## Triangulated ternary disc packings that maximize the density

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supervised by

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Packing $P$ : (in $R^{2}$ )


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- To make compact materials


Binary and ternary superlattices self-assembled from colloidal nanodisks and nanorods. Journal of the American Chemical Society, 137(20):6662-6669, 2015.

2D hexagonal $\bigcirc$-packing:


$$
\delta=\frac{\pi}{2 \sqrt{3}}
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Lagrange, 1772
Hexagonal packing maximize the density among $\square$ lattice backings.

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3D hexagonal $\bigcirc$-packing:

$$
\delta=\frac{\pi}{3 \sqrt{2}}
$$

Gauss, 1831
Hexagonal packing maximize the density among lattice $\bigcirc$ packings.
Hales, Ferguson, 1998-2014
(Conjectured by Kepler, 1611)
Hexagonal packing maximize the density.

Two discs of radii 1 and $r$ :


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Upper bound on the density:
Florian, 1960
The density of a packing never exceeds the density in the following triangle:


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Kennedy, 2006
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Heppes 2000,2003
Kennedy 2004
Bedaride, Fernique, 2019:
All these 9 packings maximize the density


## Conjecture (Connelly, 2018)

If a finite set of discs allows a saturated triangulated packing then the density is maximized on a saturated triangulated packing.


True for $\bigcirc$ and $\bigcirc \bullet$.

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## What happens with $\bigcirc$ ○ ?

- $164(r, s)$ with triangulated packings:
(Fernique, Hashemi, Sizova 2019)
- 15 non saturated
- Case 53 is proved (Fernique 2019)
- 14 more cases
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## Idea of the proof for

A Delaunay triangulation of a packing: no points inside a circumscribed circle

$\delta^{*}=\delta_{\Delta^{*}}=\frac{\pi}{2 \sqrt{3}}$

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- The density of a triangle $\Delta: \delta_{\Delta}=\frac{\pi / 2}{\operatorname{area}(\Delta)}$
- The area of a triangle $A B C$ with the largest angle $\hat{B}$ is $\frac{1}{2}|A B| \cdot|B C| \cdot \sin \hat{B}$ which is at least $\frac{1}{2} \cdot 2 \cdot 2 \cdot \frac{\sqrt{3}}{2}=\sqrt{3}$

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- Thus the density of $A B C$ is less or equal to $\frac{\pi / 2}{\sqrt{3}}$

Delaunay triangulation $\rightarrow$ weighted by the disc radii


Triangles have different densities:


What to do?

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The sparsity of a triangle $\Delta \in \mathcal{T}: S(\Delta)=\delta \times \operatorname{area}(\Delta)-\operatorname{cov}(\Delta)$ $S(\Delta)>0$ iff the density of covering of $\Delta$ is less than $\delta$ $S(\Delta)<0$ iff the density of covering of $\Delta$ is greater than $\delta$

To prove that $\mathcal{T}$ is no denser than $\mathcal{T}^{*}$, we show that $\sum_{\mathcal{T}} S(\Delta) \geq 0$
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To prove that $\mathcal{T}$ is no denser than $\mathcal{T}^{*}$, we show that $\sum_{\mathcal{T}} S(\Delta) \geq 0$
1: Introduce a potential $U$ such that for any triangle $\Delta \in \mathcal{T}$,

$$
S(\Delta) \geq U(\Delta)
$$

and

$$
\begin{equation*}
\sum_{\Delta \in \mathcal{T}} U(\Delta) \geq 0 \tag{U}
\end{equation*}
$$

2: Instead of proving a global inequality

$$
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we define the vertex potential: for a triangle $\triangle$ with vertices $A, B$ and $C$,

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U(\Delta)=\dot{U}_{\Delta}^{A}+\dot{U}_{\Delta}^{B}+\dot{U}_{\Delta}^{C}
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and prove a local inequality for each vertex $v \in \mathcal{T}$ :

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\sum_{\Delta \in \mathcal{T} \mid v \in \Delta} \dot{U}_{\Delta}^{v} \geq 0
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$$
4 \dot{U}_{\Delta_{1}}^{v}+2 \dot{U}_{\Delta_{2}}^{v}+\dot{U}_{\Delta_{3}}^{v}=0 \quad \quad \dot{U_{\Delta_{1}^{\prime}}^{v^{\prime}}}+\dot{U_{\Delta_{2}^{\prime}}^{v^{\prime}}}+\dot{U_{\Delta_{3}^{\prime}}^{v^{\prime}}}+\dot{U_{\Delta_{4}^{\prime}}^{v^{\prime}}}>0
$$

Delaunay triangulation properties $\rightarrow$ finite number of cases $\rightarrow$ verification by computer

To store and perform computations on transcendental numbers (like $\pi$ ), we use intervals.

A representation of a number $x$ is an interval / whose endpoints are exact values representable in a computer memory and such that $x \in I$.

```
sage: x = RIF (0,1)
sage: (x+x).endpoints()
(0.0, 2.0)
sage: x < 2
True
```

```
# Interval [0,1]
```


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    # [0,1]+[0,1]
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(0.0, 2.0)
sage: x < 2
True
sage: Ipi = RIF(pi) # Interval for }
(3.14159265358979, 3.14159265358980)
sage: sin(Ipi).endpoints() # Interval for sin(\pi)
(-3.21624529935328e-16, 1.22464679914736e-16)
sage: sin(Ipi) >= 0
False # Interval for }\operatorname{sin}(\pi)\mathrm{ contains 0
```

Defining $U$, we try to make it as small as possible keeping it locally positive around any vertrex $(\bullet)$.

3: How to check

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S(\Delta) \geq U(\Delta)
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on each triangle $\Delta$ ? (There is a continuum of them).

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## Interval arithmetic!

Delaunay triangulation properties $\rightarrow$ uniform bound on edge length:

$$
\begin{gathered}
\text { Verify } S\left(\Delta_{e_{1}, e_{2}, e_{3}}\right) \geq U\left(\Delta_{e_{1}, e_{2}, e_{3}}\right) \text { where } \\
e_{1}=\left[r_{a}+r_{b}, r_{a}+r_{b}+2 s\right] e_{2}=\left[r_{c}+r_{b}, r_{c}+r_{b}+2 s\right] e_{3}=\left[r_{a}+r_{c}, r_{a}+r_{c}+2 s\right]
\end{gathered}
$$

Not precise enough $\rightarrow$ dichotomy

## What was done and what will be done...

- 14 cases proved
- 133 cases to prove (Connelly's conjecture)
- maximal density for other disc sizes
(which do not allow triangulated packings)
various techniques: computer-assisted proofs, interval arithmetic, optimisation, combinatorics, discrete geometry
for this: good comprehension of the density redistribution, more optimisation
deformations of triangulated packings keep the density high $\rightarrow$ good lower bound on the maximal density

