Computer-assisted proofs: Kepler conjecture and 2-sphere packings

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- Sphere packings in 3D
- ② Optimality proofs for ○|○••|●
- Salt packings
- Oensity bound: from disks to spheres
- Conclusion
- 6 Homework

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Kepler conjecture: -packings

3D close —packings







Kepler conjecture: -packings

3D close —packings









Kepler conjecture: -packings

3D close —packings









Sphere packings in 3D

Kepler conjecture: -packings

3D close —packings $\delta^* = \frac{\pi}{3\sqrt{2}} \approx 74\%$



close packings are optimal among lattice packings









Gauss. 1831

Hales, Ferguson, 1998-2014

(Conjectured by Kepler, 1611)

Forum of Mathematics, Pi 2017

Close packings are optimal.

s close backings are obtained among lattice backings	00000, 1001
• 18th problem of the Hilbert's list	1900
 6 preprints by Hales and Ferguson 250 pages and > 180000 lines of code 	ArXiv 1998
• reviewing: 13 reviewers, 4 years "99% certain"	1999–2003
 published proof: 300 pages, 3 computer programs 	DCG 2006
Flyspeck project: formal proof (HOL Light proof assistant)	2003-2014

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Steps of the proof

 δ^* denotes the maximal density



oooloo partition space into "small" cells

FM-triangulation

 $\circ|\circ\circ|$ \circ find a suitable function to represent the density

emptiness E

Optimality proofs for • • • •

Steps of the proof

 δ^* denotes the maximal density



oloo partition space into "small" cells

FM-triangulation

oloo find a suitable function to represent the density

emptiness E potential \dot{U}

oo o distribute the density among the vertices in each cell

check all possible local configurations

(•) choice of m in U run through all coronas

••• • treat special cases configurations close to local optima ϵ -triangles

coronas of \mathcal{T}^*

Optimality proofs for • | • • • | •

Steps of the proof

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ooo oo partition space into "small" cells

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potential U

our opening verify that the redistributed density $\leq \delta^*$ check all possible local configurations

(•) choice of m in U

ooo| treat special cases
configurations close to local optima

 ϵ -triangles coronas of \mathcal{T}^*

oo oo verify that the sum of vertex densities in a cell \geq its density check all possible cells

interval arithmetic

Space partition

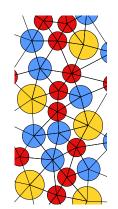




Delaunay triangulation



FM-triangulation \mathcal{T} (weighted Delaunay triangulation)



3D, 🥚

Voronoi cells + Delaunay simplices

HF-partition \mathcal{P}

consists of several types of simplices and modified Voronoi cells

(Sphere packings II. A formulation of the Kepler Conjecture)

only Voronoi cells or only Delaunay simplices

 \Downarrow

local configurations denser than δ^*

regular dodecahedron for Voronoi cells (as in dodecahedral conjecture)





Hales and McLaughlin 1998

Optimality proofs for • | • • • | •

Space partition

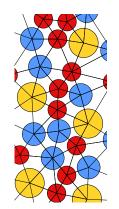




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(Sphere packings II. A formulation of the Kepler Conjecture)

pentagonal prism for Delaunay simplices

only Voronoi cells or only Delaunay simplices \Downarrow local configurations denser than δ^*





Ferguson 2006

Suitable function to measure the density



2D, 🔵

2D, **○●●**

3D, 🥚

density δ

emptiness

 $E(\Delta) := \delta^* \times area(\Delta) - area(\Delta \cap P)$

compression

compression

$$\Gamma(R) := vol(R \cap P) - \delta_{oct} \times vol(R)$$

 $\delta_{\mathsf{oct}} := \delta(\mathsf{tight\ regular\ octahedron}) < \delta^*$

$$\delta^* = rac{\delta_{ ext{tet}}}{3} + 2rac{\delta_{ ext{oct}}}{3}$$

Suitable function to measure the density

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An additive function reflecting the density:

$$\Gamma(R) < 0$$
 iff the density of R is less than $\delta_{\rm oct}$
 $\Gamma(R) > 0$ iff the density of R is greater than $\delta_{\rm oct}$

$$\delta \leq \delta^* \Leftarrow \Gamma$$
 is "low enough" on each small region



vertex potential

for
$$\Delta \in \mathcal{T}, v \in \Delta$$
, $\dot{U}^{v}_{\Delta} = V_{xyz} + m \times |\hat{v} - \hat{v}_{xyz}|$

where x,y,z are disc radii of Δ \hat{v} is the angle of Δ in v and $V_{\rm xyz},m,\hat{v}_{\rm xyz}$ are constants

3D, 🥚

score

for $R \in \mathcal{P}, v \in R$, $\sigma(R, v)$ depends on the type of R

if R is a Voronoi cell of v (R = Vor(v)), then $\sigma(R, v) = 4\Gamma(R)$ and $\sigma(R, w) = 0$ for $w \neq v$

if R is a simplex, σ varies in function of its properties and depends on Γ

2D, 🔘 💿 •

vertex potential

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$$U(\Delta) = U_{\Delta}^{A} + U_{\Delta}^{B} + U_{\Delta}^{C} \leq E(\Delta)$$

i.e. U is easy to manipulate and is at most E (lower approximation)

score

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if R is a simplex, σ varies in function of its properties and depends on Γ

$$\sum_{v \in R} \sigma(R, v) = 4\Gamma(R)$$

i.e. score of a region always equals to $4 \times \text{compression}$

(Sphere packings II. A formulation of the Kepler Conjecture)

Verify that redistribution $\leq \delta^*$ around each vertex

Ooo

for each $v \in \mathcal{T}$,

$$\sum_{\Delta \in C_{\nu}} \dot{U}_{\Delta}^{\nu} \ge 0 \qquad (\bullet)$$

configuration around a vertex – corona C

combinatorial representation of C – symbolic corona S(C)

choose m to satisfy

$$\sum_{\substack{x,y,z\\ \text{disc, radii of}\\ \Delta \in C}} V_{xyz} + m \times |2\pi - \sum_{\substack{x,y,z\\ \text{disc, radii of}\\ \Delta \in C}} \widehat{xyz}| \ge 0$$

for all coronas C

FM-triangulation \Rightarrow bounded |S(C)| \Rightarrow finite number of inequalities on n \Rightarrow computer search

3D, 🥚

for each
$$v \in \mathcal{P}$$
, $\sum_{R \in D_v} \sigma(R, v) \leq 8pt$

configuration around a vertex – decomposition star \boldsymbol{D}

combinatorial representation of D – graph G(D)

conditions on geometry of D "easily" implying $\sigma(D) \leq 8pt$ (interval arithmetic branch&bound)

(Sphere packings IV. Detailed bounds)

tame graphs – 25 000 graphs of the remaining D have restricted geometry \Rightarrow max $\sigma(D) \leq 8$ pt (linear programming)

(Sphere packings VI. Tame graphs and linear programs, except pentagonal prism graph,

(Sphere packing V. Pentahedral prisms,

6 / 15

CC graph and HCP graph

Verify that redistribution $\leq \delta^*$ **around each vertex**



for each
$$v \in \mathcal{T}$$
,
$$\sum_{\lambda \in \mathcal{L}} \dot{\mathcal{U}}^v_{\Delta} \geq 0 \qquad \qquad (ullet)$$

choose *m* to satisfy

$$\sum_{\substack{x,y,z\\ X \in C}} V_{xyz} + m \times |2\pi - \sum_{\substack{x,y,z\\ \text{disc radii} \text{ of } \\ \Delta \in C}} \widehat{xyz}| \ge 0$$

for all coronas C

FM-triangulation \Rightarrow bounded |S(C)| \Rightarrow finite number of inequalities on m ⇒ computer search

3D, 🦲

$$\mathcal{T}, \qquad \qquad \text{for each } v \in \mathcal{P}, \ \sum_{R \in \mathcal{D}_v} \sigma(R, v) \leq 8pt$$

$$\sum_{\Lambda \in \mathcal{C}} \dot{\mathcal{U}}_{\Delta}^v \geq 0 \qquad \qquad \text{(\bullet)} \qquad \text{configuration around a vertex} -$$

conditions on geometry of D "easily" implying $\sigma(D)$ < 8pt (interval arithmetic, branch&bound)

(Sphere packings IV. Detailed bounds)

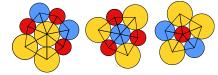
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(Sphere packings VI. Tame graphs and linear programs) except pentagonal prism graph,

(Sphere packing V. Pentahedral prisms)

FCC graph and HCP graph



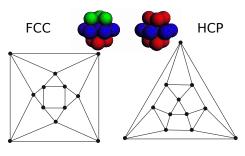


for the coronas of \mathcal{T}^* , $\sum_{\substack{x,y,z\\\text{disc radii of}\\ \Lambda \in V \text{-corona}}} V_{xyz} := 0$

for tight triangles, $U(\Delta_{xyz}) := E(\Delta_{xyz})$

€-triangles – triangles close to tight⇒ potential close to emptiness

3D, 🥚



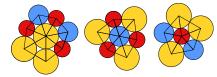
FCC and HCP decomposition stars have maximal score

 \Rightarrow close configurations have high score

Extremal cases







for the coronas of \mathcal{T}^* , $\sum_{\substack{x,y,z\\\text{disc radii of}\\\Lambda \subseteq Y_x \text{corona}}} V_{xyz} := 0$

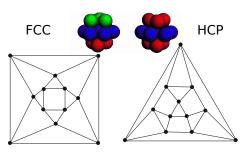
for tight triangles, $\mathit{U}(\Delta_{\scriptscriptstyle \mathit{XYZ}}) := \mathit{E}(\Delta_{\scriptscriptstyle \mathit{XYZ}})$

←-triangles – triangles close to tight⇒ potential close to emptiness

derivatives on side lengths x_i :

$$\min_{T_{\epsilon}} \frac{\partial E}{\partial x_i} \Delta x_i \ge \max_{T_{\epsilon}} \frac{\partial U}{\partial x_i} \Delta x_i$$
(interval arithmetic)

3D, 🥚



FCC and HCP decomposition stars have maximal score

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derivatives to prove that FCC and HCP are local maxima

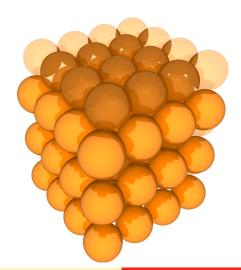
(Sphere packings III. Extremal cases)

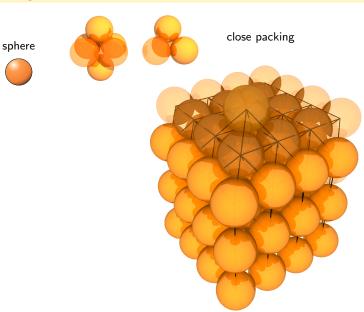
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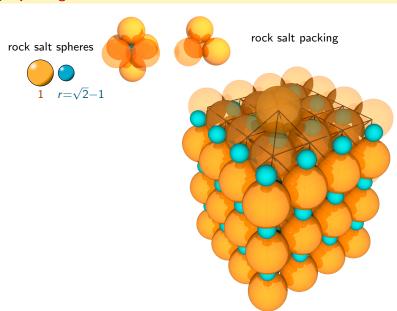


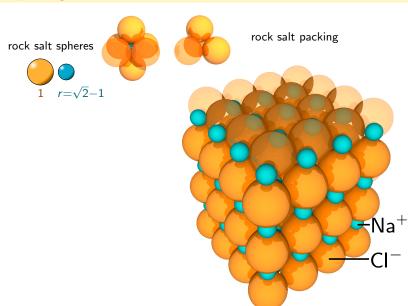


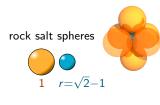
close packing







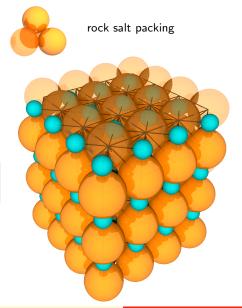




 $\begin{array}{l} {\sf triangulated} \to {\sf simplicial} \\ {\sf (contact\ graph\ is\ a\ "tetrahedration")} \end{array}$

Fernique, 2019

The only simplicial 2-sphere packings in 3D are rock salt packings.





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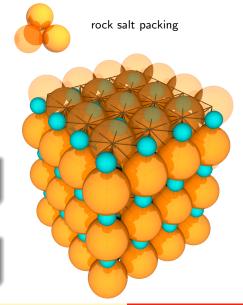
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The only simplicial 2-sphere packings in 3D are rock salt packings.

Salt conjecture

open problem

Rock salt packings are optimal $\delta^* = (\frac{5}{3} - \sqrt{2})\pi \approx 79\%$.



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Upper density bound for opposition on 2D

Florian, 1960

The density of a packing never exceeds the density in the following triangle:



Upper density bound for opposition on 2D

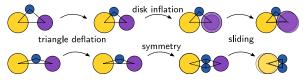
Florian, 1960

The density of a packing never exceeds the density in the following triangle:



Proof:

• Reduce the dimension of the set of triangles $(3 \to 1)$ Fejes Tóth, Mólnar, 1958 For any triangle, there is a denser triangle with at least two contacts between discs.



Upper density bound for o-packings in 2D

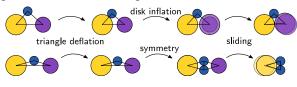
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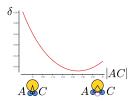


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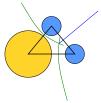


Function analisys

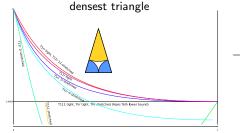


Upper density bound for o-packings

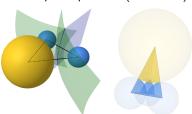
FM-triangulation (triangles)

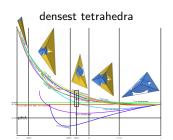


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FM-simplicial partition (tetrahedra)





Upper density bound for ___o-packings

Theorem, $r = \sqrt{2} - 1$

in progress

Each of the following tetrahedra is densest among the tetrahedra with the same spheres:











 $\delta_{1111}\approx 0.7209$

 $\delta_{11rr} \approx 0.8105$

 $\delta_{1\text{rrr}}\approx 0.8065$

 $\delta_{\textit{rrrr}}\approx 0.7847$

$$\delta_{111r} \approx 0.8125$$

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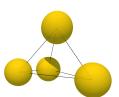
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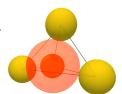
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Proof:



Upper density bound for oppositions

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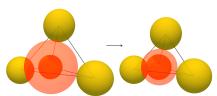
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Proof:



Upper density bound for __o-packings

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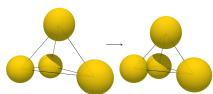
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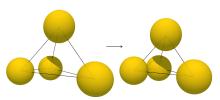
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$$\delta_{111r} \approx 0.8125$$

Proof:

• Reduce the dimension of the set $(6 \rightarrow 5)$: move spheres towards support sphere center



• Computer-assisted proof for tetrahedra with one contact: recursive subdivision + interval arithmetic ≈ 1000 lines of code

75 hours of CPU time

Why the computations are so slow

interval arithmetic + huge formulas \rightarrow loss of precision

Why the computations are so slow

interval arithmetic + huge formulas \rightarrow loss of precision

Example: to compute the support sphere radius, we need to solve $Ar^2 + Br + C = 0$

 $A = -4a^2b^2d^2 + 4a^2c^2d^2 + 4b^2c^2d^2 - 4c^2d^2 - 4c^2d^2 + 4a^2b^2c^2 - 4b^2c^2 - 4a^2c^2c^2 + 4b^2c^2c^2 + 4b^2c^2c^2c^2 + 4b^2c^2c^2 + 4b^2$

 $B = -4c^2d^4r_1 + 4b^2d^2r_1^2r_1 + 4c^2d^2r_1^2r_1 + 4d^2d^2r_1^2r_1 + 4d^2r_1^2r_1 + 4d^2r_1^2r_1 - 8d^2r_1^2r_1 + 4d^2r_1^2 - 8d^2r_1^2r_1 + 4d^2r_1^2 - 8d^2r_1^2r_1 + 4d^2r_1^2 - 8d^2r_1^2r_1 + 4d^2r_1^2 - 8d^2r_1^2r_1 + 4d^2r_1^2r_1^2 - 4d^2r_1^2r_1^2 + 4d^2r_1^2r_1^2 - 4d^2r_1^2r_1^2 -$

 $C = c^4 d^4 - 2b^2 c^2 d^2 + b^4 b^4 - 2a^2 c^2 d^2 f^4 - 2a^2 b^2 c^2 f^4 + a^4 f^4 - 2c^2 d^2 f^2 f^2 + 2b^2 d^2 f^2 f^2 + 2a^2 d^2 f^2 f^2 f^4 + 2b^2 d^2 f^2 f^2 f^4 - 2a^2 d^2 f^2 f^2 f^4 - 2b^2 d^2 f^2 f^2 - 2b^2 f^2 f^2 - 2b^2 f^2 f^2 f^2 - 2b^2 f^2 f^2 - 2b^2 f^2 f^2 f^2 - 2b^2 f^2$

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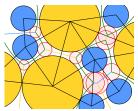
Thanks to dimension reduction: 85'd pra+86'd pra-185'd p

compute with fixed radii and edge lengths, then "simplify"

$$\begin{split} &r_{X} = r_{Y} = f_{Z} = r_{W} = 1, \quad a = 2; \\ &A = 4 \left(b \left((c-4) \left(d-f \right) - \left(b-c-d+e-f-4 \right) e \right) - \left(\left(c+d-e-f-4 \right) d+4 \left(e-f \right) \right) c - f \left(d \left(e-4 \right) - 4 e+4 f+16 \right) \right) \\ &B = 8 \left(b \left((c-4) \left(d-f \right) - \left(b-c-d+e-f-4 \right) e \right) - \left(\left(c+d-e-f-4 \right) d+4 \left(e-f \right) \right) c - f \left(d \left(e-4 \right) - 4 e+4 f+16 \right) \right) \\ &C = b \left(4 \left(c-4 \right) \left(d-f \right) - e \left(2 c \left(d-2 \right) - b \left(e-4 \right) - 4 \left(d+e+f-4 \right) \right) \right) + \left(d-4 \right) \left(c \left(d \left(c-4 \right) + 4 \left(e-f \right) \right) - 4 f \left(e-4 \right) \right) \right) \end{split}$$

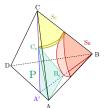
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Techniques



properties of triangulations

Geometry:

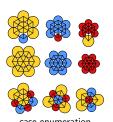


... and "tetrahedrizations"



differential geometry

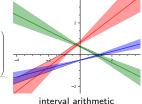
Computer assistance:



case enumeration Python, C++



symbolic calculus SageMath



interval arithmetic MPFI (RIF SageMath) Boost (C++)

- Sphere packings in 3D
- ② Optimality proofs for ○ ●
- Salt packings
- Oensity bound: from disks to spheres
- Conclusion
- 6 Homework

Homework I 16/12-6/1

The list of best-known spherical codes: https://spherical-codes.org/

- **Q** Find the maximal number M_{\max} of spheres of radius $r:=\sqrt{2}-1$ simultaneously touching a unit sphere.
- Write a function random_triangle_box which takes as input three arguments: (eps, 1b, ub) and returns a tuple of three intervals of diameter 2-eps whose centers are random numbers uniformly distributed between 1b and ub.
- Write a function area which takes as input 3 intervals (we call them a box): the 3 enclosures of lengths of the edges of a triangle (ab,ac,bc) and returns (b,v) where b=-1 iff no point from the box determines a valid triangle in \mathbb{R}^2 , b=1 if all points from the box define a triangle, and otherwise, b=0; v=RIF(-1) if $b\leq 0$, otherwise v is an enclosure of the area of the box of triangles. Write two functions area1 and area2 using two different symbolic expressions expr1 and expr2 for the area of a triangle: $s=(x+y+z)/2=\exp r1(x,y,z)=\sqrt{s(s-x)(s-y)(s-z)}$ expr $2(x,y,z)=\frac{1}{4}\sqrt{4x^2y^2-(x^2+y^2-z^2)^2}$. Compare their results on at least 1000 various boxes using random_triangle_box function. Which function is better? Why? Does expr2 change when we change the order of arguments? Write a function ultimate_area which is better than all the cited functions for any triangle.

Large except handwriting to be submitted by email to: daria.ochelina@ens-lvon.fr

Deadline: January 6, 15h45

Homework II 16/12-6/1

- An $r^{M_{\text{max}}}$ -shell around a unit sphere is the configuration of M_{max} spheres of radius r simultaneously touching the unit sphere (r, M_{max}) are the ones from the question 1). Give nontrivial upper δ_u^{T} and lower δ_l^{T} bounds on the density of the union of the FM-triangles having a vertex at the center of the unit sphere in an $r^{M_{\text{max}}}$ -shell, such that $(\delta_l^{\mathsf{T}}) > \frac{1}{(1+r)^2}$ and $\delta_u^{\mathsf{T}} < 1$. Give nontrivial upper δ_u^{Vor} and lower δ_l^{Vor} bounds on the density of a Voronoi cell of the unit sphere in an $r^{M_{\text{max}}}$ -shell. (You might find this useful: https://schoengeometry.com/a_poly.html)
- Write a function random_tetrahedron_box. Write a function vol which takes as input 6 intervals (we call them a box): the 6 enclosures of lengths of the edges of a tetrahedron (ab,ac,ad,bc,bd,cd) and returns (b,v) where b=-1 iff no point from the box determines a valid tetrahedron in \mathbb{R}^3 , b=1 if all points from the box define a tetrahedron, and otherwise b=0; v=-1 if $b\leq 0$, otherwise v is an enclosure of the volume of this tetrahedron. Try using different symbolic expression in vol function, compare them using random_tetrahedron_box.

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