Simulation of the reaction-diffusion equation

Cells contain lots of circuits: networks of genes ensure that the right proteins are produced at the right time, so a cell can react to external signals, divide and grow or fulfil special tasks. Within a circuit, the information of participating genes is dynamically read off of DNA. This process is controlled by regulatory proteins, the product of other genes. There are activating and inhibiting connections. The regulatory processes operate at the molecular level, so there is stochastic noise due to Brownian motion.

Our group develops hybrid stochastic-deterministic algorithms to simulate the temporal behaviour of complex genetic networks at molecular detail. For this, we combine Monte-Carlo approaches with analytical solutions of biochemical reactions.

A biochemical reaction typically is described by ordinary differential equations. It is assumed that all substances are distributed homogenously in the reaction volume. The reaction-diffusion equation takes into account inhomogenous concentrations for the calculation of reaction kinetics. Well-known examples for the solutions of reaction-diffusion equations are solitons and self-organization in embryogenesis.

The goal of this master thesis is to integrate realistic, diffusion-based reaction kinetics in our network simulations. You will develop numeric solutions of partial differential equations and embed these in the simulation programme. Subsequently, you will apply the programme to a biological model system.

If you are interested or have any questions, please contact
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