Parameter estimation in biochemical networks in cells

Per Lötstedt

Figure: A eukaryote cell (e.g. a mammal cell) and a prokaryote cell (e.g. a bacterium) Source: Wikipedia
Parameter estimation in biochemical networks in cells

- Monte Carlo simulation of chemical reactions and diffusion
- Reactions and diffusive jumps occur randomly
- Linear noise approximation (LNA) for the probabilities
- Estimation of parameters in the simulation model
- Bayesian framework for inference of parameters
- LNA simplification for space dependent problems with diffusion for determination of parameters

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Master Thesis projects in Computational Systems Biology

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Extending StochSS with an efficient reaction-diffusion PDE solver

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- StochSS is Software as a Service (SaaS) for simulating biochemical pathways.
- Developed in a large international collaboration (UU+UCSB)
- Implements stochastic simulation methods for reaction-diffusion models of biochemical control systems
- A PDE solver is missing

Project: Develop efficient mixed 3D/2D R-D PDE solving capabilities for StochSS using FEniCS/Dolfin (C++/Python framework for Finite Element computations).
Investigating new mechanisms in multicellular biology

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In these exploratory projects suitable for students with some biological background, we want to learn more about how to model and simulate two relatively new phenomena in multicellular biology:

- **Mechanotransduction pathways.**

  Cells in tissue sense the mechanical properties of the surrounding matrix and respond with intracellular signaling pathways, for example to remodel the extracellular matrix and change its mechanical properties. Computational methods can help understand this process, but new methods need to be developed and tested. http://www.nature.com/nrm/journal/v15/n12/abs/nrm3896.html

- **Cytonemes**

  Cytonemes are filopodia-like protrusions that communicate morphogens/signaling molecules by direct cell-to-cell contacts even at a large distances: https://en.wikipedia.org/wiki/Cytoneme. How can this relatively new discovery be incorporated in multicellular models?