



Ion Channel Mesh Generation

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Introduction

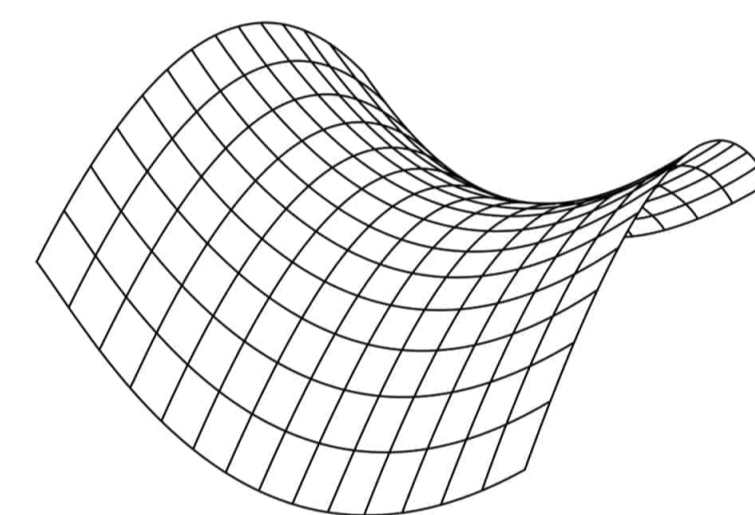
Goal

Create a package that automatically generates a model of a cell membrane around a protein in order to aid researchers studying ion channels

Currently available packages are inefficient at generating cell membrane models, either being too slow or not flexible enough to handle the myriad of proteins that researchers are studying. We created a new package that is both efficient and flexible.

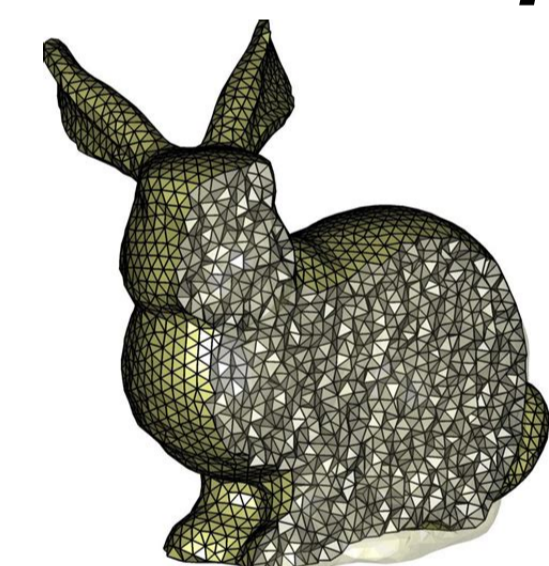
Mesh

A **surface mesh** is a way of breaking down and representing the surface of an object using a finite number of triangles such that you can model and simulate properties of that surface.



Surface Mesh [5]

A **volume mesh** is similar to a surface mesh. Instead of breaking down the surface of an object into triangles, we break down the entire object into tetrahedrons (pyramids) such that we can perform simulations on it.



Volume Mesh [6]

Package Stages

The following are the tasks our package must accomplish:

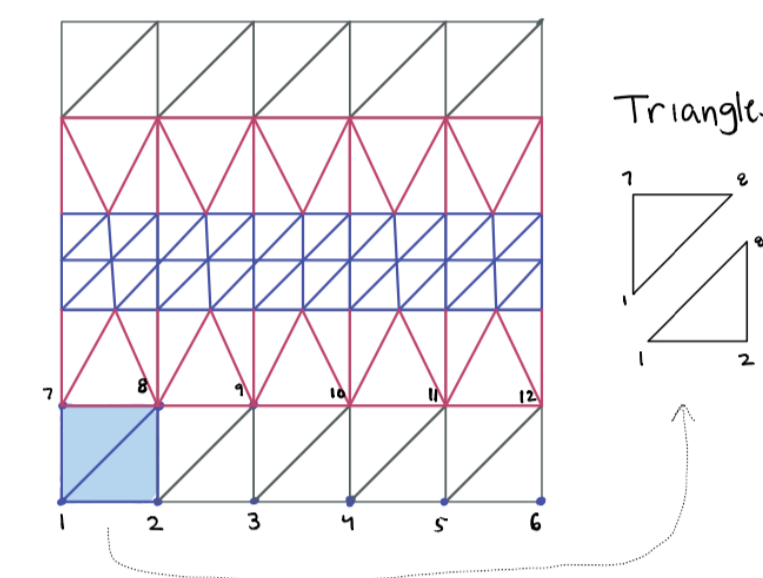
- Generate a surface mesh of the box and cell membrane surrounding the protein.
- Convert our surface mesh into a volume mesh with the help of other, open source packages.
- Split the resultant volume mesh into its different components: the cell membrane, the ion channel protein, and the solvent surrounding them.

Surface Mesh

The surface mesh is generated by combining faces into a box. The box is then set to enclose the protein.

Face Generation

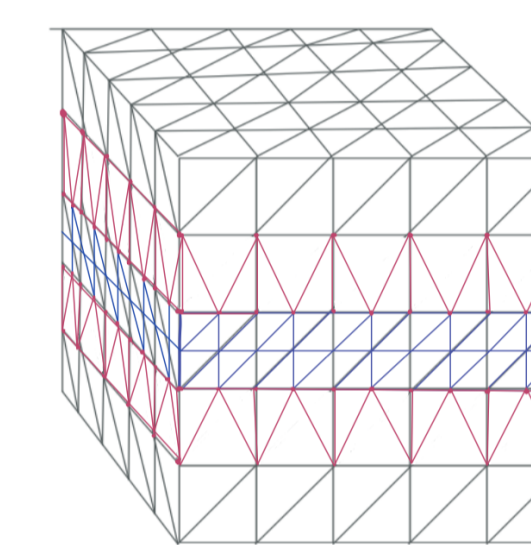
To generate a face, we recognize that triangles are identified by the 3 node ids that form the vertices. By careful assignment of node ids, we can calculate the triangles associated with a given node based on its id and the width of the face.



Nonuniform Face

Box Mesh Generation

In order to generate a nonuniform box surface mesh to enclose our protein, we combine the meshes of 6 separate faces. Once the faces are joined, we scale and shift the box to enclose our protein mesh.



Nonuniform Box

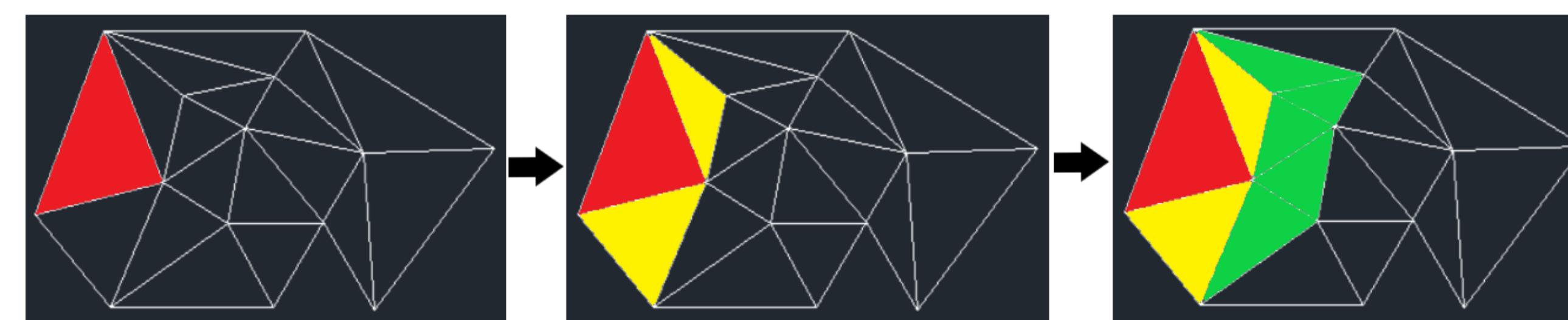
Volume Mesh

Conversion to Volume Mesh

In order to convert our nonuniform box mesh to a volume mesh, we input our surface mesh into Tetgen [1] which is a program that conveniently converts our surface mesh to a volume mesh. Tetgen [1] generates tetrahedra using the nodes in our surface mesh as vertices of the tetrahedra.

Separation of Solvent and Membrane

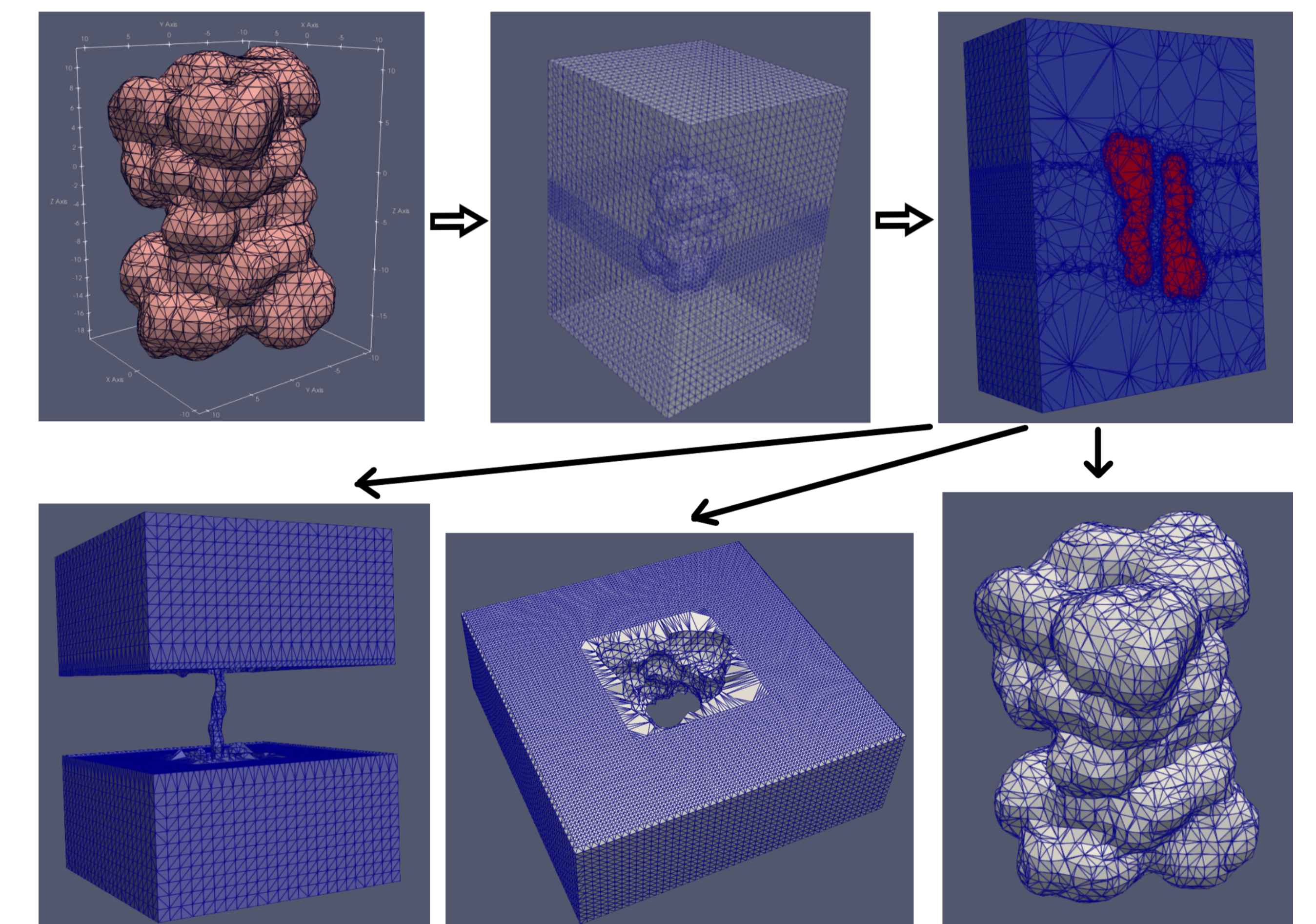
Tetgen has no knowledge of the cell membrane. It outputs a volume mesh with two regions: protein and solvent. Starting with a seed tetrahedron that lies inside the membrane, we conduct a search to find all nearby tetrahedra that also lie inside the membrane. This process is repeated until we have checked all tetrahedra in the region.



A Visualization of Breadth First Search

Conversion Process

Below is an image which shows the 4 major stages of the mesh during the conversion process. We begin with a protein surface mesh, then a box surface mesh is generated to surround the protein, then the surface mesh is converted into a volume mesh. Finally, the mesh is separated into the solvent, membrane, and protein meshes.



The Stages of Mesh Generation

References

- [1] Hang Si. 2015. *TetGen, a Delaunay-Based Quality Tetrahedral Mesh Generator*. ACM Trans. on Mathematical Software. 41 (2), Article 11 (February 2015), 36 pages. DOI=10.1145/2629697 <http://doi.acm.org/10.1145/2629697>
- [2] The FEniCS Project Version 1.5 M. S. Alnaes, J. Blechta, J. Hake, A. Johansson, B. Kehlet, A. Logg, C. Richardson, J. Ring, M. E. Rognes and G. N. Wells Archive of Numerical Software, vol. 3, 2015, [DOI]
- [3] Minxin Chen, Bin Tub, Benzhuo Lu 2012. *Triangulated Manifold Meshing Method Preserving Molecular Surface Topology*. Journal of Molecular Graphics and Modelling, 38: 411-418
- [4] Tiantian Liu, et al. *Membrane-Channel Protein System Mesh Construction for Finite Element Simulations*. Molecular Based Mathematical Biology 3.1 (2015): null. <http://eudml.org/doc/275995>
- [5] Example surface mesh. <https://cgtricks.com/wp-content/uploads/2016/07/Mesh-surface.jpg>
- [6] Volume Mesh of a Rabbit. <https://external-content.duckduckgo.com/iu/?u=https%3A%2F%2Ftse4.mm.bing.net%2Fth%3Fid%3DOIP.d1u5fkXeXS9pWdC7UY1akAHaK%26pid%3DApif=1>