Stochastic simulation of cellular reaction networks

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Modeling of reaction-diffusion systems has traditionally been based on partial differential equations governing the concentrations of the different participating chemical species. However, it is now widely appreciated that deterministic models have severe limitations when modeling reaction-diffusion processes inside the living cell, partly due to the small volumes involved. Most of the species involved will be present in very low copy numbers, and in that case a discrete, stochastic description offers a modelling advantage.

Stochastic simulation of the processes in a 3D geometry offers a great computational challenge. We have recently proposed the use of unstructured, tetrahedral meshes in the stochastic reaction-diffusion setting. It is well known that those kind of meshes is more flexible than structured, Cartesian meshes when the geometry is complicated. However, even though the meshes obtained from state-of-the art mesh generators are often adequate to use when solving the reaction-diffusion PDE numerically, the need to interpret the diffusion process as a stochastic process poses conditions on the mesh quality that are sometimes violated.

In this project we will look at the effects on mesh quality on the accuracy of the stochastic simulations. We will also investigate how different discretization methods (FEM,FVM) influences the simulations. We will be using the stochastic simulation software URDME as a basis for the experiments, but the successful completion of this project will involve extending and modifying the code.

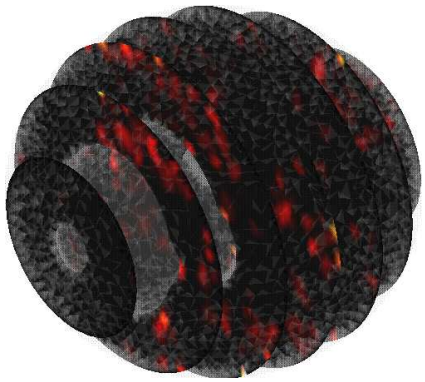

Figure 1: Example of a reaction-diffusion model simulated with URDME on an unstructured mesh. Areas with populations of a certain protein in the model are coloured red.

For more information, contact Andreas Hellander (andreas.hellander(at)it.uu.se).