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Abstract of the Doctoral Dissertation

Dynamics of far-from-equilibrium chemical systems: microscopic and mesoscopic approaches

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Many nonlinear systems under non-equilibrium conditions are highly sensitive to internal fluctuations. In this dissertation, stochastic effects in some generic reaction-diffusion models are studied using two approaches of different precision. In the mesoscopic approach, evolution of the system is governed by the master equation, which can be solved numerically or used to set up kinetic Monte Carlo simulations. On the microscopic level, particle computer simulations are used. These two stochastic approaches are compared with deterministic, macroscopic reaction-diffusion equations.

My dissertation is submitted in the form of 6 publications, preceded by an introduction into the subject area of the dissertation and a brief discussion of each publication.

In the Introduction, key information about the different approaches is presented, together with basics of nonlinear systems and a presentation of numerical algorithms used.

The first part of the Results chapter is devoted to studies on reaction-induced perturbation of particle velocity distributions in models of bistability and wave front propagation. A master equation including this perturbation is presented and compared with microscopic simulations.

The second part of the Results deals with pattern formation in reaction-diffusion systems in the context of developmental biology. A method for simulating Turing patterns at the microscopic level using the direct simulation Monte Carlo algorithm is developed. Then, experiments consisting of perturbing segmentation of vertebrate embryo's body axis are explained using the Turing mechanism. Finally, a different possible mechanism of body axis segmentation, the "clock and wavefront" model, is formulated as a reaction-diffusion model.