Utilizing Wavelets to Solve High-Dimensional Transport Equations in Nano-Devices

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Abstract

For more than three decades industrial Technology Computer Aided Design (TCAD) has been contributing to the baffling development speed of ever faster, smaller and more efficient semiconductor devices. While Drift-Diffusion (DD) equations have been the solid workhorse for TCAD engineers in the past, quantum mechanical and hot-carrier effects make this approach unreliable for the development of next generation technologies. A new challenge for TCAD also comes from the emerging 3-dimensional transistor architectures which improve the electrostatic integrity.

More rigorous simulation approaches like the Boltzmann Transport Equation (BTE) and Wigner Transport Equation (WTE) (being 6-dimensional integro-differential equations) became the focus of attention in academia and industry. Limitations of the widely applied Monte-Carlo (MC) BTE method are driving the development of alternative deterministic approaches which, in turn, suffer from the "curse of dimensionality" of the 5- and 6-dimensional phase spaces.

In this work wavelets are proposed for the deterministic solutions of the BTE and WTE for the first time. Wavelets span hierarchical, multi-scale bases and enable very efficient solution representations as well as new adaptive algorithms. The advantages of wavelets over conventional approaches are often strongly amplified in higher dimensions by the construction of so-called sparse grids. As those concepts have not been sufficiently developed for hyperbolic Partial Differential Equations (PDEs) so far, the sparse grid Multi-Wavelet Discontinuous Galerkin Method (MWDG) is derived in this thesis and its general properties are discussed. The MWDG applied to the BTE is not only flux conservative and stabilizing but, in contrast to

other BTE methods, also allows to use high-order Piecewise Polynomials (PPs) and to construct unstructured meshes in all dimensions. Although the performance of the MWDG had been very uncertain at the beginning of the work, application studies confirm a robust behavior under very coarse adaptive Multi-Wavelet (MW) sparse grid constructions which could be of more general relevance. In contrast, another approach developed during this work that combines Haar wavelets with Spherical Harmonics (SHs) turns out to be not robust enough under sparse grid constructions.
Special adaptive criteria for transport problems based on MWs properties and phase space separations are derived and demonstrated to work satisfactory for high Polynomial-Order (p-order) MWs in all phase space directions so that efficient adaptive sparse grids can automatically be found. Fully adaptive BTE N^+NN^+ simulations demonstrate savings related to the sparse MWDG grids of more than 99% (with negligible loss of accuracy) advising the further development of the MWDG.
This work proposes to efficiently represent the system matrices partly in MWs bases and partly in PPs bases by applying Fast Wavelet Transforms (FWTs) during matrix-vector multiplications. Furthermore, the transport equations show several product structures, which enables to decompose the system matrix into Kronecker products and allows matrix-vector multiplications without building the system matrices. For example the full matrices of the Wigner potential in momentum space could be overcome by this algorithm to a great extent.

Zusammenfassung

Seit über drei Jahrzehnten trägt industrielles Technology Computer Aided Design (TCAD) zu der rasanten Entwicklung immer schnellerer, kleinerer und effizienterer Halbleiter-Bauelemente bei. Bislang stellten Drift-Diffusion (DD) Gleichungen solide Werkzeuge für TCAD Ingenieure dar. Diese eignen sich jedoch nicht mehr länger um quantenmechanische Effekte und heisse Elektroneneffekte in künftigen Technologiegenerationen angemessen zu beschreiben. Eine weitere TCAD-Herausforderung stellt der derzeitige Architekturwechsel hin zu 3-dimensionalen Transistorstrukturen dar, durch welchen die elektrostatische Integrität verbessert wird.
Aktuell rücken rigorosere Formalismen wie die Boltzmann Transport Gleichung (BTG) und die Wigner Transport Gleichung (WTG) (beides 6-dimensionale Integro-Differentialgleichungen) in den Fokus von Wissenschaft und Industrie. Nachteile der weitverbreiteten Monte-Carlo (MC) BTG Methode suggerieren zudem die Entwicklung alternativer, deterministischer Lösungsverfahren welche bislang allerdings dem "Fluch der hohen Dimensionen"des 5- oder 6-dimensionalen Phasenraumes unterliegen.
In dieser Arbeit werden erstmals Wavelets für die deterministische Lösung der BTG und der WTG betrachtet. Wavelets bilden hierarchische Multiskalen-Basen und ermöglichen sehr effiziente Lösungsdarstellungen sowie neue adaptive Algorithmen. Die Vorteile von Wavelets gegenüber herkömmlichen Basen werden in hohen Dimensionen durch die Konstruktion sogenannter dünner Gitter oftmals deutlich verstärkt. Da diese Konzepte bislang nicht ausreichend auf hyperbolische Differentialgleichungen ausgeweitet wurden, werden in dieser Arbeit die Dünngitter Multi-Wavelet Discontinuous Galerkin Method

(MWDG) eingeführt und deren Eigenschaften diskutiert. Angewendet auf die BTG ist die MWDG nicht nur flusserhaltend und stabil, sondern ermöglicht im Gegensatz zu vielen anderen BTG Lösungsmethoden auch die Verwendung stückweiser Polynome höherer Ordnung, sowie die Konstruktion unstrukturierter Gitter in allen Dimensionen. Obgleich das Verhalten der MWDG anfangs sehr ungewiss war, belegen die Anwendungsstudien in dieser Arbeit ein robustes Verhalten bei sehr groben adaptiven Multi-Wavelet (MW) Dünnergitterkonstruktionen, was von allgemeiner Relevanz sein könnte.
Es werden spezielle adaptive Kriterien für Transportprobleme basierend auf Waveleteigenschaften und Phasenraumseparationen hergeleitet sowie deren erfolgreiche Anwendung mit stückweisen Polynomen hoher Ordnung in allen Richtungen des Phasenraumes demonstriert. Adaptive N^+NN^+ Simulationen weisen Einsparpotentiale (basierend auf MW Dünngittern) von über 99 % auf und legen daher die Weiterentwicklung der MWDG nahe.
Diese Arbeit schlägt eine effiziente Darstellung der Systemmatrizen teils in MW-Basis und teils in stückweiser Polynomenbasis durch Anwendung von Fast Wavelet Transforms (FWTs) während der Matrix-Vektor Multiplikationen vor. Weiterhin weisen die Transportgleichungen Produktstrukturen auf, welche Zerlegungen der Systemmatrizen in Kroneckerprodukte ermöglichen, sodass letztere auch während der Matrix-Vektor Multiplikationen nicht explizit aufgestellt werden müssen. Beispielsweise das Problem der vollbesetzten Systemmmatrizen des Wignerpotentials könnte damit zu einem Grossteil bewältigt werden.

Contents

Chapter 1

Introduction

The guiding idea behind this work is the utilization of wavelets and wavelet properties for the adaptive solution of 6-dimensional semiconductor transport equations (Boltzmann Transport Equation (BTE), Wigner Transport Equation (WTE)). The motivation to approach these integro-differential equations originates from the changing industrial Technology Computer Aided Design (TCAD) demands due to the increasing importance of quantum effects (WTE) on one hand and hot carrier effects (BTE) on the other hand.

During the last three decades, Drift-Diffusion (DD) models have been the workhorse for TCAD engineers to design faster, smaller and more efficient high-performance Field Effect Transitors (FETs). However, the approximations made by DD models are no longer justifiable due to the shrinking device sizes so that TCAD tools lost much of their predictivity during the last years. This brings more rigorous formalisms into the center of interest. Methods that solve the Schrödinger equation directly like Tight-Binding or Density Functional Theory (DFT) are still not feasible for real-world devices. Transport equations, however, imply much less approximations than the DD models and provide sufficient accuracy for next generation devices but are less complex to solve than the mentioned "first-principle" approaches. Chapter 2 gives an overview of the different formalisms to describe semiconductor transport with a strong focus on transport