Impact of Slope Limiters on DG Methods Solving Quantum-Liouville Type Equations

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Abstract

This work enhances the Discontinuous Galerkin (DG) method for solving Quantum-Liouville type equations by applying slope limiters with an approximate Riemann solver. Particularly, the moment limiter outperforms other conventional approaches in accuracy and runtime. Slope limiters applied onto the numerical results in combination with the self-consistent combination of Poisson's equation reduces the runtime by up to 31 $\%$, improving the overall computational efficiency.

I. Introduction

DG methods for the approximation are more efficient than standard methods (e.g., finite volume techniques) for solving quantum transport equations but can suffer from instabilities at cell interfaces [1]. This challenge is addressed by approximate Riemann solvers (RS), providing a unique solution [2]. This work focuses on improving an approximate RS coupled with a slope limiter (SL). Section II introduces the Liouville-von Neumann equation (LVNE), the DG method, and the SL briefly. Section III analyzes the impact of the promising candidate for SLs and summarizes the results.

II. Fundamentals

This work utilizes the Liouville-von Neumann equation (LVNE) in center-of-mass coordinates χ and ξ, expressed as $\partial_t \rho(\chi,\xi,t) = \{\imath\hbar/m \cdot \partial_\chi \partial_\xi + q/(\imath\hbar)[V(\chi+\xi/2) - V(\chi-\xi/2)]\}\rho(\chi,\xi,t)$, where ρ is the statistical density, q is the electron charge, and V represents the device potential and external bias [3]. The DG method along with a Fourier Transformation of the ξ coordinate arriving at a phase space representation, discussed in detail in [3], is then applied using an upwinding numerical flux. However, gradients at cell junctions remain and require smoothing. To address this, the problem-independent (PI), the total variation diminishing (TVD), and moment limiters will be applied and evaluated, providing varying levels of smoothing from mild to distinctive [4]. To solve the Poisson's equation, the Gummel algorithm is used ensuring self-consistency.

III. Numerical Experiments and Discussion

The foundation is a double-barrier GaAs/AlGaAs resonant tunneling diode (RTD) with a flatband potential (Fig. 1). Results from the DG algorithm were compared to the reference solution obtained via the QTBM, with the relative error calculated as the $L^p \in p = 1, 2, \infty$ norm. All simulations utilizing the DG method were carried out with a N_χ x N_ξ = 76 x 80 sized grid. Fig. 2 through 4 illustrate the effects of the PI, moment, and TVD slope limiters, respectively. Tab. I summarizes the errors and runtimes for each limiter. The moment limiter achieves both the smallest error and the fastest runtime, ensuring an efficient DG scheme. Finally, Fig. 5 presents the total runtime of the self-consistent Poisson loop. As external bias increases, fewer iterations are needed to meet the error threshold, resulting in runtime savings of up to 31 $\%$.

References

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[4] L. Zou. Understand slope limiter – graphically, 2021.

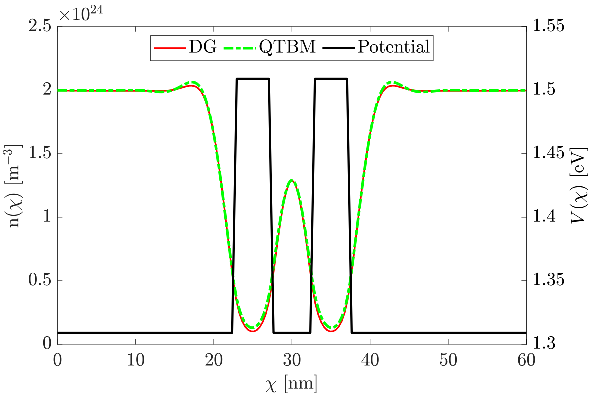

Fig. 1. Flatband potential profile of the resonant tunneling diode (RTD), as well as the statistical density derived with the QTBM (green) and DG (red). An overall good agreement between the proposed scheme and the QTBM as the reference method can be observed.

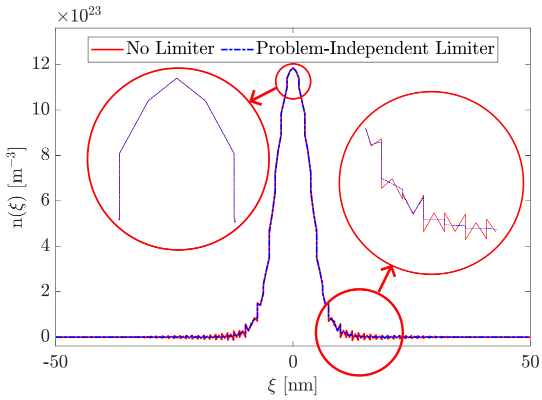

Fig. 2. Unprocessed (red) and processed (purple) results of the problem-independent limiter. The maximum at $\xi = 0$ nm is well preserved and around $\xi = 10$ nm a significant limiting of oscillations can be observed.

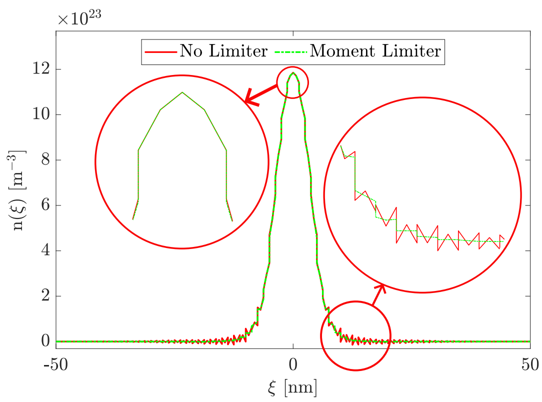

Fig. 3. Unprocessed (red) and processed (green) results of the moment limiter. The maximum at $\xi = 0$ nm is well preserved and around $\xi = 10$ nm a significant limiting of oscillations can be observed. Here, the smoothing is more distinctive than the problem-independent limiter in Fig. 2.

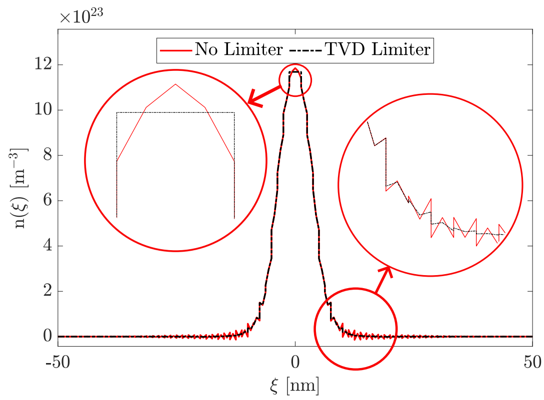

Fig. 4. Unprocessed (red) and processed (black) results of the TVD limiter. The maximum at $\xi = 0$ nm is *not* preserved and around $\xi = 10$ nm the least limiting of oscillations can be observed compared to the previous results.

TABLE I

L^p-ERROR AND RUNTIME FOR THE SLOPE LIMITERS APPLIED TO THE ξ-DOMAIN. WITH 0.06 S, THE MOMENT LIMITER IS THE MOST EFFICIENT WHILE ALSO PROVIDING THE SMALLEST ERROR.

	No Limiter	**PI**	**Moment**	**TVD**
L^1-Error	11.62 %	8.58 %	7.89 %	8.04 %
L^2-Error	7.83 %	7.38 %	7.25 %	7.46 %
L^∞-Error	8.07 %	8.07 %	8.07 %	9.36 %
Runtime		0.13 s	0.06 s	0.07 s

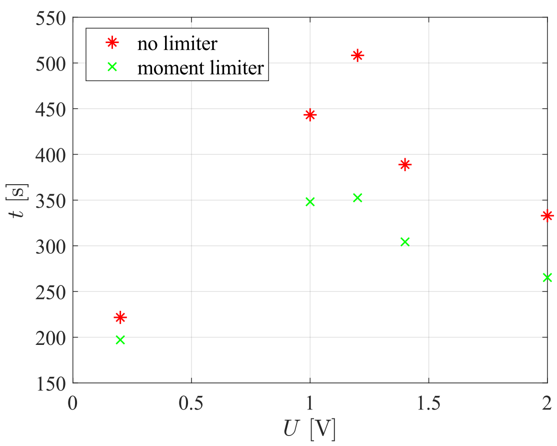

Fig. 5. Runtime comparison of the self-consistent while loop to solve Poisson's equation. Utilizing the moment slope limiter decreases the number of iterations needed to reach the desired convergence resulting in a reduction of the runtime.