Utilizing Wavelets for the Solutions of High-dimensional Semiconductor Transport Equations

Vincent Peikert and Andreas Schenk

Integrated Systems Laboratory, ETH Zürich, Gloriastr. 35, CH-8092 Zürich, Switzerland

Introduction Transport equations (Boltzmann, Wigner) on 6-dimensional phase spaces describe the behavior of charge carriers in semiconductors and form the basis for Technology Computer Aided Design (TCAD) on device level. However, the numerical solution of these high-dimensional equations involves huge matrices which practically limits contemporary direct solvers to problems with only one real space dimension. Since the integral operator in the Wigner transport equation (WTE) produces full matrices, 2-dimensional simulations are only feasible for the Boltzmann transport equation (BTE) so far. Even for the BTE the simulation of 2D devices calls for coarse meshes and geometrical simplicity which sets limitations to the accuracy and the practical application for the new TCAD challenges introduced by the rapidly increasing importance of 3D devices. By far the most established numerical BTE approach is the Spherical Harmonics Expansion Method (SHE) which is based on a representation of the momentum space in spherical coordinates and an expansion of the angular variables in SH. The SH Y_l^m build a dense basis in L_2^S on the sphere: $V_S^0 \subset V_S^1 \subset ...V_S^N \subset L_2^S$, with $V_S^N := span\{Y_l^m : l = 0,...N; m = -l,...,l\}$. Any V_S^k may be decomposed as $V_S^k = W_S^k \oplus V_S^{k-1}$, with $W_S^k \perp V_S^{k-1}$. A special property of SH is that the detail spaces W_S^k are spanned by SH Y_l^m themselves. The SH coefficients only contain the additional detail information to the orders before and decay quickly with the detail order (typically only 7 orders are necessary to simulate silicon transistors). The SH coefficient size has recently been used as an adaptive criterion for a variable order SHE expansion and the feasibility of 3D SHE simulations have been investigated [1].

Multi-Wavelets All contemporary numerical BTE approaches apply piecewise polynomials (pp) as basis functions. Usually, they apply piecewise constants (pc) in all dimensions (the SHE applies pc in the energy and real space directions). Recently, the Discontinuous Galerkin (DG) method for the BTE has been proposed [2]. The DG method is flux conserving and is (in contrast to SHE) stable with high-order pp in real space and energy directions (hp-stable) and is therefore a promising alternative. Let V_n^k be the space of all one-dimensional pp of the degree less than k on a uniform mesh (to keep the notation simple) with 2^n equidistant intervals within $[0, 1]$. By bisecting the mesh, pp build a dense basis in L_2 and fulfill the nested structure $V_0^k \subset V_1^k ... \subset V_n^k ... \subset L_2([0, 1])$. It is possible to decompose V_{n+1}^k into V_n^k and a perpendicular space W_n^k which only contains the additional details of V_{n+1}^k compared to V_n^k: $V_n^k \oplus W_n^k = V_{n+1}^k$, with $V_n^k \perp W_n^k$. Recursively, V_n^k can be decomposed by detail spaces $V_n^k = V_0^k \oplus W_0^k \oplus W_1^k \oplus ... \oplus W_{n-1}^k$. W_l^k is spanned by $2^{l-1}k$ detail functions $\psi_{l,i,j}$ which are called Multi-Wavelets (MWs) (see [3]) where l indexes the detail order, j indexes the vanishing moment order and i indexes the position.

Multi-Wavelet Discontinuous Galerkin Method Instead of using pp $\in V_n^k$ (nodal DG: NDG), the solution of the BTE Φ could be expanded in tensor products of one-dimensional MW bases (Multi-Wavelet Discontinuous Galerkin method: MWDG): $\Phi(x, y, z, \mu, \phi, \omega) = \sum_{I,J,K,L} \alpha_{I,J,K,L} \psi_I^{x,y,z} \psi_J^{\mu} \psi_K^{\phi} \psi_L^{\omega}$ (multi-indexes I are used for $\{l, i, j\}$). x,y,z are the real space coordinates, μ is the cosine of the polar angle, ϕ is the azimuthal angle and ω is the energy. Note that a tensor product is only build within the momentum space and with the real space. Within the real space, unstructured grids are typically necessary and the construction of MWs $\psi^{x,y,z}$ on unstructured grids can be done following the procedure in [4]. A strongly growing community utilizes the detail and vanishing moment properties of wavelets for the adaptive compression for different complex problems. For the solution of PDEs, hierarchical bases build the "driving force" behind modern adaptive solvers and pre-conditioners. However, of particular interest are the properties of wavelet tensor bases. The coefficient decay (as a property of the detail nature of wavelets) is strongly enhanced in multi-dimensional tensor bases so that most wavelets can be canceled. This is referred to as high-dimensional wavelets compression (HWC) here and is called adaptive sparse grids in literature [5]. Preliminary work on adaptive sparse grids concentrated on FEM formulations and on scalar wavelets rather than on the flux conserving formulations that are necessary for the solution of transport equations. Furthermore, in contrast to scalar wavelets, MWs have an additional vanishing moment hierarchy within each detail to represent high order pp and compression leads to some kind of super sparse grid. This is referred to as vanishing moment compression (VMC) here. Preliminary work on DG and MWs (e.g. [6]) use MW coefficients as adaption criterion, but always keep a full grid so that the MWDG and the NDG stay equivalent. MWDG simulations of 1D devices with pc MWs in [7] show that adaptive HWC can compress the basis by about 99 %. Furthermore, MWDG simulations of 1D devices with higher-order polynomials in [8] perform significantly better even for uncompressed MWDG (up to 96% saving for only 1.4% error in the current) and HWC and VMC can compress the basis by additional 90 %.

Future Work Even larger compression rates are expected for future full hp-adaptive MWDG simulations of 3D devices. A drawback of MWs is the higher coupling of difference operators compared to a conventional pp basis which can reduce the advantages of MWs compression. However, the product structure of the BTE within the momentum space and with the real space enables (in combination with the corresponding product basis above) to decompose the system matrix into a Kronecker product $M = M_{x,y,z} \otimes M_{\mu} \otimes M_{\phi} \otimes M_{\omega}$. Utilizing the distributive property enables to calculate a matrix vector product without building up the matrix M and with a complexity that scales with the number of unknowns only (undirectional principle [9]). Hence, an iterative solver in combination with a multi-level pre-conditioner make the problem independent of the couplings within the sub-dimensions. If quantum mechanical effects become important, the WTE has to be solved. Since the solution of the BTE and the WTE stay similar, similar high MW compression rates are expected for the WTE. MWs are advantageous for the discretization of integral operators such as the Wigner potential, since the matrices show a quasi-sparse structure. Additionally, the product structure of the Wigner potential enables the undirectional principle so that 3D MWDG WTE solvers could become feasible in the future.

[1] K. Rupp and T. Grasser, A. Jüngel, IEDM, Washington DC, USA, (2011). [2] Y. Cheng, I. M. Gamba, A. Majorana, C. Shu, Comput. Methods Appl. Mech. Engrg. 198, 3130 (2009). [3] B. Alpert, SIAM Journ. Math. Anal. 24, 246 (1993). [4] W. Sweldens, Applied and Computational Harmonic Analysis 3, 186 (1996). [5] H.-J. Bungartz, M. Griebel, Acta Numerica 13, 147, (2004). [6] A. Shelton, PhD Thesis, Georgia Institute of Technology, Atlanta (2008). [7] V. Peikert, A. Schenk, SISPAD, Osaka, Japan, (2011). [8] V. Peikert, A. Schenk, IWCE, Madison (WI), USA, (2012). [9] R. Balder PhD Thesis, TU Munich (1994).