Dissipative Discretization Schemes for Drift-Diffusion and Phase Separation Models with Applications

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For the classical van Roosbroeck equations and a binary phase separation model with global interaction and a finite number of sites finite volume discretizations on Delaunay simplex grids in two and three space dimensions are investigated.

The goal is to give a weak discrete formulation and to reproduce the essential stability properties of the analytic problems for any spatial step size h and time step τ, hence not introduce smallness assumptions on the solution variation on neighboring vertices. The main results are:

The Euler backward scheme in time and the Scharfetter–Gummel discretization of the van Roosbroeck system yields a dissipative discrete problem. Moreover for reduced equations a discrete maximum principle for the quasi Fermi potentials holds.

For the phase separation problem a Crank–Nicholson scheme in time is dissipative. Using this result and the requirement of dissipativity determine the space discretization. For that scheme a priori bounds can be proved using a weak discrete maximum principle.

The discrete equilibrium solutions for both problems are characterized by constant Fermi potentials, too. This fact can be used to simplify a numerical bifurcation analysis for the phase separation model.

Finally some numerical examples of a three dimensional semiconductor sensor are discussed, too. Here the weak form of the discretization can be used for instance to reduce the error in the functional central for that application: the contact currents. This is a joint work with Herbert Gajewski (WIAS).