

Adaptive Variable-Order Spherical Harmonics Expansion of the Boltzmann Transport Equation

Karl Rupp^{*†}, Tibor Grasser^{*} and Ansgar Jünger[†]

^{*}Institute for Microelectronics, TU Wien. Gußhausstraße 27-29/E360, A-1040 Wien, Austria

[†]Institute for Analysis and Scientific Computing, TU Wien. Wiedner Hauptstraße 8-10/E101, A-1040 Wien, Austria

Email: {rupp,grasser}@iue.tuwien.ac.at, juenger@asc.tuwien.ac.at

Abstract—The spherical harmonics expansion method provides a deterministic solution method for the Boltzmann Transport Equation for semiconductors. While first-order expansions have been used in early works, higher-order expansions are required for modern scaled-down devices. The drawback of higher-order expansion is that the number of unknowns in the resulting system of equations increases quadratically with the expansion order, leading to high memory consumptions and long simulation times. In this work we show that a considerable number of unknowns can be saved by increasing the expansion order only locally in the simulation domain. Moreover, we propose a scheme that adaptively increases the order starting from a uniform first-order expansion. For the considered n^+nn^+ -diode, savings in the number of unknowns of up to a factor of five are obtained without sacrificing any accuracy of the numerical solution.

I. INTRODUCTION

The solution of the Boltzmann transport equation (BTE) via the spherical harmonics expansion (SHE) method is in several aspects superior to the traditional and well-established stochastic Monte Carlo method [1]. As a deterministic method, it provides the favorable numerical properties of moment-based methods such as the drift-diffusion model for the solution of the full BTE. First-order expansions have been shown to yield good results in early publications [2]–[4], but with the continued miniaturization of semiconductor devices higher expansion orders are required. It has been demonstrated by Jungemann *et al.* [5] and recently by Jin *et al.* [6] that expansion orders in the range of five to seven are necessary in order to obtain accurate values for macroscopic quantities such as carrier velocities in the deca-nanometer regime.

Unfortunately, memory requirements of uniform spherical harmonics expansions up to order L on a simulation domain with N grid points are proportional to $N(L+1)^2$, even if carried out efficiently [7]. Since the total number of grid points N is already higher than for macroscopic models due to the additional energy coordinate, the quadratic dependency on the expansion order leads to huge memory requirements as already reported for fifth-order expansions in two spatial dimensions [8]. For example, considering a spatially two-dimensional simulation using 100 grid points per coordinate direction as well as 100 points along the energy coordinate, an expansion order nine leads to about $100^3 \times 10^2 = 10^8$ unknowns, whereas 4×10^6 unknowns are obtained for a first-order expansion.

For the purpose of predictive device simulation, quantities of

interest like current density, carrier densities or carrier velocities are obtained by an integration of the distribution function over energy. Due to the asymptotically exponential decay of the distribution function with energy, only contributions close to the band-edge have a large weight on these quantities. In addition, device regions that are negligible for transport do not require high-order expansions either. To reduce the total number of unknowns, we propose variable-order expansions in Sec. II, which allow for high-order SHE only in those device regions where it is actually required. The distribution of expansion orders over the simulation domain is covered by an automatic strategy and presented in Sec. III. It releases the simulator user from the tedious and possibly inefficient process of manually distributing expansion orders. Results for a spatially two-dimensional n^+nn^+ diode are presented in Sec. IV. An outlook is given and in Sec. V and finally a conclusion is drawn.

II. VARIABLE-ORDER EXPANSIONS

In all publications dealing with the SHE method, the distribution function $f(\mathbf{x}, \mathbf{p}, t)$ has so far been expanded in spherical harmonics up to a certain order L as

$$f(\mathbf{x}, \mathbf{p}, t) \approx \sum_{l=0}^L \sum_{m=-l}^l f_{l,m}(\mathbf{x}, H, t) Y_{l,m}(\theta, \varphi),$$

where \mathbf{x} denotes the spatial variable, \mathbf{p} the momentum, t time, H the total energy and θ, φ the angular components of the momentum (e.g. [1]–[8]). By projection of the BTE onto $Y_{l,m}(\theta, \varphi)$, equations for the unknown coefficients $f_{l,m}(\mathbf{x}, H, t)$ are obtained, which are then discretized in the (\mathbf{x}, H) -space.

In equilibrium, the Maxwell distribution of carriers is exactly represented by a zeroth order expansion and thus all $f_{l,m} = 0$ for $l > 0$. This is in contrast to moment methods, where higher moments of a Maxwell distribution do not vanish [9]. For small and smooth perturbations from equilibrium, the expansion coefficients are analytically known to decay rapidly [10]. At locations in the simulation domain where the carrier distribution function is far from the equilibrium state, expansion coefficients decay slowly and consequently larger expansion orders L are required to obtain a good approximation. Therefore, we set the expansion order individually for

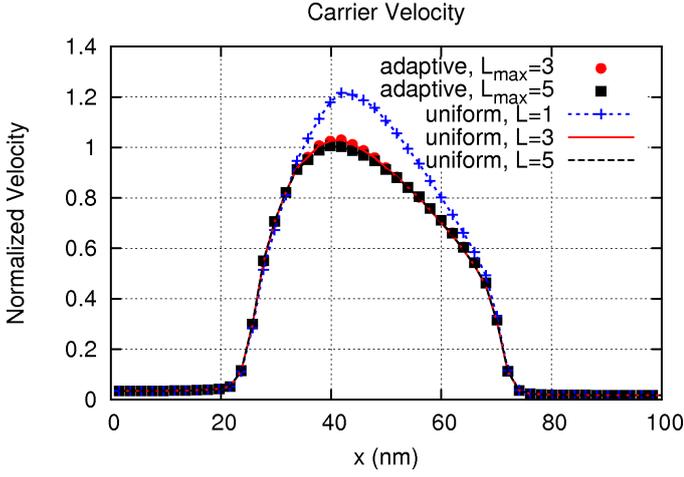


Fig. 1. Carrier velocities for different uniform and adaptive SHE orders. The seventh-order SHE results are not depicted for reasons of clarity.

each grid point (\mathbf{x}_i, H_i) in the simulation domain:

$$f(\mathbf{x}_i, \mathbf{p}_i, t) \approx \sum_{l=0}^{L_i} \sum_{m=-l}^l f_{l,m}(\mathbf{x}_i, H_i, t) Y_{l,m}(\theta, \varphi),$$

We employ the discretization using the H -transform as proposed by Hong *et al.* [8] by associating even order unknowns with mesh vertices and odd order unknowns with edges. If two vertices $\mathbf{v}_1 := (\mathbf{x}_1, H_1)$ and $\mathbf{v}_2 := (\mathbf{x}_2, H_2)$ with different expansion orders L_1 and L_2 (where without loss of generality $L_1 > L_2$) couple, the expansion order in \mathbf{v}_2 is formally considered to be increased to L_1 , but with the constraint that all expansion terms with an order above L_2 are zero. These terms at \mathbf{v}_2 are then ignored in the system matrix assembly process. The expansion order of the edge is set to the maximum of the two adjacent vertices. In an additional expansion order smoothing step we ensure that the expansion orders of two neighboring vertices do not vary by more than two, which reflects a continuous approximation of the distribution function.

III. AN ADAPTIVE SCHEME FOR SHE ORDERS

The inhomogeneous expansion orders can either be statically distributed over the simulation domain, or be distributed by an automatic adaption strategy. A static distribution allows us to incorporate additional knowledge of the user into the simulation process and full control, but can be tedious and is not preferable for every-day TCAD applications. To increase the attractiveness of the SHE method for the latter, we propose a fully-automatic adaption strategy. It is based on an analytical result (for details refer to [10]), which states that for a function g defined on the unit sphere, the rate of decay of spherical harmonics expansion coefficients is determined by the smoothness of g . More precisely, for $g = \sum_l \sum_{m=-l}^l g_{l,m} Y_{l,m} =: \sum_l Q_l$ there holds

$$|Q_l| \leq C l^{1/2-k}, \quad (1)$$

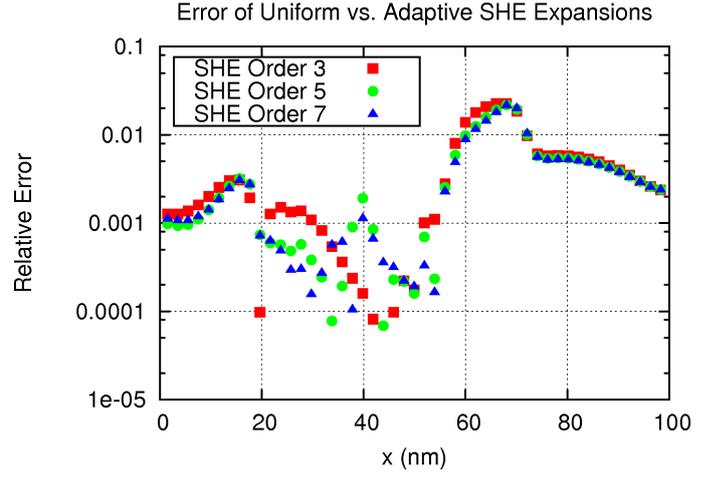


Fig. 2. Error of carrier velocities for different uniform and adaptive SHE orders.

where C is a constant and k denotes the number of continuous derivatives of g . Our indicator estimates k and increases the expansion order in regions where the decay is slow.

More precisely, on each grid point we used the estimator

$$\eta(\mathbf{x}_i, H_i) = \eta_1(\mathbf{x}_i, H_i) + \eta_2(\mathbf{x}_i, H_i),$$

where the two summands are given by

$$\eta_1(\mathbf{x}_i, H_i) = \frac{\sum_{\text{edges}} \sum_m |g_{L_i+1,m}|}{N_{\text{edges}}(\mathbf{x}_i, H_i) \log(L_i + 1) f_{0,0}(\mathbf{x}_i, H_i)},$$

$$\eta_2(\mathbf{x}_i, H_i) = \alpha \log(f_{0,0}(\mathbf{x}_i, H_i)),$$

with the number of edges N_{edges} connected to the respective grid point and L_i denoting the maximum (even) expansion order at point (\mathbf{x}_i, L_i) . The function η_1 is a slightly modified form of the inversion of Eq. 1 for k and estimates the decay of the spherical harmonics expansion at each grid point in the simulation domain. The function η_2 is an empirical term that adds extra weight closer to the band-edge, where higher contributions of the distribution function to macroscopic quantities are obtained. The parameter α was after some numerical experiments set to 0.25. If the resulting error indicator η is above a certain threshold, the expansion order at the edge and the vertices is increased for the next simulation run.

IV. RESULTS

The outlined adaption scheme has been implemented in our spatially two-dimensional simulator ViennaSHE. For demonstration purposes, we consider a spatially two-dimensional simulation of a quasi one-dimensional n^+nn^+ -diode at 0.5 V bias with an intrinsic region of 48 nm. Our simulation used 120 grid points in x -direction, two in y -direction and 120 points along the energy axis ranging up to 1.5 eV. The reason for the two-dimensional simulation is to show the memory savings using the full set of spherical harmonics, while in a one-dimensional simulation the smaller set of Legendre polynomials is used.

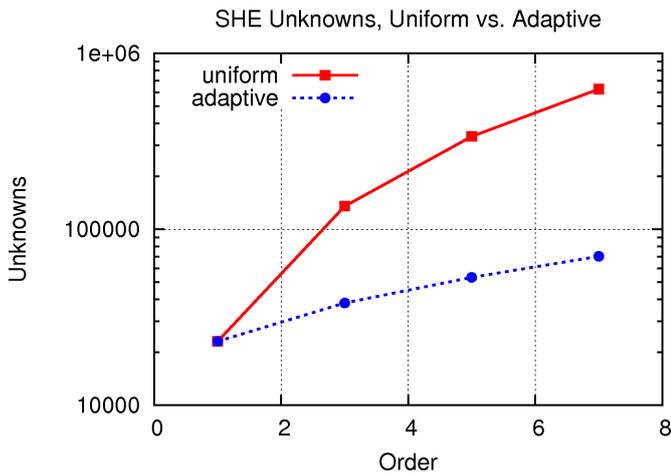


Fig. 3. Number of unknowns for different uniform and adaptive SHE orders. Savings of up to one order of magnitude are obtained.

Average carrier velocities along the device are compared for different uniform expansion orders as well as for adaptive expansion orders after one (maximum SHE order 3), two (maximum SHE order 5) and three (maximum SHE order 7) adaption steps. Fig. 1 shows the convergence of the SHE method with higher order, as well as the good agreement of the uniform and the adaptive expansions. The relative deviations of the uniform and the adaptive results are shown in Fig. 2. The error is almost uniformly below one percent, only near the end of the intrinsic region the error is slightly increased. Comparing with Fig. 1, one sees that the error is above one percent at the end of the intrinsic region. This is at least partly due to the rather large gradient of the velocity, where already small variations in the spatial direction lead to rather large differences in the velocity.

The number of unknowns using uniform SHE and adaptive SHE are depicted in Fig. 3. A considerable reduction in the number of unknowns is obtained, ranging from a factor of three for third-order expansions to a factor of nine for seventh-order expansions. It should be noted that an adaptive seventh-order expansion still uses less unknowns than a uniform third-order expansion. The savings also show a strong dependence on the considered total energy range, which depends on the applied bias. Therefore, the savings can be even higher for larger devices with a bias of several Volts, because a higher range of kinetic energies is considered.

Details of the adaption step are depicted in Fig. 4. The indicator is shifted such that the highest value equals zero. As refinement threshold, a fixed value of -5 was used. It can be seen that the expansion order is only locally increased near the band edge at the beginning of the intrinsic region. The region of increased expansion orders essentially captures the trajectories of carriers in free flight ($H = \text{const.}$) towards the right contact. It is remarkable that the expansion order is kept at lowest order towards the end of the intrinsic region near the band-edge.

It should also be noted that increased numerical stability has been observed for very coarse grids by keeping a first-order

SHE directly at the band-edge. Since the density of states is close to zero at these points anyway, there are no spurious effects on the accuracy of the solution.

V. OUTLOOK

It has to be emphasized that an efficient error indicator depends on the target quantity. The weighting $\eta_2(\mathbf{x}_i, H_i)$ used in the estimator is certainly attractive when aiming at macroscopic quantities obtained as moments of the distribution function, where the main contributions are relatively close to the band-edge. However, the η_2 term may be undesired if the high-energy tails of the distribution function are to be resolved, as it is the case for example of interest for the study of impact ionization and hot carrier degradation effects. Therefore, the proposed estimator is possibly the first out of a whole family of different adaption strategies with each strategy tailored to a different target quantity.

One drawback of the proposed indicator is that once a region is not considered for refinement, it will not be refined at a later step either (Fig. 4). This can be improved by lowering the threshold value at later adaption steps.

Instead of not only comparing the terms of highest expansion order with the zeroth-order term, the proposed error indicator can be modified to taking all available expansion orders at each vertex into account. Fluctuations of the error indicator due to sign changes of individual terms are then reduced.

The error indicator proposed in this work can also be coupled with a residual-based indicator. We expect that this is in particular an advantage at low expansion orders, where the asymptotic behavior of the analytical result in (1) does not constitute a good criterion.

VI. CONCLUSIONS

The proposed adaptive variable-order scheme allows us to solve the BTE at the accuracy of uniform high-order SHE at considerably lower computational costs, both in terms of memory and execution time. These savings of up to a factor of nine obtained for the considered n^+nm^+ diode certainly increase the attractiveness of the SHE method for TCAD tools.

In addition, the proposed scheme provides further insight into the transport contributions of individual expansion orders at various energies. In the case of average carrier velocities, high expansion orders are required near the band edge and along and below the trajectories of carriers in free flight, while lower expansion orders are sufficient at higher energies.

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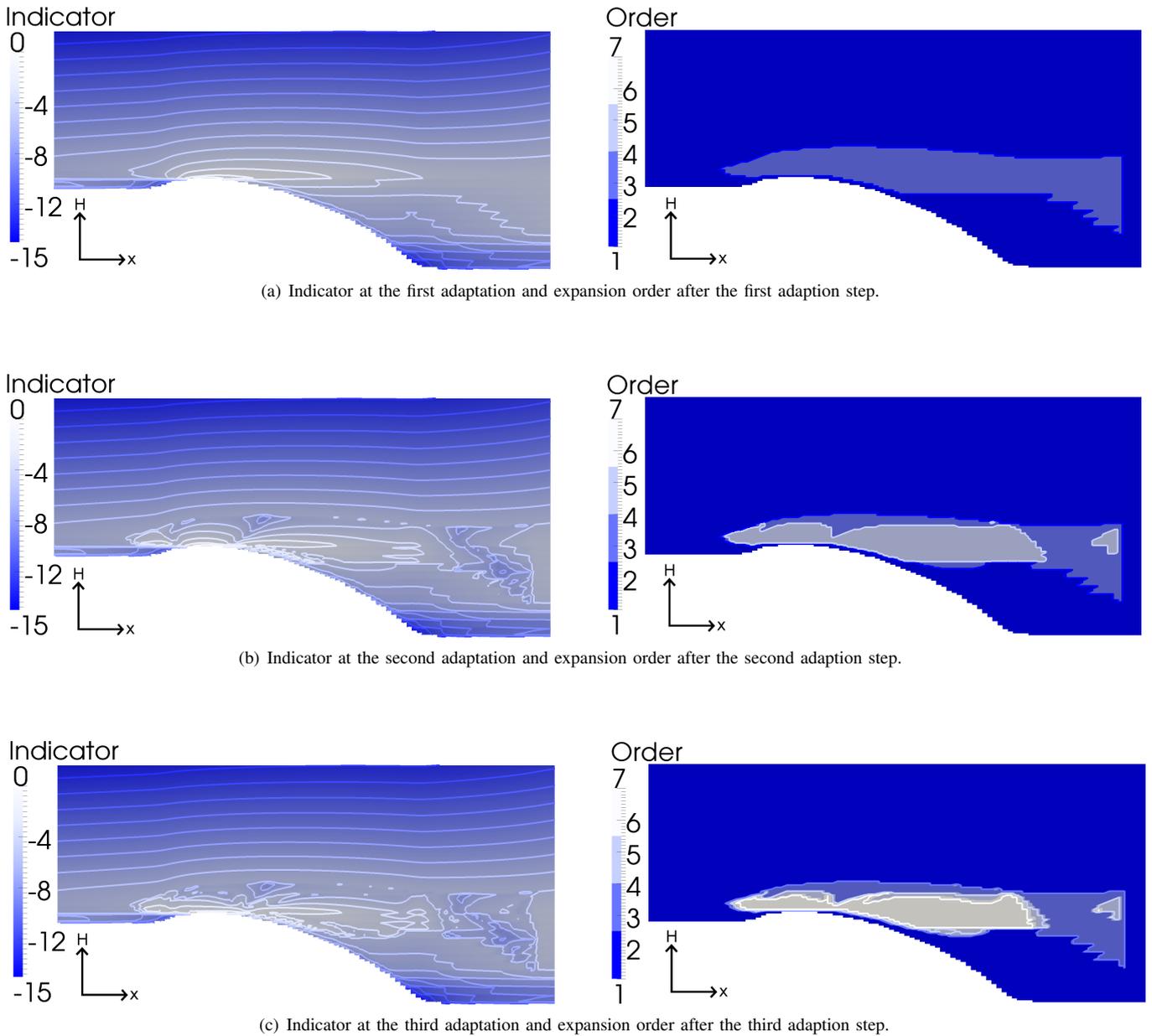


Fig. 4. Expansion indicator and expansion orders in the n^+nn^+ diode for three adaptation steps. The scheme starts with a uniform first order expansion.

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