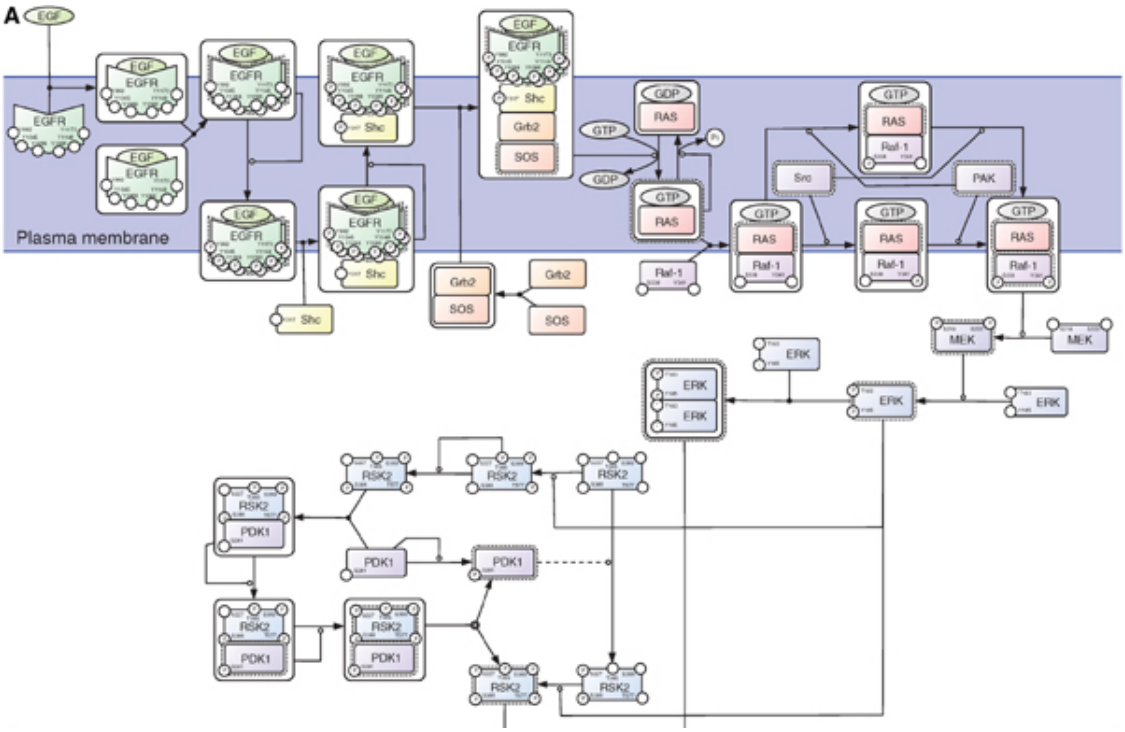
Master Thesis

INSTITUTE OF COMPUTATIONAL SCIENCE



Multiscale Stochastic Simulation

Simulate systems of bio-chemical reactions involving a wide range of time scales

Stochastic modeling of biochemical systems has become a very important research field in recent years. Theoretical and experimental work have proven the importance of stochastic processes in cellular processes and genetic regulatory networks. A simple modelization of those processes is Markovian: the time histories of the system reactants are Markov jump processes whose dynamics are described by the so-called master equation (M.E.). In 1977, Gillespie introduced an exact algorithm for the simulation of these processes, the so-called Stochastic Simulation Algorithm (SSA).

However, the SSA often proves very expensive when applied to large biological systems. In recent years, several schemes have been proposed to accelerate the SSA at the expense of accuracy.

Those accelerated schemes pertain to the so-called leaping algorithms where several reaction events are simulated over one step.

Besides, real systems can involve reactions with disparate rates (stiff systems); this drastically affects the efficiency of the leap algorithms.

This thesis will focus on these stiff systems and will aim at adapting leap algorithms to such contexts.

The first part of this project will be to understand state-of-the-art stochastic algorithms. A second part will be to investigate and develop approaches to stiff problems. Finally, the performances of the approaches will need to be evaluated on the simulation of biochemical problems.

CONTACT

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PREREQUISITES

Courses in Numerical Analysis, Probabilities
Good Programming Skills
Desire to Learn and Improvise
Independent worker

CSE LAB

Institute of Computational Science-DINFK
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In the CSE Lab we combine computational methods, computer science tools and domain specific knowledge to solve scientific and Engineering Problems in areas such as Fluid Mechanics, Nanotechnology and Life Sciences. The core computational competences of our group are in particle methods and in stochastic optimization techniques. Motivated by challenges in application fields, we focus on identifying the common elements among computational techniques and on formulating common methodological, algorithmic and software structures that facilitate their further development.