

1 The Conquest of the Kepler Conjecture

In August 1998, a message was sent out from an internet cafe in Munich that stunned the mathematical community. It stated that the writer had found “a solution to the Kepler Conjecture, the oldest problem in discrete geometry... the proof relies extensively on methods from the theory of global optimization, linear programming and interval arithmetic... well over 250 pages... computer files require over three gigabytes of space for storage...”

Two years later, a panel of twelve referees is still checking the solution provided by Tom Hales, a mathematician at the University of Michigan, and his graduate student Samuel Ferguson. No serious flaws have been found and none are expected to be found. This article gives a brief and admittedly simplistic overview of their work.

The history of the problem goes back to the early 1600s, when the astronomer-mathematician Johannes Kepler wrote about the problem of packing spheres in space. He asserted that no packing could be better than the Face Centered Cubic (FCC) packing. This is the natural one that arises from packing spheres in a pyramid, as shown in Figure 1.

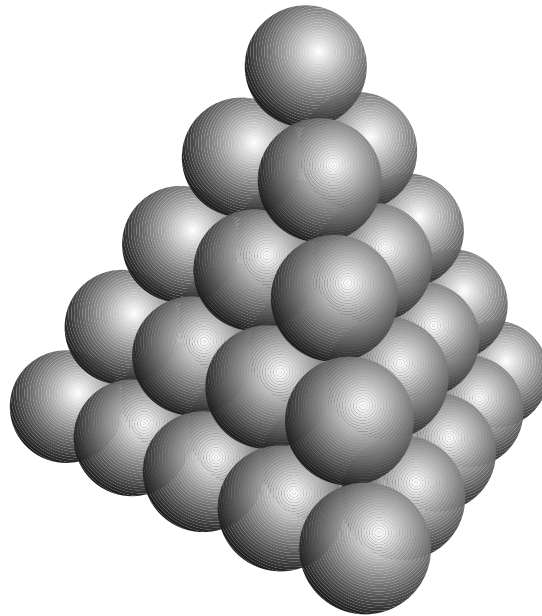


Figure 1: A pyramid in the Face Centered Cubic sphere packing

However, a proof of this simple statement is strangely elusive. A long standing result of Gauss affirms the conjecture for all lattice packings, i.e. all packings where the centers of the spheres form a lattice, but nothing says that a best packing should be of this form. There is even a 1964 conjecture of Rogers that

for the corresponding problem in a high enough dimension, the best packing will *not* be a lattice packing. Even worse, there are known non-lattice packings that are as good as FCC.

We state the problem more precisely. A n -dimensional unit sphere in R^n is composed of all points within one unit from a given center. Kepler's question deals with three dimensions, but we shall often resort to two dimensions for illustrative purposes. A sphere packing is a collection of non-overlapping spheres in R^n . All the packings we deal with will be assumed to be saturated, i.e. have no room for additional spheres. The **density** of a packing *in a finite region* is the fraction of the region occupied by spheres. The density of a packing of *space* is defined as the limit as $r \rightarrow \infty$ of the density of the packing when restricted to a sphere of radius r .

Conjecture 1 (The Kepler Conjecture) *The density of any sphere packing in three-dimensional space is at most $\frac{\pi}{\sqrt{18}}$, which is the density of the FCC packing.*

Related Problems

This question can be generalized in several directions; we give two. First, for what three-dimensional solids can optimum packing densities be found? Secondly, what is the optimum sphere packing density in n dimensions?

Surprisingly little is known about the first question. Trivial cases like cuboids aside, the first result of this sort was only found in 1990, when Andras Bezdek showed that the optimum way to pack infinitely long cylinders is in parallel columns in hexagonal fashion. The first result for a bounded solid was by his brother Karoly in 1994. He showed that the best packing involving a rhombic dodecahedron with a corner chipped off (see Figure 2) is the regular tiling of space by the original dodecahedron.

The second question has been studied a lot more. The first result was by Thue in 1890 for $n = 2$. Here is an adaptation of his proof.

Theorem 2 *The optimum packing of circles in the plane has density $\frac{\pi}{\sqrt{12}}$, which is that of the hexagonal packing.*

Proof: Start with an arbitrary packing of unit circles in the plane. Around each circle draw a concentric circle of radius $\frac{2}{\sqrt{3}}$. Where a pair of larger circles overlap, join their points of intersection and use this as the base of two isosceles triangles. The centers of each circle form the third vertex of each triangle. This induces a partition of the plane into three regions, as depicted in Figure 3.

1. The Isosceles Triangles: If the top angle of the triangle is θ radians, then its area is $\frac{2}{3} \sin \theta$ and the area of the sector is $\theta/2$, so that the packing density is

$$\frac{3\theta}{4 \sin \theta}.$$

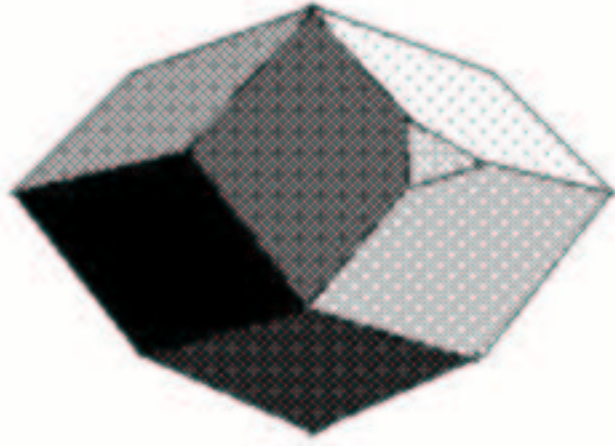


Figure 2: A chipped rhombic dodecahedron

θ ranges between 0 and $\pi/3$ radians and the maximum value of the density is $\frac{\pi}{2\sqrt{3}}$, attained at $\theta = \pi/3$.

2. Regions of the larger circles not in a triangle: Here the regions are sectors of a pair of concentric circles of radius 1 and $\frac{2}{\sqrt{3}}$ so the density is

$$\left(\frac{1}{2/\sqrt{3}}\right)^2 = \frac{3}{4} < \frac{\pi}{\sqrt{12}}$$

3. Regions not in any circle: Here the density is zero.

Thus the density of each region of space is at most $\frac{\pi}{\sqrt{12}}$. A packing can only be optimum when it causes space to be divided into equilateral triangles. This only happens for the hexagonal packing of Figure 4. ■

Unfortunately, this proof cannot be generalized to three dimensions. There are several sphere packings where the density in places is over $\frac{\pi}{\sqrt{18}}$. Experimental evidence, both from real life and computer simulations, indicates that this would be offset by lower densities in other places. The Kepler Conjecture asks whether the offset is enough.

A finite calculation

Major progress towards finding a proof of the Kepler Conjecture was made in 1953 when László Fejes Tóth showed how to reduce the problem from a global optimization involving infinitely many variables to a finite calculation.

His method requires a painstaking study of all possible local configurations, called **clusters**, that can arise in a sphere packing. A cluster around a point λ

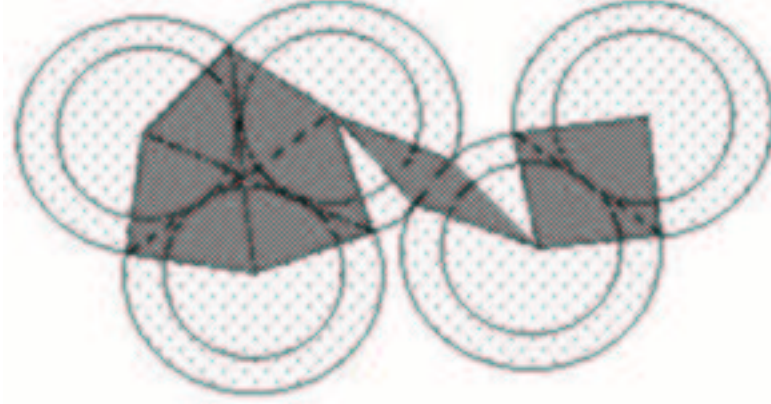


Figure 3: The plane partition induced by a sample circle packing

consists of a base sphere centered at λ and non-overlapping spheres with centers within $\tau = 2\sqrt{2}$ units of λ . The reason for the value of τ is technical and can be ignored for now. As an example, the cluster in the FCC packing is shown in Figure 5.

The set \mathcal{C} of clusters can be given a metric topology based on the coordinates of the spheres in each cluster. The idea is that if two clusters can be obtained from each other by moving spheres around the base one, then there is a finite distance between them. The less the amount of work to convert one cluster to another, the shorter the distance. Clusters involving a different number of spheres are in different components of the topological space.

The next step is to find a “correction function” f defined on \mathcal{C} that deals with the problem of certain clusters being denser than the FCC cluster. f should be continuous, so that similar clusters will have similar values of f . We shall also demand that f be **transient**, i.e. that for any packing, if Λ_r is the set of centers within r units of the origin,

$$\sum_{\lambda \in \Lambda_r} f(\lambda) = o(r^3) \quad (1)$$

This constraint keeps f from being too large a correction.

Decomposing Space with the Voronoi method

Once all clusters have been studied, attention can be turned to the task of putting them together to form larger and larger configurations that eventually fill up all of space. Building up configurations is analogous to breaking down space, and it is therefore necessary to consider different ways of performing the latter.

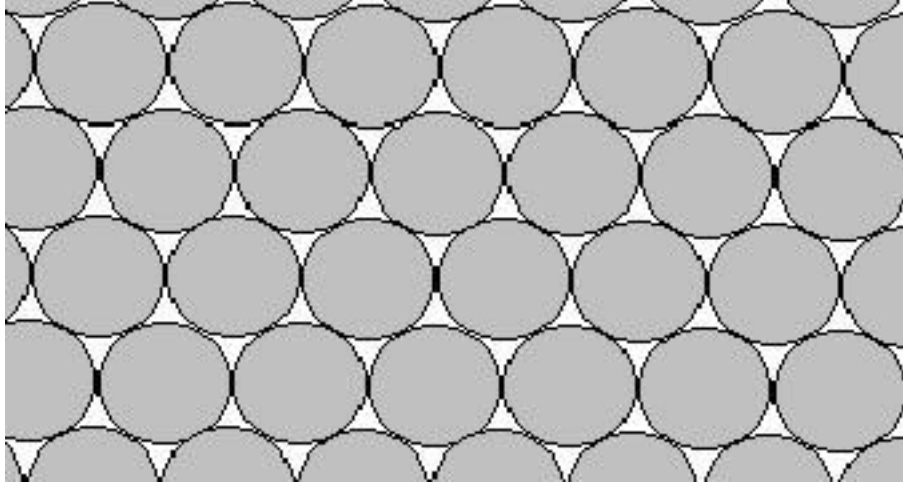


Figure 4: The hexagonal circle packing of the plane

The partition of space suggested by Fejes Tóth is the **Voronoi decomposition**. Given a sphere packing, define the **Voronoi Cell** of a sphere to be the set of points closer to it than to any other sphere. In a three (two) dimensional packing, the Voronoi cells are polyhedra (polygons) containing unit spheres (circles). However, not all such objects are candidates for Voronoi cells – no polyhedra with over sixty faces is, for example. Figure 6 gives an example of a Voronoi decomposition in two dimensions.

The density of a cell is the ratio of the volume of a unit sphere to its own volume. For example, the rhombic dodecahedron is the only Voronoi cell that occurs in the FCC packing. Its volume is $V_{fcc} = 4\sqrt{2}$ and its density is $\frac{\pi}{\sqrt{18}} \approx 0.7405$.

In two dimensions it turns out that the densest Voronoi cell is the regular hexagon. Since this tiles the plane, the optimum packing consists of circles fitted in each hexagon of the tiling. This is of course the same packing that Thue showed was optimal.

In three dimensions the densest Voronoi cell is the regular dodecahedron, which has a density of about 0.755. (This 1943 conjecture of Fejes Tóth was proved in 1998 by Sean McLaughlin, then an undergraduate at Michigan.) There are several other Voronoi cells that have densities higher than 0.7405. Like the regular dodecahedron, none of them partition space — which is a pity, because then the problem as a whole would be much easier!

Since the density of a packing is a function of the density of its cells, the Kepler Conjecture can be rephrased as the problem of showing that there are no decompositions based primarily on such highly dense cells.

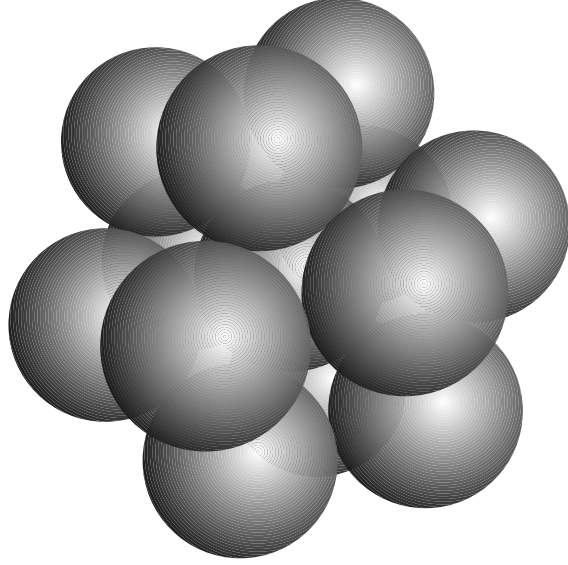


Figure 5: A cluster in the FCC sphere packing

The correction function

The use of the correction function can now be explained in more detail. For a given packing Π , let Λ be its set of centers. There is a Voronoi cell V_λ at each point $\lambda \in \Lambda$. Thus the Voronoi Decomposition is

$$\bigcup_{\lambda \in \Lambda} V_\lambda = \mathbf{R}^3$$

Now we demand that our correction function f be **FCC-compatible**, i.e. that

$$V_{fcc} \leq \text{Volume}(V_\lambda) + f(C_\lambda) \quad \forall \lambda \in \Lambda. \quad (2)$$

There are several continuous transient functions known. But finding one that is also FCC-compatible is very difficult since these functions tend to involve well over a hundred variables! However, its existence would settle the Kepler Conjecture, as we now show. If we sum (2) over Λ_r , we have

$$|\Lambda_r| V_{fcc} \leq \sum_{\lambda \in \Lambda_r} \text{Volume}(V_\lambda) + \sum f(C_\lambda) \leq \frac{4}{3}\pi(r+c)^3 + o(r^3)$$

The second inequality follows from the fact that $\bigcup_{\lambda \in \Lambda_r} V_\lambda$ is contained in a sphere of radius $r+c$ for some constant c . It should be noted that we are making use of the maximality of our packings here; the statement is certainly not true for non-saturated packings, which can have cells of infinite size.

Dividing by $r^3 V_{fcc}$, we have:

$$\frac{|\lambda_r|}{r^3} \leq \frac{4\pi}{3V_{fcc}} \left(1 + \frac{1}{r}\right)^3 + \frac{o(r^3)}{r^3}$$

and sending $r \rightarrow \infty$ we find that the density

$$\lim_{r \rightarrow \infty} \frac{|\Lambda_r| \frac{4}{3}\pi(1)^3}{\frac{4}{3}r^3} = \lim_{r \rightarrow \infty} \frac{|\Lambda_r|}{r^3} \leq \frac{4\pi}{3 \cdot 4\sqrt{2}} = \frac{\pi}{\sqrt{18}}$$

Alternative Decompositions of Space

Fejes Tóth did not pursue the Voronoi decomposition approach further since there was not enough computational power in his day to make it feasible. When Hales took it up in the 1990s, he found it was far too complicated to deal with in certain cases. He decided to try its dual, called the **Delaunay decomposition**.

Consider a network of vertices and edges, where the vertices are the centers of spheres and centers are joined by an edge if and only if their corresponding Voronoi cells have a common face. The resulting partition into simplexes is the Delaunay decomposition. An analogous decomposition in two dimensions is shown in Figure 6.

After some months of work, the Delaunay approach was also becoming too complex to deal with and Hales put the whole problem aside for a while. Insight came in November 1994 when he realized that instead of trying to dogmatically stick to one type of decomposition, it might be better to try a hybrid approach: in other words, partition each region of space into Delaunay simplexes or Voronoi cells depending on what is most convenient.

The good thing about hybrid decompositions is that there are an infinite number of them. As the months went by, Hales and Ferguson found that when the going got tough, it was quicker to change the decomposition and the correction function a bit rather than plough through with the original one. This arbitrariness certainly raised some eyebrows! What makes it permissible is the infinite-dimensionality of the problem.

Two years later, with the deadline for Ferguson's thesis submission looming, the two workers decided to stop adjusting f and the decomposition and push the proof through to the bitter end...

To follow their path, we need a few more definitions. Call a pair of centers **close** if they are within 2.51 units of each other. The choice of 2.51 was arrived at after a combination of careful planning, methodical calculation and much trial and error. Some of its uses will become clear later.

The two most interesting Delaunay simplices are the following:

1. Simplexes comprising four close centers. These are called **quasi-regular tetrahedrons**, or qr-tets for short.
2. Simplexes comprising six centers that, apart from the three opposite pairs, are pairwise close. In addition, two of the opposite pairs are over τ apart

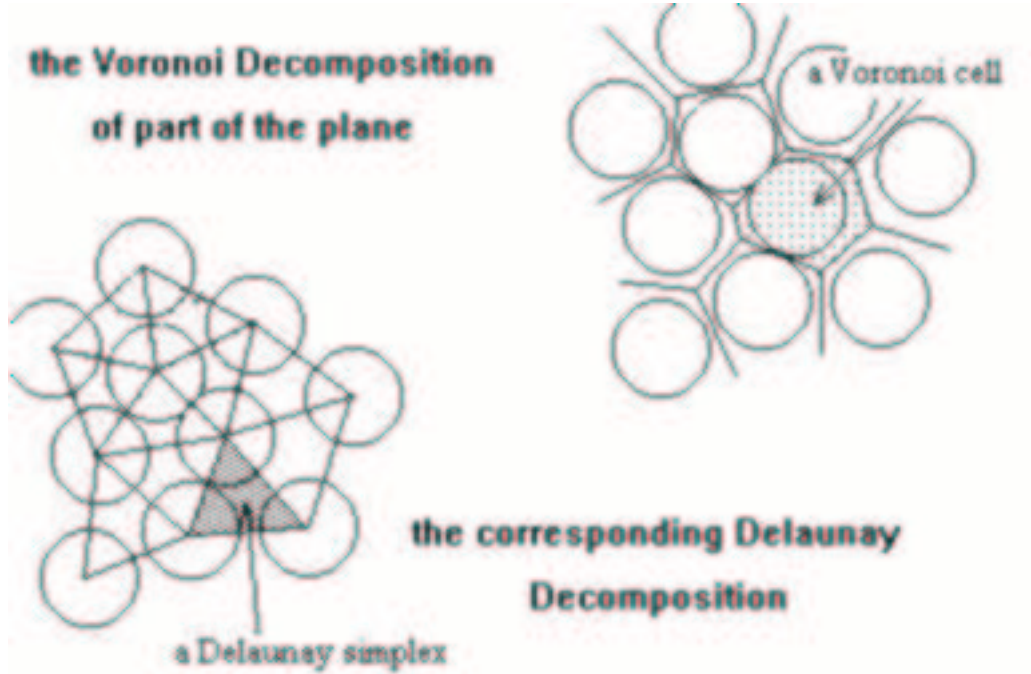


Figure 6: Two decompositions of the plane

while the third one is not. These are called **quasi-regular octahedrons**, or qr-octs for short.

The final decomposition is a little tricky to define; suffice to say it consists primarily of qr-tets, qr-octs and a host of other less interesting Delaunay simplices. The main point is that it is fixed and draws from the best features of the Voronoi and Delaunay decompositions. The correction function f is also fixed and the next step is to confirm that f is indeed FCC-compatible, i.e. that

$$f(C_\lambda) \geq V_{fcc} - Volume(V_\lambda) \quad \forall \lambda \in \Lambda \quad (3)$$

Associated Maps and Graphs

Equation (3) represents an optimization problem on f . Unfortunately the space \mathcal{C} of clusters, on which f is defined, is very complicated and can only be dealt with indirectly.

To every cluster $C \in \mathcal{C}$ associate a spherical map M_C as follows. Assume that the base sphere of C is centered at a point λ . For every other sphere S in C , draw a line from its center to λ that meets the base sphere at a point

p_S . These points form the vertices of M_C . Vertices p_R and p_S are joined by an edge of M_C iff the centers of spheres R and S are close. An example is shown in Figure 7 for the cluster called the pentahedral prism.



Figure 7: The cluster, spherical map and plane graph for the Pentahedral Prism

Lower bounds for $f(C)$ can be found by studying M_C . In many cases it is even sufficient to study G_C , which is the plane graph obtained from M_C . (G_C has a lot less information than M_C , which keeps track of geometric details like the position of the spheres relative to each other in space.) There are an infinite number of clusters for which this is not the case, but they can be grouped into a *finite* number of classes according to their maps:

n , for largest n -sided face in map	Number of maps
≤ 3	0
4	1749
5	2459
6	429
7	413
8	44
≥ 9	0
	5094

This is certainly the most labor-intensive stage of the problem. To each map is associated a non-linear optimization problem involving up to 160 variables and over 1000 inequalities. At first sight things look hopeless, till it is realized that most constraints are linear and hence standard methods from linear programming can be applied to cut down the number of cases to a more manageable 189.

To better appreciate the amount of human toil that went into this stage, an excerpt from a report by Hales in 1996 is in order:

Of the 537 ... [remaining] maps with only triangles and quadrilaterals, 531 can be discarded by linear programming methods. Five more can be discarded by a refinement of the linear programming

methods. This leaves one case. This remaining case is still giving a bound of about 8.25 points and needs to be nudged a bit more before we are finished with this case.

[Footnote, some months later:] We were down to one case, but we continue to fiddle with the scoring rules and inequalities. We are temporarily back up to 33 cases...

The one remaining map referred to above is the pentahedral prism of Figure 7. It turned out to be unbelievably difficult and became the primary focus of Ferguson's doctoral thesis.

Better methods of linear programming bring the number of cases down to 88, at which stage ad hoc computer programs can be written to deal with each. The entire solution contains about 100 000 such calculations.

The End of the Adventure

Ferguson completed his doctorate in August 1997 and returned to Ann Arbor for three months in mid 1998 to help Hales bring the project to its completion:

Theorem 3 (The Kepler Theorem) *The density of any sphere packing in three-dimensional space is at most $\frac{\pi}{\sqrt{18}}$, which is the density of the FCC packing.*

This was not the only outcome of the project however. For example, chemists have known for ages that a packing scheme that is as good as the FCC packing both locally and globally is the Hexagonal Closed Packed one. This is made of the same layers as the FCC, but the layers are arranged differently, as shown in Figure 8.



Figure 8: The difference between the FCC and HCP packings

Hales and Ferguson showed that the HCP is the only such packing. Furthermore, they were able to determine that all packings which are as good (globally only!) as the FCC look like the FCC or HCP locally for a sufficiently large percentage of space.

What's next?

There are several interesting open problems in discrete geometry that involve packing unit spheres. Here are a few.

1. It was proved by Van der Waerden and Leech in 1956 that the maximum number of spheres that a sphere could touch in three dimensions is 12. What is the answer in 4 dimensions?
2. What is the minimum volume that can be contained by N planes tangent to a sphere in three dimensions?
3. The Sausage Conjecture is an open question asked by Fejes Tóth in 1975. The problem is that of packing m spheres in R^n , $n \geq 5$ so that the volume of the convex hull generated by the spheres is minimized. The conjecture is that the optimal packing is of spheres next to each other in a straight line, i.e. 'a sausage'. It was confirmed by Betke and Henk for $n \geq 42$ in 1998.
4. The Sausage Catastrophe deals with the above problem for $n = 3, 4$. Wills suggested in 1983 that the optimal solution for small m is indeed a one-dimensional sausage, but for m larger than a certain critical value k_n the optimal configurations are n -dimensional arrangements. He conjectured that $k_3 \approx 56$ and $k_4 \approx 75000$.

References

- S. Ferguson, Sphere Packings V, LANL e-print archive `math.MG/9811077`; <http://xxx.lanl.gov/>
- T. Hales, Cannonballs and Honeycombs, Notices of the AMS, Volume 47, No. 4, pp 440 - 449.
- T. Hales, An overview of the Kepler Conjecture, LANL e-print archive `math.MG/9811071`; <http://xxx.lanl.gov/>
- T. Hales, The Kepler Conjecture, LANL e-print archive `math.MG/9811078`; <http://xxx.lanl.gov/>
- T. Hales, personal communication.
- C. Zong, Sphere Packings, 1999 Springer-Verlag, New York.

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