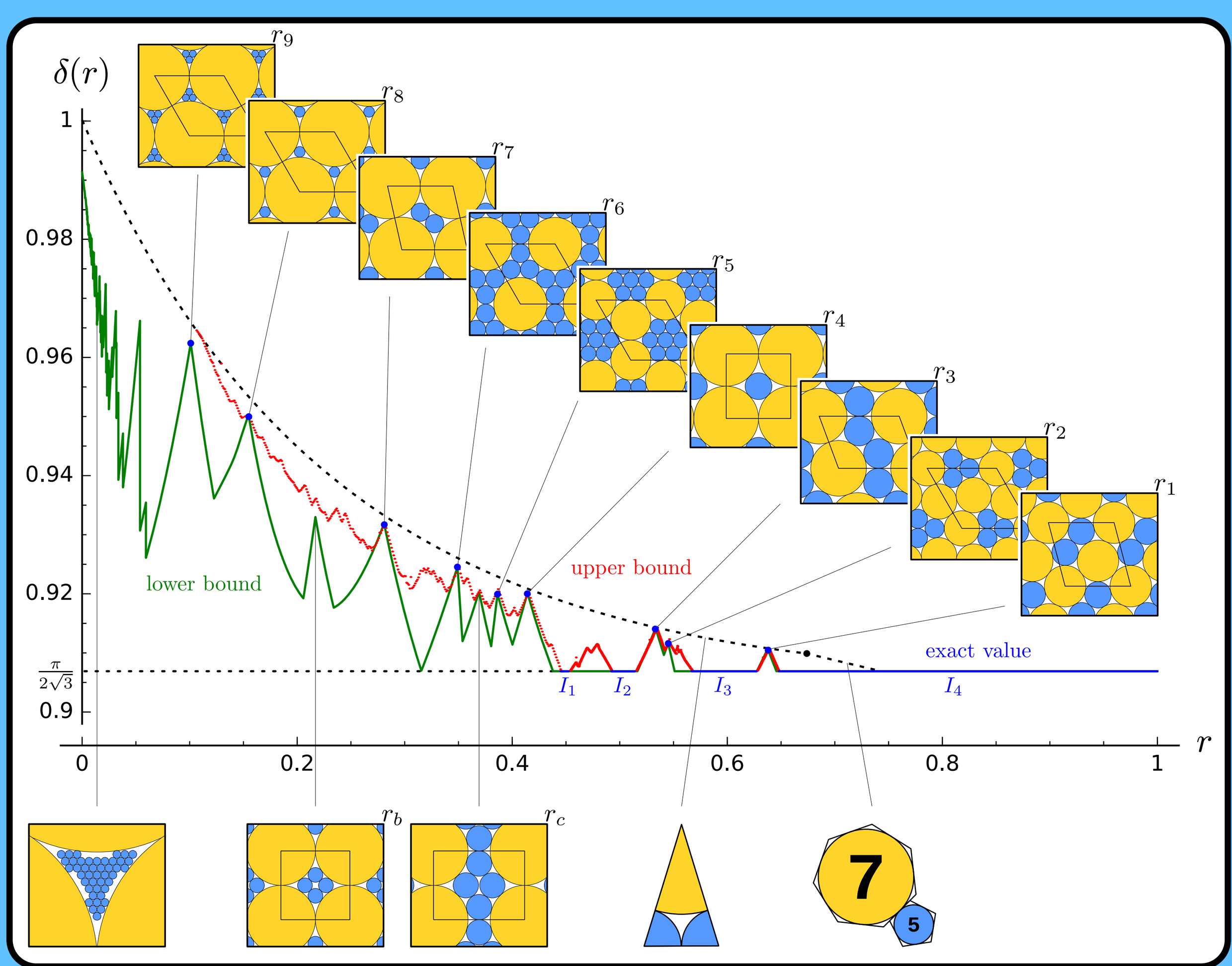
1. consider a packing of unit disks;
2. assume it is **saturated**, that is, no disk can be added;
3. consider the **Delaunay triangulation** of the centers of the disks;
4. prove that the largest angle of any triangle is between $\frac{\pi}{3}$ and $\frac{2\pi}{3}$;
5. deduce that the area of any triangle is at least $\sqrt{3}$;
6. since each triangle contains half a disk, this yields density at most $\frac{\pi}{2\sqrt{3}}$.



Proof of step 4:

- consider a triangle ABC and assume $\widehat{A}$ is its largest angle;
- $\widehat{A} \geq \frac{\pi}{3}$ otherwise the sum of the three angles would not reach π;
- if $\widehat{A} > \frac{2\pi}{3}$, then the smallest angle, say $\widehat{B}$, is at most $\frac{\pi}{6}$;
- the diameter of the circumscribed circle is $\frac{AC}{\sin \widehat{B}} \geq 2$ (law of sines);
- there is no disk center in the interior of this circumscribed circle (Delaunay);
- a disk centered as this circumscribed circle can be added to the packing;
- this contradicts saturation $\rightsquigarrow \widehat{A} \leq \frac{2\pi}{3}$.

One More Size



What if there are two sizes of disks? Can we find denser packings? For which size ratios?

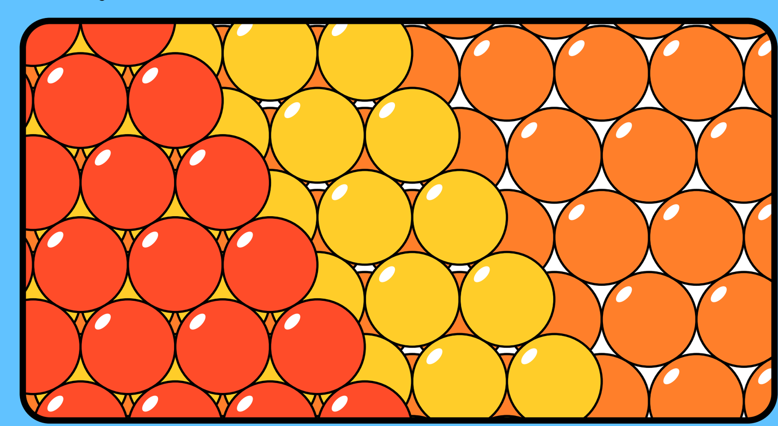
What can be said about the maximal density $\delta(r)$ of packings of disks of size 1 and $r < 1$?

- it is bounded from below by $\frac{\pi}{2\sqrt{3}}$;
- this lower bound is reached (I_1 to I_4);
- every "good packing" yields a lower bound, which can be extended by continuous deformations (green line);
- it is (Lipshitz) continuous but not decreasing (and the limit in 0 is not 1);
- upper bounds have been proven "by hand" in the 1960's (dotted black line)
- as well as by a computer assisted proof in the last 20 years (red line);
- its exact value is known for some very specific values of r (r_1 to r_9)...

One More Dimension

In 1610, Kepler conjectured that, with a density of $\frac{\pi}{3\sqrt{2}} \approx 0.74$, hexagonal layers maximize the density among packings of equal spheres.

Theorem (Hales-Ferguson, 1998)
The Kepler conjecture is true.

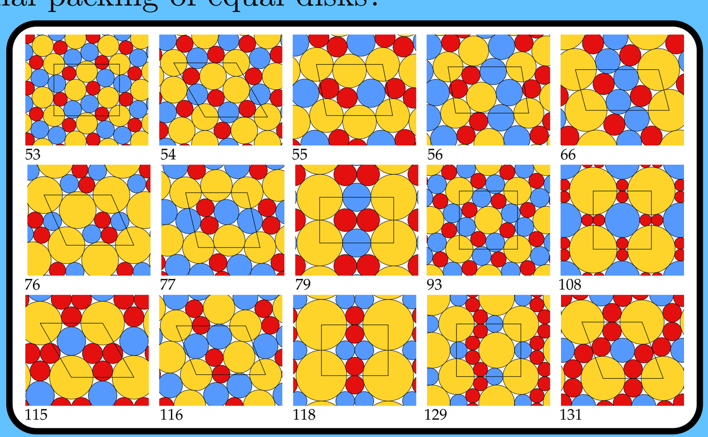


A long history:

- true among **lattice packings** (Gauss, 1831)
- 18th Hilbert problem (1900)
- sketch proof by Hales (1992)
- 6 preprints (300 pages+137000 lines of code) by Hales (1998)
- 13 reviewers, 4 years, "99% certain" (1999-2003)
- Formal proof (flyspeck project) (2003-2014)

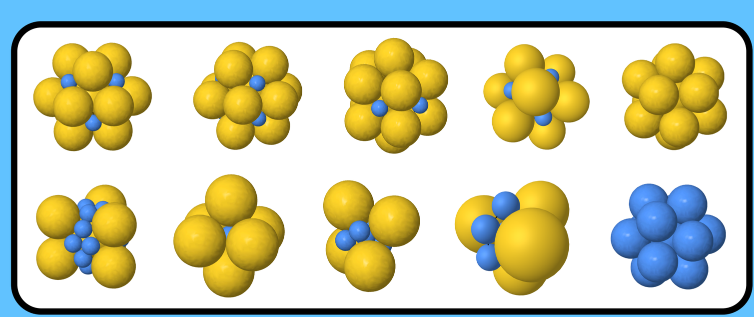
More Sizes and more Dimensions

What are the densest packings of k **different disks**? What if we allow every sizes in $[u,1]$? What is the largest u which allows density higher than the hexagonal packing of equal disks?



Some ternary packings proven to maximize the density.

What about packings with **two sizes of spheres**? In particular, in the optimal packing of unit spheres, spheres of radius $\sqrt{2}-1$ can be inserted in the holes between two layers. This yields the ubiquous fcc-structure and is conjectured to maximize density.



Some "problematic" configurations of spheres of size 1 and $\sqrt{2}-1$.

For equal spheres in **higher dimension**, some good candidates to maximize the density are known. Many are based on **laminated lattice** Λ_n, that is a lattice which admits Λ_{n-1} as a sublattice, with $\Lambda_1 = \mathbb{Z}$. Indeed, Fejes Tóth and Hales-Ferguson proved the optimality of Λ_2 and Λ_3. And further:

Theorem (Vyazovska, 2016)
The Gosset lattice Λ_8 and the Leech lattice Λ_{24} maximize the density.

The density has no reason to be always reached by a lattice or even a periodic packings...

What for **very high dimensions**? On the one hand,

Theorem (Kabatiansky-Levenshtein, 1978)
Any packing of equal spheres in $\mathbb{R}^n$ has density at most $2^{-0.599n}$.

On the other hand, any saturated packing of equal spheres in $\mathbb{R}^n$ has density at least 2^{-n}. Indeed, doubling the radius multiplies the volume by 2^n and cover the whole space.

This has (hardly) been improved to $n2^{-n}$ (1992), $\frac{6}{e}n2^{-n}$ (2011), $n\log n2^{-n}$ (2023)... But no **explicit packing** that yields density at least 2^{-n} is known for $n > 520$ (current record).

Proof Strategy I

The Kepler conjecture and packing of disks have been proven by the **localization** method. Sketch:

1. partition $\mathbb{R}^n$ in uniformly bounded sets (**cells**);
2. if some cells are "too dense": **redistribute** density excess among "close" cells;
3. we show that, eventually, the density of **every possible cell** is low enough.

A bit more details:

1. typical cells are a combination or modification of **Voronoï** cells and **Delaunay** simplices;
2. the redistribution has to be **very local** (typically around cells sharing a vertex) to avoid an unmanageable case study;
3. **interval arithmetic** is used to prove inequality on an infinite but compact set of cells.

```
sage: pi=RealDoubleField()(4*arctan(1))
sage: pi
3.141592653589793
sage: sin(pi)
1.2246467991473515e-16
sage: pi=RealIntervalField()(4*arctan(1))
sage: pi
3.141592653589794?
sage: pi.endpoints()
(3.14159265358979, 3.14159265358980)
sage: sin(pi).endpoints()
(-3.21624529935328e-16, 1.22464679914736e-16)
```

Interval arithmetic with SageMath.

```
x=RIF(1,2)
y=RIF(-3,-2)
I=x*y+3*x+2*y
J=(x+2)*(y+3)-6
```

All expressions are equal, but some are more equal than others...

```
def is_f_positive_over_X(f,X):
    if f(X).lower()>0:
        return True
    elif f(X).upper()<=0:
        return False
    else:
        (X1,X2)=X.bisection()
        return self(f,X1) and self(f,X2)
```

Checking an inequality over a compact set.

Proof Strategy II

Theorem (Cohn-Elkies, 2003)
Assume $f : \mathbb{R}^n \to \mathbb{R}$ satisfies the conditions:

1. $f(x) \leq 0$ for $|x| \geq 2$;
2. $\widehat{f}(t) \geq 0$ for all t.

Then, the density of a packing of unit spheres in $\mathbb{R}^n$ is at most $B_n \frac{f(0)}{\widehat{f}(0)}$, where $B_n = \frac{2\pi}{n} B_{n-2}$ is the volume of the unit sphere.

Cohn and Elkies used that to get **new upper bounds** for $n = 4, \ldots, 24$.

For $n = 8$ and $n = 24$, their bounds were within a factor less than 1.001 from the conjectured values. Vyazovska later relied on **modular forms** to obtain two (explicit) optimal functions.

Optimal functions **may not exist** for other values of n, in particular for $n = 3$ (or even for $n = 2$).

The technique has been extended to **several sizes** of spheres. In particular, an upper bound has been obtained for sizes 1 and $\sqrt{2}-1$ (within a factor 1.3 of the conjectured maximal density).

Proof:

1. Periodic packings get arbitrarily close to the maximal density.
2. Consider a periodic packing of unit spheres centered on $\Lambda + V$, where Λ is a lattice and $V = \{v_1, \ldots, v_N\}$ are in $\mathbb{R}^n$.
3. **Poisson summation** formula yields, for any $v \in \mathbb{R}^n$:
$$\sum_{x\in\Lambda} f(x+v) = \frac{1}{|\Lambda|}\sum_{t\in\Lambda^*} e^{-2\pi i\langle v,t\rangle}\widehat{f}(t).$$
4. Left hand side summed over $V - V$:
$$\sum_{j,k}\sum_{x\in\Lambda} f(x+v_j-v_k).$$
No sphere overlap $\rightsquigarrow |x+v_j-v_k| \geq 2$, except when $x = 0$ and $j = k$. Condition 1 yields the upper bound $Nf(0)$.
5. Right hand side summed over $V - V$:
$$\frac{1}{|\Lambda|}\sum_{t\in\Lambda^*}\left|\sum_j e^{2\pi i\langle v_j,t\rangle}\right|^2 \widehat{f}(t).$$
Condition 2 allows to bound from below by the summand for $t = 0$, i.e. $\frac{N^2}{|\Lambda|}\widehat{f}(0)$.