Surface reconstruction using Delaunay triangulation for applications in life sciences

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The big picture:
There are many different approaches to study biological systems...

- Agent-based model, non-spatial
- Representation of internal state
- Averaging
- Differential Equations
- Discretizing
- Agent-based model, spatial
- Representation of physical space
- We are here!
- Celular Automata
- Finite differential Equations
- Partial differential Equations
- Averaging
- Scaling
Basic questions:

• How do cells move?
• How do cells shape?
• How do cells signal?
• How do cells interact?
• How does the cell internal structure relate to these processes?
Our take on it:

To develop a method to mechanically study cell shaping, taking into consideration the cell’s internal structure.

How?

By discretizing the cell and using force based equations.
What kind of particles?

➡ Particles representing the cell membrane

Elastic potential
What kind of particles?

Particles representing internal volume elements of the cell

Lennard-Jones potential
What kind of particles?

Membrane and internal particles also interact via Lennard-Jones potential.
Question: How do we define the neighborhood relations between the particles?

Answer: Via a Delaunay triangulation
Problem:
A 3D Delaunay triangulation is not a good way to define the neighborhood relations between membrane points...

Why not?
Because of the biological properties of the cell membrane
Membrane points should only interact with each other on a surface!
And here the talk becomes technical...

How to, from the original 3D Delaunay triangulation, get a triangulation of the membrane points restricted to a surface?
Surface reconstruction is not an unknown problem...
What’s the difference?

General methods in surface reconstruction allow the deletion of points...
...and we can’t have our membrane varying in size...

at least not unintentionally!
The method
Step 1: Eliminate all connections between points that don’t belong to the membrane
Step 2: Identify all non-triangulated clusters on the membrane
Smallest 3D structure: simplex
Step 3: Identify the boundary of each cluster
A connection is in the cluster boundary when its two endpoints have a common neighbor outside the cluster.
Step 4: re-triangulate each cluster
There are 2 types of clusters!
Type 1: clusters without internal points
Which connections to keep?

For sure: the connections on the boundary
We start with a:
Is a neighbor of c?
No!
Restart with the next particle!
Is b a neighbor of d?
Yes!
Keep this connection!
The boundary of the part of the cluster not yet triangulated will be d-e-a-b
Start again with any particle in the new boundary
Is $d$ neighbor of $a$?
Keep this connection!
Throw away the connections that were not selected
The cluster is re-triangulated!
Any re-triangulation is a good re-triangulation!
Type 2: clusters with internal points
Get all connections between 1 and the boundary points
They will belong to the re-triangulation
The boundary of the part of the cluster not yet triangulated will be 1-i-a-b-c-d-e-f
Are there internal points left?
Get the second internal point
Get all connections between 2 and the points in the updated boundary
Keep all of them (they are all consecutive)
The boundary of the part of the cluster not yet triangulated will be 2-1-i-a-b.
Are there internal points left?
No!
Re-triangulate the rest following the method for clusters without internal points
Throw away the connections that were not selected.
The cluster is re-triangulated!
Step 5: You have a brand new re-triangulated surface!
What now?
Improvements to the method

Solving non-convex surfaces

Algorithm able to treat local changes
Simple experiments
Inclusion of diffusion

Spatial resolved simulation of chemicals inside the cell
MELC: experimental method
Calcium dynamics

- Responsible for important cell behavior, like vesicle exocytosis in neurons
- Not uniformly distributed inside the cell
- Inhomogeneity relevant
- Suitable to be simulated with our model
Thank you!