BULLETIN (New Series) OF THE
AMERICAN MATHEMATICAL SOCIETY
http://dx.doi.org/10.1090/bull/1502
Article electronically published on June 9, 2015

Dense sphere packings: a blueprint for formal proofs, by Thomas C. Hales, London Mathematical Society Lecture Note Series, Vol. 400, Cambridge University Press, Cambridge, 2012, xiv+271 pp., ISBN 978-0-521-61770-3

1. Sphere packings

The Kepler Conjecture states that the maximum density for packing three-dimensional space by equal spheres is attained by the face-centered cubic lattice packing (FCC packing), which has density $\frac{\pi}{\sqrt{18}} \approx 0.74048$. It was stated by Johannes Kepler in 1611, whose booklet [31, pp. 14–17] included a woodcut of the packing. Another periodic packing of density $\frac{\pi}{\sqrt{18}}$, the hexagonal close packing (HCP), was proposed by Barlow [1] in 1883 as a model for certain crystals. In 1900 the three-dimensional sphere packing problem was raised as part of Problem 18 on Hilbert's famous problem list [29].

A general approach to the Kepler Conjecture was suggested in the 1950s by L. Fejes-Tóth [5, pp. 174–181], which he made more detailed in the 1960s in [6, pp. 295–299]. It proposes to prove a local density inequality around each sphere center. The simplest form of such an inequality starts with a sphere packing and gives a recipe to partition space $\mathbb{R}^3$ into cells each containing one sphere, with the volume of the cell assigned to the sphere, and then proving a lower bound on the volume of every possible individual cell. More complicated forms of such inequalities can be thought of as allowing cells to overlap, assigning a weight to points in the cell, in effect sharing the volume of the overlaps between the spheres in overlapping cells. A local density inequality proves the total weight assigned to any possible cell that can be so constructed is bounded below by a particular constant. It is "local" in the sense that the shape of the cell assigned a given sphere center should depend only on the sphere centers within a fixed finite distance K of it. (In practice, for spheres of radius 1, the distance K will be less than 3.) The number of "nearby" sphere centers within this distance will be finite, call it N, and this data can be specified by $3N$ coordinates, reducing the analysis to a finite-dimensional optimization problem. This problem is that of maximizing the amount of (weighted) covered volume possible in a cell assigned to a given sphere center, taken over all possible cell shapes determined by the nearby sphere centers. It is a nonlinear optimization problem in that the total weight assigned to a cell might be a very complicated nonlinear function of the nearby sphere centers, definitely not continuously differentiable. Each such optimization problem, if solved, provides an upper bound on the (local) sphere packing density, which then implies an upper bound on the asymptotic sphere packing density. In 1958 Rogers [38] obtained in this way an upper bound of ≈ 0.7797, using a division of space into tetrahedra.

Call a local density inequality *optimal* if the bound it gives will imply the Kepler Conjecture. A priori it is not clear that optimal inequalities should exist. A local density inequality makes a logically stronger statement than an asymptotic density bound, in that removing a finite number of spheres does not change asymptotic

2010 *Mathematics Subject Classification.* Primary 52C17, 68T15; Secondary 51M20, 51Mxx, 65Kxx, 90C05, 90C26.

densities, but would change local densities. One only verifies that an optimal local density inequality exists after the fact, by establishing an upper bound, and simultaneously finding a packing giving a matching lower bound.

The difficulty of the Kepler problem is that the simplest decompositions of space do not yield optimal inequalities. There are two natural partitions of space associated to sphere centers, the *Voronoi cell decomposition* and the *Delaunay decomposition*. The Voronoi cell assigned to a sphere center is the set of points in space closer to it than to any other sphere center. The *Delaunay decomposition* cuts space into simplices (i.e., tetrahedra) with corners at sphere centers. (It is unique for generic locations of centers but has some nonuniqueness for nongeneric point locations which must be resolved.) The simplest local density inequalities associated to these would be the ratio of the amount covered by the intersection of unit spheres with the cell to the total volume of the cell. The difficulty of the sphere-packing problem is that neither of these local density inequalities is optimal. For Voronoi cells it was conjectured in 1943 by L. Fejes-Tóth [4] that for unit spheres the Voronoi cell of minimal volume is a regular dodecahedron, associated to twelve touching spheres arranged at the vertices of a regular icosahedron; the fraction of this cell occupied by the sphere is ≈ 0.75469, exceeding the Kepler bound. (The *Dodecahedral Conjecture* was proved in 2010 by Hales and McLaughlin [26].) For a Delaunay tetrahedron with sphere centers at its four vertices, a conjecturally worst tetrahedron (for a saturated packing) has four edges of length 2 and two adjacent edges of length $\sqrt{2(3+\sqrt{6})}$. It has circumradius 2 and sphere packing density ≈ 0.78469, exceeding the Rogers bound [22]. The search for optimal local inequalities needs to consider hybrid partitions of space assigned to sphere centers that choose Voronoi cells some of the time, Delaunay tetrahedra some of the time, and perhaps something in between in other cases.

In the period 1998–2005 T. Hales, together with S. Ferguson, proved the Kepler Conjecture by constructing an optimal inequality and verifying it, as described below. Subsequent work indicates there exist many different optimal local density inequalities for three-dimensional sphere packing, each giving the Kepler Conjecture as a corollary, while giving different information on local packing densities.

Local density inequalities can be studied in any dimension (see [32]). At present it is unknown whether optimal local density inequalities exist in dimensions other than $1, 2$, and 3. It is also not known in which dimensions there exists a densest packing that is *periodic*, meaning a packing having its sphere centers located at a finite set of translates of a full-dimensional lattice. It is expected that the latter will be true in dimensions $n = 8$ and $n = 24$, with densest packings attained by scaled versions of the E_8 and Leech lattice, respectively. For detailed results on sphere packings in all dimensions, consult Conway and Sloane [3].

2. Proof of the Kepler Conjecture

In 2005 and 2006 T. Hales, together with S. Ferguson, published a proof of the Kepler Conjecture. An abridged version of the proof appeared in *Annals of Mathematics* [12] in 2005, and a more detailed version of the proof appeared as [13], [14], [15], [16], [17], [18]. In 2010, in the process of developing machinery towards a formal proof, a small revision to this proof was found necessary, which is described in Hales et al. [25]. All the papers in this proof are collected in the volume [24], including the revision, some earlier work of Hales [10], [11], and an overview [33].

A major part of their achievement was the design of a local inequality which is now known to be optimal, and which has the important property of being checkable with computer assistance in a reasonable computation time. Their partition of space and assignment of weights underlying this inequality is extremely complicated to formulate. The proof that their local recipe yields an admissible partition of space is itself difficult to check. Once this is done, analytic methods are used to verify that two particular families of local configurations contain isolated local minima, corresponding to Voronoi cells of the FCC and HCP packings, respectively. Then thousands of other families of local configurations were shown to be suboptimal by obtaining bounds saying the maximal packing density was strictly below the minimum. The complicated form of the local inequality has features allowing the nonlinear optimization problem to decompose into sums of simpler problems, each of which separately could be bounded by linear inequalities encodable as linear programs. This decomposition property permitted a classification of cases labeled by auxiliary graphs and was key in reducing the computational verification to a feasible size.

Call a packing *extremal* for a local density inequality if it achieves equality in every cell of the decomposition. The extremal packings for the Hales–Ferguson local density function were determined to be those packings in which every Voronoi cell matches those of the HCC or FCP packing. There exist uncountably many distinct extremal packings, obtained by stacking plane layers of spheres whose centers are packed in a two-dimensional equilateral triangular lattice arrangement ("hexagonal layers"), with a choice of two ways to stack each subsequent layer, after the first two layers are fixed.

3. Formal proof

Since 2006 T. Hales has engaged in a project to produce a formal proof of the Kepler Conjecture, terming the project Flyspeck [21].

A *formal proof* is a proof written in a formal logical system, which has been verified by computer by a proof assistant that checks the proof logically line by line. The program for the computer to check is called a *proof script*. Formal proofs are more reliable than proofs written in mathematics journals; the latter are like computer program specifications, while a formal proof is analogous to a computer program itself.

There have been great advances in the last few years in obtaining formal proofs of landmark mathematical results. These include formal proofs of the Four-color theorem, and of the Feit–Thompson theorem, stating that all finite nonabelian simple groups have even order, cf. [9]. A Seminar Bourbaki exposé of Hales [20] reports on the current state of the art of large formal proofs.

The book under review forms part of a project to give a formal proof of the Kepler Conjecture. Some statements in this formal proof will consist of inequalities checked by computer, and certificates for the inequalities are provided as input to the final formal proof. Preparing a proof script for a formal proof of the Kepler Conjecture requires formalizing some parts of Euclidean geometry going beyond Hilbert's *Grundlagen der Geometrie* [30]. (Much of Hilbert's work was itself formalized by Meikle and Fleuriot [36] in 2003.) Such a formalization, which includes some notions of point set topology, is described in work of J. Harrison [28]. A more detailed description of this formal proof project is given in Hales et al. [25].

The goal of the book is to present a blueprint version of the planned formal proof: A *blueprint version* extracts mathematical ideas and formalizes them in a structure that is part way towards a formal proof. It serves as a mathematical scaffolding in constructing the detailed formal proof, organized to facilitate conversion to a formal proof script. The proof script is designed to be checked using the proof assistants Isabelle [37] and HOL Light [35] and [27].

4. The book

The book is entirely mathematical, presenting proofs in a conventional manner. It is self-contained and does not require any knowledge of the previous proof of the Kepler Conjecture. The proofs presented are designed to facilitate their conversion to a formal language. The book presents a history of the Kepler problem, details of the blueprint version, and additionally proves some new results which will follow from the formal proof.

An important feature is that this book formulates a new local density inequality. Proof of optimality of this new inequality will constitute a second generation proof of the Kepler Conjecture, independent of the previous proof. The new local density inequality reduces to the following simple form. Let the spheres have radius 1, so in a packing sphere centers are at distance at least 2 apart. Let V be the set of sphere centers of a saturated sphere packing ("saturated" means no hole in the packing is large enough to admit a new sphere; any packing is a subset of some saturated packing). Consider the piecewise linear function $L : [0, \infty) \to [0, \infty)$ having $L(t) = 1$ for $t \leq 1$, $L(t) = 0$ for $t \geq 1.26$ and linear interpolation between these values. Using this function, associate to a sphere packing with centers at V and a given center $\mathbf{v}$ the local quantity $\mathcal{L}(V, \mathbf{v}) = \sum_{\mathbf{w} \in V \setminus \mathbf{v}} L(||\mathbf{w} - \mathbf{v}||/2)$. The sum is finite since it only involves sphere centers $\mathbf{w}$ at distance at most 2.52 from $\mathbf{v}$. The local density inequality actually assigns to a given sphere center $\mathbf{v}$ the "local nearby volume" $H(\mathbf{v}) = 8m_1 - 8m_2\mathcal{L}(V, \mathbf{v})$, where $m_1 \approx 1.012, m_2 \approx 0.0254$ are explicit exact constants given in Definition 6.70, and the local inequality asserts $H(\mathbf{v}) \geq 4\sqrt{2}$. This inequality is equivalent to the assertion that $\mathcal{L}(V, \mathbf{v}) \leq 12$.

The new local inequality builds on recent work of C. Marchal [34] on the Kepler Conjecture. Marchal associates to a given saturated packing of spheres a new partition of space into cells of four kinds, plus possibly some unused extra volume. (The cells are closed and overlap on volume zero sets.) The Marchal partition of space is much simpler than the one used in the original inequality of Hales with Ferguson. Marchal's cells of type 1 are tetrahedra with vertices at four different sphere centers. The Marchal cells of type 2 are tetrahedra with vertices at three sphere centers plus one extra vertex strictly outside any sphere. The Marchal cells of type 3 are unions of two truncated half-cones having two vertices at sphere centers. The cells of type 4 are truncated half-cones with a vertex at a sphere center (and edge length $\sqrt{2}$). The cells of each type touching a sphere center together cover the entire sphere.

The Marchal approach has as a main ingredient a specific choice of weight function $f(h)$ defined for $h \geq 0$ which is compactly supported, which weights nearby volume, and which is allowed to be negative on part of its domain. Associated to a sphere center $\mathbf{v}$ is the set of all Marchal cells having $\mathbf{v}$ as a vertex. These cells fill out the whole solid angle at $\mathbf{v}$, and each one of them will be assessed for volume proportional to their solid angle at $\mathbf{v}$, using the weight function. Then to prove the Kepler Conjecture, two types of inequalities are required to be satisfied. The first local inequality says that the assessed volume at each sphere center will total up to at least the amount required by the Kepler Conjecture; it is actually expressed in a negative form, that a certain amount of "given up" volume is not too large. It takes the form that $\mathcal{L}_f(V, \mathbf{v}) \le 12$, where

$$\mathcal{L}_f(V, \mathbf{v}) = \sum_{\mathbf{w} \in V \setminus \mathbf{v}} f(||\mathbf{w} - \mathbf{v}||/2).$$

The second type of local inequality says that for each Marchal cell X the total volume assessed to it by all the sphere centers at its vertices is at most the total volume of the cell X. For type 1 and type 2 cells this inequality is expressed as $\gamma(X, f) \ge 0$, with

$$\gamma(X, f) := \mathrm{vol}(X) - \frac{2m_1}{\pi}\mathrm{tsol}(X) + \frac{8m_2}{\pi} \sum_{\text{edge } e} \mathrm{dih}(X, e) f(\frac{||e||}{2}),$$

where $||e||$ is the edge length. Here $\mathrm{tsol}(X)$ is the total solid angle of the sphere center vertices (up to 4π), while $\mathrm{dih}(X, e)$ is the dihedral angle (up to π), and $f(\cdot)$ is the weight function. Marchal proposes a function $f(h) = M(h)$, which is positive up to $h_+ = 1.3254$ and is zero above $h = \sqrt{2}$, and presents evidence that both types of inequalities above should hold for this function. This is Marchal's proposed local density inequality to prove the Kepler Conjecture, but the details he provides are not complete to show it is optimal.

The formal proof blueprint presented in the book under review uses the Marchal partition of space into cells, but reverses the numbering of cells; a Hales cell of type k is a tetrahedron with vertices at k different sphere centers, and it corresponds to a Marchal cell of type $5-k$. It formulates and studies a different score function than Marchal, taking $f(h)$ to be the piecewise linear function $L(h)$ mentioned above. This function importantly has the cutoff $L(h) = 0$ for $h \ge h_0 = 1.26$ (smaller than Marchal's positivity cutoff 1.3254), which greatly reduces the number of cases to be considered in the later analysis. It implies the upper bound $N = 15$ for the number of nearby spheres. For Hales's simplified function $L(h)$, the second set of Marchal inequalities on each cell, stating $\gamma(X, L) \ge 0$, does not always hold. The book presents in section 6.4 a method to deal with this difficulty. The bad cases concern cells having an edge with $||e||/2$ between $[h_-, h_+] \approx [1.23175, 1.3254]$, which are termed *critical edges* in Definition 6.89. The bad cells are weighted and grouped into *clusters* sharing a common critical edge; the weights for cells with several critical edges are such that their contributions to different clusters add up to 1. The replacement for the second inequality $\gamma(X, L) \ge 0$ in this case is Theorem 6.93, which asserts nonnegativity for a sum of weighted $\gamma(X, L)$ over clusters, after an additional correction term is included. Lemma 6.92 handles other cases.

The proof of the first local inequality $\mathcal{L}_L(V, \mathbf{v}) \le 12$ (stated as Lemma 6.95) is the heart of the proof. It is to be proved by contradiction, embodied in Corollary 6.100, concerning a putative counterexample local configuration of sphere centers. It reduces the proof to a finite-dimensional nonlinear optimization problem. The book develops and formalizes ideas used in the earlier proof, to systematize finding and discarding a large number of cases. It shows that a counterexample configuration with $\mathcal{L}_L(V, \mathbf{v}) > 12$ can be taken to have several extra desirable properties, called a *contravening configuration* (Lemma 8.16). These include, after fixing $\mathbf{v} = 0$ and letting W denote the finite set of sphere centers having $2 \leq ||\mathbf{w}|| \leq 2h_0 = 2.52$, the properties: (i) W globally maximizes the function $\mathcal{L}_L(W, \mathbf{v})$ over finite packings; (ii) W has cardinality 13, 14, or 15; (iii) the projected points $\overline{\mathbf{w}} = \mathbf{w}/||\mathbf{w}||$ of W onto the surface of the unit sphere, with pairs $\overline{\mathbf{w}}_1, \overline{\mathbf{w}}_2$ connected with geodesic arcs whenever $||\mathbf{w}_1 - \mathbf{w_2}|| \leq 2.52$, cut the surface of the unit sphere into geodesic polygons having all angles less than π. Property (iii) defines an abstract planar graph, and the argument then classifies all such planar graphs with some extra structure, called a *hypermap.* (The earlier proof of the Kepler Conjecture used graphs without this extra structure; the use of hypermaps facilitates the arguments.) The proof establishes that there is a finite list of such hypermaps and determines them all. To each such hypermap it associates a family of linear programs to obtain upper bounds on $\mathcal{L}(W)$. The linear programs are now shown to imply the contradiction that $\mathcal{L}(W, \mathbf{v}) < 12$, i.e., the linear program is infeasible. This can be certified by a certificate of infeasibility (using dual variables) to be input into the proof checker. The linear programs are constructed using many auxiliary geometric properties of such sphere center configurations W, detailed in Chapter 7.

The book is divided into three parts. Part I of the book, Chapter 1, presents a historical overview of work on the problem in Sections 1.1 to 1.5, finishing in Section 1.6 with a sketch of the planned blueprint proof.

Part II, Chapters 2 to 5, gives geometric foundations for the proof, comprising geometric and trigonometric equalities and inequalities, Chapter 4 treats the structure of hypermaps. Chapter 5 introduces a notion of “fan” to further describe hypermaps; this notion is different from that of “fan” in toric varieties. The book's foundations go beyond the treatment of Hilbert's *Grundlagen der Geometrie* in the treatment of Voronoi cells for individual sphere centers and of Delaunay triangulations.

Part III, Chapters 6 to 8, presents a detailed description of the steps to establish the new local density inequality. Section 6.3.2 gives an informal discussion of the tradeoffs involved between the Voronoi cells and Delaunay simplices that motivate the Marchal decomposition.

The book establishes new mathematical results. Section 8.6 proves the *strong Dodecahedral Conjecture* of Bezdek [2], which asserts that the Voronoi cell having the smallest surface area is the regular dodecahedron of unit radius. A corollary is a new proof of the Dodecahedral Conjecture of Fejes-Tóth [4]. The methods of this book also suffice to prove another conjecture of Fejes-Tóth [7], [8], stating that any packing of space by unit balls such that each ball is touched by twelve others necessarily consists of hexagonal layers; see Hales [19].

Note. In August 2014 Hales announced by email that the Flyspeck project has been completed. A formal proof of the Kepler Conjecture based on a proof script based on this blueprint has been accomplished, with two separate computer validations; cf. Hales et al. [23].

Acknowledgments

The reviewer received support from NSF grant DMS-1401224, the Clay Foundation and from ICERM. He thanks R. Kusner and W. Kusner for helpful comments.

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