

FAKULTÄT FÜR MATHEMATIK Dekan Univ.-Prof. Dr. Christian Krattenthaler

Einladung zur öffentlichen Defensio von

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Thema der Dissertation:

Uncertainty Quantification with Applications in Nanotechnology

Abstract:

In recent years, nanoscale devices such as silicon nanowire sensors, field-effect transistors (FETs), and nanopores have been promising devices in medicine and engineering. Silicon nanowire sensors have been used to detect minute concentrations of biomolecules e.g., DNA oligomers, tumor markers, toxic gases and diffusion of ions through transmembrane proteins. FETs have become a very widely used device within the electronics industry. These devices are cutting-edge technologies and, at the same time, an interesting model system for stochastic partial differential equations (PDEs).

Various sources of noise and fluctuations are included in the model equations here. Doping of semiconductor devices is inherently random and results in a random number of impurity atoms placed at random positions. These effects due to the random location of dopants are of increasing importance, as the devices have been shrunk into the nanometer scale and billions of them are required to work together despite the unavoidable process variations. In field-effect sensors, target molecules bind to randomly placed probe molecules in a stochastic process so that the detection mechanism is inherently stochastic. The Brownian motion of the target molecules also results in changes in charge concentration and permittivity which propagates through the self-consistent transport equations and finally results in noise in the sensor output.

These considerations motivate the development of advanced stochastic numerical methods to model the uncertainty in nanoelectronic devices. We develop stochastic drift-diffusion-Poisson system of equation to model the effect of randomness on charge transport. To that end, existence and local-uniqueness theorems for weak solutions of the are presented and for the stochastic PDE an efficient computational technique (Scharfetter-Gummel iteration) is used to solve it. In order to calculate the ionic currents through various transmembrane proteins a transport equation for confined structures is employed. The computational significance of this continuum model is that the (6 + 1)-dimensional Boltzmann equation is reduced to a (2 + 1)-dimensional diffusion-type equation and ionic currents through confined structures can be calculated immediately.

We address the numerical challenge by using state-of-the-art methods, such as multilevel Monte Carlo method, and improve on it by determining the discretization parameters in the numerical approach such that the computational work is minimized for a prescribed total error. In this way, the various sources of error are balanced optimally. To further improve the computational efficiency, a randomized low-discrepancy sequence such as a randomly shifted rank-1 lattice are applied.

Prüfungssenat:

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