MCell and DReAMM Simulations of Catecholamine Release Detected using a Patch Clamp Technique

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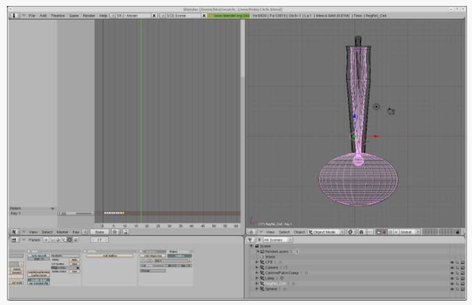
Abstract

Patch clamp amperometry is a technique for the electrochemical detection of catecholamine ions across a cell membrane. Using the computer aided design tool, Blender, various models of the patch clamp, with the carbon fiber electrode and vesicle were constructed. Simulations of objects were then run in MCell. Finally, DReAMM (Design, Render, and Animate MCell Models) was used to display the MCell simulations, showing how the fusion pore formed and how ions were detected by the carbon fiber electrode.

Introduction

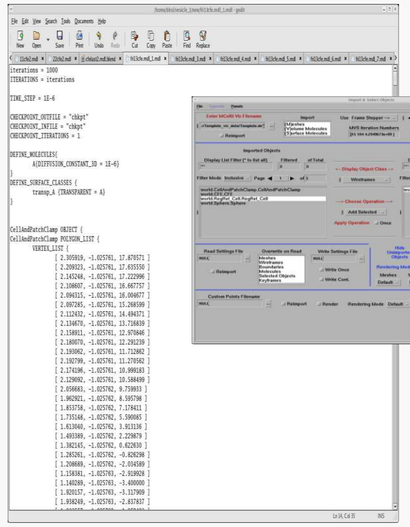
Simulations were created to demonstrate the process of exocytosis and the catecholamine detection on the carbon fiber electrode. Models were constructed to show how a vesicle forms the fusion pore to release such ions. Varying the distance of the carbon fiber electrode inside the patch clamp directly affected the number of ions detected.

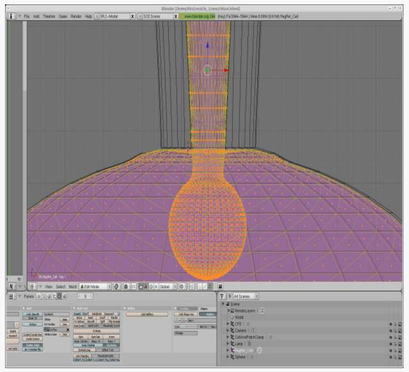


Blender was the 3D visualization tool which used basic shapes to create the cell, patch clamp, carbon fiber electrode, and vesicle for mesh generation. Files were exported as MDL (Model Description Language), which were then run in MCell3. The files were then imported into DReAMM where the meshes were visualized and edited. Final changes to individual meshes such as size, opacity, and color were accomplished in DReAMM.

Method

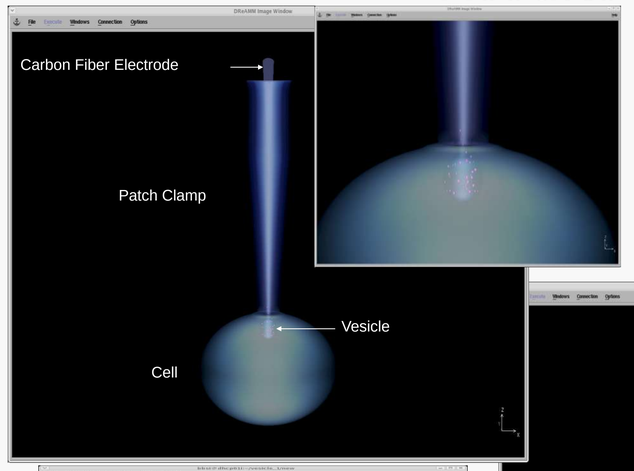
Blender files were exported as MDL files, each of which had to be edited to display the appropriate viz output. Animation files were exported separately, which created an individual file for each frame.



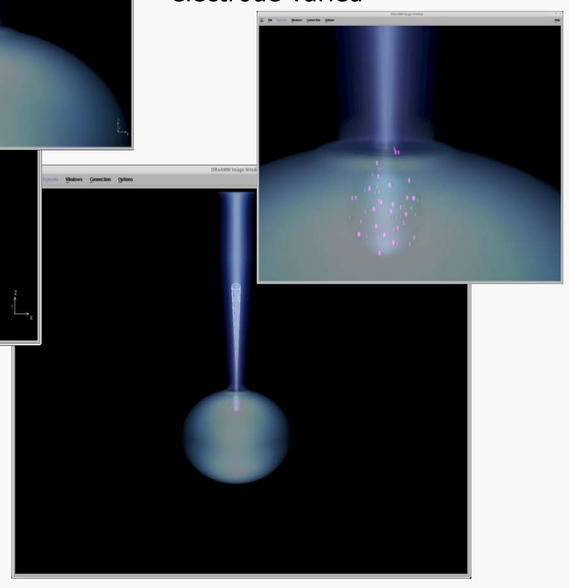


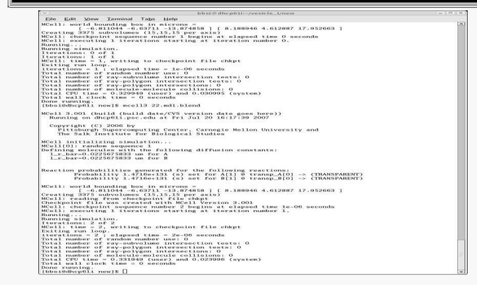
Using Monte Carlo algorithms, MCell3 generated the simulations based upon iterations and time-steps. Region-release for molecules and surface classes of objects were defined within specific MDL files. Animations created in Blender were represented in MCell3 using checkpoints—creating a file onto which viz input and output data was accumulated.

Results



Two different DReAMM simulations were created, with the distance of the carbon fiber electrode varied





MCell3 generating the simulation for one MDL file

Conclusion

Additional simulations may be created for variables such as patch clamp solution concentration, and an intracellular matrix. Each of these factors will affect the rate at which molecules are detected. For further research, fusion pore size may also be varied.

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