Stochastic PDEs for Modeling Transport in Nanoscale Devices

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Abstract. The understanding of charge transport plays an essential role in the design of many electronic and nanoscale devices such as electrical-impedance tomography (EIT) sensors, nanowire field-effect (bio- and gas) sensors and nanopore sensors for instance in medical applications and nanotechnology. Thus, carefully and realistic modeling and analysis of charge transport in nanoscale devices are of great importance. In this regard, we extend the transport model, namely the drift-diffusion-Poisson system to the frequency domain and analyze the existence and local uniqueness of its solution in the alternating-current (AC) small-signal regime, which were only demonstrated experimentally recently. To further improve the model, we develop the stochastic drift-diffusion-Poisson system in order to model uncertainty in the nanoscale devices. To this end, we first analyze the stochastic PDE system by presenting existence and local uniqueness of its solution, and then develop optimal stochastic numerical methods such as multilevel Monte-Carlo and multilevel randomized quasi Monte-Carlo finite-element methods to model randomness in charge transport. In fact the total errors of the presented stochastic methods including different (statistical and discretization) sources have to be balanced in order to improve the computational efficiency of the methods. This leads to finding the optimal discretization parameters and number of samples and consequently optimal stochastic methods. Realistic modeling of medical and electronic devices such as EIT sensors is also essential in this field. In this dissertation, we develop an EIT inverse model problem in an infinite-dimensional setting by extending the standard forward model to a nonlinear elliptic partial differential equation. The uncertainty in the presented nonlinear EIT model is due to the material and inclusion properties such as permittivities, charges and sizes of inclusions in the main body, which are essential in medicine, EIT and bioimpedance tomography to screen the interior body and to detect tumors or to determine body composition. These geometrical and physical governing parameters are extracted simultaneously by solving the resulting EIT inverse problem by means of an adaptive Markov-chain Monte-Carlo finite-element method (MCMC-FEM), including an MCMC sampling technique for the probability space and a Galerkin finite-element approximation for the discretization of the physical space. Furthermore, we formulate the EIT inverse model in a measure-theoretic framework and prove well-definedness and well-posedness of the posterior measure and the Bayesian inversion. The Bayesian inference also proves its ability to interpret the statistical variability in the measured outputs of biofilms growth and degradation. To this end, we present a system of PDEs as a mathematical model for biofilms, which describes the time dependent evolution of the size of the biofilm including quorum sensing and cooperation of bacteria against antibiotics. The results of biofilm inverse problem prove the ability of the proposed uncertainty quantification method to accurately estimate relevant system parameter in the model.