Project Title:

Simulation of molecular signaling during synaptic plasticity, in Purkinje neuron.

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Description of the project

1. Background and purpose of the project, relationship of the project with other projects

The project is to use a stochastic simulation engine (MesoRD) to evaluate models of cellular signaling processes underlying synaptic plasticity in cerebellar neurons. This approach complements and uses the results of our experimental measurements, obtained from living brain tissue.

2. Specific usage status and calculation method.

Simulations of mid-level complexity have been successfully run on the RCCC system, with previous version of the MesoRD 0.2 simulation engine. In FY 2011 we decided to switch to MesoRD 0.3, which implements more complete support of SBML and more accurate computation of molecular interactions than the previous version.

3. Result

MesoRD 0.3 was found to be stable on the RCCC but we uncovered significant problem in the Constructive Solid Geometry module, that was modified in this version. Specifically, the CSG module seems to suffer from numerical instabilities under icc optimisation. It seems the problem is related to near-singular matrices. The problem is currently looked into by MesoRD developers.

4. Conclusion

Models are being developed for this project and test runs are done on workstation running MS-Windows. We expect that the problems that we identified will be fixed in the next release of the software, due this spring.

5. Schedule and prospect for the future

See above.

6. If you wish to extend your account, provide usage situation (how far you have achieved, what calculation you have completed and what is yet to be done) and what you will do specifically in the next usage term.

One major task with the new release will be to test that previously obtained simulation results will all be reproduced with the more accurate simulation engine. Since the model description format has been significantly altered, we are now recoding previous models for this purpose. In parallel, we will initiate simulations with more complex models (up to 35500 molecules and > 1 million subvolumes).

7. If you have a “General User” account and could not complete your allocated computation time, specify the reason.

8. If no research achievement was made, specify the reason.

We have been working with the simulation engine developers (J. Elf lab at Uppsala Univ.) to identify bugs in the current software release. In parallel, model components are developed and tested separately but have not yet been assembled into a complete simulation on RCCC.