#### **Graphs in Nature**

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#### **General theme**

Geometric structure

 $\Rightarrow$ 

Graph-theoretic structure

 $\Rightarrow$  Algorithms

... and clearer understanding of graph structure leads to better algorithms

# I. Crystals and polyhedra

## Prototypical example: Steinitz's theorem

Purely combinatorial characterization of geometric objects:



Graphs of convex polyhedra are exactly 3-vertex-connected planar graphs [Steinitz 1922]

## Algorithmic Steinitz not entirely understood

Given a 3-connected planar graph, we can find a polyhedron representing it, with integer coordinates, in polynomial time



Best known upper bound on these coordinates (based on lifting Tutte spring embeddings) is singly exponential [Ribó Mor et al. 2011; Buchin and Schulz 2010]

Can we do better?

## Non-convex crystal polyhedra

Some materials (here, bismuth) crystallize into orthogonal polyhedra instead of convex polyhedra



Image: Bilovitskiy [2015]

## Steinitz-like theorem for orthogonal polyhedra

The graphs of *3-regular, topologically spherical* orthogonal polyhedra are exactly 2-connected planar cubic bipartite graphs where no 2-vertex cut separates the graph into three pieces [Eppstein and Mumford 2014]

Hard part: Construct polyhedron from dually-4-connected graph

Main ideas: Represent polyhedron combinatorially as special coloring and orientation of dual graph

Induction proof that dual coloring always exists

Topological order of bichromatic subgraphs  $\Rightarrow$  coordinates



## Algorithms for realizing orthogonal polyhedra



Can find orthogonal realization of graph in randomized O(n)time, deterministic  $O(n(\log \log n)^2 / \log \log \log n)$ 

Bottleneck: Decompose 4-connected Eulerian maximal planar graphs by

- Splitting on 4-cycles
- Suppressing pairs of adjacent degree-4 vertices
- Contracting pairs of opposite neighbors of isolated degree-4 vertices

## **II. Bubbles and Foams**

## Soap bubbles and soap bubble foams



Image: woodleywonderworks [2007]

Soap molecules form double layers separating thin films of water from pockets of air

A familiar physical system that produces complicated arrangements of curved surfaces, edges, and vertices

What can we say about the mathematics of these structures?

#### **Planar soap bubbles**

3d is too complicated, let's restrict to two dimensions



Image: Keller [2002]

Main result: graphs of 2D soap bubble clusters = 3-regular 2-connected planar graphs [Eppstein 2014]

## **Plateau's laws**

In every 3D soap bubble cluster:

- Each surface has constant mean curvature
- Triples of surfaces meet along curves at 120° angles
- These curves meet in groups of four at equal angles

Observed in 19th c. by Joseph Plateau Proved by Taylor [1976]



Image: Unknown [1843]

## Young-Laplace equation



Thomas Young Image: Adlard [1830]

For each surface in a soap bubble cluster:

mean curvature = 1/pressure difference (with surface tension as constant of proportionality)

Formulated in 19th c., by Thomas Young and Pierre-Simon Laplace



Pierre-Simon Laplace Image: Feytaud [1842]

## Plateau and Young–Laplace for planar bubbles

In every planar soap bubble cluster:

- Each curve is an arc of a circle or a line segment
- Each vertex is the endpoint of three curves at 120° angles
- It is possible to assign pressures to the bubbles so that curvature is inversely proportional to pressure difference



 $120^{\circ}$  angles  $\Rightarrow$  must be 3-regular

## Geometric reformulation of the pressure condition



For arcs meeting at  $120^{\circ}$  angles, the following three conditions are equivalent:

- We can find pressures matching all curvatures
- Triples of circles have collinear centers
- Triples of circles form a "double bubble" with two triple crossing points

## Möbius transformations

Fractional linear transformations

$$z \mapsto \frac{az+b}{cz+d}$$

in the plane of complex numbers

Take circles to circles and do not change angles between curves

Plateau's laws and the double bubble reformulation of Young–Laplace only involve circles and angles

so the Möbius transform of a bubble cluster is another valid bubble cluster



## Proof that bubbles are 2-connected

Equivalently: They do not have a bridge, an edge that has the same face on both of its sides



Image: Unknown [1940]

Main ideas of proof:

- A bridge that is not straight violates the pressure condition
- A straight bridge can be transformed to a curved one that again violates the pressure condition

## Bridges are the only obstacle

For planar graphs with three edges per vertex and no bridges, we can always find a valid bubble cluster realizing that graph

Main ideas of proof:

- 1. Handle 3-connected components separately, separately and use Möbius transformations to glue results together
- 2. Use Koebe-Andreev-Thurston circle packing to find a system of circles whose tangencies represent the dual graph
- **3.** Construct a novel type of Möbius-invariant *power diagram* of these circles, defined using 3d hyperbolic geometry
- 4. Use symmetry and Möbius invariance to show that cell boundaries are circular arcs satisfying the angle and pressure conditions that define soap bubbles

## **Circle packing**



After separating into components we have a 3-connected 3-regular graph

Koebe–Andreev–Thurston circle packing theorem guarantees the existence of a circle for each face, so circles of adjacent faces are tangent, other circles are disjoint

Can be constructed by efficient numerical algorithms [Collins and Stephenson 2003]

## Möbius-invariant Voronoi diagram

Circle packing  $\Rightarrow$  hemispheres in 3D  $\Rightarrow$  planes in upper halfplane model of hyperbolic space



Construct the hyperbolic Voronoi diagram of these planes and restrict Voronoi cell boundaries to 2D plane

Symmetries of hyperbolic space restrict to Möbius transformations of the plane  $\Rightarrow$  diagram is invariant under Möbius transformations

## Step 4: By symmetry, these are soap bubbles



 $\begin{array}{l} \text{M\"obius} \Rightarrow \text{transform any triple of} \\ \text{tangent circles to equal radii} \end{array}$ 

Power diagram boundaries become rays meeting at  $120^{\circ} \Rightarrow$  they obey all local requirements on soap bubble clusters

Local pressure differences at each triple  $\Rightarrow$  global system of pressures fulfilling Young–Laplace equation

## **Algorithmic application**

Lombardi drawing: Visualize graphs with circular-arc edges, equally spaced angles

Soap bubble realization  $\Rightarrow$  all 3-regular planar graphs have Lombardi drawings

(even when not 2-connected)

Depicted: a 46-vertex graph from Grinberg [1968], illustrating Wikipedia article on Grinberg's theorem on Hamiltonicity of planar graphs



## **III. Cracks and Needles**

#### **Gilbert tessellation**



Image: Rocchini [2012b]

#### Gilbert [1967]:

Choose random points in  $\mathbb{R}^2$ 

Start growing line segments in opposite (random) directions and equal speeds at each point

Stop growing each segment when it hits another one

## Modeling the growth of needle-like crystals

(Gilbert's original motivation)



Image: Lavinsky [2010]

## Cracks in dried mud

"Most mudcrack patterns in nature topologically resemble" Gilbert tesselations [Gray et al. 1976]



Image: Grobe [2007]

## Combinatorial structure of a Gilbert tessellation

Represent as a graph:

Vertex for each segment

Edges to the segments at its endpoints



## **Contact graphs**

# $\label{eq:Vertices} \begin{array}{l} {\sf Vertices} = {\sf non-overlapping geometric objects of some type} \\ {\sf Edges} = {\sf pairs that touch but do not overlap} \end{array}$



E.g. Koebe–Andreev–Thurston circle packing theorem: Planar graphs are exactly the contact graphs of disks

## **Contact graphs of line segments**

These graphs are:

#### Planar

(2,3)-sparse

(Each *k*-vertex subgraph has at most 2k - 3 edges)

- 2k because each segment has 2 ends
- -3 because the convex hull has  $\geq 3$  vertices



## **Recognizing** (2,3)-sparse graphs



Pebble game:

Start with all vertices, no edges, 2 pebbles/vertex

If a missing edge has > 3 pebbles, remove one pebble and draw edge directed away from removed pebble

If you need more pebbles, pull them backwards along directed paths, reversing the path edges If (2, 3)-sparse, draws all edges If not: will get stuck

[Lee and Streinu 2008]

#### From pebbles to line segments

# Theorem: Contact graphs of line segments are exactly the planar (2,3)-sparse graphs

Proof outline:

Edge directions from pebbling indicate which segment crashed into which other

Embed the graph using Tutte spring embedding Straighten segments using infinitesimal weights

(2,3)-sparsity  $\Rightarrow$  cannot degenerate to a line

[Thomassen 1993; de Fraysseix and Ossona de Mendez 2004]

(With planar separators, can pebble and recognize in time  $O(n^{3/2})$ )

## Gilbert tessellations with restricted angles

E.g., random points with axis-aligned pairs of motorcycles:



Mackisack and Miles [1996]; Burridge et al. [2013] Image: Rocchini [2012a]

#### **Cellular automata**

In some simple 2D cellular automata, sparse random initial conditions produce patterns that look like (or are provably) orthogonal Gilbert tessellations [Eppstein 2010, 2021]



## **Recognizing axis-parallel contact graphs**

Contact graphs of axis-parallel segments = planar bipartite graphs



[Hartman et al. 1991]

#### **Gilbert tessellations vs contact graphs**

Segment contact graphs: Fully characterized Gilbert tessellation graphs are a special case, but...

All unterminated line segments must be on the outer face



Unknown extra constraints from equal growth rate of segments

#### **Algorithms for Gilbert tessellation**

Define asymmetric distance: Time when one segment would crash into another Repeatedly find closest pair and eliminate blocked segment Use dynamic closest pair data structure of [Eppstein 1995]

 $O(n^{3/2+\epsilon})$  [Eppstein and Erickson 1999] Improved to  $O(n^{4/3+\epsilon})$  [Vigneron and Yan 2014] Additional log speedup using mutual nearest neighbors instead of closest pairs [Mamano et al. 2019]

## Algorithmic application: Roof design

Input: Outline of a building

Trace cross-sections of constant-slope roofline

Line segments along ridge lines grow inwards until they run into another part of the roof

Can be constructed using (non-random) Gilbert tessellations [Cheng and Vigneron 2007; Huber and Held 2012] Image: Huber [2012]







# **IV. Crumples and Folds**

## Patterns in crumpled paper



Image: Pruitt [2011]

Studied experimentally [Andresen et al. 2007] (e.g. ridge lengths appear to obey power laws) but not well-understood theoretically

## Similar patterns at nanoscale

Crumpled graphene has applications including power storage [Stoller et al. 2008] and artificial muscles [Zang et al. 2013]



Image: Duke University [2013]

## A discrete model of paper folding

Fold a piece of paper arbitrarily so that it lies flat again (without crumpling)



## A discrete model of paper folding

Unfold it again and look at the creases from its folded state



## A discrete model of paper folding

It looks like a graph!



#### Local constraints at each vertex

Maekawa's theorem: at interior vertices, |# mountain folds - # valley folds| = 2



So all vertex degrees must be even and  $\geq$  4 [Murata 1966; Justin 1986]

#### Local constraints are not enough



Some tree-structured folding patterns are locally-foldable at each vertex, but have no global flat folding [Hull 1994]

At the central crossing, two opposite creases nest tightly

The extra folds farther out on these two creases are incompatible with nesting

#### ...but all even-degree trees are realizable

Given an abstract tree with even-degree internal vertices, we can find a flat-foldable folding pattern in the shape of that tree

[Eppstein 2018]



#### Main idea of tree realization

Construct tree top-down from root

Maintain buffer zones to prevent creases from nearing each other



## Alternative graph model for infinite paper

Instead of interpreting infinite rays as leaves, add a special vertex at infinity as their shared endpoint



Image: Hossain [2015]

...so trees become series-parallel multigraphs

## Some combinatorial constraints

The graphs of flat folding patterns with a vertex at infinity are:

- 2-vertex-connected
- 4-edge-connected
- not separable by removal of any 3 finite vertices

Proof ideas: convexity of subdivision rigidity of triangles



An unrealizable graph

[Eppstein 2018]

## Return to finite paper sizes

On circular or square paper, every folding pattern without interior vertices can be flat folded [Eppstein 2018]

(Not true for equilateral triangles!)



Corollary: All outerplanar graphs are realizable as folding patterns

## Summary

#### Polyhedra Well characterized; fast recognition and reconstruction

Planar soap bubble foams Well characterized; fast recognition and reconstruction What about 3d?

Contact graphs of segments: Well characterized; fast recognition and reconstruction Combinatorial model missing some features of Gilbert tessellations

Flat-folded surfaces:

Partial characterization

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