Application of Discontinuous Galerkin Methods onto Quantum-Liouville type Equations

V. Ganiu, D. Schulz
Chair for High Frequency Techniques, TU Dortmund, Friedrich-Woehler-Weg 4, 44227 Dortmund, Germany
e-mail: valmir.ganiu@tu-dortmund.de

***Abstract*—High performance computing methods are needed for the time-dependent analysis of carrier transport within nano structures when using density matrix formulations. For this purpose, a discontinuous Galerkin (DG) method for the numerical approximation of Quantum-Liouville type equations is presented.**

INTRODUCTION

The main advantage of the DG method is its dependency on matrix-vector-multiplications when performing transient calculations allowing a parallelization of the resulting algorithms. This has already been successfully demonstrated in other fields of research like in computational fluid dynamics [1]. Hence, the aim of this work is to propose an algorithm based on a Quantum-Liouville type equation not only considering a spatially constant but spatially varying effective mass distribution and a self-consistent Hartree-Fock potential as well.

METHODOLOGY

Starting with the von Neumann equation in center-mass coordinates χ and ξ, a Finite Volume (FV) technique is applied onto the center mass coordinate ξ, followed by an expansion of the density matrix based on plane waves, arriving at a Quantum-Liouville type equation [2]. The DG method is used in χ-direction resulting in a hybrid method [3]. Along with the spatially varying effective mass different numerical fluxes [1] occur, which in combination with boundary conditions as well as the complex absorbing potential (CAP) [4] have a critical influence on the stability of a transient DG method.

DISCUSSION

To assess the stability, the eigenvalues of the resulting system matrix must be analyzed. As depicted in Fig. 1a-1d in combination with Tab. I, two factors have a crucial influence on the stability of the DG scheme: the numerical flux and the CAP. The CAP pushes the eigenvalue spectrum towards the negative half of the real axis. The choice of an upwind flux further ensures stability by avoiding eigenvalues with a positive real part. Finally, stability can be achieved. To asses the numerical validity of the proposed scheme, a resonant tunneling diode (RTD) is analyzed as depicted in Fig. 2. The self-consistent analysis for the thermal equilibrium is performed for the case of a spatially constant and a spatially varying effective mass. Evidently, from Fig. 3 it can be concluded that the inhomogeneous effective mass leads to a higher local maximum, which is in agreement with the results in [5]. Furthermore, the self-consistent transient simulation of the RTD with a spatially constant effective mass is depicted in Fig. 4 confirming convergence. Finally, from Fig. 5 it can be concluded that performing a transient simulation, a noticeable reduction in computation time compared to a conventional FV approach, as described in [5], can be achieved with the DG and fourth order Runge-Kutta (DGRK4) algorithm.

ACKNOWLEDGMENT

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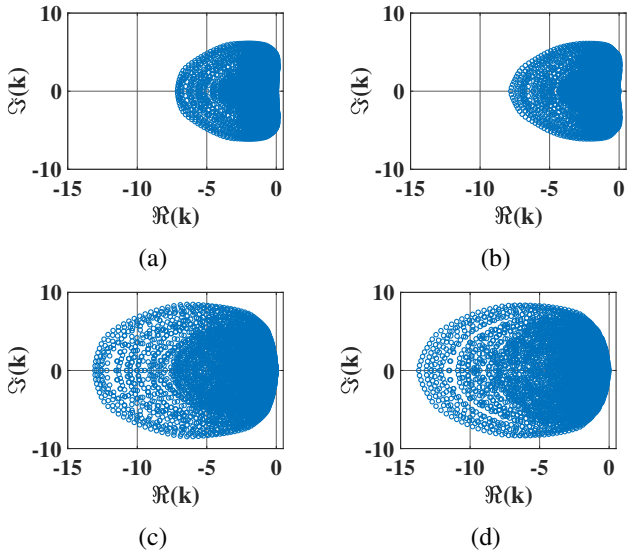

Fig. 1: Stability analysis for the central flux with no CAP (a), central flux with CAP (b), upwind flux with no CAP (c), and upwind flux with CAP (d). The real part of the eigenvalues must be exclusively located in the second and third quadrant of the complex plane. The right vertical line indicates the imaginary axis.

	Fig. a	Fig. b	Fig. c	Fig. d
$\Re_{max}(k)$	0.1265	0.0504	$-3.18e-7$	-0.0015
$\Re_{min}(k)$	-7.1083	-7.7918	-13.0494	-13.6978

TABLE I: Maximum and minimum real part of the eigenvalues from Fig. 1a-1d.

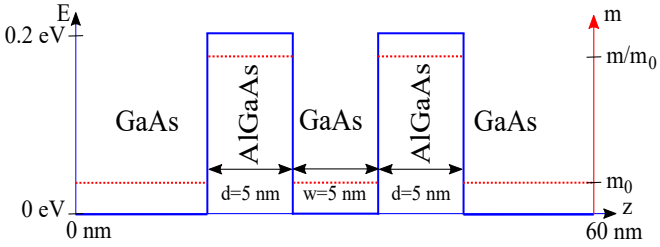

Fig. 2: Schematic representation of a resonant tunneling diode showing the band edge potential and the spatially varying effective mass m_0.

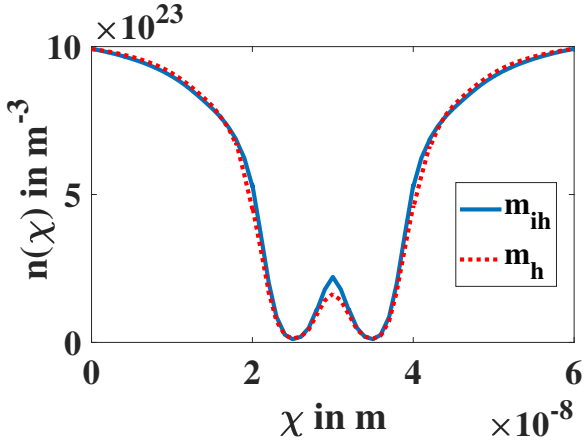

Fig. 3: Self-consistent carrier distribution $\boldsymbol{n}$ dependent on χ in a RTD with homogeneous mass distribution (m_h) and inhomogeneous mass distribution (m_{ih}).

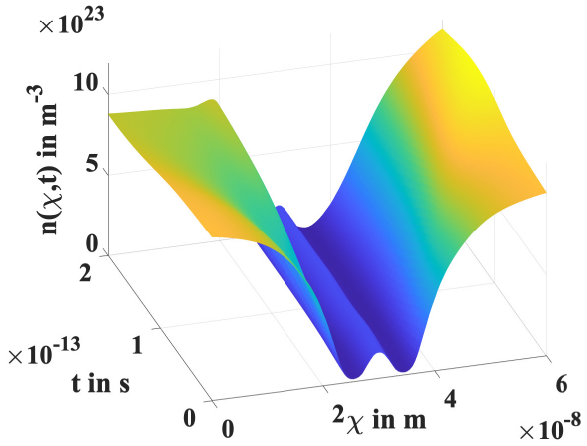

Fig. 4: Spatially time dependent self-consistent carrier distribution n for a mass distribution m_h, dependent on χ.

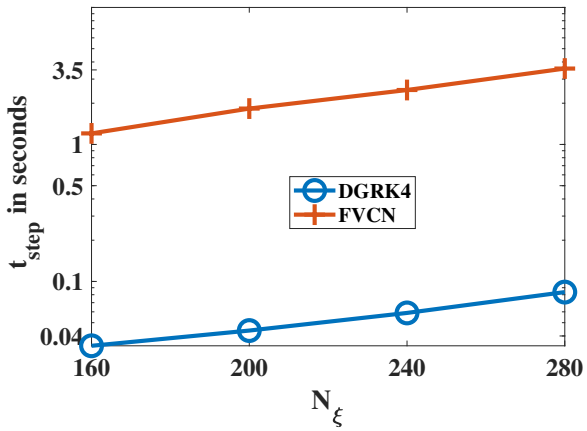

Fig. 5: Comparison of the computation time between the DGRK4 algorithm and the FV-Crank Nicolson (FVCN) scheme [5]. N_ξ indicates the number of ξ-elements.