Framework for an Ensemble-based Topological Entropy Calculation in Three Dimensions

Eric Roberts[1], Suzanne Sindi[1], Spencer Smith[2], Kevin Mitchell[1]

[1]*University of California, Merced*

[2]*Mount Holyoke College*

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In a Nutshell

We build an algorithm for computing topological entropy that:

1. requires only an **ensemble** of trajectories
2. requires **no knowledge** of governing equations
3. scales **favorably in runtime** compared to other 2D ensemble-based approaches
4. can be **generalized to higher dimensions**

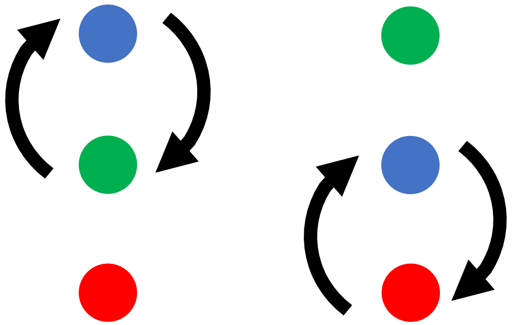
Topological Entropy in Rod-Stirring System

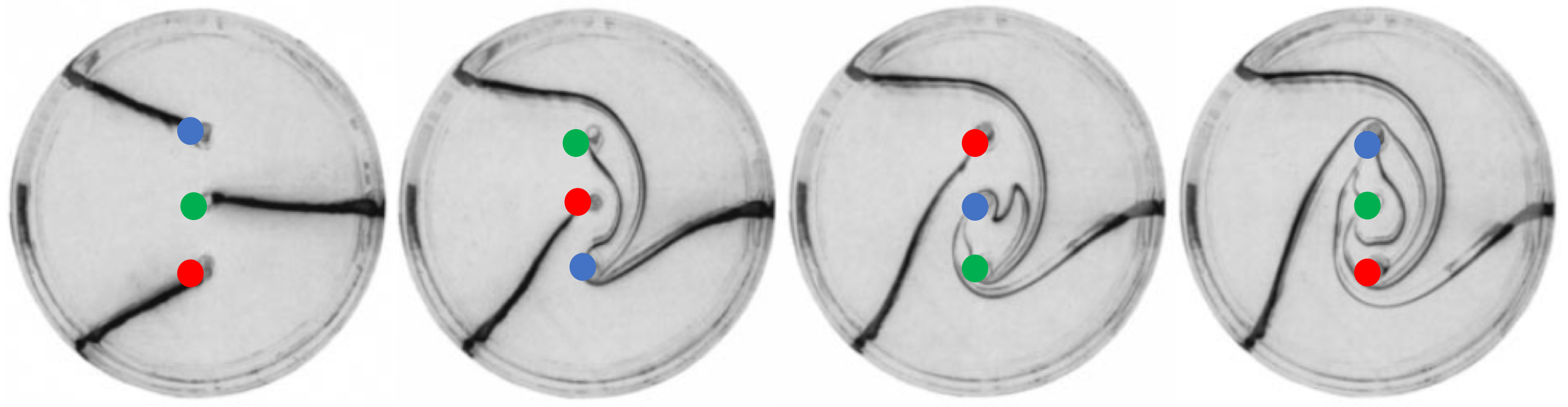
Topological entropy given by exponential growth rate of an advected material line

Bad mixing protocol

Rod stirring process gives low topological entropy

One Period





Four periods

Source: Boyland, P. L., Aref, H. & Stremler, M. A. (2000).

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Rod stirring process gives high topological entropy

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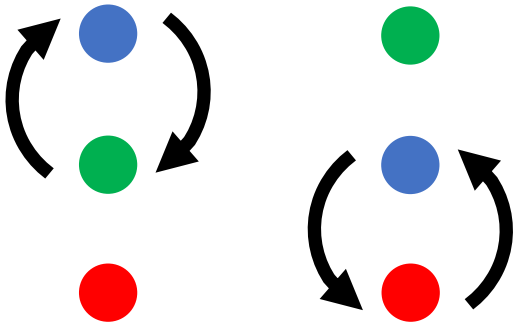

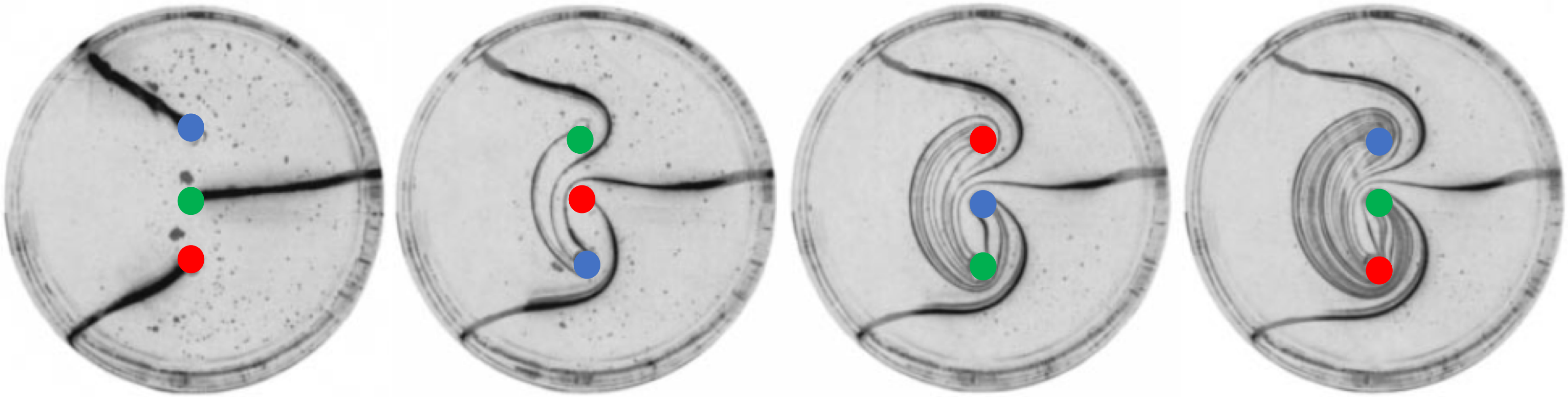

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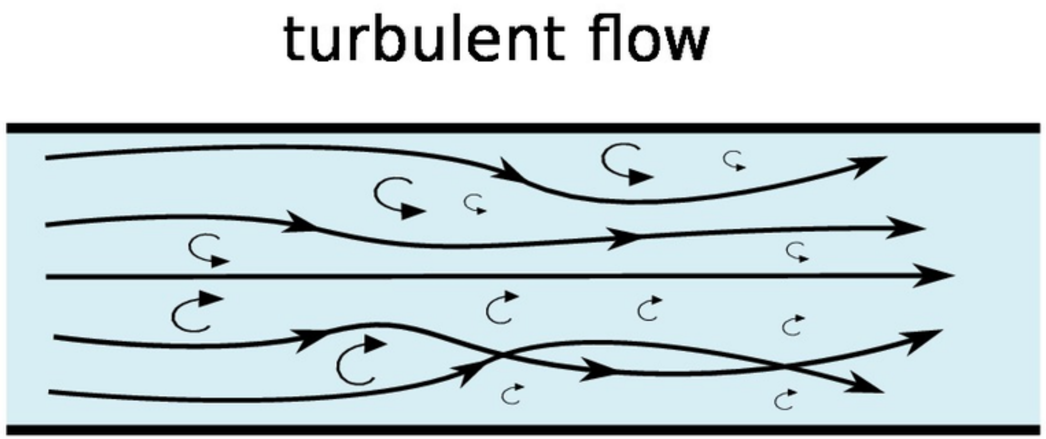
Motivation for Studying Topological Entropy

Everyday Mixing

We typically think of turbulence when discussing fluid mixing

- Characterized by formation of eddies and vortices in high Reynold's number regimes
- Scalar (cream) is mixed in fluid (coffee) quickly



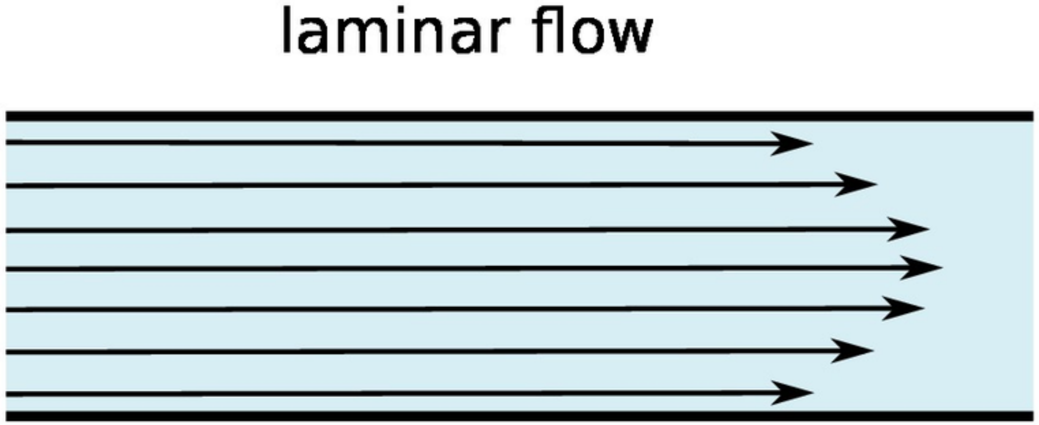
http://www.albaniles.org

Source: https://www.flickr.com/photos/kidmissile/4427545035/

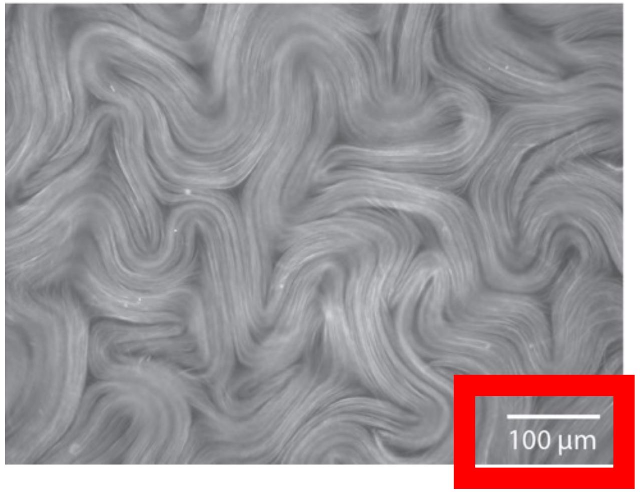
Everyday Mixing

Turbulence doesn't occur when Reynold's number is low

- Low Reynold's number results from viscous flows or small length scales **(bottom right)**
- Scalar (oil) mixing in fluid (peanut butter) requires more work



Source: *http://www.homemadeeats.com*



Courtesy of *Dogic Lab*, UC Santa Barbara

Mixing from Chaotic Advection

Chaotic advection arises from from repeated *stretching* and *folding* of fluid.

- Produces an effective stirrer/mixer in laminar flows
- Commonly exploited in industry settings (paint mixing, food processing)
- We use chaotic advection to study mixing of a bio material on cellular scale

Video Credit: ah clem, *"Depoe Bay, Oregon-salt water taffy pulling machine."* <https://www.youtube.com/watch?v=Y7tlHDsquVM>

Chaotic Advection and Topological Entropy

Chaotic advection implies positive topological entropy (TE)

- TE is common proxy for quality of mixing
- What if velocity field or governing equations are unknown

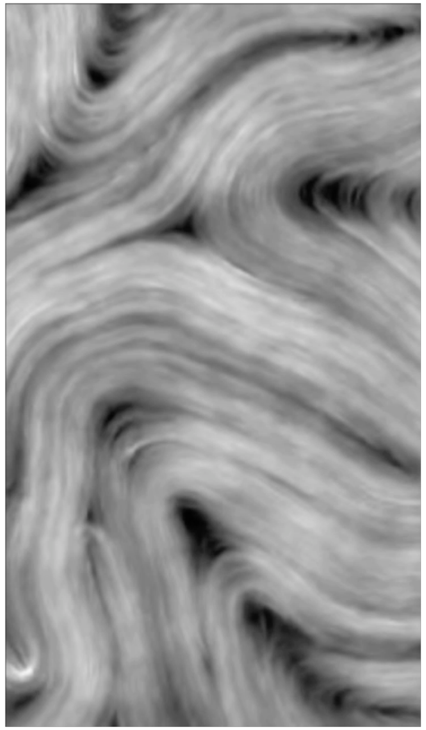
Can we compute TE from *only* trajectory data?

In collaboration with the *Hirst Lab*, UC Merced

Can we compute TE from only a sparse set of trajectories?

Ref: *Thiffeault, (2010)*

How well do densely-packed bundles of microtubules mix?

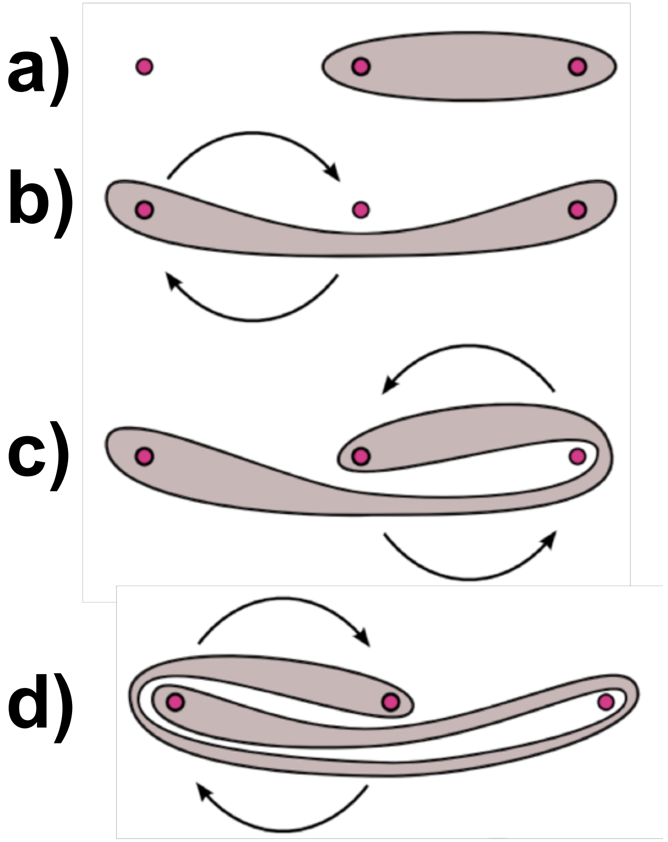


Courtesy of *Dogic Lab*, UC Santa Barbara

Topological Entropy from Trajectory Data

Use trajectories as stirrers to deform and braid an “elastic loop”

Growth of loop gives topological entropy lower bound



Ref: Thiffeault, Jean-Luc. "*Braids of entangled particle trajectories*." (2010)

Topological Entropy from Trajectory Data

Use trajectories as stirrers to deform and braid an “elastic loop”

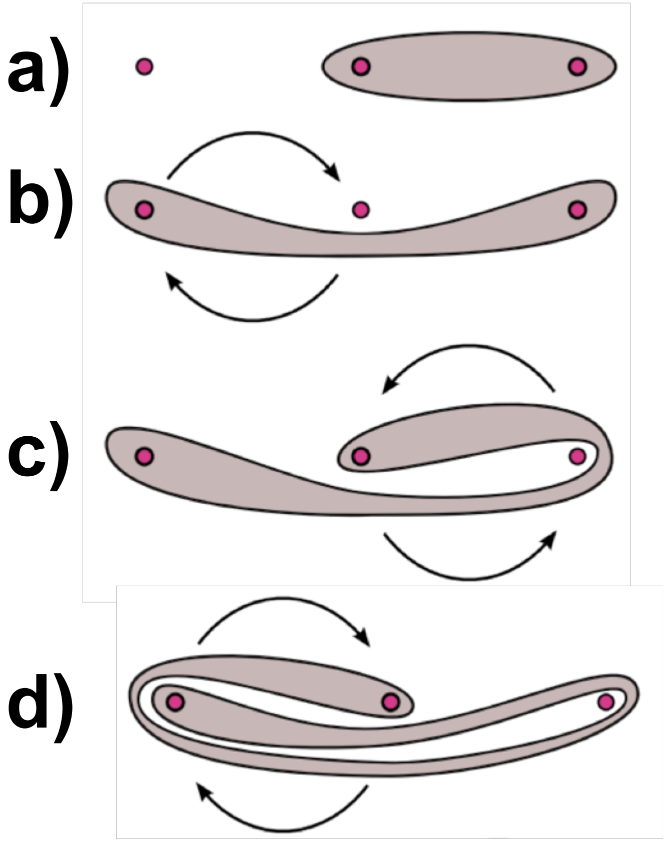
We are motivated by trajectory braiding work of Thiffeault, Budišić, Finn, and Allshouse

Finite Time Braiding Exponents (FTBE)

Encodes trajectories as braids and uses actions of braids to stretch loops

- Pros
  - i) Works for open, aperiodic trajectories
- *Cons*
  - *i) Slow for high point densities*
  - *ii) No higher dimensional generalization*

See Budišić and Thiffeault. "*Finite-time braiding exponents.*" (2015)



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Topological Entropy from Trajectory Data

Use trajectories as stirrers to deform and braid an “elastic loop”

Our contribution: Motivated by Marc Lefranc, we use a computational geometric approach to encode the loop and overcome the hardships below

<u>**Finite Time Braiding Exponents (FTBE)**</u>

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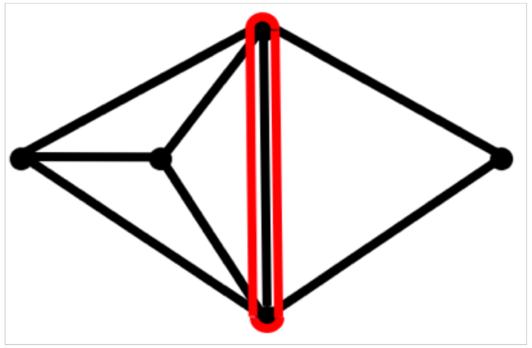

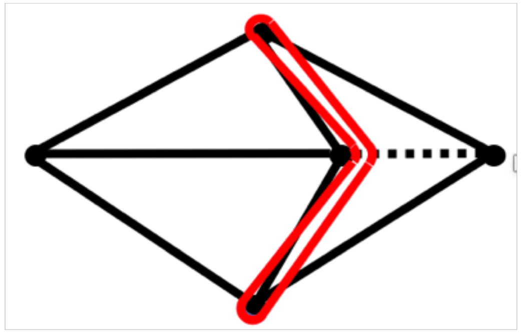

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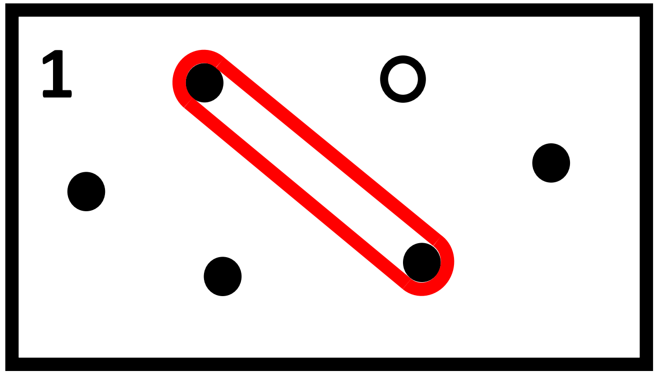
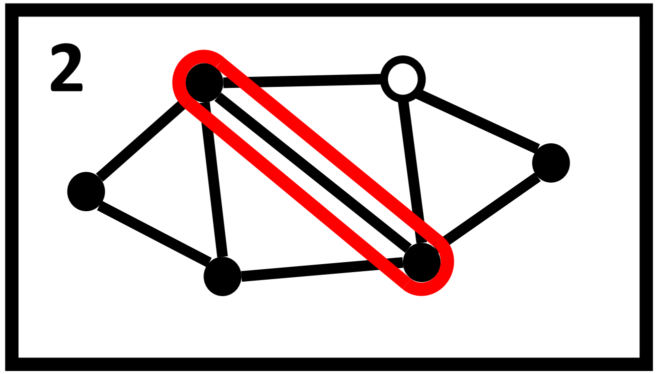
E-tec: Ensemble-based Topological Entropy Calculation

E-tec Snapshot

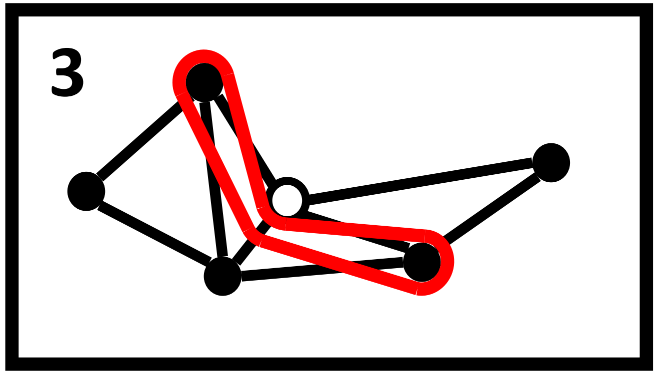
E-tec: Ensemble-based Topological Entropy Calculation (*Roberts, Sindi, Smith, Mitchell. Chaos.* ***29****, 13124 (2019)*)



1. Choose trajectories to anchor loop



2. Triangulate initial points
   (constrained to choice of
   initial band)

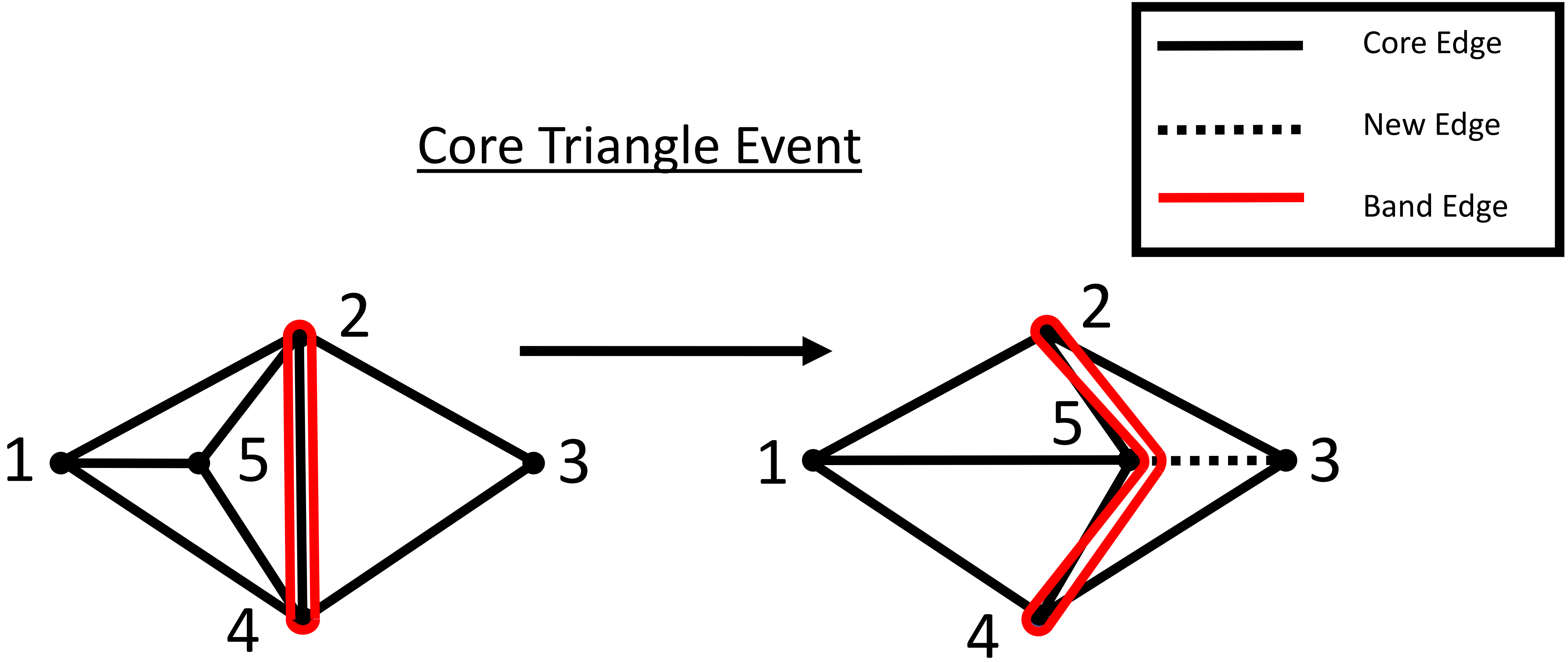


3. Evolve trajectories, stretching band and locally updating triangulation upon each point-triangulation edge collision. (Hollow point moves for reference.)

Detecting Trajectory-Band Collisions

We track two different types of **triangle collapse events:**

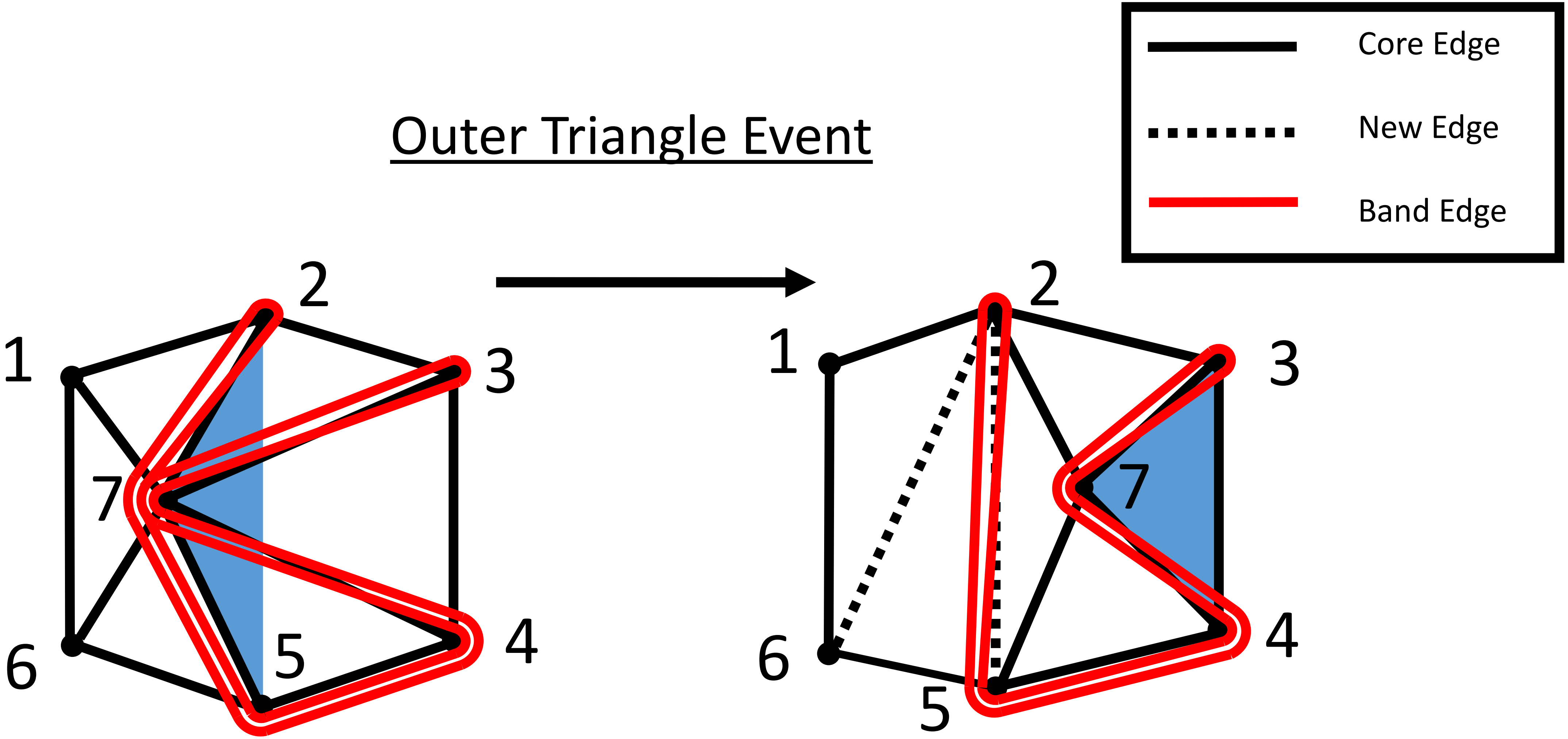
Core Triangle Event



Detecting Trajectory-Band Collisions

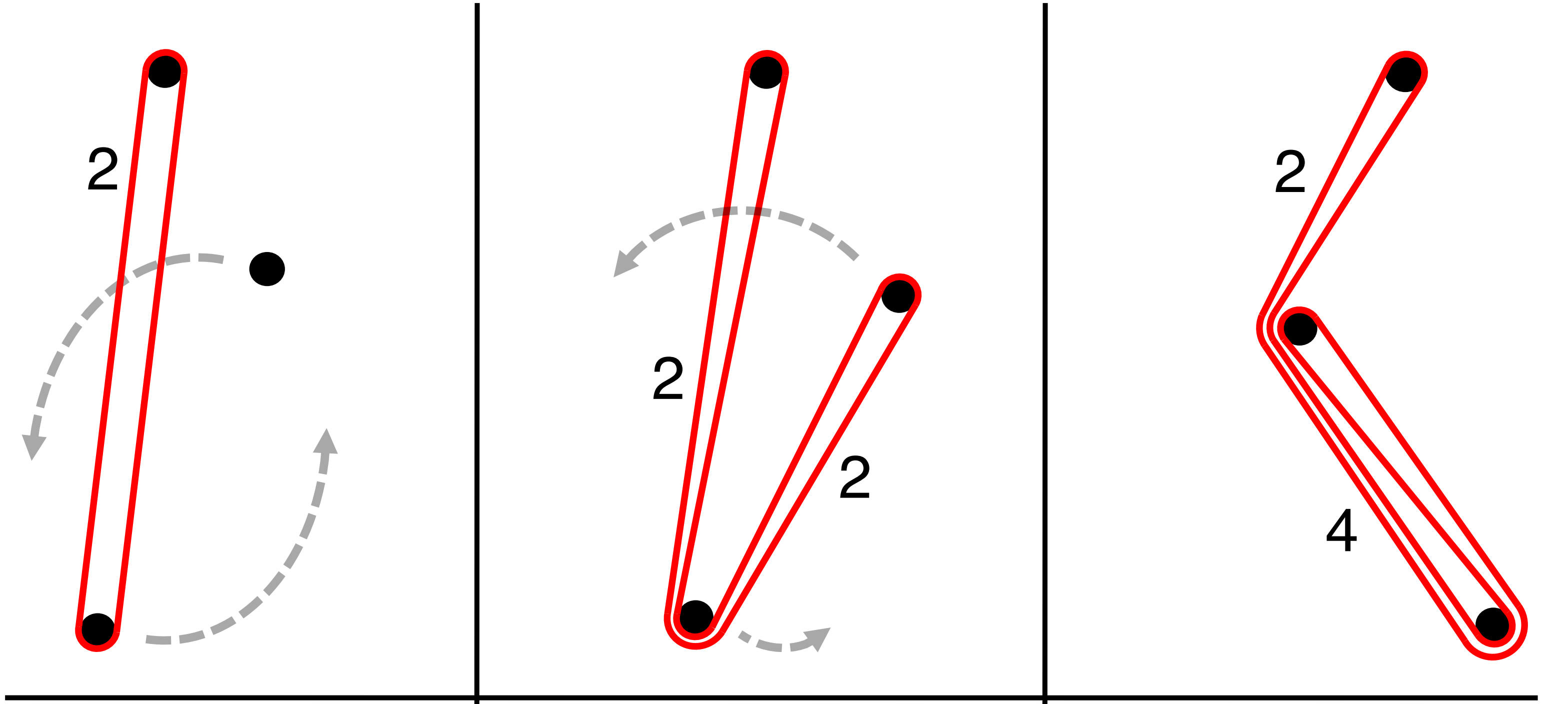
We track two different types of **triangle collapse events:**

Outer Triangle Event



Tracking Loop Growth

- We compute the topological length in the number of edges
- Loop complexity is hidden in exponentially growing integer weights
- **Triangulation** is used to detect point-band collision events



Total Number of Edges = 2 | Total Number of Edges = 4 | Total Number of Edges = 6

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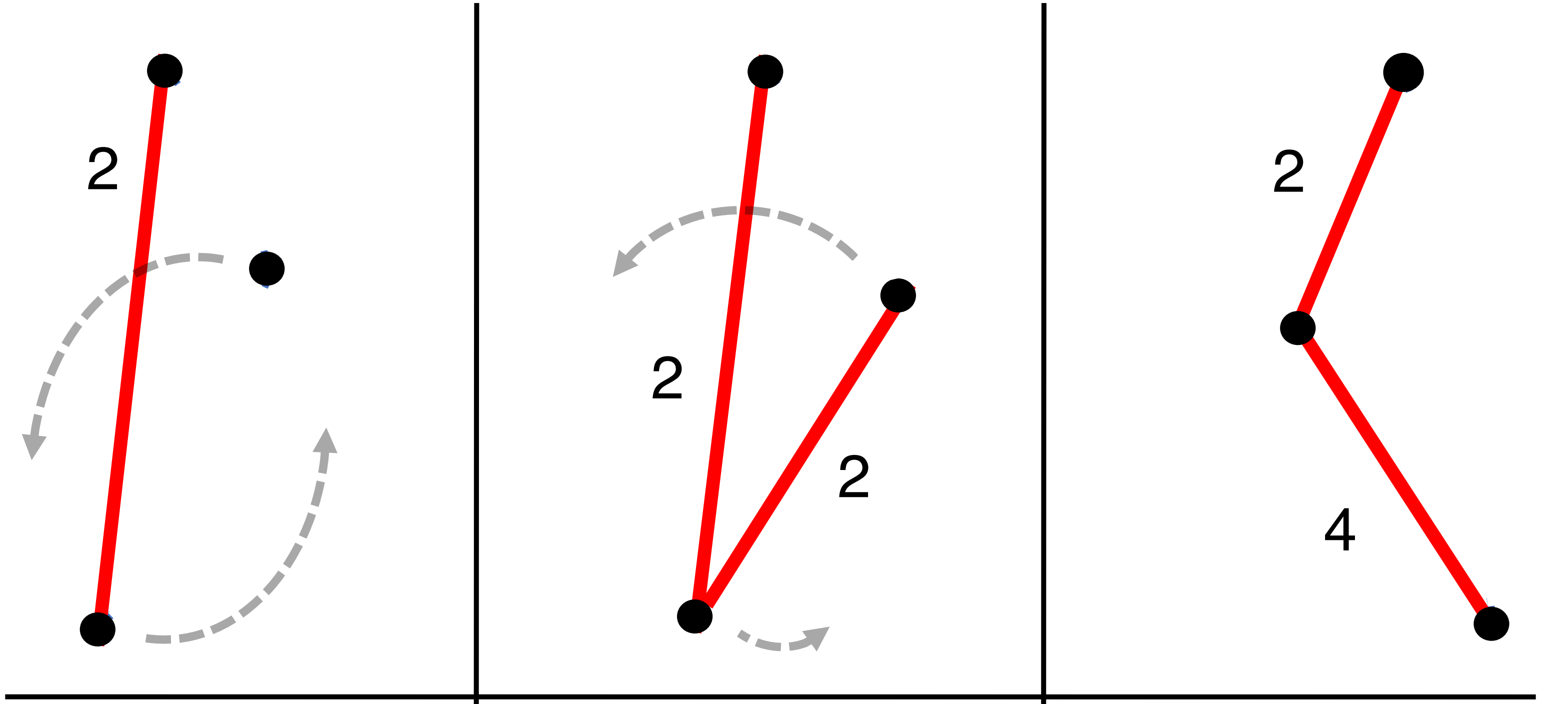

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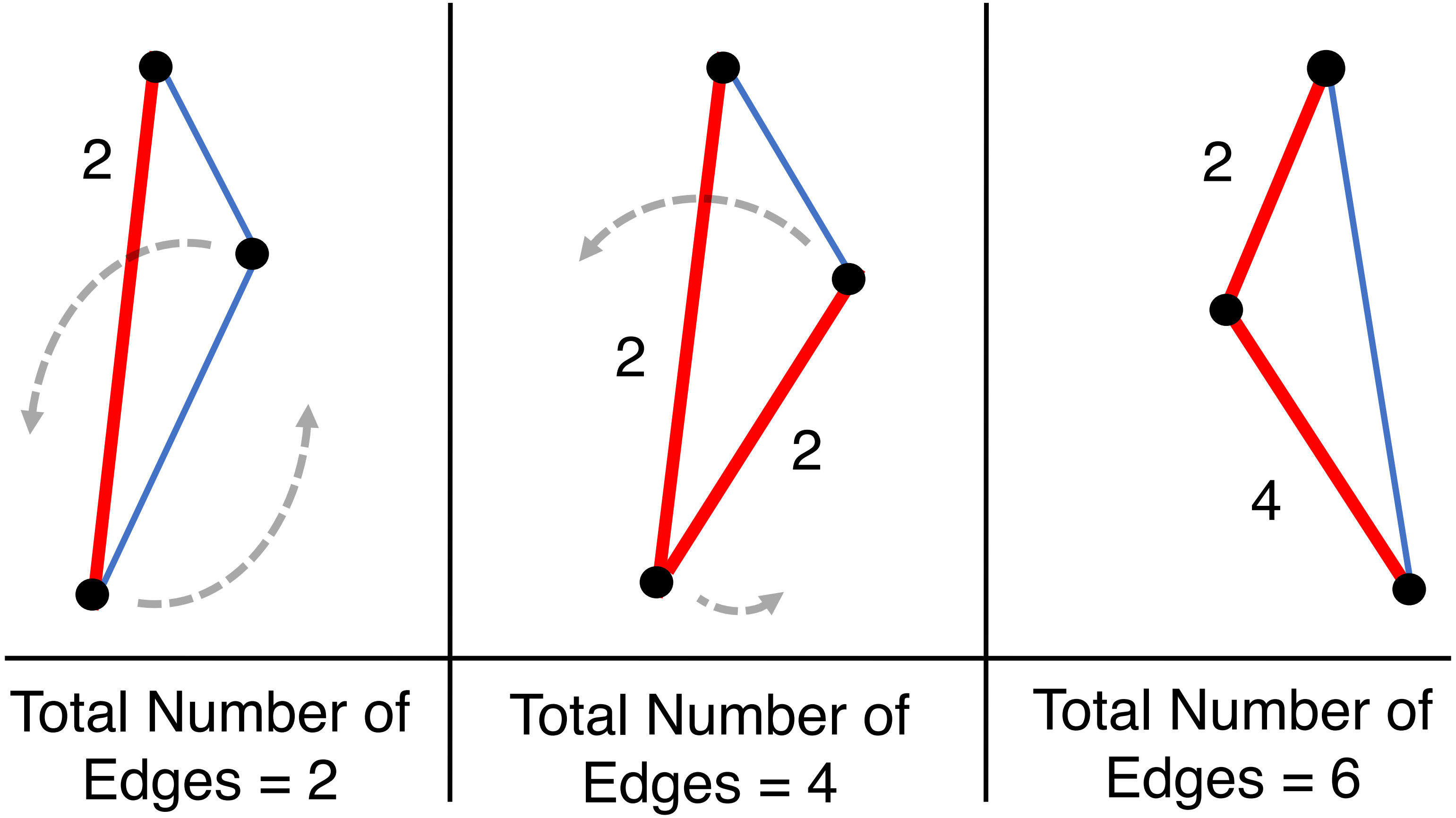
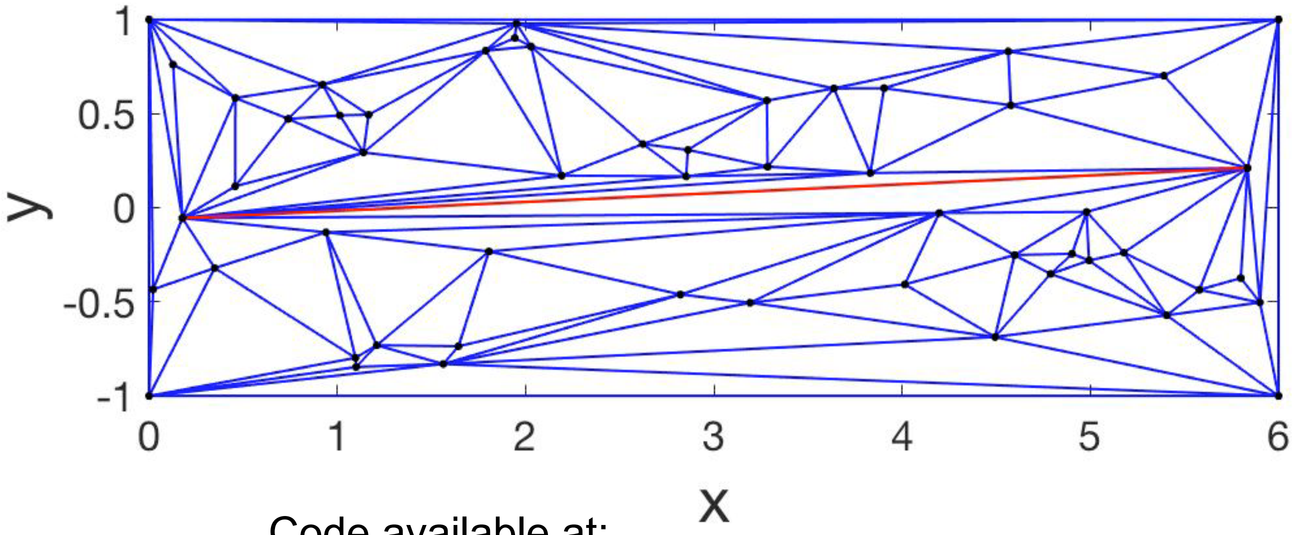


Example in 2D

- Blue edges denote core triangulation of points

- Red edges denote core triangulations with nonzero loop 'weight'

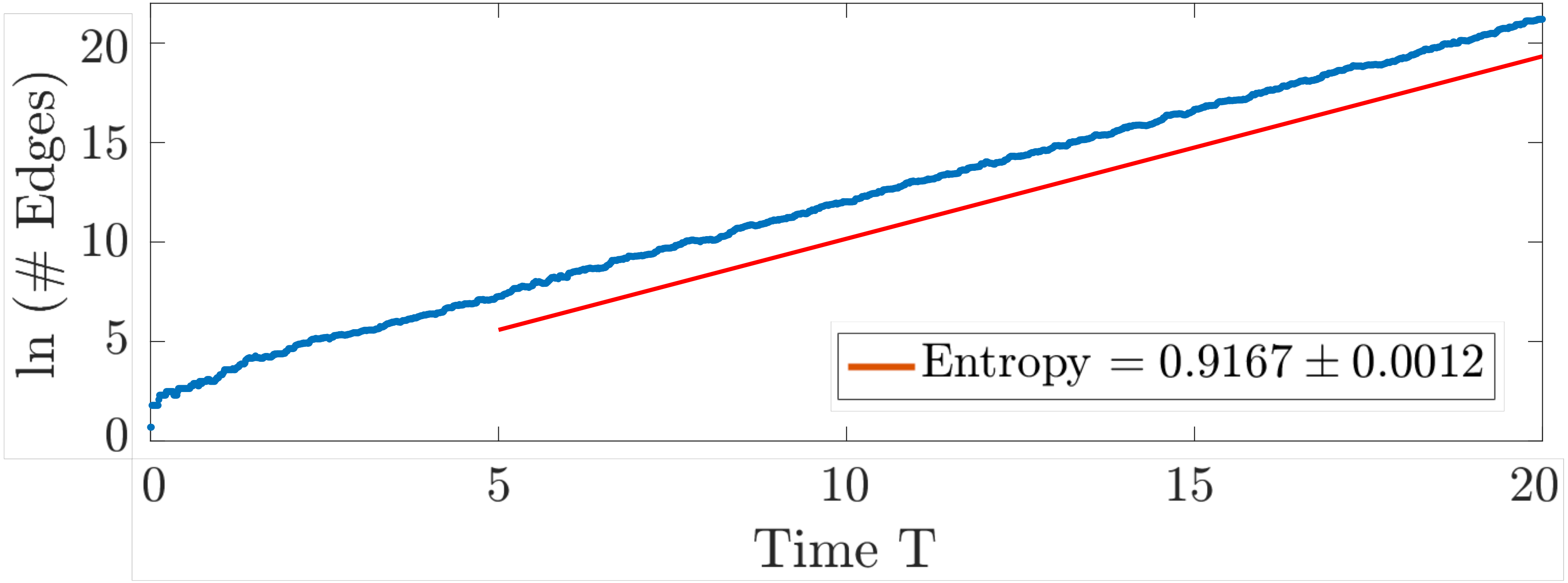


Code available at:
https://zenodo.org/record/1406200#.XH2vzlNKjdR

A final band configuration

E-tec Output

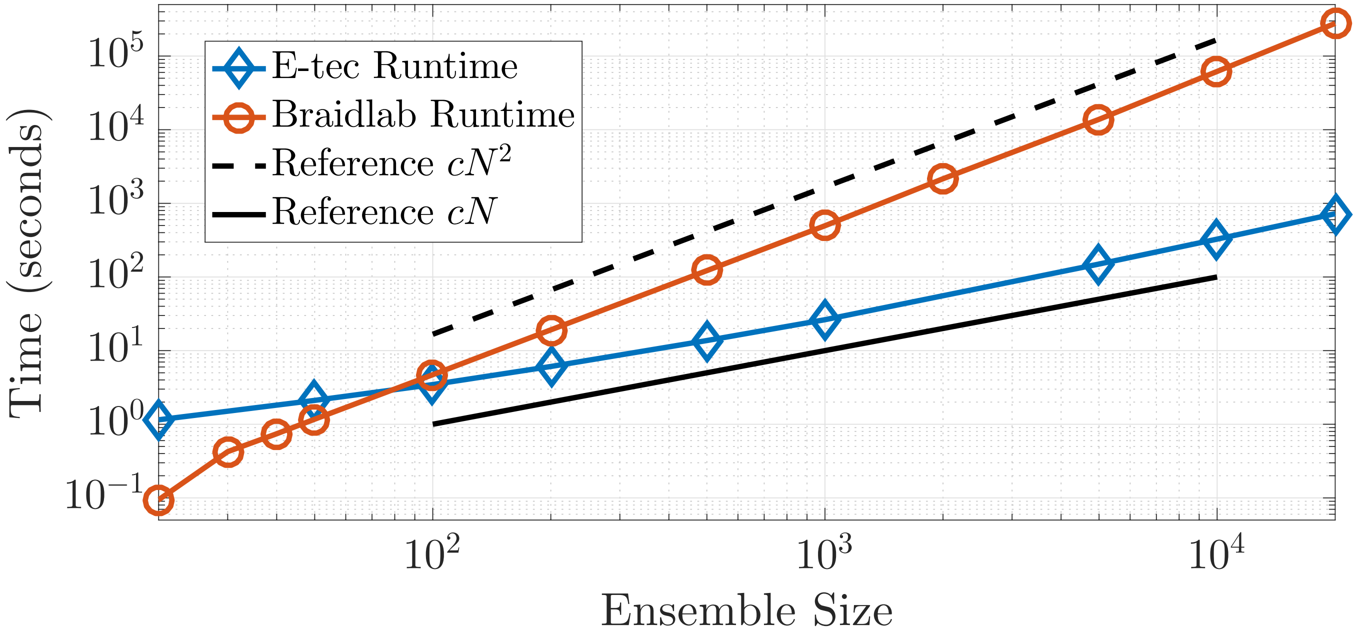
Topological entropy estimate is the growth of sum of total band edge weights as a function of time



Why use E-tec?

Two major advancements:

1) Runtime scales nearly-linearly in size of ensemble



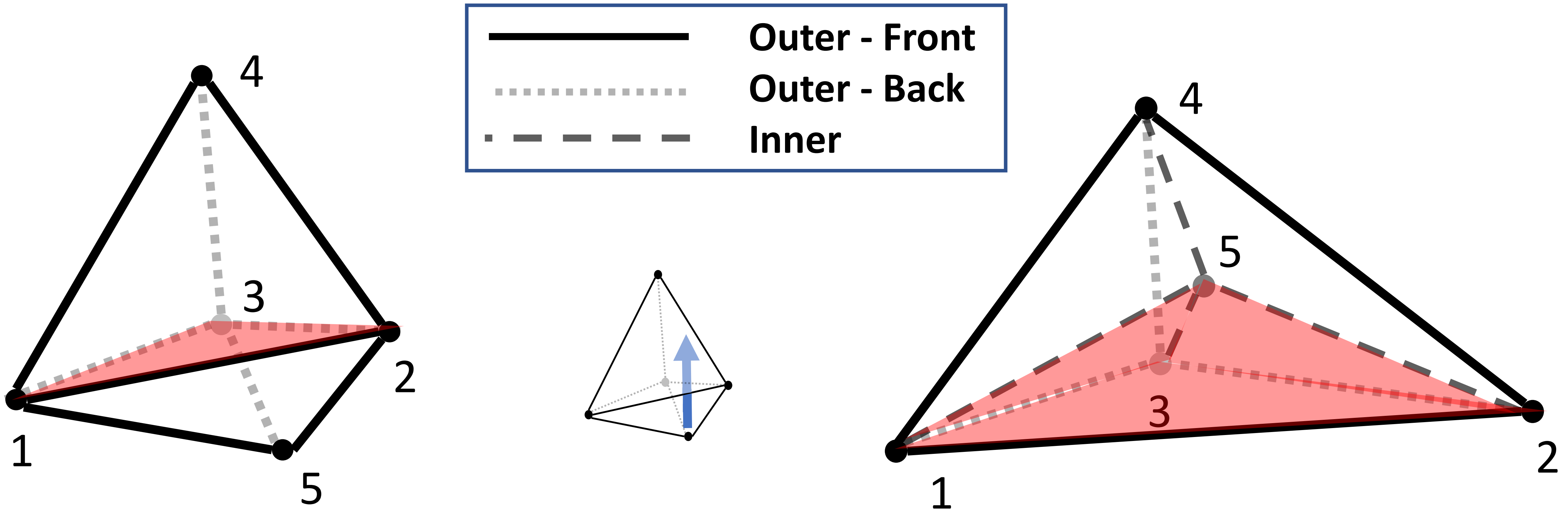
2) Triangulations generalize to **higher dimensions**

E-tec in 3D

3D Framework

We replace loop with an elastic sheet (red)

- Below, point 5 moves up, collapsing tetrahedron <1,2,3,5> with a point-face collision
- Local re-triangulation results in three new tetrahedra

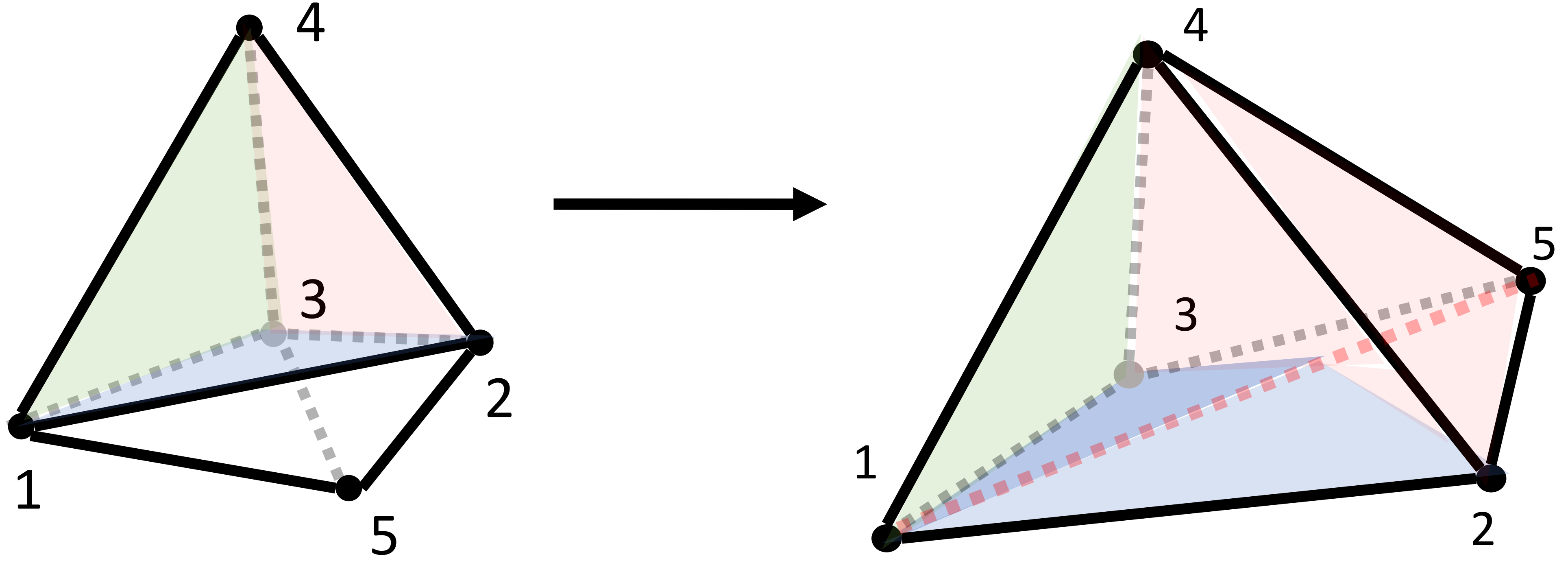


Main Difficulty Generalizing to 3D

Edge-edge collisions are tricky

- Point 5 moves to the right and up
- Edges 2-3 and 1-5 collide

By re-thinking how to record the structure of the elastic sheet, we may sidestep this difficulty.



Dual E-tec

Dual E-tec in 2D

Original E-tec: counts number of times the loop **crosses over** each edge

Dual E-tec: counts number of times the loop **intersects** each edge

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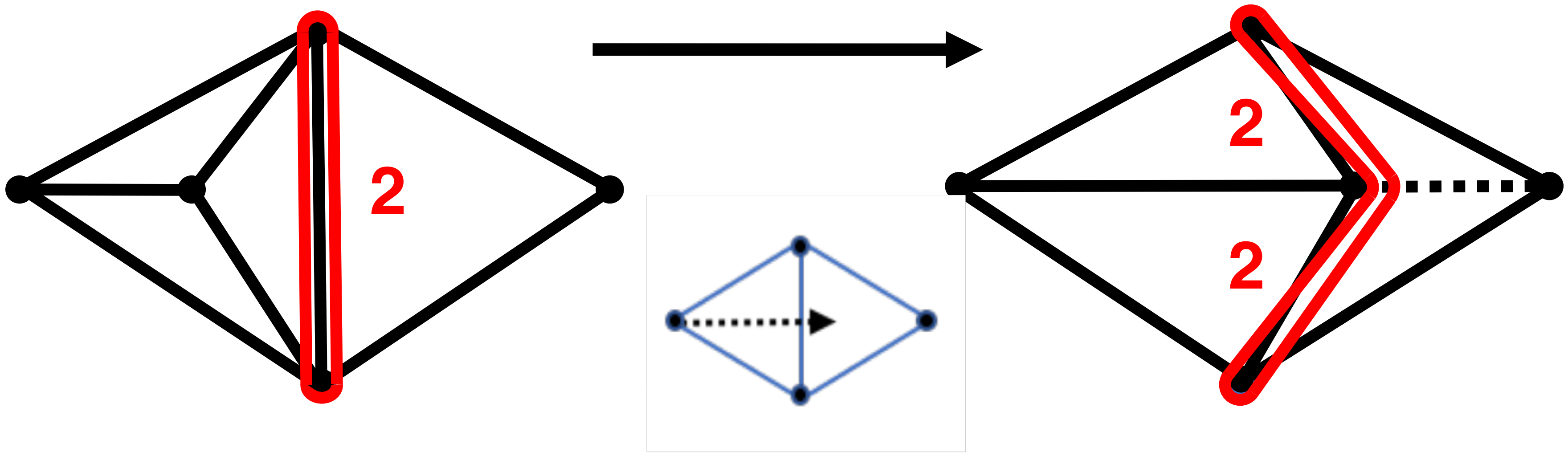
Original E-tec: Weighted edges in **red** with corresponding edge weights



Dual E-tec in 2D

Original E-tec: counts number of times the loop **crosses over** each edge

Dual E-tec: counts number of times the loop **intersects** each edge

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Dual E-tec: Weighted edges in **blue** with corresponding edge weights

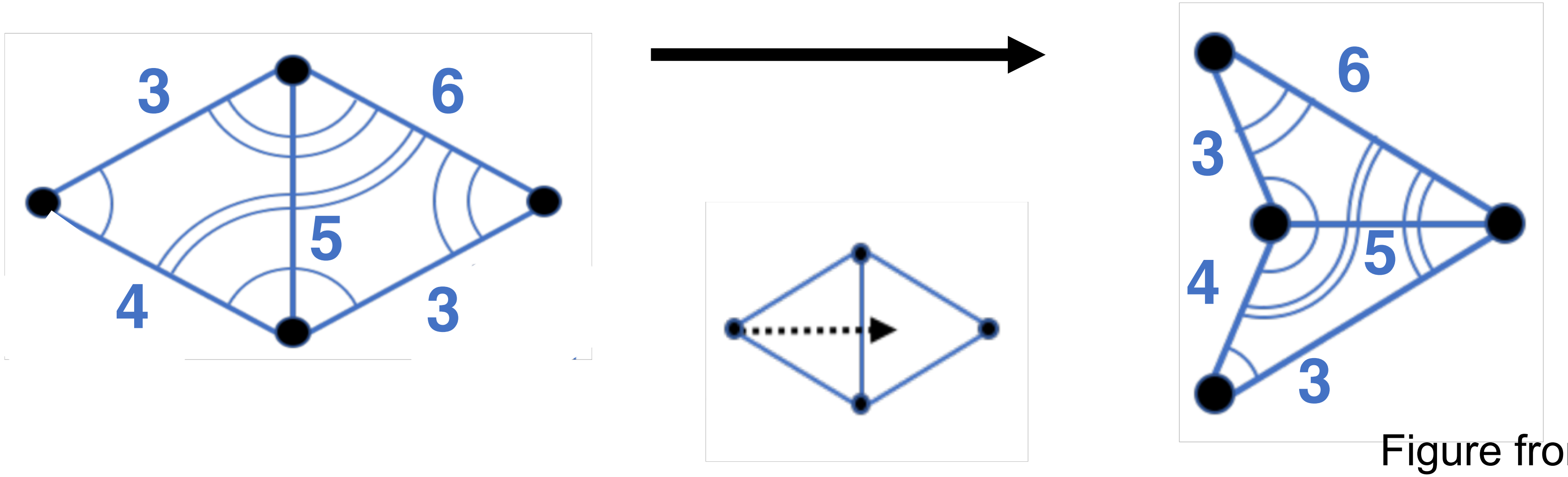


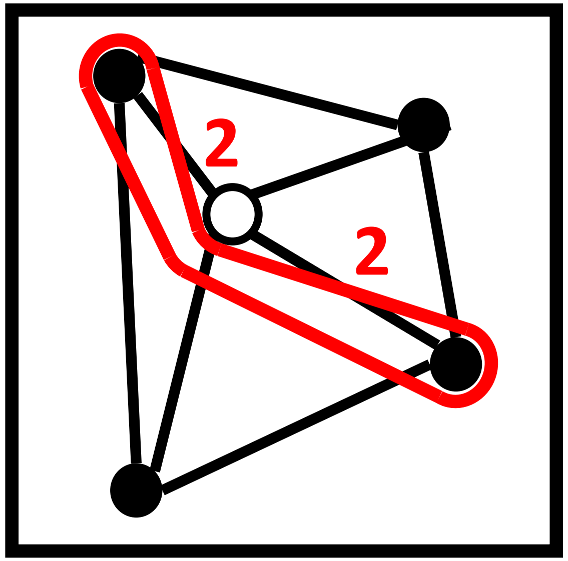
Figure from Spencer Smith

Dual E-tec Advantages

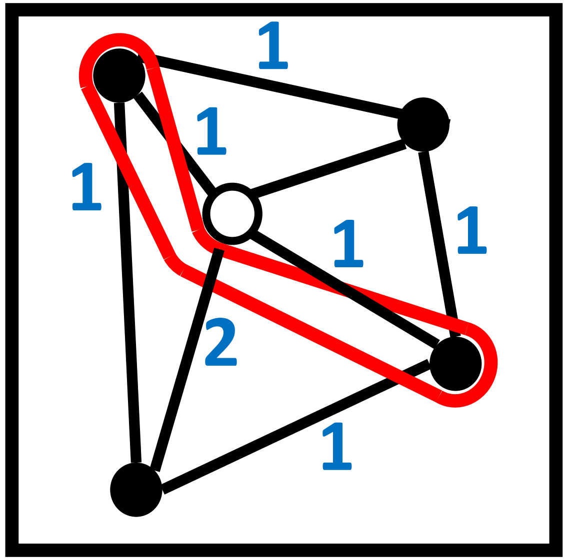
Loop or sheet may be represented at **any** time with **any** triangulation

- Band and triangulation are decoupled

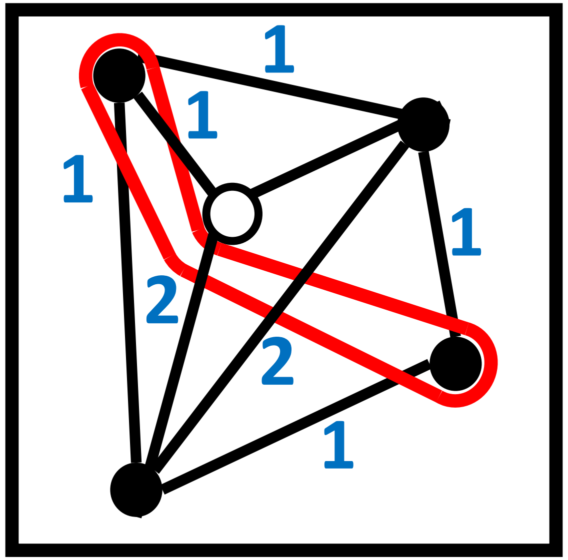
Original E-tec



Dual E-tec 1



Dual E-tec 2



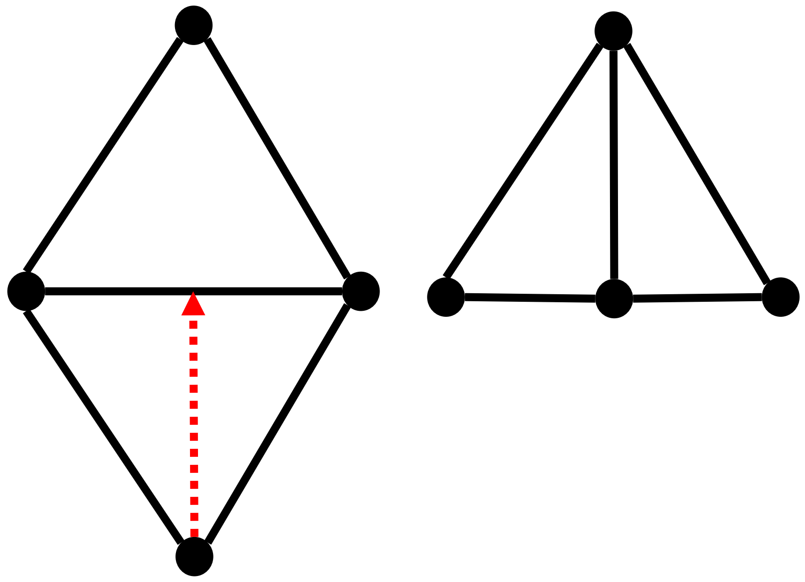
Next Steps

Maintaining a Delaunay Triangulation

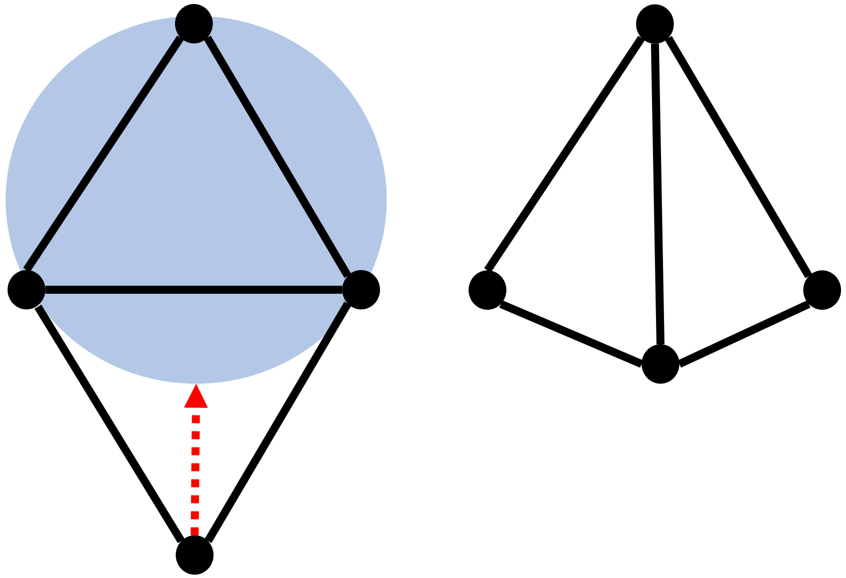
If 3D triangulation in Delaunay, edge-edge collisions will not occur

- Let’s locally re-triangulate in a smarter way

Current local triangulation update



New triangulation update

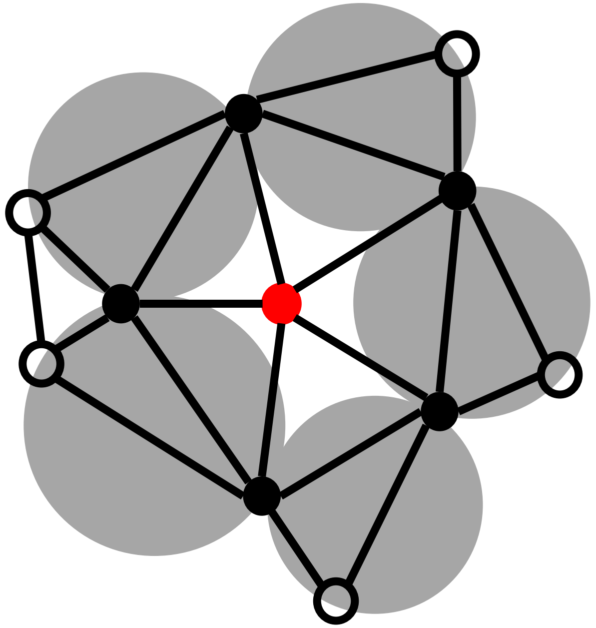


Maintaining a Delaunay Triangulation

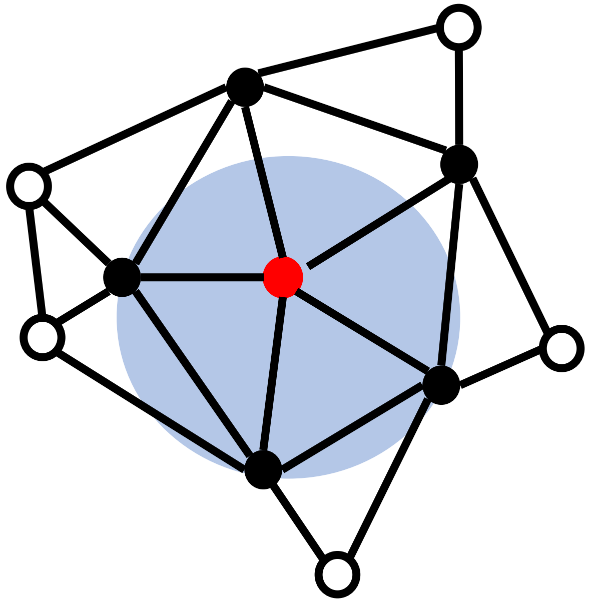
Inspired by Hugo Ledoux, we re-triangulate at all topological events

- Move a point step-by-step to closest event, locally updating structures each time
- Bypasses current CGAL implementation that involves roots of 8^{th} order polynomial

Must locally re-triangulate if neighboring '*real*' circumspheres are broken



Must locally re-triangulate if '*imaginary*' circumspheres are broken



Discussion

- E-tec is the fastest algorithm for computing topological entropy from an ensemble of trajectories
- Verified with experimental biofluid results (*Tan, Roberts, et.al. Topological chaos in active nematics. (Submitted to Nature Physics)*)
- First ensemble-based calculation generalizing to higher dimensions

Near Future Work: Implement Ledoux idea in 3D

- Interested in 3D coherent set detection (similar to Allshouse work using 2D braiding)
- 3D active matter microflows is a rich area ready to be investigated through the lens of chaotic advection

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Thank You. Questions?

CCBM
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