Simulation of the currents through nanopore sensors

G. Tulzer[1] and C. Ringhofer[2] and C. Heitzinger[1,2,*]

[1] Institute for Analysis and Scientific Computing
Vienna University of Technology (TU Wien)
Wiedner Hauptstraße 8–10, A-1040 Vienna, Austria

[2] School of Mathematical and Statistical Sciences
Arizona State University
Tempe, AZ 85287-1804, USA
Clemens.Heitzinger@TUWien.ac.at, http://Clemens.Heitzinger.name/

ABSTRACT

Introduction. Nanopores are the ultimate Coulter counters. The principle of a Coulter counter is that the translocation of a particle through a small channel separating two reservoirs of electrolyte solution briefly changes the electrical resistance of the liquid. This change indicates the number and size of the particles. Since the diameters of nanopores are comparable to the size of the particles to be detected in the most advanced experiments, nanopores are indeed the ultimate Coulter counters.

The experimental progress in this field in recent years [1–4] motivates simulations of nanopores acting as sensors in order to provide quantitative understanding and to enable rational design. Among the applications of nanopores are single-molecule detection and DNA sequencing. There are several open questions regarding physically correct modeling and efficient numerical methods.

The model equations. Here our basic model equations are the stationary drift-diffusion-(Navier-)Stokes-Poisson system. The (Navier-)Stokes equations describe the transport of water acting as the background medium; the drift-diffusion equations describe the transport of anions and cations; and the Poisson equation ensures self-consistency of all charge carriers. The two transport subsystems, namely drift-diffusion and (Navier-)Stokes, are coupled as well: The flow of the background medium results in a third term for the fluxes in the modified drift-diffusion equations, and the (Navier-)Stokes equations contain an additional force term due to the effect of the ions on the background medium.

The drift-diffusion-(Navier-)Stokes-Poisson system is a phenomenological model, and we discuss its derivation from a system of coupled Boltzmann equations as the most general description.

Numerical method. In order to simulate realistic nanopores, it is mandatory to resolve their geometry. Therefore we use the finite-element method on an unstructured mesh. The mesh is finer near the nanopore and coarser away from it. The simulation domain is chosen sufficiently large to diminish the effect of the boundary conditions. The model equations are solved in a self-consistent loop using a Newton iteration.

Simulation results. Since this model includes the interactions of the background medium with the ions that are driven through the pore by the applied potential, it includes all the physics of the problem. These interactions are highly relevant to understand the sensing mechanism [5]. We present numerical results of nanopores that have been fabricated and used as sensors and we discuss how the currents through the nanopores affect the translocation of analyte molecules, also by calculating the forces acting on the molecules.

Acknowledgment. The first and last authors acknowledge support by the FWF (Austrian Science Fund) START project no. Y660 *PDE Models for Nanotechnology*.

REFERENCES

[1] H. Bayley and P.S. Cremer. Stochastic sensors inspired by biology. *Nature*, 413:226–230, September 2001.

[2] S. Howorka, S. Cheley, and H. Bayley. Sequence-specific detection of individual DNA strands using engineered nanopores. *Nature Biotechnology*, 19:636–639, July 2001.

[3] J. Clarke, H.-C. Wu, L. Jayasinghe, A. Patel, S. Reid, and H. Bayley. Continuous base identification for single-molecule nanopore DNA sequencing. *Nature Nanotechnology*, 4:265–270, 2009.

[4] M. Ayub, S.W. Hardwick, B.F. Luisi, and H. Bayley. Nanopore-based identification of individual nucleotides for direct RNA sequencing. *Nano Lett.*, 13(12):6144–6150, 2013.

[5] Y. Liu, K. Lilja, C. Heitzinger, and R.W. Dutton. Overcoming the screening-induced performance limits of nanowire biosensors: a simulation study on the effect of electro-diffusion flow. In *IEDM 2008 Technical Digest*, pages 491–494, San Francisco, CA, USA, December 2008.