A Computer Verification of the Kepler Conjecture

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Abstract

The Kepler conjecture asserts that the density of a packing of congruent balls in three dimensions is never greater than $\pi/\sqrt{18}$. A computer assisted verification confirmed this conjecture in 1998. This article gives a historical introduction to the problem. It describes the procedure that converts this problem into an optimization problem in a finite number of variables and the strategies used to solve this optimization problem.

2000 Mathematics Subject Classification: 52C17.
Keywords and Phrases: Sphere packings, Kepler conjecture, Discrete geometry.

1. Historical introduction

The Kepler conjecture asserts that the density of a packing of congruent balls in three dimensions is never greater than $\pi/\sqrt{18} \approx 0.74048\ldots$. This is the oldest problem in discrete geometry and is an important part of Hilbert’s 18th problem. An example of a packing achieving this density is the face-centered cubic packing (Figure 1).

A packing of balls is an arrangement of nonoverlapping balls of radius 1 in Euclidean space. Each ball is determined by its center, so equivalently it is a collection of points in Euclidean space separated by distances of at least 2. The density of a packing is defined as the lim sup of the densities of the partial packings formed by the balls inside a ball with fixed center of radius $R$. (By taking the lim sup, rather than lim inf as the density, we prove the Kepler conjecture in the strongest possible sense.) Defined as a limit, the density is insensitive to changes in the packing in any bounded region. For example, a finite number of balls can be removed from the face-centered cubic packing without affecting its density.

Consequently, it is not possible to hope for any strong uniqueness results for packings of optimal density. The uniqueness established by Lemma 2.8 is nearly as

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strong as can be hoped for. It shows that certain local structures (decomposition stars) attached to the face-centered cubic (fcc) and hexagonal-close packings (hcp) are the only structures that maximize a local density function.

1.1 Hariot and Kepler

The modern mathematical study of close packings can be traced to T. Hariot. Hariot’s work—unpublished, unedited, and largely undated—shows a preoccupation with packings of balls. He seems to have first taken an interest in packings at the prompting of Sir Walter Raleigh. At the time, Hariot was Raleigh’s mathematical assistant, and Raleigh gave him the problem of determining formulas for the number of cannonballs in regularly stacked piles. Shirley, Hariot’s biographer, writes that this study “led him inevitably to the corpuscular or atomic theory of matter originally deriving from Lucretius and Epicurus [25, p.242].”

Kepler became involved in packings of balls through his correspondence with Hariot in the early years of the 17th century. Kargon writes, in his history of atomism in England,

\begin{quote}
According to Hariot the universe is composed of atoms with void space interposed. The atoms themselves are eternal and continuous. Physical properties result from the magnitude, shape, and motion of these atoms, or corpuscles compounded from them. . . .
\end{quote}

Probably the most interesting application of Hariot’s atomic theory was in the field of optics. In a letter to Kepler on 2 December 1606 Hariot outlined his views. Why, he asked, when a light ray falls upon the surface of a transparent medium, is it partially reflected and partially refracted? Since by the principle of uniformity, a single point cannot both reflect and transmit light, the answer must lie in the supposition that the ray is resisted by some points and not others . . .

It was here that Hariot advised Kepler to abstract himself mathematically into an atom in order to enter ‘Nature’s house’. In his reply of 2 August 1607, Kepler declined to follow Hariot, ad atomos et vacua. Kepler preferred to think of the reflection-refraction problem in terms of the union of two op-
posing qualities—transparence and opacity. Hariot was surprised. “If those assumptions and reasons satisfy you, I am amazed.” [14, p.26]

Despite Kepler’s initial reluctance to adopt an atomic theory, he was eventually swayed, and in 1611 he published an essay that explores the consequences of a theory of matter composed of small spherical particles. Kepler’s essay was the “first recorded step towards a mathematical theory of the genesis of inorganic or organic form” [28, p.v].

Kepler’s essay describes the face-centered cubic packing and asserts that “the packing will be the tightest possible, so that in no other arrangement could more pellets be stuffed into the same container.” This assertion has come to be known as the Kepler conjecture. This conjecture was verified with computer assistance in 1998 [15].

1.2 Newton and Gregory

The next episode in the history of this problem is a debate between Isaac Newton and David Gregory. Newton and Gregory discussed the question of how many balls of equal radius can be arranged to touch a given ball. This is the three-dimensional analogue of the simple fact that in two dimensions six pennies, but no more, can be arranged to touch a central penny. This is the kissing-number problem in $n$-dimensions. In three dimensions, Newton said that the maximum was 12 balls, but Gregory claimed that 13 might be possible. B. L. van der Waerden and Schütte in 1953 showed that Newton was correct [24].

The two-dimensional analogue of the Kepler conjecture is to show that the honeycomb packing in two dimensions gives the highest density. This result was established in 1892 by Thue, with a second proof appearing in 1910 (26, 27).

In 1900, Hilbert made the Kepler conjecture part of his 18th problem [16]. The third part of that problem asks, “How can one arrange most densely in space an infinite number of equal solids of given form, e.g. spheres with given radii . . . , that is, how can one so fit them together that the ratio of the filled to the unfilled space may be as great as possible?”

1.3 The literature

Past progress toward the Kepler conjecture can be arranged into four categories: (1) bounds on the density, (2) descriptions of classes of packings for which the bound of $\pi/\sqrt{18}$ is known, (3) convex bodies other than balls for which the packing density can be determined precisely, (4) strategies of proof.

Various upper bounds have been established on the density of packings. A list of such bounds appears in [10]. Rogers’s bound of 0.7797 is particularly natural [29]. It remained the best available bound for many years.

1.4 Classes of packings

If the infinite dimensional space of all packings is too unwieldy, we can ask if it is possible to establish the bound $\pi/\sqrt{18}$ for packings with special structures.
If we restrict the problem to packings of balls whose centers are the points of a lattice, the packings are described by a finite number of parameters, and the problem becomes much more accessible. Lagrange proved that the densest lattice packing in two dimensions is the familiar honeycomb arrangement \[21\]. Gauss proved that the densest lattice packing in three dimensions is the face-centered cubic \[9\]. The enormous list of references in \[4\] documents the many developments in lattice packings over the past two centuries.

### 1.5 Other convex bodies

If the optimal packings of balls are too difficult to determine, we might ask whether the problem can be solved for other convex bodies. To avoid trivialities, we restrict our attention to convex bodies whose packing density is strictly less than 1.

The first convex body in Euclidean 3-space that does not tile for which the packing density was explicitly determined is an infinite cylinder \[1\]. Here A. Bezdek and W. Kuperberg prove that the optimal density is obtained by arranging the cylinders in parallel columns in the honeycomb arrangement.

In 1993, J. Pach exposed the humbling depth of our ignorance when he issued the challenge to determine the packing density for some bounded convex body that does not tile space \[22\]. (This challenge was met by A. Bezdek \[2\].)

### 1.6 Strategies of proof

In 1953, L. Fejes Tóth proposed a program to prove the Kepler conjecture \[5\]. A single Voronoi cell cannot lead to a bound better than the dodecahedral bound. (The dodecahedral bound is the ratio of the volume of a inscribed ball to the volume of the containing dodecahedron.) L. Fejes Tóth considered weighted averages of the volumes of collections of Voronoi cells. These weighted averages involve up to 13 Voronoi cells. He showed that if a particular weighted average of volumes is greater than the volume of the rhombic dodecahedron, then the Kepler conjecture follows. The Kepler conjecture is an optimization problem in an infinite number of variables. L. Fejes Tóth’s weighted-average argument was the first indication that it might be possible to reduce the Kepler conjecture to a problem in a finite number of variables. Needless to say, calculations involving the weighted averages of the volumes of several Voronoi cells are complex.

L. Fejes Tóth made another significant suggestion in \[6\]. He was the first to suggest the use of computers in the Kepler conjecture. After describing his program, he writes,

Thus it seems that the problem can be reduced to the determination of the minimum of a function of a finite number of variables, providing a programme realizable in principle. In view of the intricacy of this function we are far from attempting to determine the exact minimum. But, mindful of the rapid development of our computers, it is imaginable that the minimum may be approximated with great exactitude.

A widely publicized attempt to prove the Kepler conjecture was that of Wu-Yi Hsiang \[17\], \[18\]. Hsiang’s approach can be viewed as a continuation and extension
of L. Fejes Tóth’s program. Hsiang’s work contains major gaps and errors [3]. A list of published materials relating to these errors can be found in [10].

2. Structure of the proof

This section describes the structure of the proof of the Kepler Conjecture.

Theorem 2.1. (The Kepler Conjecture) No packing of congruent balls in Euclidean three space has density greater than that of the face-centered cubic packing.

Here, we describe the top-level outline of the proof and give references to the sources of the details of the proof ([8], [11], [12], [13], [14], [7], [15]).

Consider a packing of congruent balls of unit radius in Euclidean three space. The density of a packing does not decrease when balls are added to the packing. Thus, to answer a question about the greatest possible density we may add non-overlapping balls until there is no room to add further balls. Such a packing will be said to be saturated.

Let $\Lambda$ be the set of centers of the balls in a saturated packing. Our choice of radius for the balls implies that any two points in $\Lambda$ have distance at least 2 from each other. We call the points of $\Lambda$ vertices. Let $B(x,r)$ denote the ball in Euclidean three space at center $x$ and radius $r$. Let $\delta(x,r,\Lambda)$ be the finite density, defined by the ratio of $A(x,r,\Lambda)$ to the volume of $B(x,r)$, where $A(x,r,\Lambda)$ is defined as the volume of the intersection with $B(x,r)$ of the union of all balls in the packing. Set $\Lambda(x,r) = \Lambda \cap B(x,r)$.

The Voronoi cell $\Omega(v)$ around a vertex $v \in \Lambda$ is the set of points closer to $v$ than to any other ball center. The volume of each Voronoi cell in the face-centered cubic packing is $\sqrt{3}/2$. This is also the volume of each Voronoi cell in the hexagonal-close packing.

Let $a: \Lambda \to \mathbb{R}$ be a function. We say that $a$ is negligible if there is a constant $C_1$ such that for all $x \in \mathbb{R}^3$ and $r \geq 1$, we have

$$\sum_{v \in \Lambda(x,r)} a(v) \leq C_1 r^2.$$  

We say that the function $a$ is fcc-compatible if for all $v \in \Lambda$ we have the inequality

$$\sqrt{3}/2 \leq \text{vol}(\Omega(v)) + a(v).$$

Lemma 2.2. If there exists a negligible fcc-compatible function $a: \Lambda \to \mathbb{R}$ for a saturated packing $\Lambda$, then there exists a constant $C$ such that for all $x \in \mathbb{R}^3$ and $r \geq 1$, we have

$$\delta(x,r,\Lambda) \leq \pi/\sqrt{18} + C/r.$$  

Proof. The numerator $A(x,r,\Lambda)$ of $\delta(x,r,\Lambda)$ is at most the product of the volume of a ball $4\pi/3$ with the number $|\Lambda(x,r+1)|$ of balls intersecting $B(x,r)$. Hence

$$A(x,r,\Lambda) \leq |\Lambda(x,r+1)|4\pi/3. \quad (2.1)$$
In a saturated packing each Voronoi cell is contained in a ball of radius 2 centered at the center of the cell. The volume of the ball $B(x, r + 3)$ is at least the combined volume of Voronoi cells lying entirely in the ball. This observation, combined with fcc-compatibility and negligibility, gives

$$
\sqrt{32}|\Lambda(x, r + 1)| \leq \sum_{v \in \Lambda(x, r + 1)} (a(v) + \text{vol}(\Omega(v))) \\
\leq C_1(r + 1)^2 + \text{vol} B(x, r + 3) \\
\leq C_1(r + 1)^2 + (1 + 3/r)^3\text{vol} B(x, r).
$$

(2.2)

Divide through by $\text{vol} B(x, r)$ and eliminate $|\Lambda(x, r + 1)|$ between Inequality (2.1) and Inequality (2.2) to get

$$
\delta(x, r, \Lambda) \leq \frac{\pi}{\sqrt{18}}(1 + 3/r)^3 + C_1 \frac{(r + 1)^2}{r^3\sqrt{32}}.
$$

The result follows for an appropriately chosen constant $C$.

**Remark 2.3.** We take the precise meaning of the Kepler Conjecture to be a bound on the essential supremum of the function $\delta(x, r)$ as $r$ tends to infinity. Lemma 2.2 implies that the essential supremum of $\delta(x, r, \Lambda)$ is bounded above by $\pi/\sqrt{18}$, provided a negligible fcc-compatible function can be found. The strategy will be to define a negligible function, and then to solve an optimization problem in finitely many variables to establish that it is fcc-compatible.

The article [8] defines a compact topological space $X$ and a continuous function $\sigma$ on that space.

The topological space $X$ is directly related to packings. If $\Lambda$ is a saturated packing, then there is a geometric object $D(v, \Lambda)$ constructed around each vertex $v \in \Lambda$. $D(v, \Lambda)$ depends on $\Lambda$ only through the vertices in $\Lambda$ at distance at most 4 from $v$. The objects $D(v, \Lambda)$ are called decomposition stars, and the space of all decomposition stars is precisely $X$.

Let $\delta_{\text{tet}}$ be the packing density of a regular tetrahedron. That is, let $S$ be a regular tetrahedron of edge length 2. Let $B$ the part of $S$ that lies within distance 1 of some vertex. Then $\delta_{\text{tet}}$ is the ratio of the volume of $B$ to the volume of $S$. We have $\delta_{\text{tet}} = \sqrt{8} \arctan(\sqrt{2}/5)$.

Let $\delta_{\text{oct}}$ be the packing density of a regular octahedron of edge length 2, again constructed as the ratio of the volume of $S$ to the volume of the octahedron. We have $\delta_{\text{oct}} \approx 0.72$.

Let $pt = -\pi/3 + \sqrt{2}\delta_{\text{tet}} \approx 0.05537$.

The following conjecture is made in [8]:

**Conjecture 2.4.** The maximum of $\sigma$ on $X$ is the constant $8pt \approx 0.442989$.

**Lemma 2.5.** An affirmative answer to Conjecture 2.4 implies the existence of a negligible fcc-compatible function for every saturated packing $\Lambda$. 


Proof. For any saturated packing $\Lambda$ define a function $a : \Lambda \rightarrow \mathbb{R}$ by
\[
-\sigma(D(v, \Lambda))/(4\delta_{oct}) + 4\pi/(3\delta_{oct}) = \text{vol}(\Omega(v)) + a(v).
\]
Negligibility follows from [8, Prop. 3.14 (proof)]. The upper bound of $8 \text{ pt}$ gives a lower bound
\[
-8 \text{ pt}/(4\delta_{oct}) + 4\pi/(3\delta_{oct}) \leq \text{vol}(\Omega(v)) + a(v).
\]
The constant on the left-hand side of this inequality equals $\sqrt{32}$, and this establishes fcc-compatibility.

Theorem 2.6. Conjecture 2.4 is true. That is, the maximum of the function $\sigma$ on the topological space $X$ of all decomposition stars is $8 \text{ pt}$.

Theorem 2.6, Lemma 2.5, and Lemma 2.2 combine to give a proof of the Kepler Conjecture 2.1.

Let $t_0 = 1.255$ ($2t_0 = 2.51$). This is a parameter that is used for truncation throughout the series of articles on the Kepler Conjecture.

Let $U(v, \Lambda)$ be the set of vertices in $\Lambda$ at distance at most $2t_0$ from $v$. From a decomposition star $D(v, \Lambda)$ it is possible to recover $U(v, \Lambda)$ (at least up to Euclidean translation: $U \mapsto U + y$, for $y \in \mathbb{R}^3$). We can completely characterize the decomposition stars at which the maximum of $\sigma$ is attained.

Theorem 2.7. Let $D$ be a decomposition star at which the maximum $8 \text{ pt}$ is attained. Then the set $U(D)$ of vectors at distance at most $2t_0$ from the center has cardinality 12. Up to Euclidean motion, $U(D)$ is the kissing arrangement of the 12 balls around a central ball in the face-centered cubic packing or hexagonal-close packing.

2.7 Outline of proofs

To prove Theorems 2.6 and 2.7 we wish to show that there is no counterexample. That is, we wish to show that there is no decomposition star $D$ with value $\sigma(D) > 8 \text{ pt}$. We reason by contradiction, assuming the existence of such a decomposition star. With this in mind, we call $D$ a contravening decomposition star, if
\[
\sigma(D) \geq 8 \text{ pt}.
\]
In much of what follows we will assume that every decomposition star under discussion is a contravening one. Thus, when we say that no decomposition stars exist with a given property, it should be interpreted as saying that no such contravening decomposition stars exist.

To each contravening decomposition star, we associate a (combinatorial) plane graph. A restrictive list of properties of plane graphs is described in [15, Section 2.3]. Any plane graph satisfying these properties is said to be tame. All tame plane graphs have been classified. (There are several thousand, up to isomorphism.) Theorem 15 Th 2.1] asserts that the plane graph attached to each contravening decomposition star is tame. By the classification of such graphs, this reduces the
proof of the Kepler Conjecture to the analysis of the decomposition stars attached to the finite explicit list of tame plane graphs.

A few of the tame plane graphs are of particular interest. Every decomposition star attached to the face-centered cubic packing gives the same plane graph (up to isomorphism). Call it $G_{fcc}$. Likewise, every decomposition star attached to the hexagonal-close packing gives the same plane graph $G_{hcp}$. Let $X_{crit}$ be the set of decomposition stars $D$ such that the set $U(D)$ of vertices is the kissing arrangement of the 12 balls around a central ball in the face-centered cubic or hexagonal-close packing. There are only finitely many orbits of $X_{crit}$ under the group of Euclidean motions.

In [8, Lemma 3.13], the necessary local analysis is carried out to prove the following local optimality.

**Lemma 2.8.** A decomposition star whose plane graph is $G_{fcc}$ or $G_{hcp}$ has score at most 8 pt, with equality precisely when the decomposition star belongs to $X_{crit}$.

In light of this result, we prove 2.6 and 2.7 by proving that any decomposition star whose graph is tame and not equal to $G_{fcc}$ or $G_{hcp}$ is not contravening.

There is one more tame plane graph that is particularly troublesome. It is the graph $G_{pent}$ obtained from the pictured configuration of twelve balls tangent to a given central ball (Figure 3). (Place a ball at the north pole, another at the south pole, and then form two pentagonal rings of five balls.) This case requires individualized attention. S. Ferguson proves in [7] that if $D$ is any decomposition star with this graph, then $\sigma(D) < 8$ pt.

To eliminate the remaining cases, more-or-less generic arguments can be used. A linear program is attached to each tame graph $G$. The linear program can be viewed as a linear relaxation of the nonlinear optimization problem of maximizing $\sigma$ over all decomposition stars with a given tame graph $G$. Because it is obtained by relaxing the constraints on the nonlinear problem, the maximum of the linear problem is an upper bound on the maximum of the original nonlinear problem. Whenever the linear programming maximum is less than 8 pt, it can be concluded that there is no contravening decomposition star with the given tame graph $G$. This linear programming approach eliminates most tame graphs.

When a single linear program fails to give the desired bound, it is broken into a series of linear programming bounds, by branch and bound techniques. For
every tame plane graph $G$ other than $G_{hcp}$, $G_{fcc}$, and $G_{pent}$, we produce a series of linear programs that establish that there is no contravening decomposition star with graph $G$. When every face of the plane graph is a triangle or quadrilateral, this is accomplished in [13]. The general case is completed in the final sections of [15].

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