

Topology of Random Cell Complexes

Ben Schweinhart

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December 10, 2014

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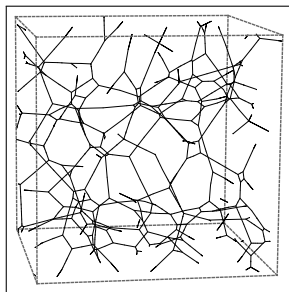
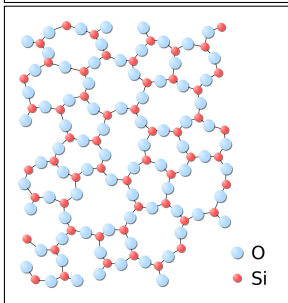
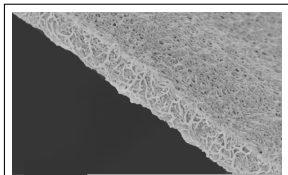
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Open Cell Foams

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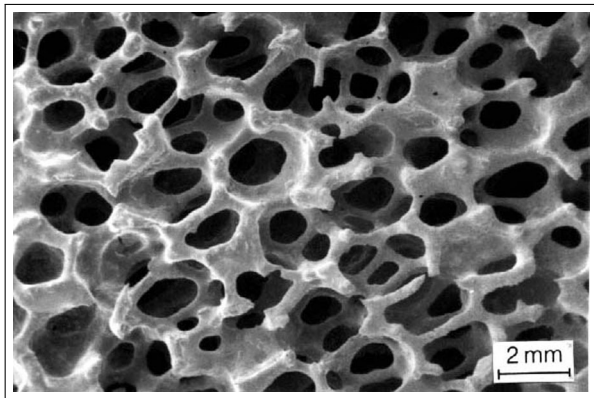
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- Interesting topology
- Very important material in practice, not well understood

Grain Growth

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- Show movie
 - Steady state for which scale-free properties have converged? Dependence on initial conditions?
 - Need metric - a nice one is given by considering the local topology.

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- These systems have interesting topology, but they have not yet been studied using topological methods.*
- Crystallography doesn't apply to disordered materials.
- Plan: First, I will introduce a new, general method to quantify the topology of cell complexes.
- Then I will talk about a case study, and discuss computational results - strong evidence of existence of a steady state.
- If I have time, I will briefly describe two other topological methods.

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Idea of Swatches

Key Idea

Quantify the local topology of cell complexes by using probability distributions of local configurations.

- Used to define a distance on cell complexes. The distance can be used to, e.g., quantify the variability of cell complexes generated in a particular way, compare two cell complexes (i.e. experimental results with simulations), or test convergence to a steady state
- Applicable to many different physical systems, computable.
- Joint work with Jeremy Mason (Boğaziçi University) and Bob MacPherson (Institute for Advanced Study)
- Paper on the arxiv: Topological Similarity of Random Cell Complexes, and Applications to Dislocation Networks.

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Regular Cell Complexes

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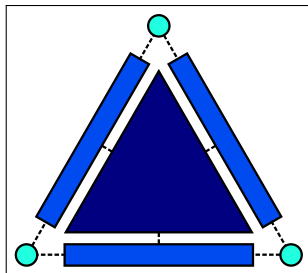
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Definition

A **Regular Cell Complex** is a space built inductively by attaching cells in each dimension (points, line segments, disks, etc). Each cell is glued on by homeomorphisms from their boundaries into the existing structure.

Graph Representation

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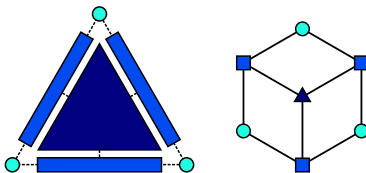
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- Represent a regular cell complex by the adjacency graph of the cells, labeled by dimension.
- Captures all topological properties.

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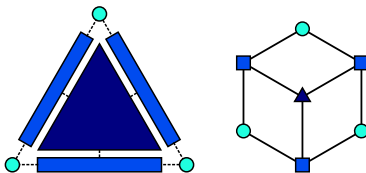
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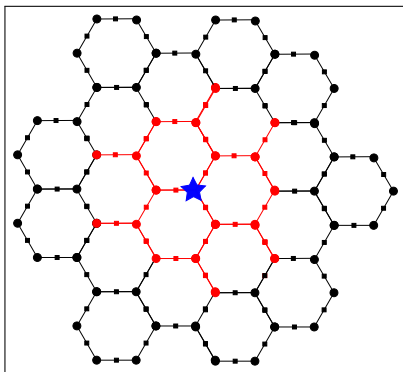
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Swatches



Definition

The **swatch at vertex v of radius r** is the neighborhood of v of radius r in the graph distance (every edge has length one).

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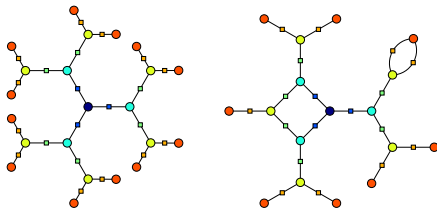
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- Two swatches have the same **swatch type** if they represent the same topological configuration.
- Sub-swatch of a swatch: swatch of smaller radius at the same root (central vertex).

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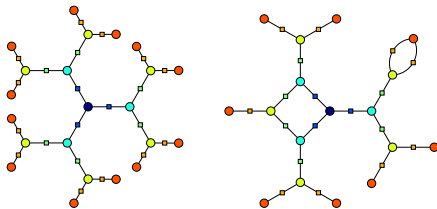
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Cloth

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Collaborators

- For each r , consider the probability distribution of swatch types of radius r at the vertices of a cell complex.
- This family of probability distributions is called the **cloth** of the cell complex.
- Captures all local topological properties of the cell complex.

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Tree of Swatches

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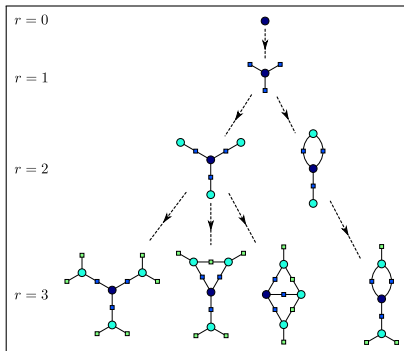
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Collaborators



- Connect swatch type of radius r with all subswatch types of radius $r - 1$.
- The cloth is a weighting on this tree, subject to consistency conditions.

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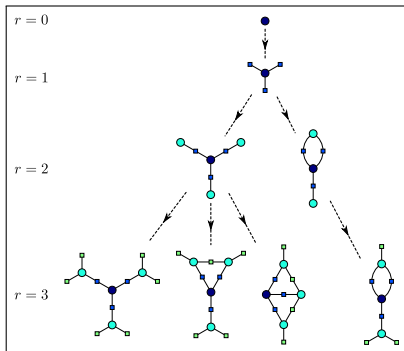
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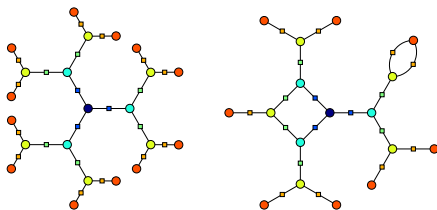
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- Distance between two swatches = one over order (# cells) of largest common subswatch, or 0 if they are equal.
- $d(S_1, S_2) = \frac{1}{13}$

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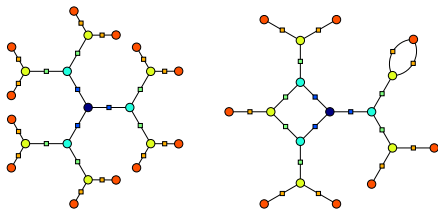
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If C_1 and C_2 are cell complexes, $d_r(C_1, C_2)$ is the Earth Mover's Distance between the probability distributions at radius r induced by distance on swatches.

- Earth Mover's Distance = the infimum of the costs of transformations between the two probability distributions on swatch types of radius r .
- Cost = amount of probability mass moved between swatch types, weighted by swatch distance.
- Distance can be used to compare different structures, test convergence to steady state, iteratively modify structures to reach a desired state

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Convergence of Cell Complexes

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- **Limit distance** = $d(C_1, C_2) = \lim_{r \rightarrow \infty} d_r(C_1, C_2)$.
- A sequence $\{C_i\}$ of cell complexes converges if it is a Cauchy sequence in d .
- Equivalent to all swatch frequencies converging.

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Theorem

(Benjamini-Schramm Graph Limit) A convergent sequence of cell complexes gives rise to a limit distribution on the space of countable, connected cell complexes a root specified. The distance can be extended to the space of these distributions.

- Also implies convergence of all local topological properties: those that can be defined in terms of maps from a fixed labeled graph H into the diagram of C_j .
- Reference: Large Networks and Graph Limits

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Collaborators

- Simulate curvature-driven evolution of dimension one network in 3-space.
 - Represent network as one-dimensional cell complex.
 - Compute cloth (swatch distributions) for radius $r < 10$
 - Track distance d_r to candidate steady state
 - Discuss other applications of topology to the case study.

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Collaborators

- Curvature-driven evolution of polygonal curves in \mathbb{T}^3 .
- The polygonal curves meet each other at vertices of degree three.
- The curves are composed of line segments meeting at nodes.
- Evolves by energy minimization, assuming constant energy γ per unit length.
- This can be viewed as a very simple model of a dislocation network in the process of recovery.

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Movie

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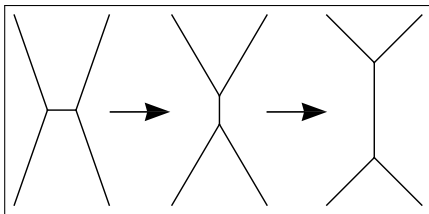
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- Edge Flip
- Digon Deletion
- Edge Intersection

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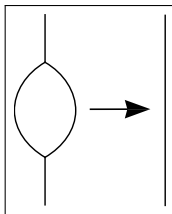
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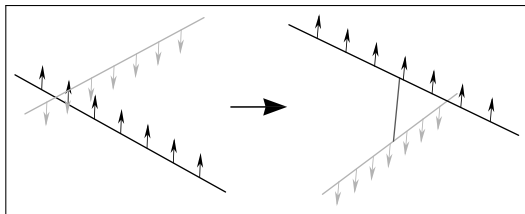
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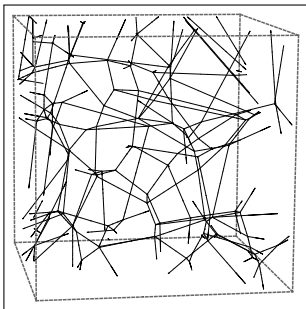
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- **Voronoi Graph:** modified 1-skeleton of Voronoi tessellation for random points in the three-torus.
- **Random Graph:** Place random points on the three-torus. Randomly create edges between pairs that are close enough.
- Both evolve to “steady state”.

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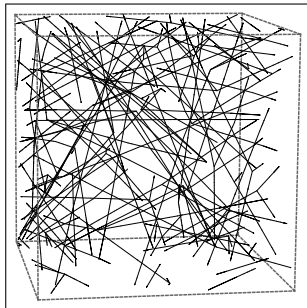
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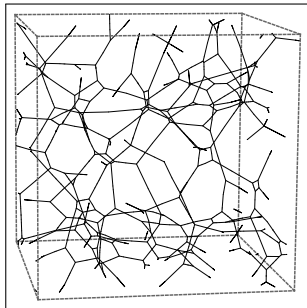
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- Simulate curvature-driven evolution of dimension one network in 3-space.
- Represent network as one-dimensional cell complex.
- Compute cloth (swatch distributions) for radius $r < 10$
- Find candidate steady state for which many scale-free properties appear to have converged.
- Track distance d_r to candidate steady state

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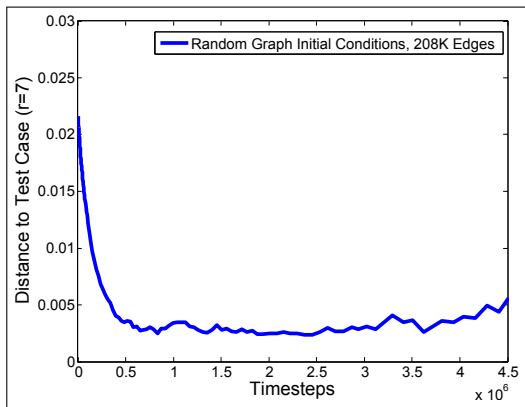
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- Track distance to large, steady state test case as system evolves.
- Change coordinates to aid comparison of systems.

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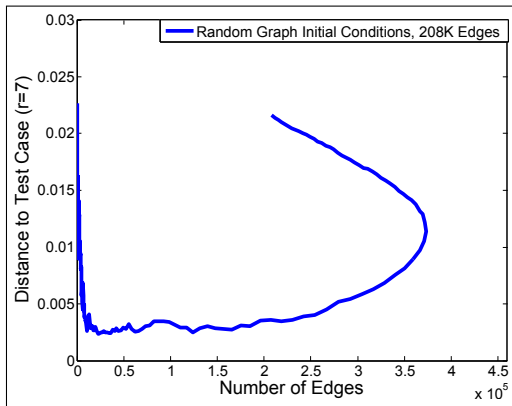
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- Track distance to large, steady state test case as system evolves.
- Change coordinates to aid comparison of systems.

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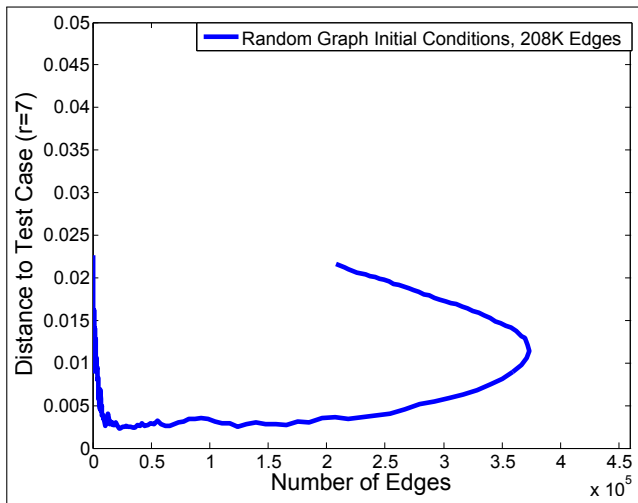
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- First Case: Random Graph Initial Conditions

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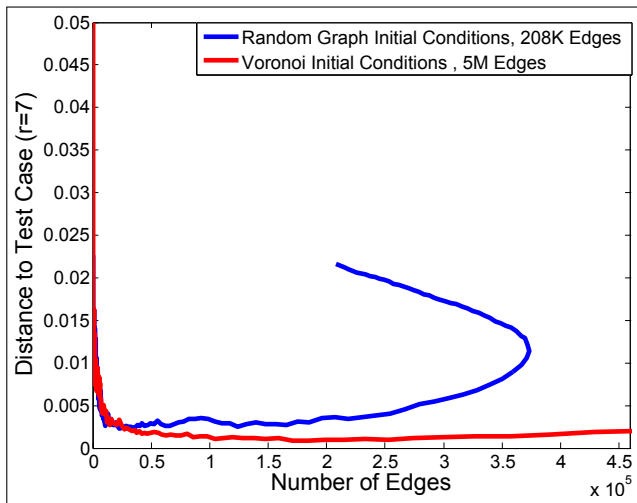
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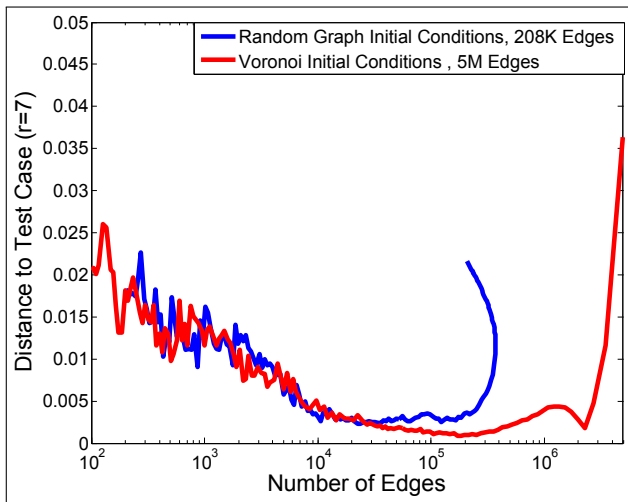
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- Second Case: Large Voronoi

Convergence Results, II



- Second Case: Large Voronoi

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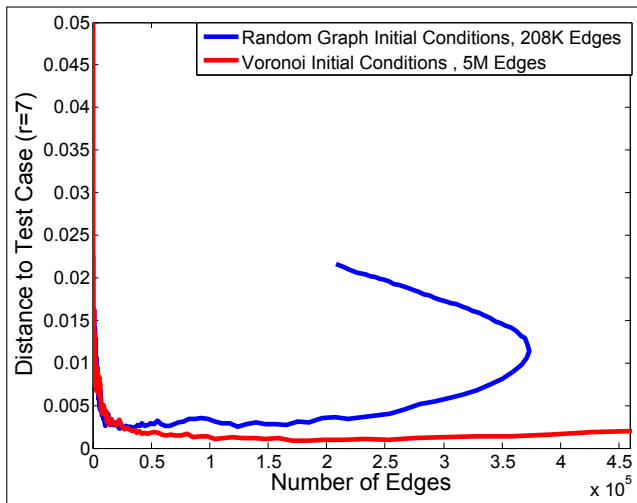
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- Second Case: Large Voronoi

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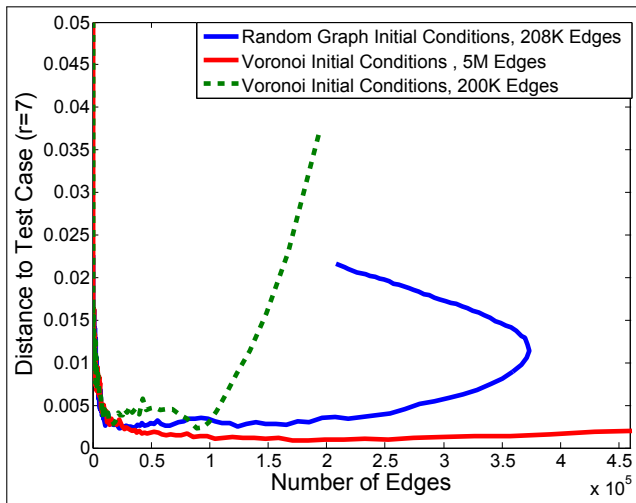
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■ Third Case: Small Voronoi

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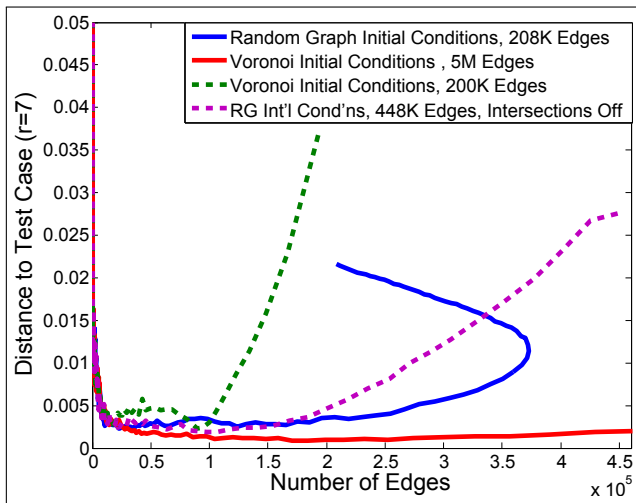
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- Fourth Case: Random Graph with Intersections Disabled

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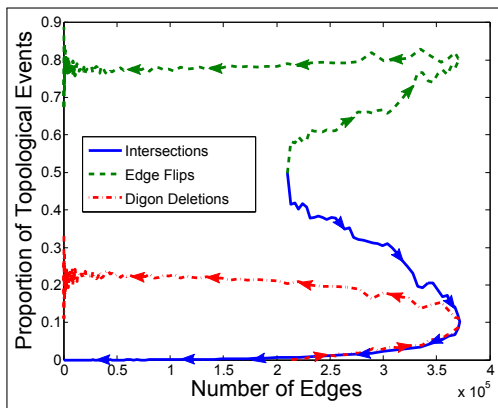
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- Plot preponderance of different topological changes as simulation proceeds.
- Intersections computationally expensive; can disregard for better steady state statistics.

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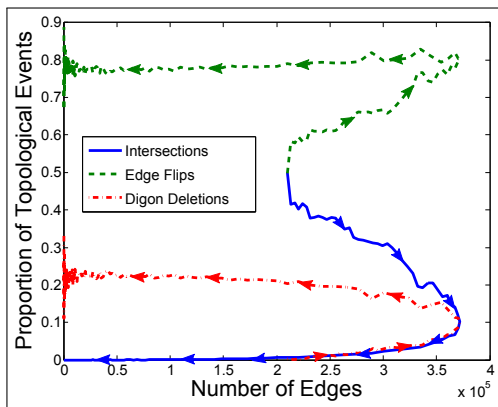
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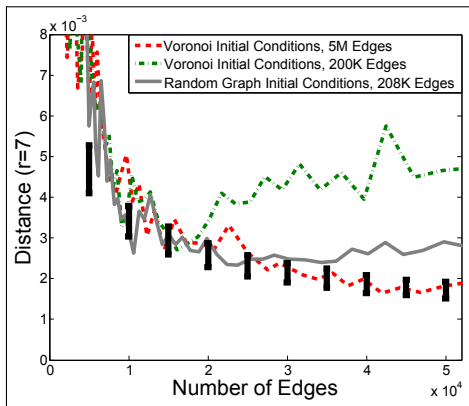
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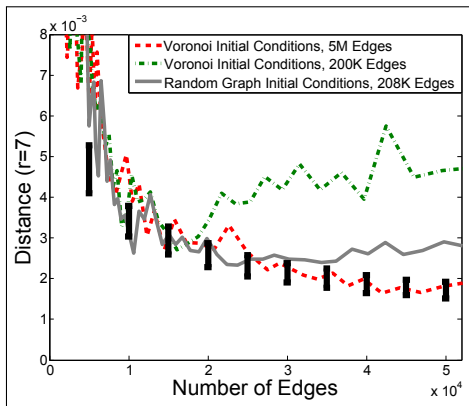
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Collaborators



- Hard to estimate statistical error for cloth: complicated interdependencies of swatch frequencies
- Idea: compare simulation to representative subsamples of test case

Error Estimation



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- Idea: compare simulation to representative subsamples of test case

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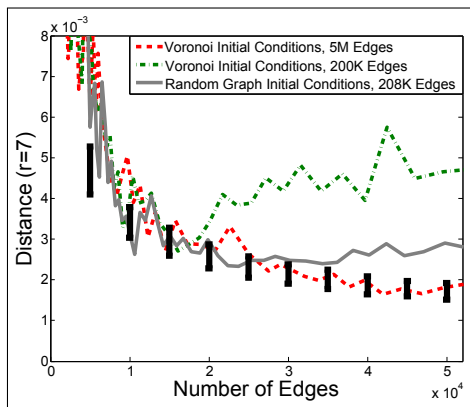
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- System has converged to state represented by test case if it is statistically indistinguishable from a subsample of it.
- Within one standard deviation of subsamples: good evidence of convergence.

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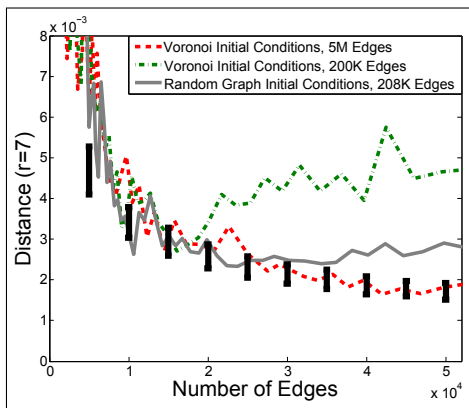
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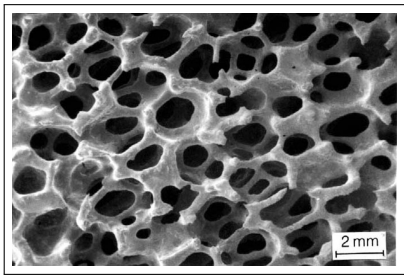
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Collaborators



- Consider ϵ -neighborhoods of $X \subset \mathbb{R}^3$, X_ϵ .
- As ϵ increases, holes form and disappear.
- Persistent Homology tracks these holes as ϵ increases.
- Look at figures in Mathematica

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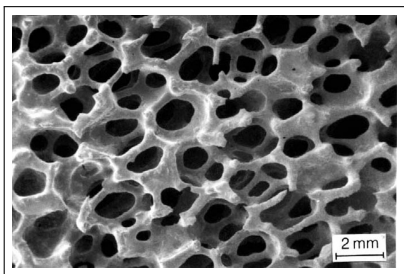
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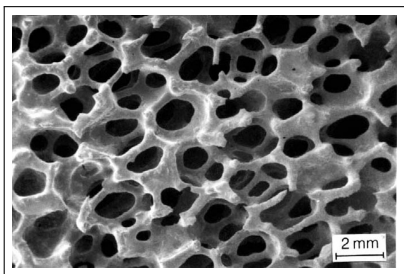
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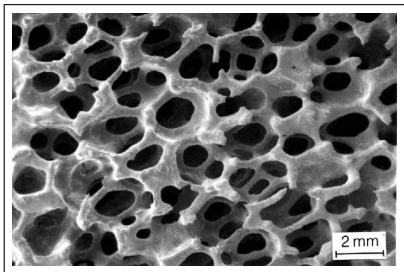
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Collaborators

- **Philosophy:** use persistent homology to study geometry of fixed object.
- Paper - “Measuring Shape with Topology” (Journal of Mathematical Physics, joint with R. MacPherson)
- Holes in X_ϵ correspond to voids in X
- Find voids in materials

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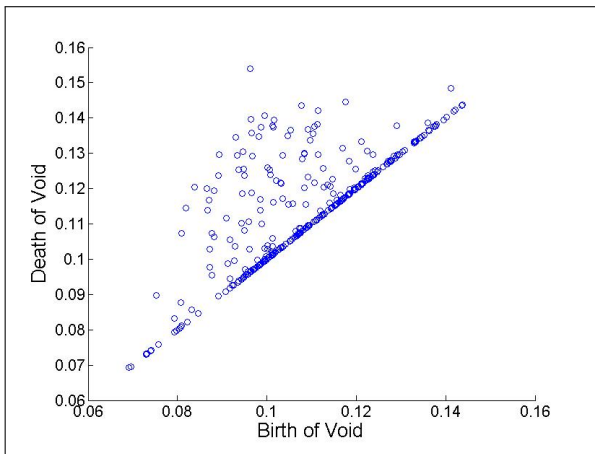
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- Plot time when hole appears vs time when it disappears
- Points on $x=y$ line are noise

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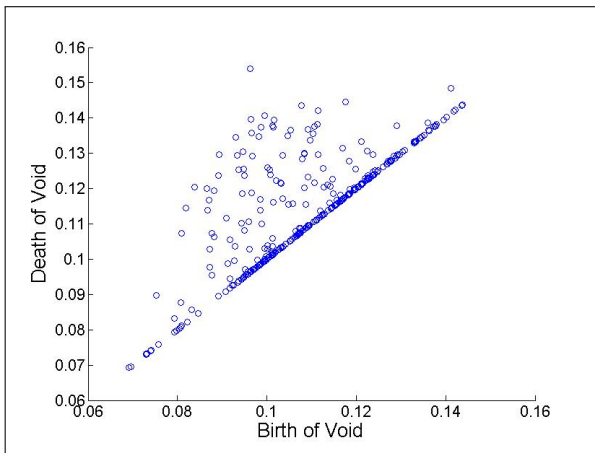
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1-skeleton of Voronoi Decomposition

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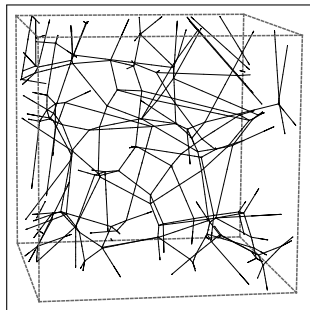
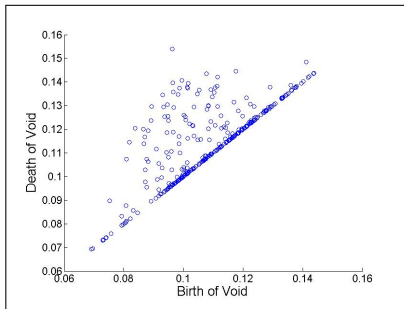
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- Persistent Homology recovers the cells.

Steady State of CDE Simulation

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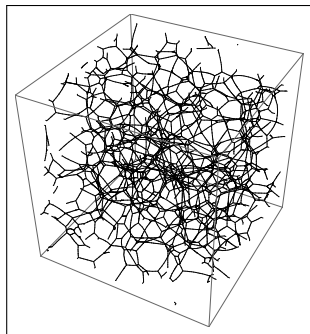
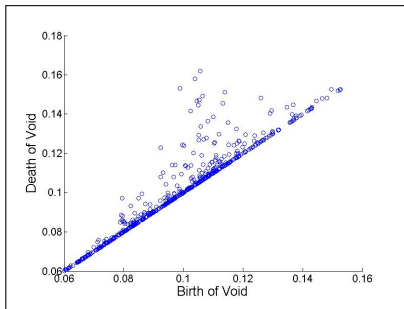
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■ More surprising voids!

Minimal Cycles

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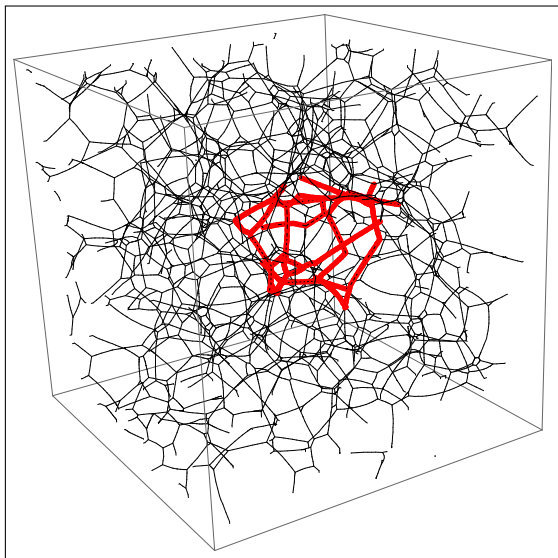
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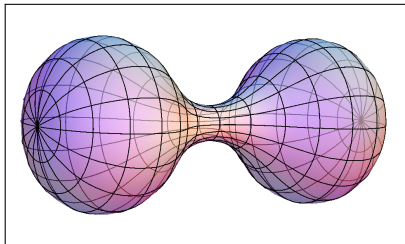
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- Usual interpretation of Persistent Homology represents this as two points for two voids
 - Correct structure: Persistence Tree
 - Adjacency of minimal cycles?

Persistence Tree

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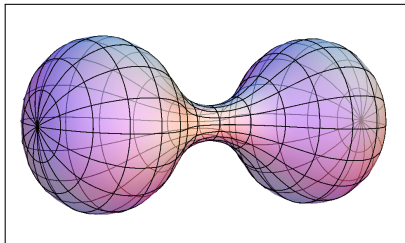
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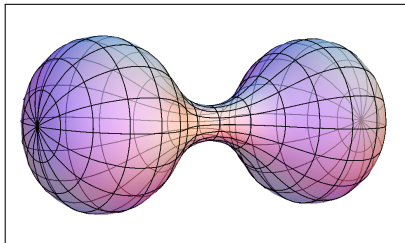
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Unknotted Networks

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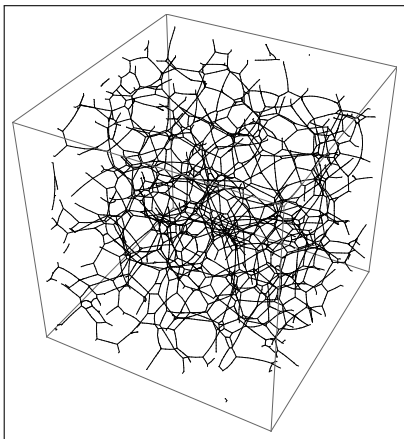
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- Many embedded graphs from physical systems appear to be unknotted.
- How to measure this?

Unknotted Networks

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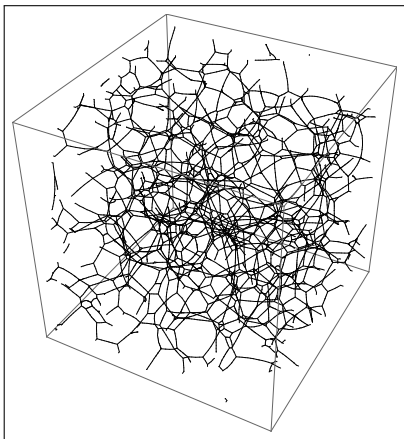
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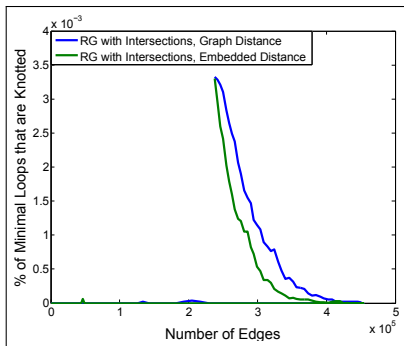
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- Look at shortest cycle containing each edge. Is it knotted?
- Start with knotted network, track # of knotted minimal cycles as system evolves.
- Curvature-driven evolution appears to unknot networks.

Minimal Cycles

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Ben
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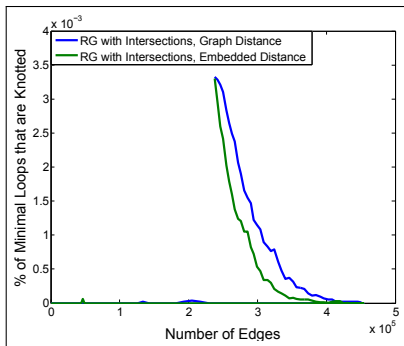
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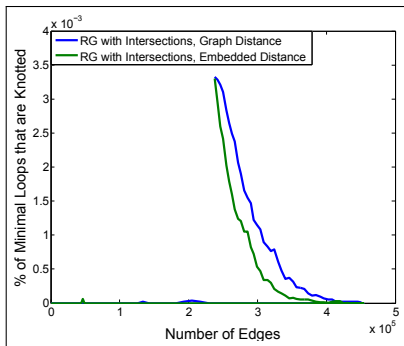
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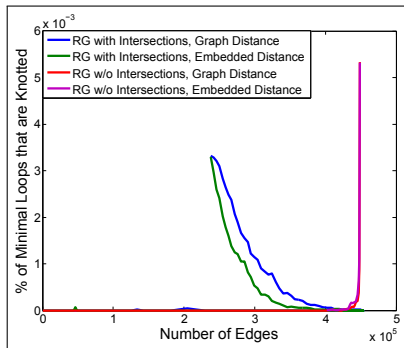
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- Look at shortest cycle containing each edge. Is it knotted?
- Start with knotted network, track # of knotted minimal cycles as system evolves.
- Curvature-driven evolution appears to unknot networks.
- Network unknots even faster if intersections turned off.

Unknottedness

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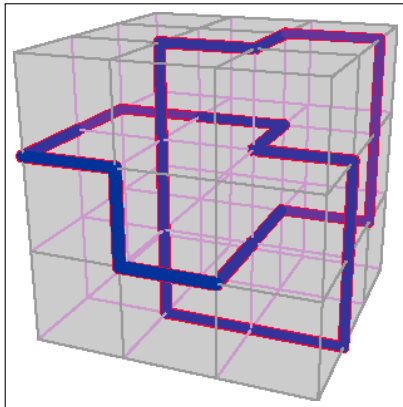
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- Unknotted networks can contain knots.

Defining Unknottedness

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Definition

An embedded graph is **unknotted** if its complement has the homotopy type of a graph.

- Physical interpretation: equivalent to existence of dual network (important for, i.e., open cell foams).
- I'm working on several theoretical questions surrounding this definition.
- Is it equivalent to π_1 of the complement being free?

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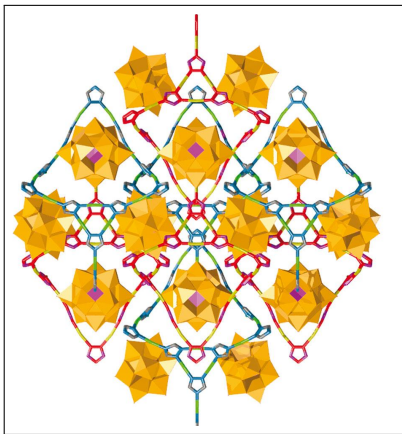
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- Knotted materials may have interesting, useful properties.
- Metal-organic frameworks: new, exotic, sometimes knotted

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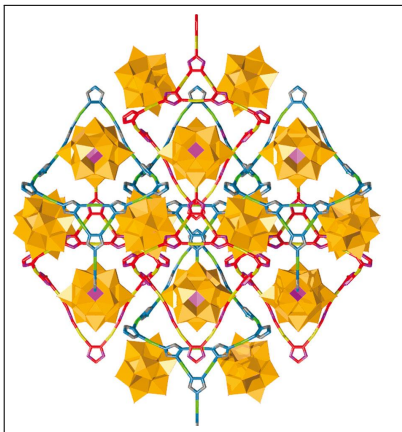
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- Interesting topology abounds in materials science and physics.
- Topology could be useful for understanding structures that are currently not well-understood using any methods.
- Many applications to work on, many new methods to be developed.
- Perhaps the study of these applications will also provide new ideas for topology.

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- Robert MacPherson (Institute for Advanced Study) - PhD Advisor
- Jeremy Mason (Boğaziçi University) - Swatches