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# **NOTETAKER CHECKLIST FORM**

**(Complete one for each talk.)**

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**Speaker's Name:\_** Martin Cramer Pedersen

**Talk Title:\_** Polyhedra and packings from hyperbolic honeycombs

Date: <u>10 /02 /2018</u> Time:1<u>1 :00 Can</u>h / pm (circle one) Date: 10 /02 /2018

Please summarize the lecture in 5 or fewer sentences:

T<u>he EPINET project explores 2D hyperbolic tilings as a source of crystalline fra</u>meworks i<u>n 3D Euclidean space. The goal is to establish the simplest nets in hyperbolic s</u>pace, fr<u>om which Euclidean counterparts can be generated. The guiding principal is o</u>ne of h<u>yperbolic surface tiling, where the 3D crystallinity of an underlying surface induces</u> 3<u>–periodic networks. The extraordinary wealth of hyperbolic tilings allows us to enumerate</u> networks and their spatial realizations with greater breadth than conventional approaches.

# **CHECK LIST**

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Polyhedra and packings from hyperbolic honeycombs Hot Topics: Shape and Structure of Materials MSRI, UC Berkeley, 1<sup>st</sup> - 5<sup>th</sup> of October, 2018

Martin Cramer Pedersen & Stephen Hyde Niels Bohr Institute & Australian National University

#### In this talk



#### Welcome to the EPINET project

The EPINET project explores 2D hyperbolic (HP) filings as a source of crystalline frameworks (or networks) in 3D euclidean (EP) space. Our aim is to enumerate networks with a broad spectrum of properties that are of possible interest to peopeless, shortunal chemists, and statistical physicists. The quiding principal is one of hyperbolic surface Ming, where the 3D crystallinity of an underlying surface induces 3-periodic networks. The extraordinary wealth of hyperbolic tilings allows us to equipmente networks and their spatial realisations ("embeddings") with greater breadth than conventional approaches.

#### Search the databases

- . Hyperbolic Subgroup Tilings
- U-Tilings
- Hyperbolic Nets
- System Nats

#### Explore the databases

· Structure Taxonomy

#### **Site Information**

- $\bullet$  About
- $-$  Changelon
- Contacts
- Acknowledgements
- Future Changes

**Background Information** 

#### EPINET - Euclidean Patterns in Non-Euclidean Tilings



Ramsden et al. (2009), EPINET, http://epinet.anu.edu.au/

# In this talk

The goal of this talk is to establish the simplest nets in hyperbolic space, from which we can generate Euclidean counterparts.

Specifically, we chase highly symmetric, infinite (i.e. 3-periodic) deltahedra in Euclidean space.

Our motivation:

- · Templates for reticular chemistry
- · Optimal packing geometries
- · Enumeration of these structures



Cowpea Mosaic Virus PDB 2bfu



MOF-399 Furukawa et al. (2012)

### In this talk

Agenda:

- · Establish a bit of notation about nets and their symmetries
- · Present a pipeline for generating nets in Euclidean space from nets in hyperbolic space
- · Show a bunch of interesting nets generated from this pipeline
- · Analyze and compare a subset of the generated nets





# Platonic solids

Described by Plato around 360 B.C. (regular nets on  $\mathbb{S}^2$ ):



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In this talk, we are particularly interested in the tetrahedron, the octahedron, and the icosahedron as they are composed of equilateral triangles; they are (regular) "deltahedra".

 $\mathbb{H}^2$  and  $\mathbb{S}^2$  allow for nets that are forbidden in  $\mathbb{E}^2$  - i.e. so-called non-crystallographic symmetries.



A few words about the Poincaré disk model of  $\mathbb{H}^2$ :



- · A conformal model of the hyperbolic plane Angles are preserved!
- · Geodesics appear as circle arcs (or straight lines through the center)
- · These triangles are congruent and equilateral



The usual crystallographic notation will not work for  $\mathbb{H}^2$ .

We use the orbifold notation for symmetry groups:

- · N means that our pattern has a unique N-fold symmetry point
- · A ∗ means a mirror symmetry. ∗N means that N mirror lines meet in a point
- $\cdot$   $\times$  means that our pattern has glide symmetry
- · means that there is a translational symmetry in our pattern





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Escher (1955)



333 (or p3)



Escher (1955)







∗3333



Conway et al. (2008), Escher (1960)





Conway et al. (2008), Escher (1960)

We can think of the embeddings from before as generalizations of the famous "penny packing" in  $\mathbb{E}^{2}$  with  $*2\bar{3}$ N symmetry:



The density,  $\rho$ , of an *N*-contact packing is summed up beautifully in L. F. Tóth's formula:

$$
\rho\left(N\right)=\frac{3\csc\left(\frac{\pi}{N}\right)-6}{N-6}
$$

The groups with orbifold symbols  $*23N$  are called "honeycombs".

Tóth (1940)



Most honeycombs are hyperbolic:



# 3-periodic minimal surfaces

Minimal surfaces are surfaces that locally minimize area (usually subjected to specific boundary conditions). The most symmetric 3-periodic minimal surfaces in  $\mathbb{E}^{3}$  are known (for genus 3):



Their covering space is  $\mathbb{H}^2$  . And importantly,  $*246$  symmetries in  $\mathbb{H}^2$  can be lifted to symmetries in  $\mathbb{E}^{3}$  via these surfaces.

Schwartz (1890), Schoen (1970), Bai et al. (2016)



### 3-periodic minimal surfaces

By identifying the opposing edges of a (hyperbolic) dodecagon, we can construct the TPMS.

Here, the P-surface:



We have the unit cell of the P-surface:

- $\cdot$  in universal cover,  $\mathbb{H}^2$ , on the left (6 lattice vectors)
- · as a 3-periodic surface in the middle (3 lattice vectors)
- · as a 3-torus on the right (0 lattice vectors)



# Lifting a net from  $\mathbb{H}^2$  to  $\mathbb{E}^3$

As a first example, we can decorate a  $*246$  orbifold like this:



The pattern in  $\mathbb{H}^2$  shares the symmetries of the P-surface,  ${\it Im} \bar{3} {\it m}$  and  $*{\rm 246}$  and is known as sod in databases. It outlines the cage-like structure of the mineral sodalite.

This works because the symmetries of the net in  $\mathbb{H}^2$  are "commensurate" with the symmetries of the surface.

O'Keee et al. (2008), RCSR - http://rcsr.anu.edu.au
# Lifting a net from  $\mathbb{H}^2$  to  $\mathbb{E}^3$

If we lift the same net from  $\mathbb{H}^2$  onto the D-surface, we get a completely different net:



Here, we recover the well-known net nbo (named after the compound NbO) with extrinsic symmetry  $Pn\overline{3}m$  and intrisic symmetry  $*246$ .

In general, for a commensurate decoration we get 4 nets in  $\mathbb{E}^{3};$  1 from the  $P$ and D− surface, and 1 from each of the 2 embeddings of the Gyroid.





#### Relaxing a net

We usually distinguish between the emerging net and a relaxed version of the net (called the equilibrium placement).



In this case, the two structures are quite similar, but this process might change the structure quite a bit. Symmetries are preserved.

Delgado-Friedrichs & O'Keeffe (2005)



## Commensurate symmetries

We know that the most symmetric periodic decoration of these surfaces we can construct will have symmetry ∗246.

And the least symmetric one will just have translational symmetry (i.e. space group P1 and ∘∘∘).

So we need to know all symmetry groups, G, for which:

∗246 ≤ G ≤ ◦◦◦





 $000$ 

## Commensurate symmetries

Robins and collaborators did this and ended up with 131 commensurate symmetry groups:



Slide 20/41

We now have the pieces needed to bring realise our hyperbolic disk packings in  $\mathbb{E}^{3}$  via the TPMS.



All we need to do is deform the pattern on the left (with ∗239 symmetry) to be commensurate with the symmetries our TPMS (with \*246/○○○ symmetry).



Index 1,  $y = -1/30$ 

## Getting frustrated













Visualizing the cosets of the subgroup can aid us a further:

• Starting with a<br>tesselation of  $\mathbb{H}^2$  of ∗23(10) domains...



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- · and recover the orbifold symbol of the subgroup - here 3∗22...
- · and see how a single orbifold can be visualized...
- · as well as the decoration needed to build the  $[3, 10]$ -net.



Now we know how to deform the  $\{3,10\}$  net into a net we can lift to  $\mathbb{E}^3$  via the TMPS and ∗246:

 $\cdot$  Starting from a<br>tesselation of  $\mathbb{H}^2$  of ∗246 domains...



- · Starting from a tesselation of  $H^2$  of ∗246 domains...
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- · Starting from a tesselation of  $H^2$  of ∗246 domains...
- · we can construct a tesselation of commensurate 3∗22 domains...
- · and decorate the tesselation with the motif we just found...
- and get a  $[3, 10]$ commensurate with the symmetries of our TMPS.
- · We can think of the pattern as an 8-connected packing of disks.









Due to the commensurate symmetry, we can visualize this as a net on the TMPS:





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Slide 26/41

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Using Systre, we compute equilibrium placements for all of our nets generated using the different surfaces.

Delgado-Friedrichs & O'Keeffe (2005)



Generally, we get 4 different nets from each pattern in  $\mathbb{H}^2.$ 

However, in this case, our mirror symmetry does not lift to the Gyroid, so the resulting nets from the two embeddings via the Gyroid are identical.



Note that the net on the P is 9-valent. Edges may merge when computing canonical embeddings.

Hyde et al. (2014)



#### A note on enumeration

 $\cdot$  We can "name" out honeycomb nets by their parent hyperbolic net, their (subgroup) orbifold symbol, and the surface on with which we lift them to  $\mathbb{E}^{3}$  .



Ramsden et al. (2009), Evans et al. (2015), Kolbe & Evans (2018)



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- · However:
	- · Two subgroups can have the same orbifold symbol
	- $\cdot$  Some subgroups "sit" in the ∗246 lattice in innitely many ways
	- · Some orbifolds have non-trivial symmetries (i.e. symmetries not in the ∗246 lattice)



 $[3, 7]$  on  $2223_{11}$ 

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	- · Some orbifolds have non-trivial symmetries (i.e. symmetries not in the ∗246 lattice)
- · Enumeration is hard. Computations get hard for very elongated orbifolds.





#### For  $N \in \{7, 8, 9, 10, 12\}$ , we:

· Determined all subgroups of 23N down to and including those that could be found as index-4 subgroups in ∗246



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- We found 10 infinite deltahedra in our search. 5 are not reported elsewhere. Maybe?
- · As well as many other interesting structures



 $[3, 9]$  on 2223 $_{31}$  via P





Slide 30/41

#### FACULTY OF SCIENCE

# From  $\mathbb{H}^2$  to  $\mathbb{E}^3$


# From  $\mathbb{H}^2$  to  $\mathbb{E}^3$

Other structures are nearly deltahedra:





 $[3, 7]$  on 2223<sub>11</sub> via P (svn-x)



Slide 32/41



famous graphs

**Google Search** 

I'm Feeling Lucky

Google offered in: Dansk Føroyskt

#### The 7-valent Klein graph [edit]

This graph is a 7-regular graph with 24 vertices and 84 edges, named after Felix Klein.

It is a Hamiltonian graph. It has chromatic number 4, chromatic index 7, radius 3. diameter 3 and girth 3.

It can be embedded in the genus-3 orientable surface, where it forms the dual of the "Klein map", with 56 triangular faces, Schläfli symbol {3,7}<sub>8</sub>.<sup>[4]</sup>

It is the unique distance-regular graph with intersection array  $\{7, 4, 1, 1, 2, 7\}$ ; however, it is not a distance-transitive graph.[5]

#### Algebraic properties [edit]

The automorphism group of the 7-valent Klein graph is the same group of order 336 as for the cubic Klein map, likewise acting transitively on its half-edges.

The characteristic polynomial of this Klein graph is equal to  $(x - 7)(x + 1)^7(x^2 - 7)^8$  $[6]$ 

#### References Ledit1

1. ^ Wolz, Jessica; Engineering Linear Layouts



**Named after** Felix Klein **Vertices** 24 **Edges**  $84$ **Radius** R **Diameter**  $\overline{\mathbf{z}}$ Girth  $\overline{3}$ **Automorphisms** 336 **Chromatic**  $\overline{a}$ number **Chromatic index**  $\overline{7}$ **Properties** Symmetric Hamiltonian Table of graphs and parameters

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Table of graphs and parameters

Due to computational constraints, we generated these [3, 7]-nets on the three-torus as well the Klein graph:

> $\cdot$  2223<sub>01</sub>  $\cdot$  2223<sub>41</sub>  $\cdot$  2223<sub>11</sub>  $\cdot$  2223<sub>12</sub>  $\cdot$  2223<sub>13</sub>  $\cdot$  2223<sub>32</sub>  $\cdot$  2223<sub>14</sub>  $\cdot$  2223<sub>21</sub>  $\cdot$  2223<sub>23</sub>  $\cdot$  2223<sub>31</sub> · Klein  $\cdot$  23 $\times$  (A)





Dress (1987)

Due to computational constraints, we generated these [3, 7]-nets on the three-torus as well the Klein graph:



Using an invariant representation of the surface embedding (and double-checking with Delaney-Dress symbols), these embeddings are equilavent.

Nauty and GAP can establish the group of automorphisms for each of our nets. Nauty classifies our  $[3, 7]$  nets as:





As before, we see that the [3,7] net built via  $2223_{31}$  is indeed the Klein graph.



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And in conclusion, we have produced four 3-periodic embeddings of the 7-valent Klein graph.

The prettiest ones is built via one of the embeddings of the Gyroid:



## **Outlook**

#### Next steps:

· Very symmetric Schwarzites i.e. the surface duals of the triangulations





#### **Outlook**

Next steps:

- · Very symmetric Schwarzites i.e. the surface duals of the triangulations
- · Embeddings via sub-periodic surfaces (and other surfaces) e.g. the [3, 7] on 2223 on an HCB-surface on the right

RCSR, http://rcsr.anu.edu.au, EPINET, http://epinet.anu.edu.au/



#### Outlook

#### Next steps:

- · Very symmetric Schwarzites i.e. the surface duals of the triangulations
- · Embeddings via sub-periodic surfaces (and other surfaces) e.g. the [3, 7] on 2223 on an HCB-surface on the right
- · Curating and comparing our nets to existing databases such as RCSR and EPINET



RCSR, http://rcsr.anu.edu.au, EPINET, http://epinet.anu.edu.au/

References

Polyhedra and packings from hyperbolic honeycombs Pedersen & Hyde Proc. Natl. Acad. Sci. 115, 6905-6910 (2018)

Surface embeddings of the Klein and the Möbius-Kantor graphs Pedersen, Delgado-Friedrichs, & Hyde Acta Crystallogr. Sect. A 74, 223-232 (2018)

Hyperbolic crystallography of two-periodic surfaces and associated structures Pedersen & Hyde Acta Crystallogr. Sect. A 73, 124-134 (2017)

### Acknowledgements

Funding:

From Australian National University:

- · Stephen Hyde
- · Stuart Ramsden
- · Vanessa Robins
- · Olaf Delgado-Friedrichs

From Technische Universität Berlin:

- · Myfanwy Evans
- · Benedikt Kolbe



Software:



