Numerical methods and hybrid models for chemical master equations

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Many processes in biology, chemistry and physics can be regarded as reaction systems in which different species interact via a number of reaction channels. In the approach of *deterministic reaction kinetics*, such systems are modelled by ordinary differential equations which describe how the concentrations of the species change in time. This model is simple and computationally cheap, but fails if the influence of stochastic noise cannot be ignored, and if certain species have to be represented in terms of integer particle numbers instead of real-valued concentrations.

In *stochastic reaction kinetics*, the system is considered as a Markov jump process on a high-dimensional, discrete state space. Each state is a vector of integers which correspond to the particle numbers of the different species. The goal is to compute the associated time-dependent probability distribution which evolves according to the chemical master equation. Due to the curse of dimensionality, however, solving this equation numerically is a considerable challenge.

In the first part of the talk an adaptive wavelet method for the chemical master equation will be presented. This methods allows to reduce the large number of degrees of freedom considerably by representing the solution in an adaptively chosen sparse wavelet basis. The accuracy of the method is discussed, and its efficiency is illustrated by a numerical example.

In the second part of the talk, hybrid models for reaction systems are discussed. In these models only the "critical" species are represented by the accurate but computationally costly master equation, whereas the other species are represented by the simple but coarse deterministic description. In this talk, we discuss the properties of several hybrid models and present bounds for the modelling error.