Hybrid models and numerical methods for high-dimensional master equations

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Biochemical reaction systems can be modelled in different ways. If all species are present in abundance, the effects of fluctuations and the discreteness of individual particles can be neglected. In this case the dynamics of the system can be reasonably described with the traditional reaction-rate approach, i.e. by solving a set of d ordinary differential equations for the concentrations of the species.

The reaction-rate approach is simple and computationally cheap, but not appropriate if the transcription of genetic information in a gene regulatory network is investigated. In gene regulatory networks some of the species contain only a very low number of particles, and small-scale stochastic fluctuations caused by inherent stochastic noise can cause large-scale effects. These effects can only be reproduced if the system is represented by a time-dependent probability distribution $p(t, x_1, \ldots, x_d)$ which indicates the probability that at time t exactly x_i particles of the i-th species exist. It is well-known that p is the solution of the chemical master equation, but solving this equation numerically is only possible for rather small systems because the number of degrees of freedom grows exponentially with the number of species.

This dilemma has motivated a number of attempts to construct a hybrid model which combine the simple but coarse reaction-rate approach with the precise but expensive stochastic kinetics. A particularly appealing hybrid model has recently been proposed by A. Hellander and P. Lötstedt. In this talk, the pros and cons of their model will be discussed, and an extension of the Hellander-Lötstedt model will be derived. Moreover, it will be sketched how the chemical master equation appearing in the stochastic part of the model can be solved numerically. Our method decreases the huge number of unknowns by representing the solution in a sparse wavelet basis combined with an iterative procedure which in each time-step detects the essential degrees of freedom.