E-Cell Sprint 2016

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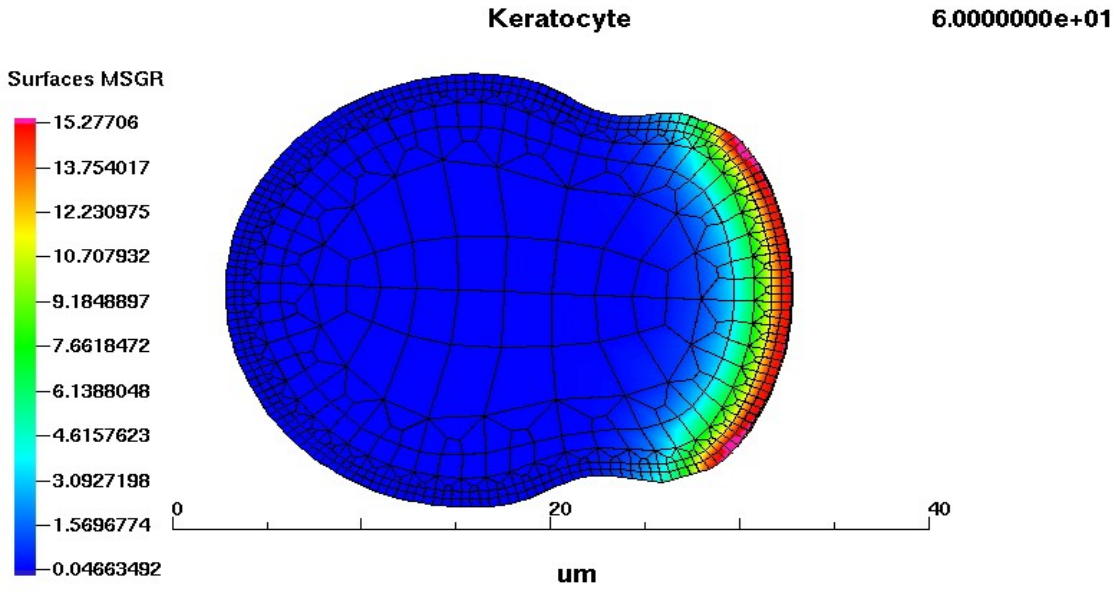
- Cytopede – a simulation tool which allow cell motility (mechanics) to be simulated in 3 dimension using mesh based technique.

- We have reproduced the model in Spatiocyte, a particle based reaction diffusion simulator, which Is more efficient in investigating interactions between single molecule in living cells.

Cytopede – 3D mesh tool for Cell motility



Spatiocyte – Lattice based Particle Simulator

Task

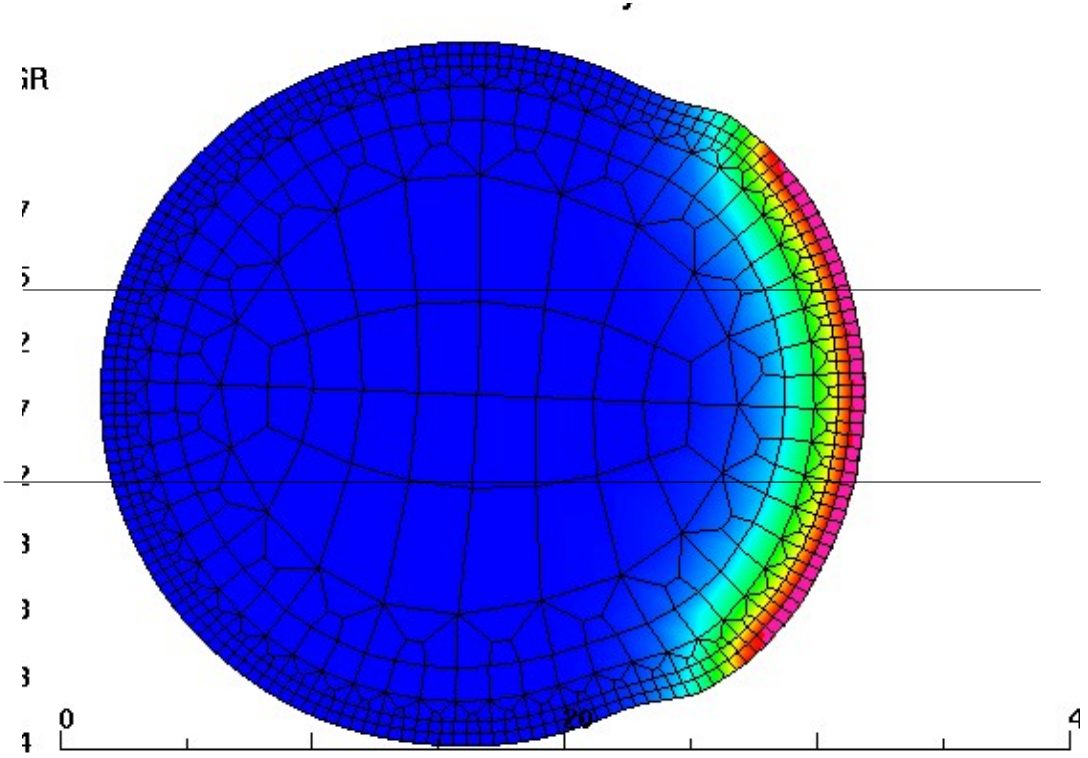
- Although we are able to reproduce the exact movement of Cytopede model, we did not reproduce the species concentration and reaction based on Cytopede.

- What we want to do here is to carry out some analysis on the Cytopede output such as plotting graph of species concentration against axes over a time frame.

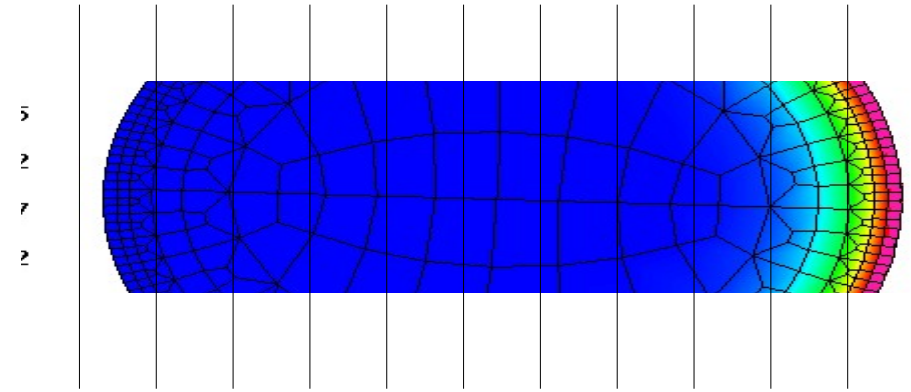
- We also need to reproduce the species concentration in Spatiocyte based on Cytopede.

Messenger Concentration Profile for Cytopede

- We created a concentration profile for Messenger in Cytopede.
- Messenger is the “signal” created in the cytopede method to define the protrusion area in the cell.
- In Cytopede simulation, the messenger concentration has been fixed at the right edge of the cell so it could has a fix movement towards the right side.



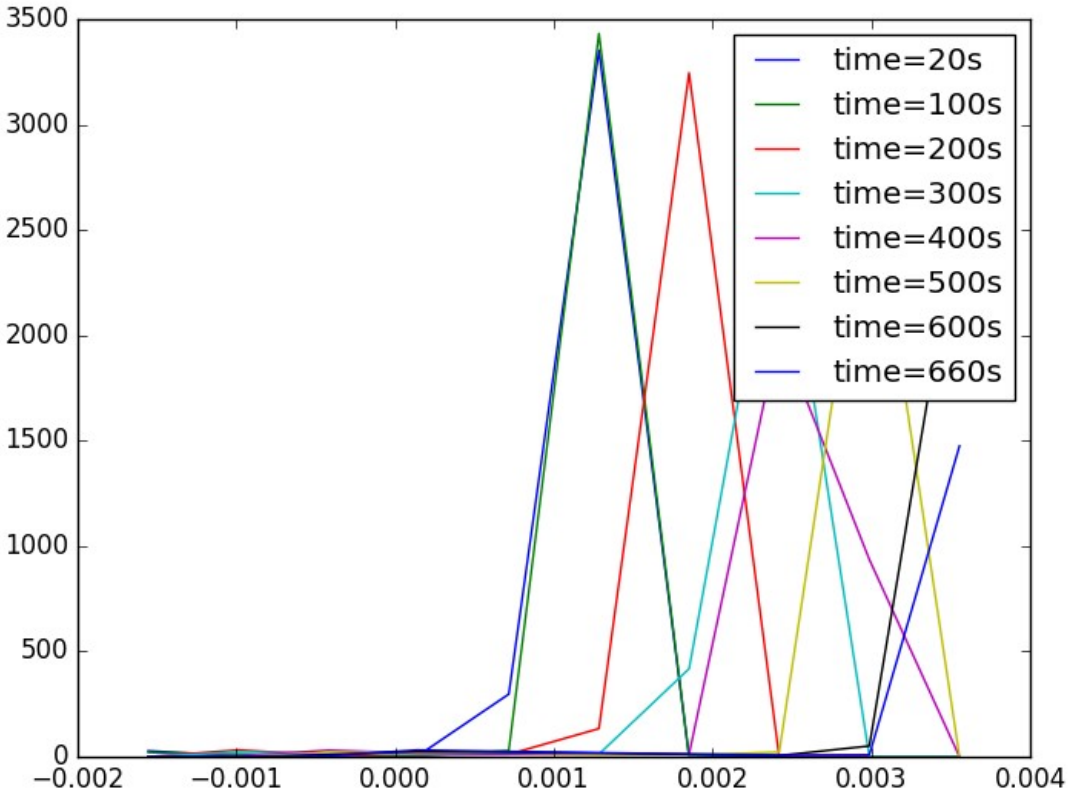
We first select the middle part of Y-axis.



Then we break the x-axis into parts and calculate the total messenger concentration in each part.

We obtain the minimum and maximum coordinates of the system and plotted multiple line graphs based on different time frame.

Since the messenger concentration is fixed at the right edge, we expect the graph will be converging to the right side.



The initial location of the cell is slightly to the left of the modeled system.
It can be seen that at 20s, There is a high concentration of messenger at the center of the coordinates which is where the right edge of the cell is located at.

While advancing through the time frame, it can be seen that the max concentration of Messenger is shifting towards the right side, consistently showing the messenger concentration is always fixed at the right edge of the cell. At t=600s, it can be seen that All of messenger are accumulated at the right edge of the system.

Problem and Future Work.

- The same analysis need to be done on Spatiocyte simulation of the same model.
- We have derive the area based on the mesh in Cytopede. In order to reproduce the same concentration, we have to be able to accurately populate the number of molecules in the each area defined in Spatiocyte.
- Spatiocyte currently can populate molecules on the cell surface randomly as non HD molecules.
- There is a need to configure a way such that the population of molecules on each defined area is fixed to the concentration found in the same mesh in Cytopede (not randomly).
- Also, more analysis can be carried out on both methods such as diffusion rate once we are able to populate the accurate concentration in Spatiocyte.

THE END