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Numerical Methods for Innovative Semiconductor Devices

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Few discoveries have shaped our modern society like semiconductors have. Despite of (or rather due to) several decades of research, several emerging semiconductor technologies and materials have the potential for disruptive innovation. Among them are highly-efficient perovskite solar cells, resource-efficient nanowires as well as quantum technologies. Starting from a classical nonlinear drift-diffusion model for charge transport via electrons and holes in a self-consistent electric field (the van Roosbroeck system), we present several necessary extensions. Mathematically, the challenges amount to (i) including thermodynamically consistently nonlinear diffusion in discretizations; (ii) modeling and simulating considerably slower ion movement and surface effects; (iii) coupling hyperelasticity with charge transport; (iv) incorporating atomistic effects into a macroscopic model and (v) solving an inverse problem.

Orateur: FARRELL, Patricio (Weierstrass Institute Berlin)