A High Polynomial-Order Wavelet Method for Semiconductor Transport Equations

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INTRODUCTION

Recently, wavelets have been proposed as basis functions for the solution of 6-dimensional semiconductor transport equations (Boltzmann Transport Equation (BTE), Wigner Equation) for the first time [1]. The main advantage of wavelets are their hierarchical compression and adaptation properties enabling an adaptive solution with a fraction of the coefficients that are necessary with a conventional basis. Since the advantages of wavelets increase in higher dimensions, they could enable uniquely accurate TCAD tools for 2- and 3-dimensional devices. Hence, in [1] the Multi-Wavelet (MW) Discontinuous Galerkin (DG) method (MWDG) has been proposed and shown to reduce the number of coefficients by about 99 % with piecewise constant MWs. As a next step and in order to further reduce the coefficients, the MWDG for high polynomial orders (POs) is demonstrated in this work for the first time.

HIGH PO MWDG PERFORMANCE STUDY

MWs build a hierarchical basis for all piecewise polynomials (pps) so that the MWDG and the usual DG can be equivalent (uncompressed case). However, in the MWDG method it is possible to select only a small, relevant subspace of a pp space (compression). Wavelet compression strongly reduces the number of coefficients at a small expense of accuracy. In this study the proof of principle for the uncompressed and the compressed high PO MWDG method as well as a fair comparison between different POs (here for the orders 0,1, and 3) in all dimensions is presented. First, a grid for the uncompressed 0th order MWDG with 66,304 coefficients is created by careful manual adaptation. From that the grids for higher POs are naively generated by directly replacing grid points with high polynomial order so that the "coefficient density" stays the same everywhere in the phase space. Finally, the solutions are compressed to 6000 coefficients and solved by MWDG. The same well-studied n^+nn^+ structure as in [1] is simulated and the same well-benchmarked uncompressed 0th PO MWDG simulation with 1,147,904 coefficients as in [1] is used as a benchmark reference.

RESULTS

Figs. 1 and 2 show that the uncompressed MWDG is stable with all POs (no spurious oscillations, distribution function Φ is positive). All high-orders in x (physical space), μ (velocity in transport direction) and ω (energy) perform significantly better than the 0th order in both, density and current. Surprisingly, the high x orders "100" (PO in x: 1, PO in μ: 0, PO in ω: 0) and "300" perform best: At $x = 0.5$ the "000" error in the current is 21.3 %, whereas the "100" and "300" errors are only 1.47 %. Furthermore, since the discontinuities of the solutions within the n^+n junctions are strongly suppressed, the over-estimations of the currents within the n^+n regions (which appear in all upwinding formulations for the BTE) are strongly reduced. The high ω orders "013" and "033" show the second best behavior (5.88 % error both), whereas the high μ orders "011" and "031" are not acceptable (12.5 % error). Note: The spherical harmonics expansion method uses high POs in μ direction. For compression, Φ should be decomposed in $\Phi = \Phi_E + \Phi_V$. Φ_E lives on a subspace composing all MWs that are constant in μ direction and containing the energy and density information. The energy is a density normed quantity. Hence, the contribution of the wavelets to the norm $|\frac{\Phi_E}{n}|_{L^2}$ should be chosen as adaptation criterion. Φ_E contains steep gradients so that thresholds should be chosen carefully (Fig. 3). Φ_V, on the other hand, contains i.a. the current information. Since the current is of absolute relevance, the contribution of the wavelets to the norm $|\Phi_V|_{L^2}$ should be chosen. Consequently, high compression rates are possible for Φ_V. Following these new adaptation rules, in Figs. 1 and 2 Φ_E is compressed to 1000 coefficients (from 4736) and Φ_V is compressed to 5000 coefficients (from 61,568). The compression of high-order μ,ω MWDG performs well so that over 90 % compression is possible without much loss of accuracy (Figs. 2 and 4). However, the compressions for high x orders show local inaccuracies in the density. Applying 8000 coefficients (Fig. 1) or improved current weighted adaptation rules can already solve that problem.

CONCLUSION

High-order polynomials perform significantly better than piecewise constants for uncompressed MWDG (up to 96% coefficient saving for only 1.4% error in the current). A new wavelet compression rule applying a phase space separation can compress the solution additionally by over 90 %. Even larger compression rates are expected for future full hp-adaptive MWDG simulations in 6-dimensional phase spaces.

ACKNOWLEDGMENT

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REFERENCES

[1] V. Peikert and A. Schenk, Proc. 11th Int. Conf. on Simulation of Semiconductor Processes and Devices (SISPAD), Osaka, Japan, Sep. 8 - 10, 2011, pp. 299 - 302.

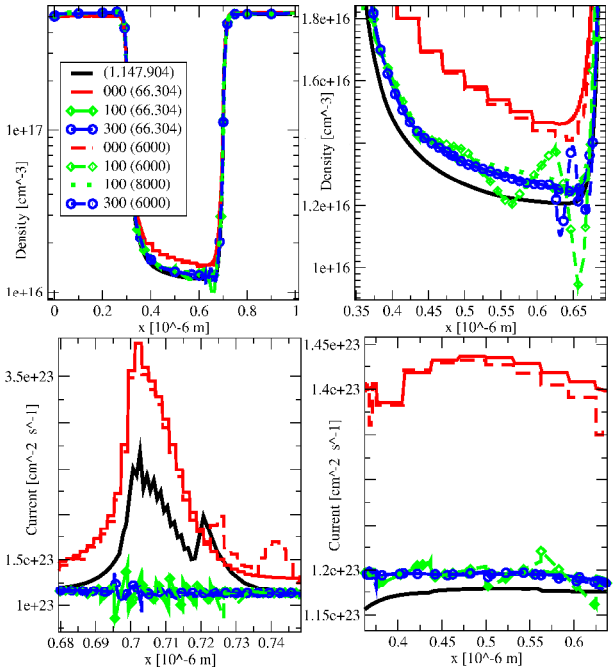

Fig. 1. n^+nn^+ simulations at 1V drain with high POs in x direction. Note: The shown currents are not the upwinding fluxes (which would be conserved), but calculated from the solutions of the BTE Φ directly.

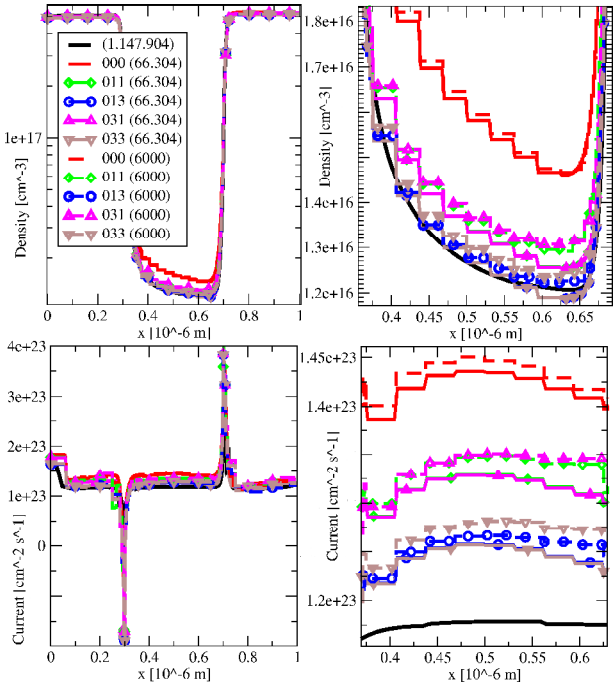

Fig. 2. n^+nn^+ simulations at 1V drain with high POs in μ and ω directions in analogy to Fig. 1.

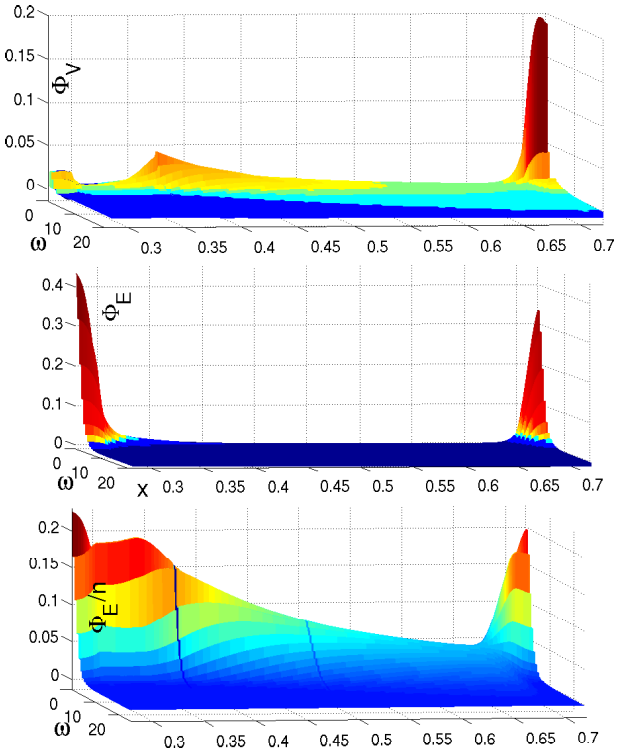

Fig. 3. The Figs. illustrate the phase space separation of the "300 (6000)" simulation at $\mu = 1$, $x = [0.25, 0.75]$ (n^+n junctions are at $x = 0.3$ and $x = 0.7$) and $\omega = [0, 25]$. Top: Φ_V is partly even larger in the channel region than in the left contact region. Middle: Φ_E ranges over many orders of magnitude. Bottom: Adaptation for Φ_E should be based on $\frac{\Phi_E}{n}$.

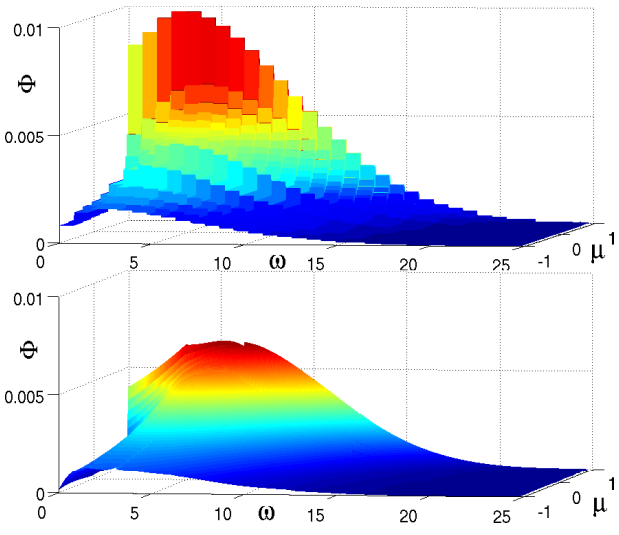

Fig. 4. The Figs. show the "000 (6000)" (upper panel) and "033 (6000)" (lower panel) simulations at $x = 0.6\mu m$.