Intrinsic Geometries of Fullerenes

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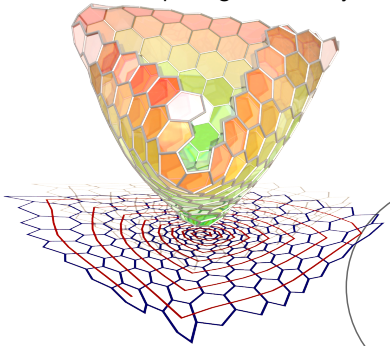
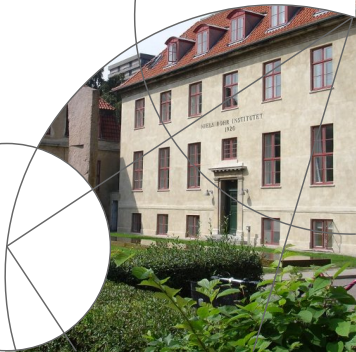
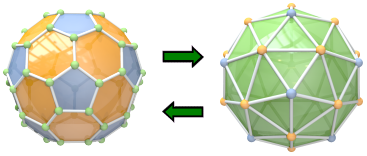




Fullerenes

Fullerenes are carbon molecules that form polyhedral cages. Their bond structures are exactly the planar cubic graphs that have *only pentagon and hexagon* faces. These are called *fullerene graphs*.

A wealth of information can be derived directly from the fullerene graphs. This talk will focus on fullerene *manifolds* or *intrinsic surfaces* and how these embed naturally in space.



A fullerene graph's *dual* is the planar graph for which faces become vertices and vice versa. This representation is easiest to work with for reasoning about their surface properties.

Fullerenes come in many shapes and sizes. On N vertices, there are $\mathcal{O}(N^9)$ distinct isomers.

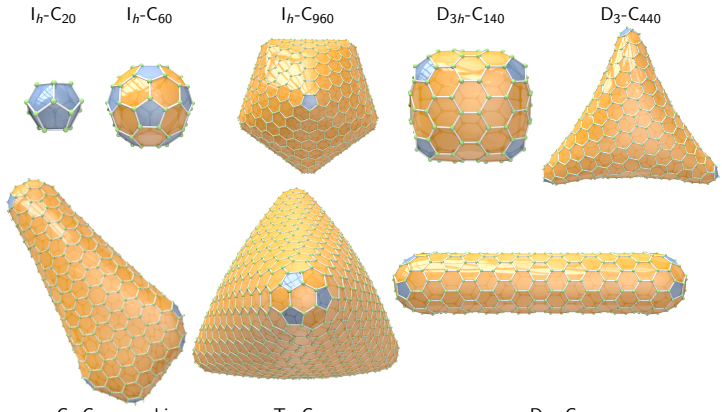
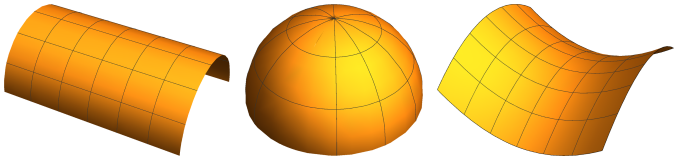


Table: A selection of a few fullerenes

Gaussian curvature

Gaussian curvature $K = \kappa_1 \kappa_2$ is the product of *principal curvatures* and describes *how a surface bends*.



$K = 0$ $K > 0$ $K < 0$

It is an *intrinsic* and *local* property of the manifold, and is independent of how it may be embedded.

The Gauss-Bonnet theorem

Integrating the Gaussian curvature over an orientable surface yields:

$$\int_S d\mathbf{s}\ K(\mathbf{s}) = 2\pi(2 - 2g)$$

Sphere	Plane / Torus	Genus 2	$\cdots$
4π	0	-4π	$\cdots$

Fullerene surfaces have spherical topology, i.e. a total of curvature of 4π.

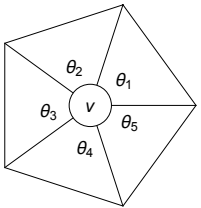
Discrete Gauss-Bonnet theorem

Discrete version of Gauss-Bonnet:

$$\sum_{v=1}^{N} K_v = 2\pi(2-2g)$$

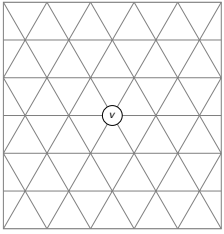
For a point v, the Gaussian curvature K_v is the difference between 2π and the angle of a circle around the point:

$$K_v = 2\pi - \textstyle\sum_i \theta_i$$

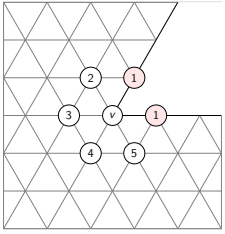


Fullerenes have total curvature 4π like the sphere, i.e. always exactly 12 pentagons, each contributing $\frac{2\pi}{6}$.

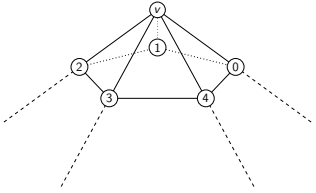
Folding and unfolding positive curvature surfaces



Deg. 6 patch



Deg. 5 vertex
$\frac{2\pi}{6}$ cut out.



Deg. 5 cone
Gauss. curvature $\frac{2\pi}{6}$

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Folding and unfolding positive curvature surfaces

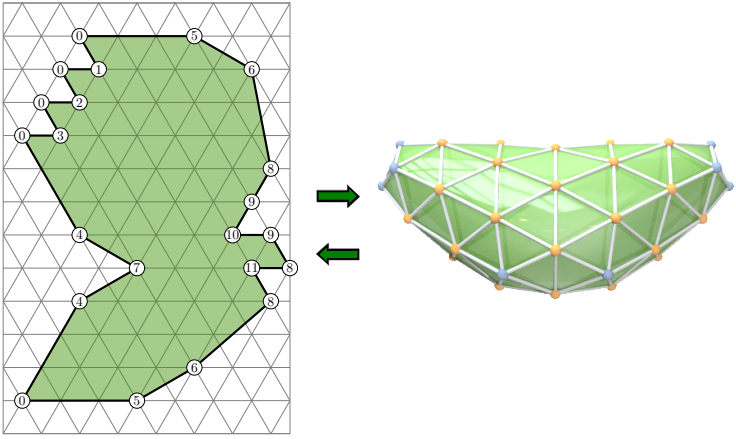


Figure: C_{2v}-C_{102} Eisenstein plane unfolding and 3D-embedding.

Ideal fullerene embedding in space

Given a fullerene dual graph, can we find an isometric embedding, i.e., one that doesn't stretch or twist its surface metric? This is true when all the triangles remain equilateral in the embedding.

This is the natural embedding of the fullerene dual, and modulo a slight distortion due to physical effects, it closely resembles the physical fullerene structure.

Does the ideal embedding always exist?

Yes! By Alexandrov's Theorem:

Theorem

Let M be a convex polyhedral metric on the sphere. Then there exists a convex polyhedron $P \subset \mathbb{R}^3$ such that the boundary of P is isometric to M. Moreover, P is unique up to a rigid motion.

A fullerene surface defines a convex polyhedral metric, so a isometric convex embedding exists and is unique.

Can we find it?

Usually, but not always. We have used numerical force-field optimization, which sometimes breaks down due to large forces; increasingly often as fullerenes grow in size.

Idea: Degree-5 vertex placement uniquely decides shape. Thin out, and find ideal twelve-cornered shape using surface distances.

Problem 1: Triangulation of coarse surface is important, most triangulations yield garbage.

Solution 1: Delaunay triangulation ensures faces without Gaussian curvature; surface lengths approximate spatial lengths. Need to perform *intrinsic* Delaunay triangulation, since we don't have embedding. Algorithm by Fisher et al. (2007).

Problem 2: How to obtain full fullerene given coarse structure?

Solution 2: Unfolding to Eisenstein plane determines which deg. 6 nodes are inside each triangle. Unfold and interpolate.

Distances along fullerene surfaces

The surface metric is only piecewise flat: Multiple straight lines connect the same two points. Three points do not define a unique triangle.

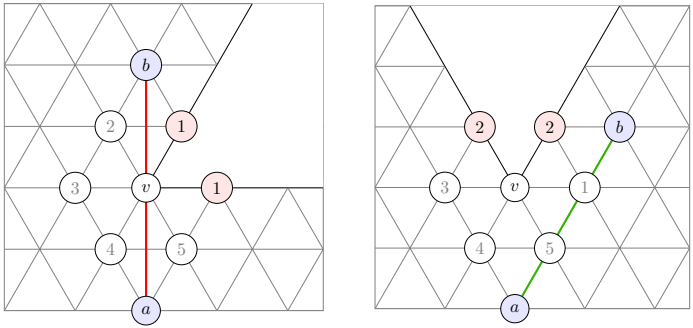
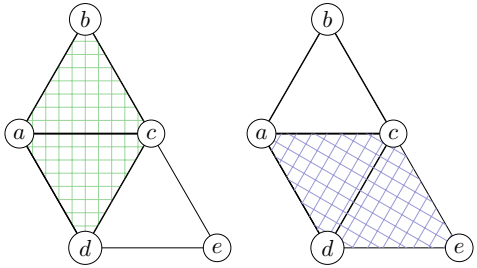


Figure: Length of red path is $2\sqrt{3}$. Length of green path is 3.

It is impossible to equip the surface with a global, isometric 2D-coordinate system.

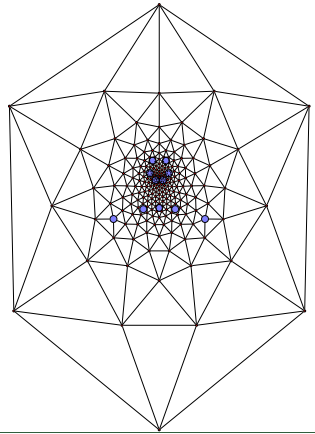


However, any pair of adjacent simplices can share a Cartesian coordinate system. *Inside* such a pair, lengths and angles are "flat", and we can calculate them in the usual manner. *Outside* the pair, the coordinate system is invalid if neighbouring a cone point. But a region containing only deg. 6 vertices are "flat" and can be equipped with a common coordinate system.

Procedure

Given fullerene dual graph:

D_{6d}-C_{480}

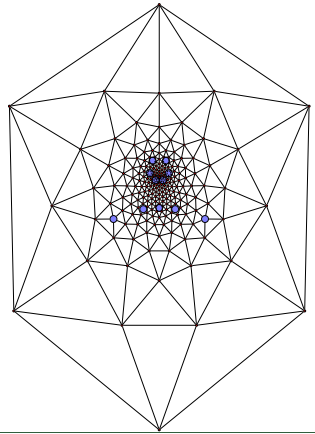


Procedure

Given fullerene dual graph:

1 Compute coarse intrinsic Delaunay triangulation of surface.

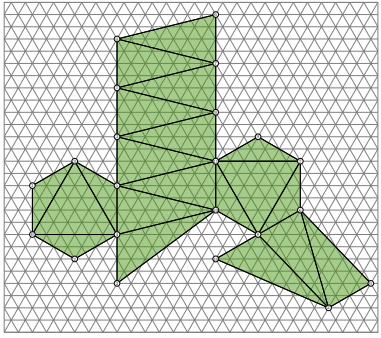
D_{6d}-C_{480}



Procedure

Given fullerene dual graph:

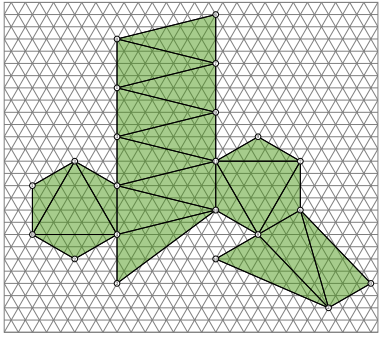
1. Compute coarse intrinsic Delaunay triangulation of surface.
2. Unfold triangles to Eisenstein plane.



Procedure

Given fullerene dual graph:

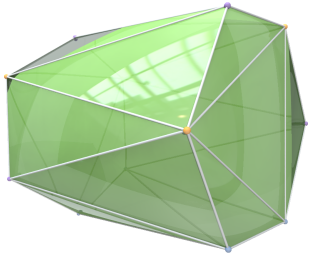
1. Compute coarse intrinsic Delaunay triangulation of surface.
2. Unfold triangles to Eisenstein plane.
3. "Rasterize" triangles to find degree-6 nodes in each triangle.



Procedure

Given fullerene dual graph:

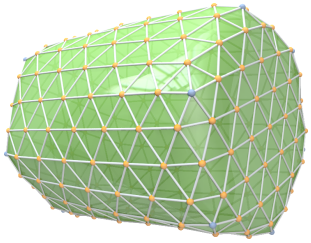
1. Compute coarse intrinsic Delaunay triangulation of surface.
2. Unfold triangles to Eisenstein plane.
3. "Rasterize" triangles to find degree-6 nodes in each triangle.
4. Compute coarse polyhedron from Delaunay triangulation and surface distances.



Procedure

Given fullerene dual graph:

1. Compute coarse intrinsic Delaunay triangulation of surface.
2. Unfold triangles to Eisenstein plane.
3. "Rasterize" triangles to find degree-6 nodes in each triangle.
4. Compute coarse polyhedron from Delaunay triangulation and surface distances.
5. Interpolate degree-6 node positions.



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4. Compute coarse polyhedron from Delaunay triangulation and surface distances.
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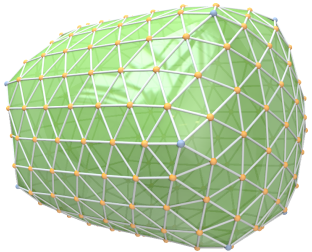
6a. For ideal deltahedron: relax using force-field optimization.



Procedure

Given fullerene dual graph:

1. Compute coarse intrinsic Delaunay triangulation of surface.
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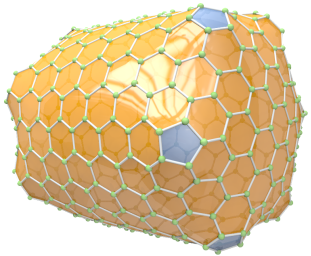
4. Compute coarse polyhedron from Delaunay triangulation and surface distances.
5. Interpolate degree-6 node positions.

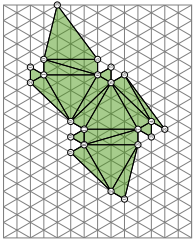
6a. For ideal deltahedron: relax using force-field optimization.

6b. For physical fullerene structure: dualize and optimize.

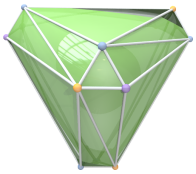


Results

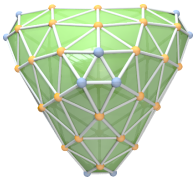
Unfolding



Coarse polyhedron



Interpolated deltahedron



Optimized fullerene

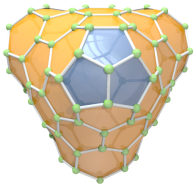
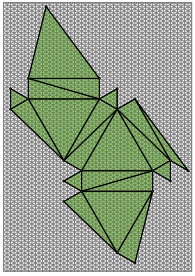


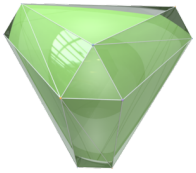
Table: Result for T_d-C_{100}.

Results

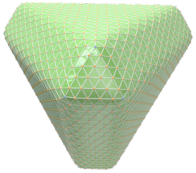
Unfolding



Coarse polyhedron



Interpolated deltahedron



Optimized fullerene

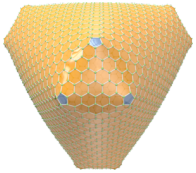
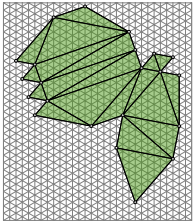


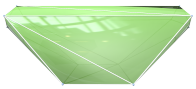
Table: Result for T_d-C_{2500}.

Results

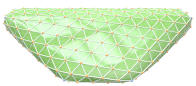
Unfolding



Coarse polyhedron



Interpolated deltahedron



Optimized fullerene

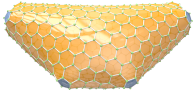


Table: Result for C_{2v}-C_{714}.

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Results

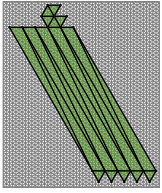
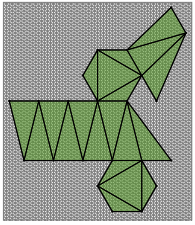
Unfolding	Coarse polyhedron	Interpolated deltahedron	Optimized fullerene
			

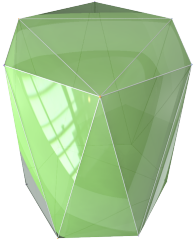
Table: Result for D_{5d}-C_{1680}.

Results

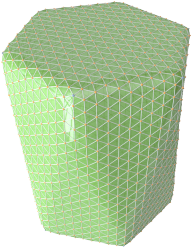
Unfolding



Coarse polyhedron



Interpolated deltahedron



Optimized fullerene

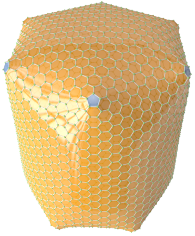


Table: Result for D_{6d}-C_{3000}.

Software

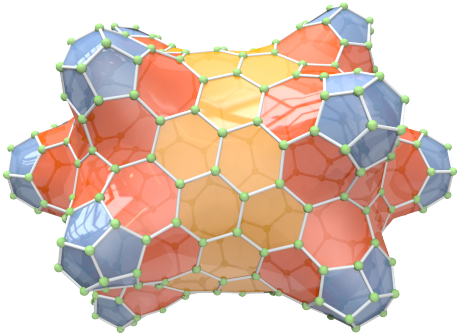
`Fullerene`: A software package for constructing and analyzing structures of fullerenes.

Schwerdtfeger, Wirz, and Avery

http://tinyurl.com/fullerenes

Implements a huge variety of tools for geometric, topological, physical, and chemical analysis of fullerenes.

Gracias por su atención!



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