diffusion in porous media. High-order approximation of the $\alpha = 2(1-\sigma)$ fractional derivative is applied. Numerical comparison results are discussed.

Valuation of European Options with Liquidity Shocks Switching by Fitted Finite Volume Method

M. N. Koleva, L. G. Vulkov

We consider a regime-switching Markov model of market liquidity with two states - liquid state and the illiquid state, which is formulated by a non-linear coupled system of one parabolic and one ODE. We develop a fitted finite volume method for pricing European options with switching liquidity shocks. As the parabolic equation is degenerate, in order to obtain second-order accuracy in space, we refine the mesh locally near the degenerate point. We investigate some basic properties of the numerical solution and establish convergence in maximal discrete norm. An efficient algorithm for implementation of the discrete schemes is proposed. Results from various numerical experiments with different European options are provided.

A Revised Wigner Function Approach for Stationary Quantum Transport

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Quantum electron transport in modern semiconductor devices is described by a Wigner equation formally similar to the classical Liouville equation (also called Vlasov equation).

The Wigner equation describing stationary quantum transport has a singularity at the point $k=0$. Deterministic solution methods usually deal with the singularity by just avoiding that point in the mesh (e.g., Frensley's method). Results from these methods are known to depend strongly on the discretization and meshing parameters. The method is not stable under mesh refinement and results can even be unphysical.

We propose a revised approach which explicitly includes the point $k=0$ in the mesh. For this we give two equations for $k=0$. The first condition is an algebraic constraint which ensures that the solution of the Wigner equation has no singularity for $k=0$. If this condition is fulfilled we then can derive a transport equation for $k=0$ as a secondary equation. The resulting system with two equations for $k=0$ is overdetermined and we call it the constrained Wigner equation.

We give a theoretical analysis of the overdeterminacy by relating the two equations for $k=0$ to boundary conditions for the sigma equation, which is the inverse Fourier transform of the Wigner equation (or equivalently the von Neumann equation in a linearly transformed coordinate system).

Finally, we show results from a prototype implementation of the constrained Wigner equation which gives good agreement with results from the quantum transmitting boundary method. The revised method is stable under mesh refinement. No parameter fitting is needed.

On a Bolza Problem

M. Krastanov, N. Ribarska

The classical problem of the calculus of variations is studied under the assumption that the integrand is a continuous function. Under suitable ad- ditional assumptions, a non-smooth version of the classical Euler equation is proved.

Adaptive Finite Element Method for the Nonlinear Poisson-Boltzmann Equation Applied to the SecYEG Membrane Channel

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In this work, we consider the Poisson-Boltzmann equation (PBE) which gives a mean field description of the electrostatic potential of a system of molecule(s) in ionic solution. In order to pose a standard weak formulation with a regular right hand side and a solution in $H^1(\Omega)$, two and three term splittings of the potential are utilized (see Holst, 2012). In this way, the irregular distribution on the right hand side, represented by a linear combination of delta functions, is transformed to another irregular distribution supported on the interface between the molceular and ionic solution, which this time is also a bounded linear functional on H_0^1. We derive explicitly computable bounds on the error in energy norm for the regular H^1 part of the solution of the PBE. A patchwise equilibrated flux reconstruction technique (see Braess and Schöberl, 2006) is used to obtain a conforming approximation of the dual variable. Thus, the evaluation of the error indicator in the adaptive algorithm can be realized in a very efficient manner in parallel.
This methodology is applied to study the electrostatic potential in the membrane channel SecYEG. The channel is located in the plasma membrane of bacteria and provides a lateral exit into the bilayer for membrane proteins, while simultaneously offering a pathway into the aqueous interior for secreted proteins. The molecular mechanisms that determine the functionality of the channel for these two pathways and driving forces of the translocation are not comprehensively understood. Important contribution to both may come from the electrostatic interactions between the SecYEG and translocated peptide. The system consists of 46 373 atoms, 9563 of which belong to the SecYEG. Moreover, an ion excluded layer with a tickness of 2