10 May Report:

## Summary of progress

|  |
| --- |
| **20th April – Meeting with Joe:**   * Discussed persistent problem where dropping z in the middle compartment resulted in a higher voltage in that compartment at the end of the simulation, which contradicts Kira’s multicompartmental model. * In my single compartmental model, the voltage drops appropriately, so it is something in the electrodiffusion implementation that is causing the problem. * Joe and I changed the diffusion constants (sped them up) and found that we could replicate Kira’s phenomena like that. |
| **21st April – Meeting with Kira:**   * Discussed the problem with Kira. * She told me she changed the time step in her last few multicompartmental experiments for the same reason that she was getting odd electrodiffusion results. * Once she changed the time step from 10^-3 to 10^-6 (like in Sejnowski’s experiments) the problem was solved. |
| **22nd April – 27th April: A 10^-6 timestep was taking too long (order of days)**   * Needed to find ways to speed up my implementation: * Changed total structure of the program in terms of which values are stored in which classes. Goal was to minimize repeated information and simplify the code as much as possible. Ideally the compartment class should only hold information that it needs at that time, otherwise it needs to dump old variables. * Implemented generator functions and maximized use of list comprehension techniques to increase code speed. * Reduced lines of python code by +- 40% * Made a new version of the Jupyter notebook (V4) to utilize all the changes made. |
| **27th April – 06th May: Challenges with RAM**   * New code now designed to speed up the simulation. Successfully managed to run short trial simulations at significantly faster speeds. * Once I started making the simulations slightly longer the CPU RAM usage would go through the roof. I capped the RAM on pycharm (IDE) to 14Gb. This cap was reached at about 6 minutes when running 4 compartments with a dt of 10^-5. * To overcome the RAM issue, I wanted to minimize the number of items stored in arrays that are not being currently active but still find a way to keep all this information which would be needed for graphing at a later point. * I spent a few days learning about the HDF5 (Hierarchical Data Format 5) file type which is a hyper compressed file that can interface well with python and used in many genetics and cosmological studies with big data. * Implemented the HDF5 framework to the project so that the simulation will save the simulation arrays to the hard drive at specific intervals, and then dump the arrays from RAM. * I used the online NEXUS HDF5 file viewer to view the file afterward. * Simulations now appear to be using substantially less RAM (+- 1.5Gb) even when more compartments are added or the timestep is reduced. |
| **06th May – 10 May: Aligning new data storage system with Jupyter.**   * Construction of the interface between the Jupyter framework and the new file system. * All figures and most of code had to change to accommodate it. * Started running rudimentary tests (e.g. Experiment 1A) * Experiment 1B is a 30-minute simulation with 3 compartments, where z is altered in the middle. The estimated completion time is just over 3 hours. Currently at home running simulation on the beast so cant check RAM usage easily but simulation appears to be running without error. |
|  |
|  |

|  |  |
| --- | --- |
| **Title** | **Experiment A1** |
| Aim | Trial experiment to assess whether new version of the multicompartmental model would result in a drop in voltage if we dropped z in the middle compartment. |
| Summary | Three compartments all starting at default. |
|  |  |
|  |  |
| Conclusions | * Apparent success at dt = 0.01 ms * Boundary graphs not fully completed for new model so not shown here. * Later identified that there were electrodiffusion errors in the code so unsure of how robust this is. |

|  |  |
| --- | --- |
|  | **Experiment A2** |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  | * Problem of rasied Vm in compartment 2 occuring again even with dt = 10^-5 * Next step, try run with time step 10-6 * If that fails I know there is something wrong with my electrodiffusion. * Electrodiffusion figure doesn’t seem to be working, there is definitely ion flux at the end (order of magnitudes for these values are too low) |

|  |  |
| --- | --- |
|  | **Experiment A3** |
|  |  |
|  | Repeat of the same experiment above just with dt = 10^-6 |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  | * Not the result I was hoping for… ended up still with a higher membrane potential in the second compartment than in the other 2 compartments * The chloride reversal potentials in my simulations drop much lower than they do in Kira’s. * Next steps are to review the electrodiffusion equations again, and possibly review the chloride diffusion constants and see if that is correct.   Equilibrium values too low |

|  |  |
| --- | --- |
| **Title** | **Experiment B1**  Made fix to electrodiffusion |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  | * The Vm is finally dropping which is great * The impermeant charge change here was extremely low so difficult to see the true effects * Simulation still running very slowly. Might be solved with PyPy * Would be interesting to go back to my old model and make the electrodifusion changes to code to see if I would get the same results |