MULTISCALE SIMULATION METHODS FOR LIVING CELLS

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Background

In living cells, the number of chemically active molecules is often low and an accurate model is stochastic. The cell is partitioned into compartments at a mesoscopic level and the state of the system is given by the copy number of each species in every compartment. Trajectories or realizations of the system are generated by a Monte Carlo method by simulating the reactions between the molecules and their motion by diffusion. One such computational method has been devised in [1]. When a more detailed description is needed e.g. because the mesoscopic model is not known, single molecules are tracked when they react and diffuse in Brownian motion in a microscopic model [4]. By coupling the mesoscopic model with the microscopic model, the efficiency of the meso description is combined with the accuracy of the micro description [3].

Project

We are interested in investigating the coupling between the mesoscopic model and the microscopic model. Assume that a molecular species is treated microscopically on one side of a plane and mesoscopically on the other side. How should a molecule in the micro model be transfered to the meso model when it crosses the plane and where should a meso molecule be placed when it becomes microscopic? How accurate is a method when the meso molecules are first advanced one time step with frozen positions of the micro molecules and then the micro molecules are advanced with frozen meso molecules? Another way of coupling the models is proposed in [2]. What are the differences between the two approaches? These questions can be answered by generating trajectories of simple systems using `matlab` and collecting statistics from the simulations.

References

[1] S. Engblom, L. Ferm, A. Hellander, and P. Lötstedt. Simulation of stochastic reaction-diffusion processes on unstructured meshes. *SIAM J. Sci. Comput.*, 31 (2009), 1774–1797.

[2] M. B. Flegg, S. J. Chapman, R. Erban. The Two Regime Method for optimizing stochastic reaction-diffusion simulations. Manuscript, University of Oxford, Oxford, UK, 2011.

[3] A. Hellander, S. Hellander, and P. Lötstedt. Coupled mesoscopic and microscopic simulation of stochastic reaction–diffusion processes in mixed dimensions. Manuscript submitted for publication 2011.

[4] S. Hellander, and P. Lötstedt. Flexible single molecule simulation of reaction-diffusion processes. *J. Comput. Phys.*, 230 (2011) 3948–3965.

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