Enumerating tilings of triply-periodic minimal surfaces

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Overview

Preliminaries
   Motivation

Minimal surfaces and orbifolds
   Triply periodic minimal surfaces
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Enumerating isotopy classes of tilings
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Graphs in nature and materials science

- Chemical structures are often modelled as (locally finite, simple) graphs in $\mathbb{R}^3$. 
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Sodalite, an aluminosilicate, a real Zeolite in $\mathbb{R}^3$. Image courtesy of Stephen Hyde.
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**Figure**: Sodalite on the primitive surface
The central idea of the EPINET approach

- Study entangled graphs by explicit constructions of graphs on surfaces.
- **The EPINET approach**: Investigate nets by drawing graphs symmetrically on an embedded hyperbolic surface in $\mathbb{R}^3$. Then forget about the surface.
- Use special surfaces so that produced graphs are symmetric in $\mathbb{R}^3 \implies H^2$
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Figure: Hyperbolic Tiling and the corresponding drawing on the diamond surface in $\mathbb{R}^3$. 
Example of a tiling of the hyperbolic plane and the resulting net

*Figure:* The corresponding net in $\mathbb{R}^3$, representing a molecular structure grown on the diamond surface with two distinct strands.
Minimal Surfaces

- Locally minimize their surface area relative to the boundary of a small neighbourhood of any point.
- The soap film bounded by a wire is a minimal surface; many equipotential surfaces in nature are (close to) minimal; many membranes found in living tissue.

Figure: Minimal surfaces as soap films between wires left (Paul Nylander) and chips right
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- The translations are a result of more refined symmetries.
- These symmetries yield a hyperbolic orbifold (∗246).
Central definition - Orbifolds

Definition - developable orbifolds for equivariant tiling theory

Let $X = \mathbb{H}^2, \mathbb{E}^2$ and $\Gamma \subset \text{Iso}(X)$ discrete. The set of data $(X, \Gamma)$ associated with the quotient map $\pi : X \to X/\Gamma$ is a (metric) orbifold.

Figure: Hyperbolic and Euclidean Developable Orbifolds
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Take-Home Message I

- Graphs in $\mathbb{R}^3$ can be studied (effectively) by exploring graphs on TPMS.
- These are covered by the hyperbolic plane $\mathbb{H}^2$.
- Prominent TPMS exhibit a high degree of symmetry.
- Orbifolds are generalisations of surfaces that account for symmetries.
- Orbifolds with quotient space of finite area are determined, up to homeomorphism, by the isomorphism class of their symmetry group.
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- Observation: One can construct tilings with a combinatorial description depending on given special generators of a symmetry group.
- Description only defines tiling up to symmetry preserving isotopies.
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(a) Twist on an annulus.

**Figure:** Two views on the effect of a right Dehn twist.
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(b) Twist on a cylinder.

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Central theoretical result for enumerations

Generalized Dehn-Nielsen-Baer theorem (K.)

The MCG of a finite volume hyperbolic orbifold $\mathcal{O}$ with fundamental group $\Gamma$ is isomorphic to a certain subgroup of $\text{Out}(\Gamma)$, the group of outer automorphisms.
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- This means that the MCG $\text{Mod}^{\pm}(\mathcal{O})$ corresponds to special sets of generators of $\Gamma$. 
Algorithm for enumerations

Input

- Symmetry group $\Gamma$ of interest
- Highest complexity of the combinatorial tiling class up to which to enumerate
- Presentation of MCG of the orbifold associated to $\Gamma$ and word length up to which we enumerate the tilings as representatives of MCG elements
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- List of sets of generators of $\Gamma$ as isometries
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Main obstacles for enumerations of isotopy classes of tilings onto TPMS

For (useful) implementations of enumerations of tilings in $\mathbb{H}^2$, we need:

- Explicit (and nice) action of $\text{MCG}$ on sets of generators
- Combinatorial description of tiling in terms of generators for symmetry group
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- Derivations of presentations of MCGs
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- A rather lengthy presentation of the MCG in terms of 'half-twists'.
- Using the package KBmag for the programming language GAP, which provides experimental algorithms.
- By connecting the rotational centers for the generators with inserted points according to an appropriate adjacency matrix.
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Final Take-Home Message and Summary

- The mapping class group generates different decorations of a surface or orbifold starting from a given one.
- The MCG is very complicated in general, but has a nice set of generators.
- The complexity ordering for isotopy classes of tilings, given nice generators for the MCG, is ‘in line with our intuition’.
- One can overcome most computational challenges for rotational symmetry groups.
- The enumeration of isotopy classes of symmetric graph embeddings is feasible.
- Potential uses include systematically checking structures for certain physical properties, for possible synthetic materials.
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Different isotopy classes of tilings and resulting structures in $\mathbb{R}^3$
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Thanks to my collaborator
Myfanwy Evans, Technical University Berlin