From Kepler to Hales, and Back to Hilbert

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In layman's terms the Kepler Conjecture from 1611 is often phrased like "There is no way to stack oranges better than greengrocers do at their fruit stands" and one might add: all over the world and for centuries already. While it is not far from the truth this is also an open invitation to a severe misunderstanding. The true Kepler Conjecture speaks about infinitely many oranges while most grocers deal with only finitely many. Packing finitely many objects, for instance, within some kind of bin, is a well-studied subject in optimization. On the other hand, *turning* the Kepler Conjecture into a finite optimization problem was a first major step, usually attributed to László Fejes Tóth [5]. Finally, only a little bit less than 400 years after Johannes Kepler, Thomas C. Hales in 1998 announced a complete proof which he had obtained, partially with the help of his graduate student Samuel P. Ferguson [7]. There are many very readable introductions to the proof, its details, and the history, for instance, by Hales himself [8] [10]. Here I will make no attempt to compete with these presentations, but rather I would like to share an opinion on the impact of the Kepler Conjecture and its history for mathematics in general.

1 Packing Spheres

Yet we should start with the formal statement. In the following we will encode a packing of congruent spheres in 3-space by collecting their centers in a set $\Lambda \subset \mathbb{R}^3$. If $B(x,r)$ is the ball with center $x \in \mathbb{R}^3$ and radius $r > 0$ and if $c > 0$ is the common radius of the spheres in the packing then

$$\delta(r,\Lambda) \;=\; \frac{3}{4\pi r^3} \sum_{x\in\Lambda} \operatorname{vol}(B(0,r)\cap B(x,c))\,,$$

the fraction of the ball $B(0,r)$ covered by the balls in the packing Λ, is the *finite packing density* of Λ with radius r centered at the origin. Now the upper limit

$$\delta(\Lambda) \;=\; \overline{\lim}_{r\to\infty}\delta(r,\Lambda)$$

does not depend on the constant c, and it is called the *packing density* of Λ.

THEOREM (Kepler Conjecture). *The packing density $\delta(\Lambda)$ of any sphere packing Λ in $\mathbb{R}^3$ does not exceed*

$$\frac{\pi}{\sqrt{18}} \approx 0.74048 .$$

It remains to explain where the oranges are. The standard pattern originates from starting with three spheres whose centers form a regular triangle and putting another on top such that it touches the first three. This can be extended indefinitely in all directions. One way of describing this sphere packing in an encoding like above is the following:

$$\Lambda_{\text{fcc}} = \{ a(1,0,0) + b(0,1,0) + c(1,1,1) \mid a,b,c \in \mathbb{Z} \} ,$$

This amounts to tiling 3-space with regular cubes of side length 2 and placing spheres of radius $1/\sqrt{2}$ on the vertices as well as on the mid-points of the facets of each cube. This is why Λ_{fcc} is called the *face-centered cubical* packing. Figure 1 (left) shows 14 spheres (significantly shrunk for better visibility) in the cube, the black edges indicate spheres touching. To determine the packing density it suffices to measure a single fundamental domain, that is, one of the cubes. Each sphere at a vertex contributes 1/8 to each of the eight cubes which contain it while each sphere on a facet contributes 1/2. We obtain

$$\delta(\Lambda_{\text{fcc}}) = (8 \cdot \frac{1}{8} + 6 \cdot \frac{1}{2}) \cdot \frac{4\pi}{3(\sqrt{2})^3} \cdot \frac{1}{2^3} = 4 \cdot \frac{2\pi}{3\sqrt{2}} \cdot \frac{1}{8} = \frac{\pi}{3\sqrt{2}} = \frac{\pi}{\sqrt{18}} .$$

One thing which is remarkable about the Kepler Conjecture is that the optimum is attained at a *lattice packing*, that is a sphere packing whose centers form a $\mathbb{Z}^3$-isomorphic subgroup of the additive group of $\mathbb{R}^3$. This means that the optimum is attained for a packing with a great deal of symmetry while the statement itself does not mention any symmetry. It was already known to Carl Friedrich Gauß that Λ_{fcc} is optimal among all lattice packings, but the challenge for Hales to overcome was to show that there is no non-lattice packing which is more dense.

As already mentioned I will not try to explain the proof, not even its overall structure, but I would like to point out a few aspects. What also contributes to the technical difficulty is that Λ_{fcc} is by no means the only sphere packing with the optimal density $\pi/\sqrt{18}$. There are infinitely many others, including another well-known example which is called the *hexagonal-close* packing. This means that the naively phrased optimization problem

$$\sup \left\{ \delta(\Lambda) \mid \Lambda \text{ is a sphere packing in } \mathbb{R}^3 \right\} \tag{1}$$

has infinitely many optimal solutions.

A key concept in discrete geometry is the *Voronoi diagram* of a set Λ of points, say in $\mathbb{R}^3$. The *Voronoi region* of $x \in \Lambda$ is the set of points in $\mathbb{R}^3$ which is at least as close to x as to any other point in Λ. This notion makes sense for

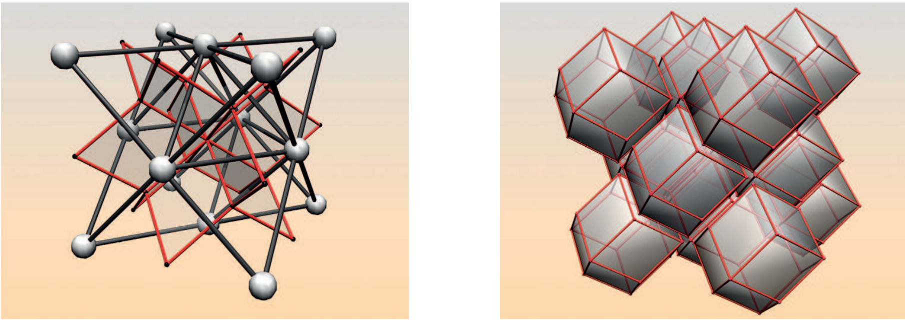

Figure 1: 14 balls of Λ_{fcc} in a cube and corresponding Voronoi regions

finite as well as infinite sets Λ. If Λ is finite or if the points are "sufficiently spread out" then the Voronoi regions are convex polyhedra. The Voronoi diagram is the polyhedral complex formed from these polyhedra. For example, the Voronoi region of any point in the face-centered cubical lattice Λ_{fcc} is a *rhombic dodecahedron*, a 3-dimensional polytope whose twelve facets are congruent rhombi. Figure 2 shows the rhombic dodecahedron, and Figure 1 (right) shows how it tiles the space as Voronoi regions of Λ_{fcc}. Some 2-dimensional cells (facets of Voronoi regions) are also shown in Figure 1 (left) to indicate their relative position in the cube.

Here comes a side-line of the story: The volume of the rhombic dodecahedron with inradius one equals $\sqrt{32} \approx 5.65685$, and this happens to be slightly larger than the volume of the regular dodecahedron of inradius one, which amounts to

$$10\sqrt{130 - 58\sqrt{5}} \;\approx\; 5.55029\,.$$

A potential counter-example to the Kepler Conjecture would have Voronoi regions of volume smaller than $\sqrt{32}$. The statement that, conversely, each unit sphere packing should have Voronoi regions of volume at least the volume of the regular dodecahedron of inradius one, is the Dodecahedral Conjecture of L. Fejes Tóth from 1943. This was proved, also in 1998, also by Hales together with Sean McLaughlin [12, 13]. Despite the fact that quantitative results for one of the conjectures imply bounds for the other, the Kepler Conjecture does not directly imply the Dodecahedral Conjectures or conversely. Not surprisingly, however, the proofs share many techniques.

We now come back to the Kepler Conjecture. The reduction of the infinite-dimensional optimization problem (1) to finite dimensions is based on these Voronoi regions. The observation of L. Fejes Tóth in 1953 was that in an optimal sphere packing only finitely many different combinatorial types of Voronoi regions can occur. This resulted in a non-linear optimization problem over a compact set. Hales simplified this non-linear problem using linear approximations. In this manner each candidate for a sphere packing more dense than the face-centered cubical packing gives rise to a linear program. Its infeasibil-

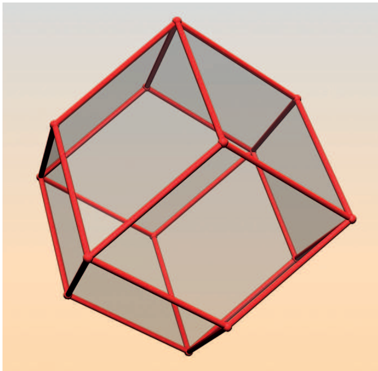

Figure 2: Rhombic dodecahedron

ity refutes the potential counter-example. This idea was improved and further extended by Hales and his co-authors such that this approach resulted in a managable computation, albeit an enormous one.

What differs mathematics fundamentally from other fields of science is the concept of a *proof*. A sequence of statements which establish the claim in a step-by-step manner by applying the rules of logic to trace the result back to a set of axioms. Once the proof is there the result holds indefinitely. The traditional way to accept a proof is to have it scrutinized by peers who review the work prior to publication in a mathematical journal. While neither the author of a proof nor its reviewers are perfect it is rather rare that results are published with a severe error. The mathematical community was content with this proof paradigm for more than 100 years, since the logical foundations of mathematics were laid at the turn from the 19th to the 20th century. The main impact of Hales' proof to mathematics in its generality is that it is about to change this paradigm, most likely forever.

After obtaining his computer-based proof Hales submitted his result to the highly esteemed journal *Annals of Mathematics*. The journal editors initiated the reviewing process which involved a team of more than a dozen experts on the subject, lead by Gábor Fejes Tóth, the son of László Fejes Tóth. It took more than seven years until an outline version of the proof was finally accepted and published [9]. To quote the guest editors of a special volume of *Discrete & Computational Geometry* on more details of the proof, Gábor Fejes Tóth and Jeffrey C. Lagarias [4]:

> The main portion of the reviewing took place in a seminar run at Eötvos University over a 3 year period. Some computer experiments were done in a detailed check. The nature of this proof, consisting in part of a large number of inequalities having little internal structure, and a complicated proof tree, makes it hard for humans to check every step reliably. Detailed checking of specific

> assertions found them to be essentially correct in every case tested. The reviewing process produced in the reviewers a strong degree of conviction of the essential correctness of this proof approach, and that the reduction method led to nonlinear programming problems of tractable size. [...] The reviewing of these papers was a particularly enormous and daunting task.

The standard paradigm for establishing proofs in mathematics was stretched beyond its limits. There is also a personal aspect to this. Hales and his co-authors had devoted a lot to the proof, and after waiting for a very long time they had their papers published but only with a warning. The referees had given up on the minute details and said so in public. The referees cannot be blamed in any way, to the contrary, their effort was also immense. This was widely acknowledged, also by Hales. But for him to see his results published with the written hint that, well, a flaw cannot be entirely excluded, must have been quite harsh nonetheless.

2 The Subsequent Challenge

It was David Hilbert who initiated a quest for provably reliable proofs in the 1920s. Ideally, he thought, proofs should be mechanized. The first trace to what later became famous as the "Hilbert Program" is maybe the following quote [16, p. 414]:

> Diese speziellen Ausführungen zeigen [...], wie notwendig es ist, das Wesen des mathematischen Beweises an sich zu studieren, wenn man solche Fragen, wie die nach der Entscheidbarkeit durch endlich viele Operationen mit Erfolg aufklären will.[1]

Hilbert's work on this subject resulted in two books with his student Paul Bernays [17, 18]. It is widely believed that the incompleteness theorems of Kurt Gödel [6] put an end to Hilbert's endeavor. However, this is not completely true.

After his proof was published with disclaimers Hales set out to start the `Flyspeck` project [2]. Its goal is to establish a formal proof of the Kepler Conjecture, quite to Hilbert's liking. The idea is to formalize the proof in a way that it can be verified by a theorem prover. Hales settled for John Harrison's `HOL Light` [14] and now also uses `Coq` [1] as well as `Isabelle` [20].

A *theorem prover* like `HOL Light` is a program which takes a human-written proof and validates that the rules of propositional logic are correctly applied to obtain a chain of arguments from the axioms to the claim, without any gap. In this way a theorem prover assists the mathematician in proving rather than finding a proof on its own. Of course, such a theorem prover itself is a

[1] These special arguments show [...], how necessary it is to study the genuine nature of the mathematical proof, if one wants to clarify questions like the decidability by finitely many operations.

piece of software which is written by humans. So, where is the catch? The actual core of a theorem prover is very small, small enough to be verified by a human, and this core verifies the rest of the system in a bootstrapping like fashion. This is already much better in terms of reliability. Moreover, if this is not enough, it is even possible to use several independent theorem provers for mutual cross-certification. This way theorem provers help to establish proofs in mathematics with a reliability unprecedented in the history of the subject. For an introduction to automated theorem proving see [21].

To get an idea how such a formal proof may look alike, for example, here is the `HOL Light` proof [15, p. 75] that $\sqrt{2}$ is irrational:

```
let NSQRT_2 = prove
 (`!p q. p * p = 2 * q * q ==> q = 0`,
  MATCH_MP_TAC num_WF THEN REWRITE_TAC[RIGHT_IMP_FORALL_THM] THEN
  REPEAT STRIP_TAC THEN FIRST_ASSUM(MP_TAC o AP_TERM `EVEN`) THEN
  REWRITE_TAC[EVEN_MULT; ARITH] THEN REWRITE_TAC[EVEN_EXISTS] THEN
  DISCH_THEN(X_CHOOSE_THEN `m:num` SUBST_ALL_TAC) THEN
  FIRST_X_ASSUM(MP_TAC o SPECL [`q:num`; `m:num`]) THEN
  ASM_REWRITE_TAC[ARITH_RULE
   `q < 2 * m ==> q * q = 2 * m * m ==> m = 0 <=>
    (2 * m) * 2 * m = 2 * q * q ==> 2 * m <= q`] THEN
  ASM_MESON_TAC[LE_MULT2; MULT_EQ_0;
       ARITH_RULE `2 * x <= x <=> x = 0`]);;
```

Modern theorem provers are already powerful enough to allow for formal proofs of very substantial results such as the Jordan Curve Theorem or the Fundamental Theorem of Algebra. However, they are nowhere near to formally verify large pieces of software such as a solver for linear programs. Yet an essential step in the proof of the Kepler Conjecture is to verify the infeasibility of thousands of linear programs. One good thing about linear programming is that infeasibility has a certificate via Farkas' Lemma. Now the idea is to check those certificates from an external LP solver (which is allowed to be unreliable) via formally verified interval arithmetic. Even if the formal proof of the Kepler Conjecture is still incomplete it is now within reach.[2] A revised version of the proof which also describes the formalization aspects appeared in 2010 [11]. An even newer approach to the Kepler conjecture, due to Christian Marchal [19] reduces the number of cases to check but still requires computer support.

Here is a side remark which may sound amusing if you hear it for the first time: Gödel's first incompleteness theorem itself has been formalized in `nqthm` by Natarajan Shankar in 1986 [3]. John Harrison's `HOL Light` version of that statement (without the proof) reads as follows:

[2]The `Flyspeck` web site claims 65 % completeness of the proof of the Kepler Conjecture by June 2010 [2].

```
|- !A. consistent A /\
       complete_for (SIGMA 1 INTER closed) A /\
       definable_by (SIGMA 1) (IMAGE gform A)
       ==> ?G. PI 1 G /\ closed G /\ true G /\ ~(A |-- G) /\
              (sound_for (SIGMA 1 INTER closed) A ==> ~(A |-- Not G))
```

3 Conclusion

A minimalistic way to tell the story about the Kepler Conjecture is: "Kepler meets Hilbert twice". The first encounter is Hilbert's 1900 address in Paris, where he specifically mentioned the Kepler Conjecture in his 18th problem. This way the Kepler Conjecture was ranked among the most eminent mathematical problems of the time. Later, at various stages in the history of the proof several different flavors of mathematical software systems played and still play a key role. The downside of the current state of affairs is that a computer based proof seems to be unavoidable. The upside, however, is that a reliable version of such a machine-assisted proof is, in fact, possible. Quite close to what Hilbert had imagined.

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References

[1] *The* `Coq` *proof assistant*, `http://coq.inria.fr/`.

[2] *The* `Flyspeck` *project*, `http://code.google.com/p/flyspeck/`.

[3] Robert S. Boyer, Matt Kaufmann, and J. Strother Moore, *The Boyer–Moore theorem prover and its interactive enhancement*, Comput. Math. Appl. 29 (1995), no. 2, 27–62. MR 1314243 (95i:68115)

[4] Gábor Fejes Toth and Jeffrey C. Lagarias, *Guest editors' foreword [The Kepler conjecture by Thomas C. Hales, with Samuel P. Ferguson]*, Discrete Comput. Geom. 36 (2006), no. 1, 1–3. MR 2229656

[5] László Fejes Tóth, *Lagerungen in der Ebene, auf der Kugel und im Raum*, Die Grundlehren der mathematischen Wissenschaften, Band 65, Springer-Verlag, Berlin, 1953, 2nd ed. 1972. MR 0057566 (15,248b), 0353117 (50 #5603)

[6] Kurt Gödel, *Über formal unentscheidbare Sätze der Principia Mathematica und verwandter Systeme I*, Monatsh. Math. Phys. 38 (1931), no. 1, 173–198. MR 1549910

[7] Thomas C. Hales, *The Kepler conjecture*, arXiv: `http://front.math.ucdavis.edu/math.MG/9811078`.

[8] ———, *Canonballs and honeycombs*, Notices Amer. Math. Soc. 47 (2000), no. 4, 440–449.

[9] ———, *A proof of the Kepler conjecture*, Ann. of Math. (2) 162 (2005), no. 3, 1065–1185. MR 2179728 (2006g:52029)

[10] ———, *Historical overview of the Kepler conjecture*, Discrete Comput. Geom. 36 (2006), no. 1, 5–20. MR 2229657 (2007d:52021)

[11] Thomas C. Hales, John Harrison, Sean McLaughlin, Tobias Nipkow, Steven Obua, and Roland Zumkeller, *A revision of the proof of the Kepler conjecture*, Discrete Comput. Geom. 44 (2010), no. 1, 1–34. MR 2639816

[12] Thomas C. Hales and Sean McLaughlin, *A proof of the dodecahedral conjecture*, arXiv: `http://front.math.ucdavis.edu/math.MG/9811079`.

[13] ———, *The dodecahedral conjecture*, J. Amer. Math. Soc. 23 (2010), no. 2, 299–344. MR 2601036 (2011d:52037)

[14] John Harrison, `http://www.cl.cam.ac.uk/~jrh13/hol-light/`.

[15] ———, *`HOL Light` tutorial (for version 2.20)*, `http://www.cl.cam.ac.uk/~jrh13/hol-light/tutorial_220.pdf`, 2011.

[16] David Hilbert, *Axiomatisches Denken*, Math. Ann. 78 (1917), no. 1, 405–415. MR 1511909

[17] David Hilbert and Paul Bernays, *Grundlagen der Mathematik. Vol. I*, J. W. Edwards, Ann Arbor, Michigan, 1944, 2nd ed. Springer-Verlag, Berlin, 1968. MR 0010509 (6,29a), 0237246 (38 #5536)

[18] ———, *Grundlagen der Mathematik. Vol. II*, J. W. Edwards, Ann Arbor, Michigan, 1944, 2nd ed. Springer-Verlag, Berlin, 1970. MR 0010510 (6,29b), 0272596 (42 #7477)

[19] Christian Marchal, *Study of the Kepler's conjecture: the problem of the closest packing*, Math. Z. 267 (2011), no. 3-4, 737–765. MR 2776056 (2012b:52032)

[20] Larry Paulson, Tobias Nipkow, and Makarius Wenzel, `http://www.cl.cam.ac.uk/research/hvg/Isabelle/`.

[21] Freek Wiedijk, *Formal proof — getting started*, Notices Amer. Math. Soc. 55 (2008), no. 11, 1408–1414.

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