Packing Space with Regular Tetrahedra

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Credits

- Thanks to Marjorie Senechal (Smith College) for providing an English translation of Dirk Struik's history paper.
- Thanks to my former student Elizabeth R. Chen, now a postdoc in the Michael Brenner lab (Harvard), for nicely finishing her PhD. (Ph.D. 2010).
- Thanks to Sharon Glotzer (Dept. of Chemical Engineering-Univ. of Michigan) for slides on her group's work.

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1. Contents of Talk

- The talk surveys the problem of packing space with congruent copies of regular tetrahedra.
- How dense can such a packing be?
- What are their packing properties?
- The problem has a very long history.

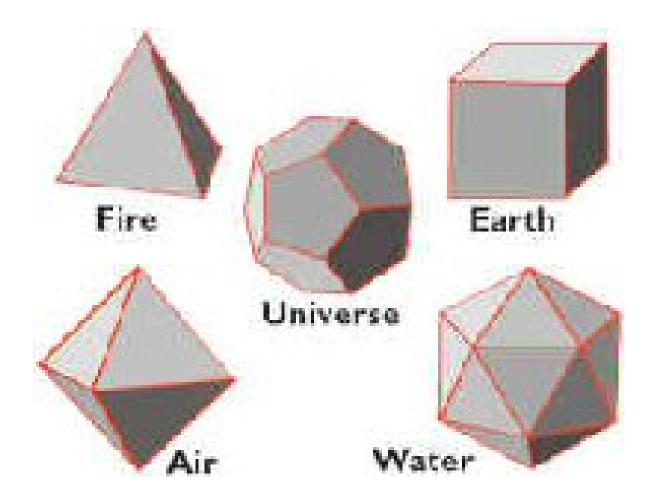
2. History to 1900

- The five regular solids (Platonic solids) are the tetrahedron, cube, octahedron, dodecahedron, icosahedron.
- At least three regular solids were known to the Pythagoreans: tetrahedron, cube and dodecahedron. (6th Centry BCE)
- Discovery of the remaining two: octahedron and icosahedron (20 sides) and proof there are only five, is sometimes attributed to Theaetetus (ca 419- 369 BCE), a contemporary of Plato.

Plato (427 BCE - 347 BCE)

- The regular solids feature in the philosophy of Plato.
- In the dialogue Timeaus Plato associates earth, air, fire, and water with the solids: cube, octahedron,tetrahedron and icosahedron.
- The dodecahedron is exceptional! Plato assigns it with the shape: "...god used for arranging the constellations in the whole heaven."

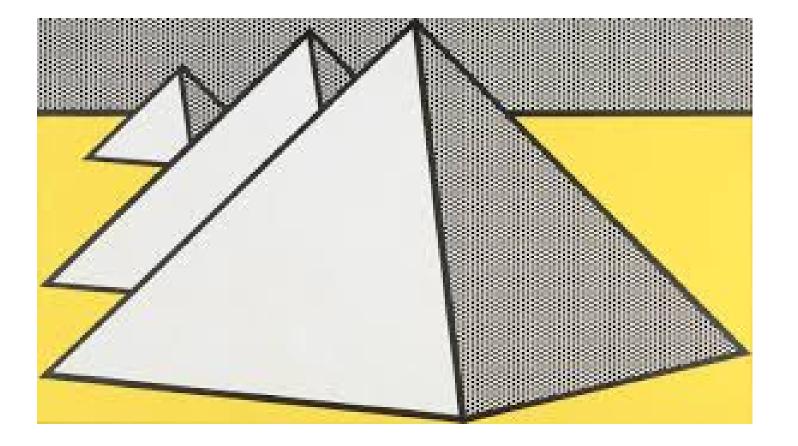
Platonic Solids



Aristotle (384 BCE - 322 BCE)

- In De Caelo (Latin title) (a.k.a. On Heavenly Bodies), Aristotle discusses the elements earth, air, fire, water etc. and the regular solids.
- He states in De Caelo, Book III, Part 8: "It is agreed that there are only three plane figures which can fill a space, the triangle, the square and the hexagon, and only two solids, the pyramid and the cube."
- In this context pyramid= regular tetrahedron. This may be taken to mean that Aristotle asserted: regular tetrahedra tile space. (If so, Aristotle made a mistake.)

Roy Lichtenstein: Pyramids II (1969)



Euclid (ca 300 BCE)

- Euclid is believed to have lived in the generation following Plato.
- Euclid's Elements, systematized geometry and number theory. It is still in print, in the Heath translation from the Greek (Cambridge University Press). (Dover reprint also available.)
- It has 13 books. Book 13 of the Elements constructs the five regular Platonic solids (Propositions 13-17). Euclid proves these are the complete list of regular solids (Proposition 18 ff.) He gives explicit constructions, producing them inscribed in a sphere.

Averroes (1126 AD- 1198 AD)

- Full name: Abu-Walid Muhammad Ibn Ahmad ibn Rushd (Cordoba, Spain–Marrakech, Morocco)
- He wrote 20,000 pages, making commentaries on most of Aristotle's works, including "De Caelo." His commentaries are based on Arabic translations of Aristotle.
- Averroes commentary & Aristotle 'De Caelo' translated from Arabic to Latin by Michel Scotus (1175– ca 1232). Much Averroes commentary survives in Latin translation, in the Justine edition of Aristotle (Venice 1562-1574).

Averroes (1126 - 1198)

- The Averroes commentary asserts that 12 tetrahedra meet at a point and fill space there. That is: Twelve pyramids (locally) fill space.
- If so, Averroes made a mistake!

Regiomontanus (1436 - 1476)

- Full name: Johannes Müller (born in Kónigsburg, Bavaria died Rome, Italy)
- Works on astronomy, plane and spherical trigonometry, calendar reform.
- He reportedly wrote a lost work titled: "On the five solids, which are called regular, and which do fill space and which do not, in contradiction to the commentator on Aristotle, Averroes."

Franciscus Maurolyctus (1494 - 1575)

- Full name: Francesco Maurolico. Born: Messina, Sicily. Of Greek origin. Benedictine monk and abbot. Became master of the mint in Messina. Gave one of earliest proofs using mathematical induction.(Arithmeticorum libri duo (1575)).
- He wrote a work called : "De qvinque solidis, qvaue vvlgo regvlaria dicvntvr, qvae videlicet eorvm locvm impleant et qvae non, contra commentatorem Aristotelis Averroem." (On the five solids, which are called regular, on which do fill space and which do not, in contradiction to the commentator on Aristotle, Averroes)

Franciscus Maurolyctus (1529)

- Colophon to work: "Libellus de Impletione loci quinque solidorum regularium per franciscum mauolycium Compositus & exararus hic finitur. Messanae In freto siculo. Decembris 9. 1529."
- This manuscript is in Rome. A transcription by Luigi de Marchi in 14 July 1883, listed a table of contents. From the table of contents we infer Maurolyctus knew: There is a periodic tiling of space whose unit cell is 6 regular octahedra plus 8 regular tetrahedra.
- The manuscript and its contents are the subject of the ongoing PhD thesis of Claudia Addabbo (Univ. of Pisa).

David Hilbert (1862-1943)

- Hilbert made major contributions in many fields: Invariant Theory ("Hilbert basis theorem") Number Theory ("Zahlbericht") Geometry ("Foundations of Geometry"), Mathematical Physics ("Hilbert spaces") Mathematical Logic ("Hilbert program") (⇒ He was a "polymath")
- Hilbert formulated at the 1900 International Mathematical Congress, held in Paris, a famous list of Mathematical Problems. (23 problems, some still unsolved.)

Hilbert's 18-th Problem (1900)

- The 18-th problem, on Hilbert's list discusses: packing and tiling of space by congruent polyhedra.
- 'I point out the following question [...] important in number theory and perhaps sometimes useful to physics and chemistry: How can one arrange most densely in space an infinite number of equal solids of given form, e.g. spheres with given radii or regular tetrahedra with given edges (or in prescribed position), that is, how can one so fit them together so that the ratio of the filled space to the unfilled space may be as great as possible."

Hilbert's 18-th Problem- Remarks

- The main part of Hilbert's 18-th problem, not considered here, concerns crystallographic packings in higher dimensions.
- It was solved by Ludwig Bieberbach (1910, 1912).

Packing Spheres versus Packing Regular Tetrahedra

• Kepler's Conjecture (1611). A densest sphere packing is given by the face-centered cubic (FCC) lattice packing ("cannonball packing").

FCC Packing Density: $\frac{\pi}{\sqrt{18}} \approx 0.74048$.

- Kepler's Conjecture was proved in 1998-2006 by Thomas
 C. Hales with Samuel P. Ferguson. It is a hard problem.
 (250+ pages). Update: Hales formal proof (2015).
- Packing regular tetrahedra is probably much harder! (Tetrahedra are not invariant under rotation!)

Hilbert: Two Packing Problems for Regular Tetrahedra (1900)

- General Packings: Pack congruent regular tetrahedra, allowing Euclidean motions.
- Translational Packings: Pack allowing copies of a single tetrahedron moved only by translations.
- A Subclass of Translational Packings: Lattice packings.

3. Interlude: Hilbert's Third Problem

- Hilbert's third problem: "The equality of the volumes of two tetrahedra of equal bases and equal altitudes" (Scissors Congruence Problem)
- Goal. To prove an impossibility result showing that the (infinite) "method of exhaustion" is needed for a satisfactory theory of 3-dimensional volume.
- To "succeed in specifying two tetrahedra of equal bases and equal altitudes which can in no way be split up into congruent tetrahedra, and which cannot be combined with congruent tetrahedra to form two polyhedra which themselves can be split up into congruent tetrahedra."

- Call the finite cutting up operation: "Scissors Congruence" (Equicomplementability)
- Solved by Max Dehn (1900, 1904). He introduced a new 3-dimensional scissors congruence invariant, which is an obstruction to polyhedra of equal volume being equivalent under scissors congruence.
- New Dehn invariant is 1-dimensional:

$$D_1(P) = \sum_e (edge \ length) \otimes (dihedral \ angle)$$

- Dehn showed that a regular tetrahedron is not scissors congurent to a cube of the same volume.
- More recently (Conjecture of Hadwiger 1963), solved 1980:
 Theorem 1. (Debrunner (1980))
 If a polyhedron P tiles three-dimensional space, then P must be scissors congruent to a cube of the same volume.
- Result rediscovered by Lagarias and Moews, Disc. Comp. Geom. 1995.

• Now we have also:

Theorem 2. (Wolfgang Schmidt (1961) If a polyhedron P does not tile space, then its packing density

 $\Delta(P) < 1.$

- Combining these results with that of Dehn, we conclude: **Corollary.** The maximal density of a packing of congurent copies of a regular tetrahedron T satisfies $\Delta(T) < 1$.
- This proof is ineffective. It gives no upper bound.

- Dehn also defined higher-dimensional invariants, one in each even codimension: codimension 0= volume, codim 2, codim 4, etc.
- There are thus $\lceil \frac{n}{2} \rceil$ such invariants in dimension n.
- Open Problem: Are Dehn's invariants a complete set of Euclidean scissors congruence invariants?
- Answer: Yes, for dimensions $n \le 4$. (Sydler (1965) for n = 3, Jessen (1969) for n = 4.) Open Problem, for $n \ge 5$.

4. More History

Hermann Minkowski (1864-1909)

- Minkowski is known for the *Geometry of Numbers* (1896), Many applications in algebraic number theory, Diophantine approximation.
- Geometry of numbers concerns interactions of: lattices and convex bodies. Specifically studies: densest *lattice packings* of congruent convex bodies.
- Minkowski (1896, 1904) obtained sharp results for centrally symmetric convex bodies (in theory).

Hermann Minkowski (1904)

- But: A regular tetrahedron is a non-symmetric convex body.
- In 1904, Minkowski showed that the densest lattice packing of non-symmetric convex bodies *C* is the same as that of their centrally symmetric difference body

$$D(C) := \frac{1}{2}(C - C) = \left\{ \frac{1}{2}(x - y) : x, y \in C \right\}$$

• He applied his method to the regular tetrahedron. He asserted that the densest lattice packing of a regular tetrahedron has density

$$\frac{9}{38} = 0.236842...$$

Helmut Groemer (1962)

• Theorem. (Groemer) There exists a lattice packing of regular tetrahedra having packing density

$$\Delta = \frac{18}{49} = 0.367346...$$

• \Rightarrow Minkowski made a mistake!

(He asserted the difference body of a regular tetrahedron is a regular octahedron; it is not.)

Douglas Hoylman (1970)

- Hoylman proved Groemer's construction is optimal.
- **Theorem.** (Hoylman) The densest lattice packing of a regular tetrahedron has packing density

$$\Delta = \frac{18}{49} = 0.367346...$$

Ulrich Betke and Martin Henk (2000)

- Betke and Henk (2000) designed an efficient algorithm to find the density of the densest lattice packing of any (symmetric or nonsymmetric) polyhedron (i.e. 3-dimensional polytope). (Discrete & Computational Geometry 16 (2000), 157–186.)
- The algorithm solves a series of linear programming problems. They make a computer implementation of the algorithm.
- Method is applied to compute the densest lattice packings of all regular polyhedra.

Elizabeth Chen (PhD student): Studies Packings of Tetrahedral Clusters 2005

Locally dense structures of tetrahedra



John H. Conway and Salvatore Torquato (PNAS 2006)-1

- John Horton Conway is a well known mathematician at Princeton, and Salvatore Torquato is a chemist, materials scientist (and much more) at Princeton. They find general packings and coverings of space with regular tetrahedra.
- (Initial packing) Pack 20 regular tetrahedra inside a regular icosahedron, with centers touching at central point. Form the convex hull of these 20 tetrahedra. This is a centrally symmetric convex body *C*. Then lattice pack *C* using the Betke and Henk algorithm. Packing density attained this way: $\Delta = \frac{45}{64} = 0.703125$.

John H. Conway and Salvatore Torquato (PNAS 2006)-2

 (Packing Improvement) ("reformed Scottish packing")
 Deform the arrangement of 20 tetrahedra slightly and repack as above. Packing density obtained is now:

 $\Delta pprox 0.7165598.$

• (From Conway-Torquato paper abstract) "Our results suggest that the regular tetrahedron may not be able to pack as densely as the sphere, which would contradict a conjecture of Ulam. The regular tetrahedron might even be the convex body having the smallest possible packing density."

Conway H J & Torquato S, PNAS 103(28): 10612 (2006).

0.7166 ^{с⊤}	"very low"cт	0.7175cт
"Icosahedral" lattice packing	Type I Clathrate	Type II Clathrate
Scottish* bubbles	Irish bubbles	Welsh bubbles

Conway and Torquato conjectured:

35

Is Ulam wrong? Are tetrahedra the worst packers of all?

The Glotzer Group @ University of Michigan

Paul M. Chaikin (2007)

- Paul Chaikin is a physics professor at New York University.
- With undergraduates, experimented with filling fishbowls and other containers with tetrahedral dice. Packings seem more dense than spheres, about 75 percent.
- No rigorous proof: the dice are not perfect tetrahedra, the container walls influence the density. Error estimate 3%.
- Talk at APS meeting (March 2007): P. Chaikin, Stacy Wang (Stuvesant High School !), A. Jaoshvili, "Packing of Tetrahedral and other Dice," BAPS.2007.MAR.S29.10

Elizabeth R. Chen (2007-2008)

- Elizabeth Chen finds a "world record" dense packing of regular tetrahedra. (Discrete and Computational Geometry 40 (2008), 214–240.) (Submitted 1 January 2007)
- Theorem. (E. Chen) There exists a packing of regular tetrahedra having density at least 0.7786.
- This disproves the speculation of Conway and Torquato, so Ulam's Conjecture remains unsolved.

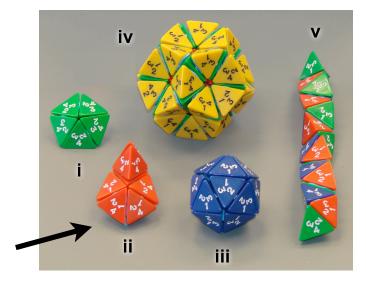
Ulam's Conjecture: The hardest 3-dimensional convex body to pack is the solid sphere (density ≈ 0.74048)

Chen "Wagon Wheel" packing-1

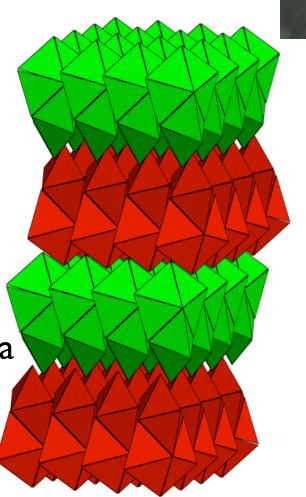
- Five regular tetrahedra sharing a common edge fill space nearly perfectly around that edge. The uncovered dihedral angle is: 0.020433... of the full dihedral angle.
- "Wagon wheels" (Nonomers) are configurations of 9 tetrahedra, having two "wagon wheels" of 5 tetrahedra on diagonally opposite edges.
- Geometric fact: diagonally opposite edges are perpendicular. This favors cubical packings.

Ulam verified for tetrahedra in 2007





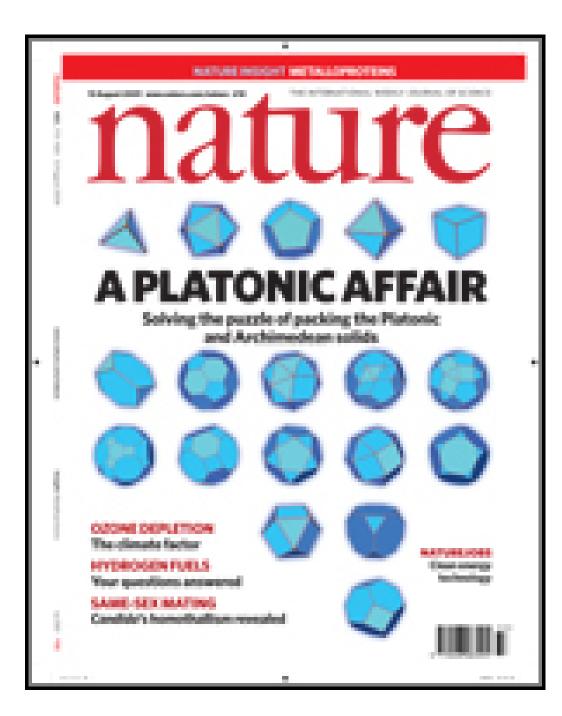
Elizabeth Chen (2007) proposed and constructed a crystal of nonamers with $\phi = 0.7786 > \phi_{rcp}!$ Discrete Comput. Geom. 40: 214 (2008)





Torquato Strikes Back. (13 August 2009)

- S. Torquato and Y. Jiao, Dense packings of the Platonic and Archimedean solids, Nature 460 (13 August 2009). (submitted 29 April 2009)
- They obtain a "world record" tetrahedral packing by "deforming" the Chen wagon-wheel packing.
- Density achieved: $\Delta \approx 0.78202$.
- Based in part on this result, the paper gets on the front cover of Nature.



Torquato Followup, Phys Rev E (arxiv 9 Sept 2009)

- S. Torquato and Y. Jiao, Dense packings of polyhedra: Platonic and Archimedean solids, Phys. Rev. E. (50 pages). arXiv:0909.0940 9 Sept 2009 (submitted June 2009)
- Paper present further deformations of the "wagon wheel packings" achieving a "world record" density $\Delta = 0.8203...$ The final packing is "disordered."

The method used a computer search, termed the "Adaptive Shrinking Cell" (ASC) optimization method. It "squeezes" uses a "simulated annealing" stochastic Monte Carlo method with acceptance rules.

Glotzer Group Packings (Nature 10 Dec 2009)

- Sharon Glotzer is a Professor of Chemical Engineering (also Materials Science, Physics and much more) at the University of Michigan. Her research group studies Computational Nanoscience and Soft Matter.
- A. Haji-Akbari, M. Engel, A. S. Keys, X. Zheng, R. G. Petsche, P. Palffy-Muhoray, S. C. Glotzer, "Disordered, quasicrystalline and crystalline phases of densely packed tetrahedra", Nature 462, 10 Dec 2009, 773–777. (submitted 5 July 2009). [Lead authors: grad student Amir Haji-Akbari and postdoc Michael Engel.]

Aside: Nanomaterials

- There is now interest in nanomaterials made of tiny tetrahedra. What properties do such materials have?
- Methods now exist to fabricate such materials. Variations: tetrahedra that are "sticky" on one face.
- Of great interest: unusual optical properties.

Glotzer Group Packing-2 (10 Dec 2009)

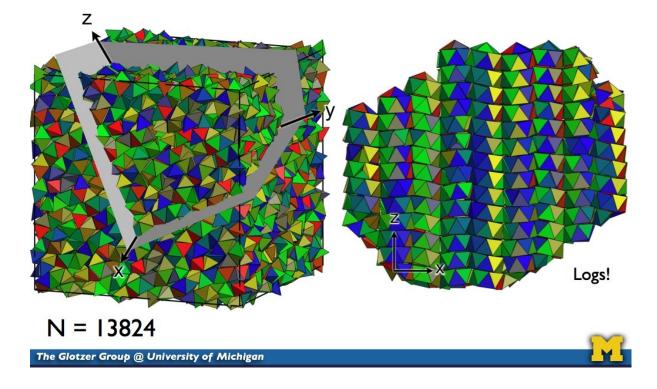
- By "squeezing" tetrahedral packings (simulation), they predict that a fluid of hard tetrahedra undergoes a first order phase transition to a dodecagonal quasicrystal having packing density approximately 0.8324. The quasicrystal property is remarkable!
- By further compression they obtain a "world record" tetrahedra packing with density

$\Delta \approx 0.8503...$

Method used Glotzer group "squeezing" computer package: Glotzilla.

Glotzer Group Dodecagonal Quasicrystal Packing-3

A dodecagonal quasicrystal!



Quasicrystals-1

- Quasicrystals are materials have diffraction patterns indicating long range order of atoms, but which have forbidden symmetries ruling out periodic atomic order. Discovered by Dan Schechtman (Technion-Haifa) while at National Bureau of Standards (= NIST) in 1982, published Phys Rev. Letters 1984.
- These materials can exhibit diffraction symmetries forbidden for crystals: 5-fold symmetry or 12-fold symmetry.
- Their discovery was initially treated with incredulity and ridicule.

Quasicrystals-2

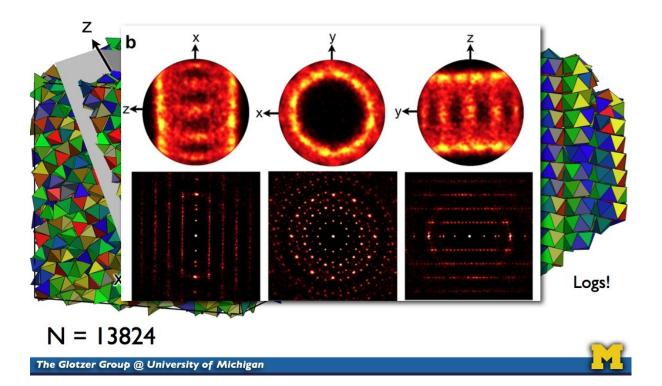
- Over 200 kinds of quasicrysalline materials are now known. Typically they are mixtures of two or three kinds of atoms (eg. AlCuFe) at suitable density.
- Some quasicrystalline phases appear to be thermodynamically stable. They can be grown to macroscopic size, e.g. 1 inch across, and then appear crystalline in the usual sense.
- Dan Shechtman awarded Nobel Prize in Chemistry 2011 for this discovery (October 2011).

Quasicrystals-3

- Regular tetrahedra are the first example known of single hard bodies which (apparently) exhibit a quasicrystalline phase.
- Note: Ideal dodecagonal quasicrystalline symmetry is aperiodic in two directions, periodic in third direction.

Glotzer Group Quasicrystal Packing: Diffraction

A dodecagonal quasicrystal!

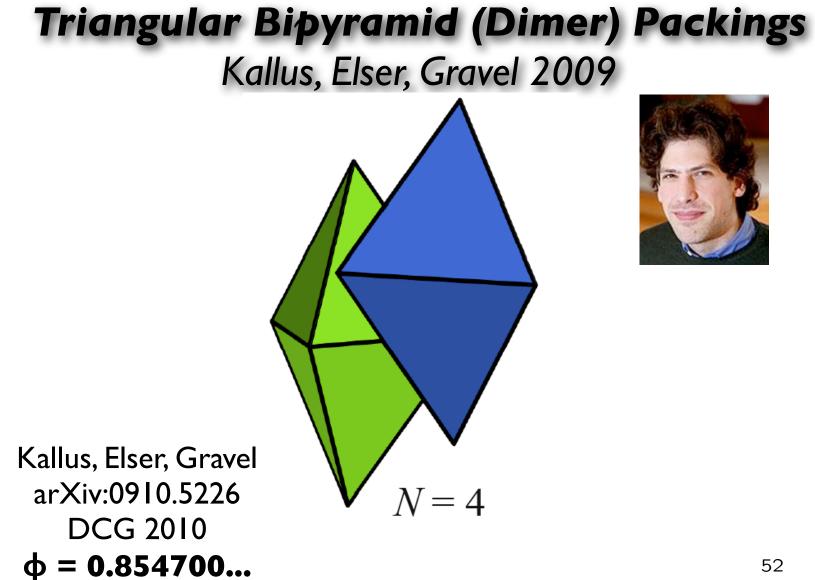


Y. Kallus, V. Elser and S. Gravel (arXiv 9 Dec. 2009)

- Yoav Kallus is a physics grad student at Cornell in the group of Veit Elser, where Simon Gravel is postdoc (as of 2009).
- They find a simple crystallographic packing having only four tetrahedra in the unit cell. These tetrahedra correspond to a dimer of two tetrahedra glued face to face, and a reflection of this dimer. The crystallographic symmetry group acts transitively on the dimers.

They achieve a new "world record" density of

$$\Delta = \frac{100}{117} \approx 0.854700...$$





Flashback: Double Lattice Packings (Kuperberg² (1990))

- The Kallus-Elser-Gravel packing uses idea of G. Kuperberg and W. Kuperberg, that *double lattice packings*, using a body *P* with its reflected body -*P*, yield good packings.
- The Kuperbergs used their idea (Disc. Comp. Geom **5** (1990), 389-397) in 2-D to show that *every convex body* S in the plane has a general packing density of at least

$$\Delta(S) \ge \frac{\sqrt{3}}{2} = 0.8660....$$

(Comparison: a circular disk *C* packs with density $\Delta(C) = \frac{\pi}{\sqrt{12}} \approx 0.9069....$)

Flashback-2: Ulam Problem in Two Dimensions

- Mini-Ulam Problem: What is the hardest convex body to pack in two dimensions?
- Answer: Definitely **NOT** a circular disk, whose packing density is $\frac{\pi}{\sqrt{12}} \approx 0.9069$
- Reinhardt (1934) found a "smoothed octagon" O that has smaller packing density

$$\Delta(O) = \frac{8 - \sqrt{32} - \log 2}{\sqrt{8} - 1} \approx 0.902414.$$

Flashback-3: Ulam Problem in Two Dimensions

- Reinhardt (1934) conjectured the "smoothed octagon" to be optimal.
- Proving the Reinhardt body is "hardest to pack" seems complicated! (There is some evidence for its optimality, in a variational approach to the problem put forward by Tom Hales (2011).)
- Best lower bound for general bodies is strictly bigger than Kuperberg bound 0.8660.... Current best lower bound for centrally symmetric convex bodies is 0.892656.. (Tammela (1970)).

Torquato and Jiao Return (arXiv 21 Dec 2009)

- S. Torquato and Y. Jiao, Analytical Constructions of a family of dense tetrahedron packings and the role of symmetry, eprint: arXiv:0912.4210 21 Dec. 2009 (Condensed Matter).
- Torquato and Jiao find a two-parameter family of deformations of the Kallus-Elser-Gravel packing. They optimize over their family and obtain a new "world-record" packing with density

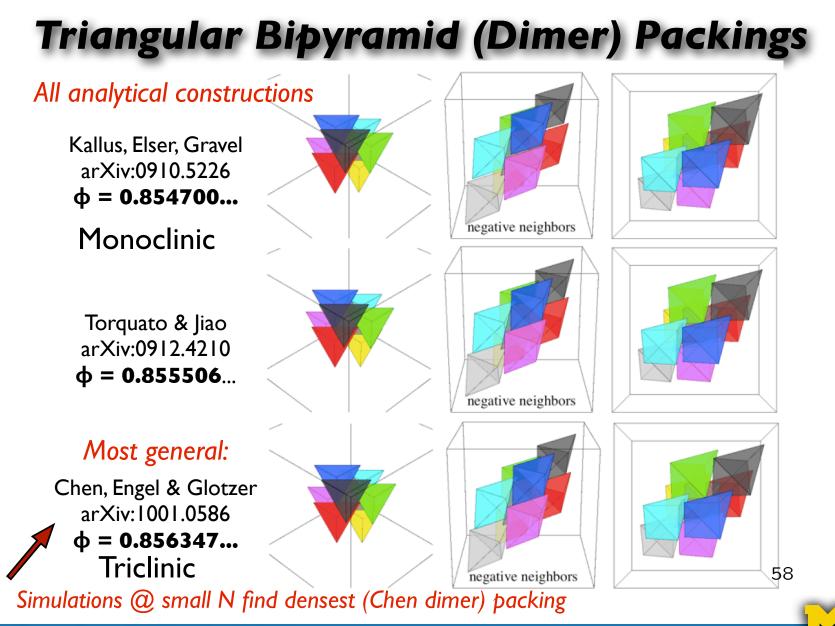
$$\Delta = \frac{12250}{14319} \approx 0.855506...$$

Chen, Engel and Glotzer (arXiv 5 January 2010)

- Elizabeth R. Chen, Michael Engel, and Sharon C. Glotzer, Dense crystalline dimer packings of regular tetrahedra, Disc. Comp. Geom 44 2010, 253–280.
 eprint arXiv:1001.0586 5 January 2010 (Condensed Matter)
- They find a three-parameter family of deformations of the Kallus-Elser-Gravel packing. They argue that that 3 is the maximum dimensional set of deformations. They optimize and obtain a new "world-record" packing with density

 $\frac{4000}{4671} \approx 0.856347...$

This is the *current champion packing!*



The Glotzer Group @ University of Michigan

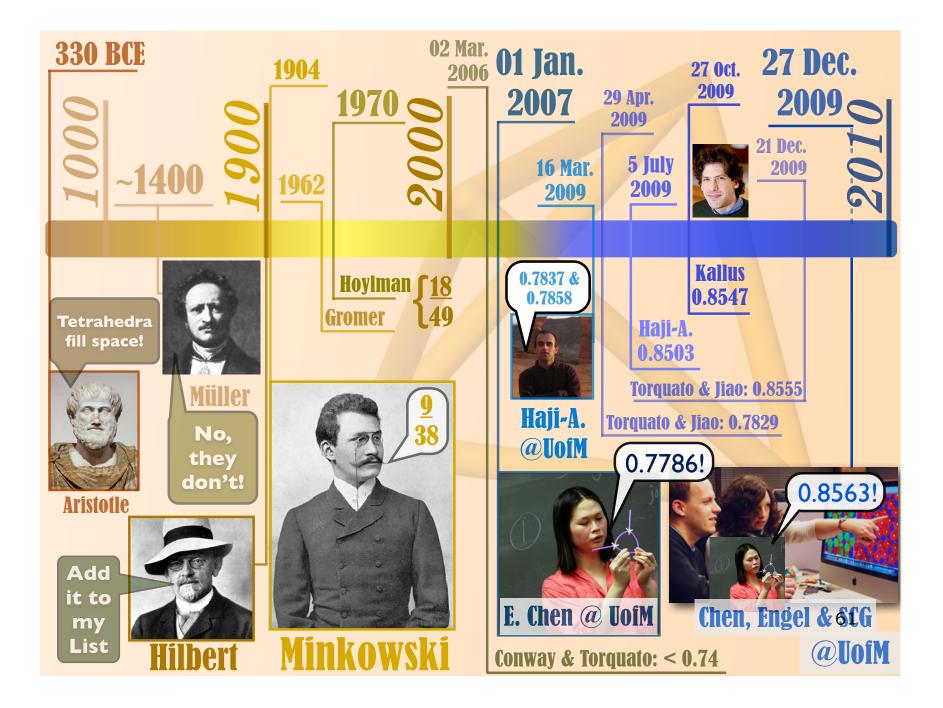
Upper Bound for Tetrahedral Packing Density

- Know abstractly that the maximal packing density $\Delta(T)$ of regular tetrahedra is some constant $c_0 < 1$.
- Problem. Obtain a numerical upper bound for this quantity.
- Y.Kallus, V. Elser and S. Gravel (Disc. Comp. Geom. 2011) obtained such a bound: It is less than 1 by a minuscule amount:

 $2.6 \times (10)^{-25}$.

Summary-1

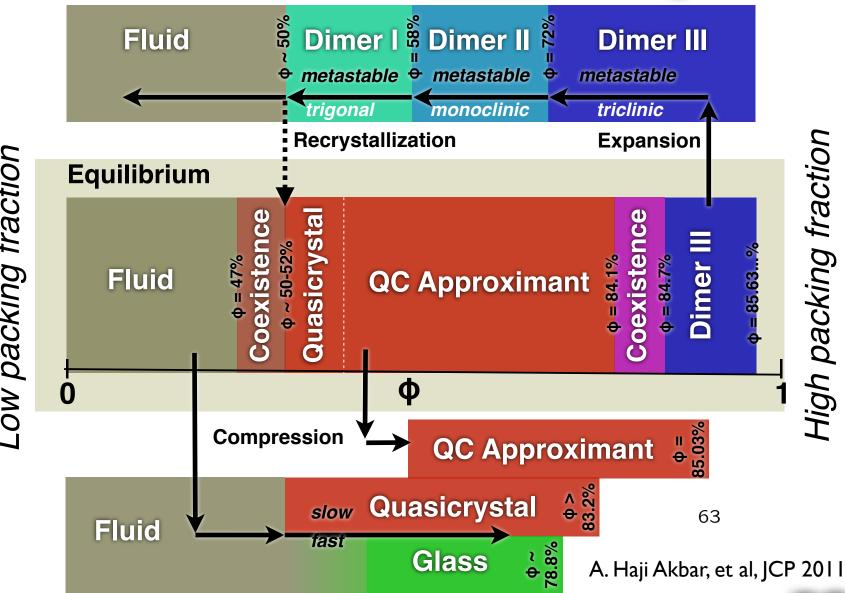
- In low-dimensional discrete geometry, mistakes eventually get uncovered and corrected.
- Large-scale computational work is valuable and useful in making progress in this area.
- The current "world record" packing may be a viable candidate for a "densest packing of regular tetrahedra."
- The progress on this problem justifies Hilbert's remark "sometimes useful in chemistry and physics," and now also in materials science!



Recent Progress

- Materials Science. Glotzer group further analyzes phase diagram of packing tetrahedra, studied sensitivity to changing shape slightly.
- Mathematical Physics. Understanding quasicrystalline phase transitions in simple models (C. Radin, U. Texas)
- (Soft) Condensed Matter Physics. General packing search algorithms (Elser, Kallus, Gravel), (Torquato et al)
- Metric Geometry. Study of densest packings of other shapes: Regular octahedra, archimedean solids.

Hard Tetrahedron Phase Diagram



Low packing fraction

High packing fraction

References

- J. C. Lagarias and Chuan-Ming Zong, *Mysteries in packing regular tetrahedra*, Notices Amer. Math. Soc. **15** (2012), no. 11, 1540–1549.
- Dirk J. Struik, *Het Probleem 'De Impletione Loci'*, Nieuw. Archief voor Wiskunde **15** (1925–1928), no. 3, 121–137 (Dutch) [Marjorie Senechal translation to be posted on arXiv at some future date.]

Thank you for your attention!