3D Solution of the Boltzmann Equation on Supercomputers

FWF Application

Category: Stand-Alone Project

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There are no ethical issues associated with this research project proposal.

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Contents

Abstract

Semiconductor device simulation relies on solving the most accurate models available, commonly constrained by the computational budget of a single machine. The recent shift from purely two-dimensional to fully three-dimensional device layouts, however, entails much higher computational cost for simulations of the same accuracy – typically orders of magnitude. A reduction of the accuracy to fit the same computational budget is highly undesirable from an engineering point of view. Instead, accuracy can be preserved by increasing the computational budget beyond what is provided by a single machine through a distributed simulation on a compute cluster or supercomputer such as the Vienna Scientific Cluster.

Unfortunately, efficient simulations on supercomputers are very challenging and require a careful exchange of data across processes. It is the aim of this project to master these challenges by developing the necessary parallel algorithms and techniques. To define a reasonable scope for this endeavor, we consider the solution of the Boltzmann Transport Equation (BTE), which is commonly considered to be the best semiclassical description of charge transport in semiconductors. Unfortunately, the conventionally employed stochastic Monte Carlo method exhibits an unfavorable square-root dependence of accuracy versus computational resources. A better alternative considered in this project is the deterministic spherical harmonics expansion method with an accuracy directly proportional to the available computational resources. We will improve the discretization and derive scalable linear and nonlinear solvers for the BTE by building on top of the generic parallel solver infrastructure provided by the software package PETSc. The result of this project will be the first deterministic large-scale solutions of the BTE, providing unprecedented accuracy for three-dimensional device simulations to stimulate for new insights in urgent modeling and engineering challenges such as hot carrier degradation.

Existing fruitful collaboration with Prof. Ansgar Jüngel, Institute for Analysis and Scientific Computing, TU Wien, and Prof. Tibor Grasser, Institute for Microelectronics, TU Wien, will be continued in this project; both will contribute their expertise and experience on discretization schemes and macroscopic models for the BTE. Funding for the PI as a senior-postdoctoral researcher and for one PhD student under the supervision of Prof. Grasser for the duration of three years is requested.

Introduction

The continued scaling of metal-oxide-semiconductor (MOS) field-effect transistors has resulted in a shift to fully three-dimensional device geometries. For example, Intel is using 3D transistors (*tri-gate* transistors) in their latest Ivy Bridge, Haswell, and Broadwell processors, resulting in higher speed and lower power consumption than earlier planar transistors. However, fully three-dimensional device simulations entail considerably higher numerical cost than two-dimensional simulations of planar devices. For example, if a two-dimensional device simulation on a 100×100-grid is to be extended to a three-dimensional device simulation on a $100 \times 100 \times 100$ grid with the same numerical resolution, 100 times more unknowns are encountered. In practice, the total numerical cost increases by even more than a factor of 100, because the unknowns are then coupled in three spatial dimensions and the cost of linear solvers typically grows faster than the number of unknowns.

The memory and processing power of current computers already allows for a simulation of three-dimensional devices using traditional macroscopic models such as the drift-diffusion model. However, feature lengths of modern scaled-down devices are below the range of validity of commonly employed macroscopic models [1], hence full solutions of the Boltzmann Transport Equation (BTE) are sought. In addition to macroscopic quantities such as the charge carrier density, a full solution of the seven-dimensional BTE also provides the distribution of charge carriers with respect to their momentum. Such additional information provides deeper insight and enables refined studies of high-energy effects such as hot carrier degradation. The most popular method for this purpose is the Monte Carlo method, which, however, leads to excessive costs due to its square-root dependence of the obtained accuracy on the total execution time [2]. Moreover, the inherent stochastic nature of the Monte Carlo method renders the simulation of rare events or those evolving on a relatively long time scale practically impossible. Examples include the floating body effect in silicon-on-insulator devices, the simulation of transistors at technologically relevant radio frequencies, or the resolution of high energy tails [3].

An attractive alternative solution approach for the stationary, six-dimensional BTE is the deterministic spherical harmonics expansion (SHE) method. It relies on an expansion of the three-dimensional momentum space into a discrete energy coordinate, while the angular

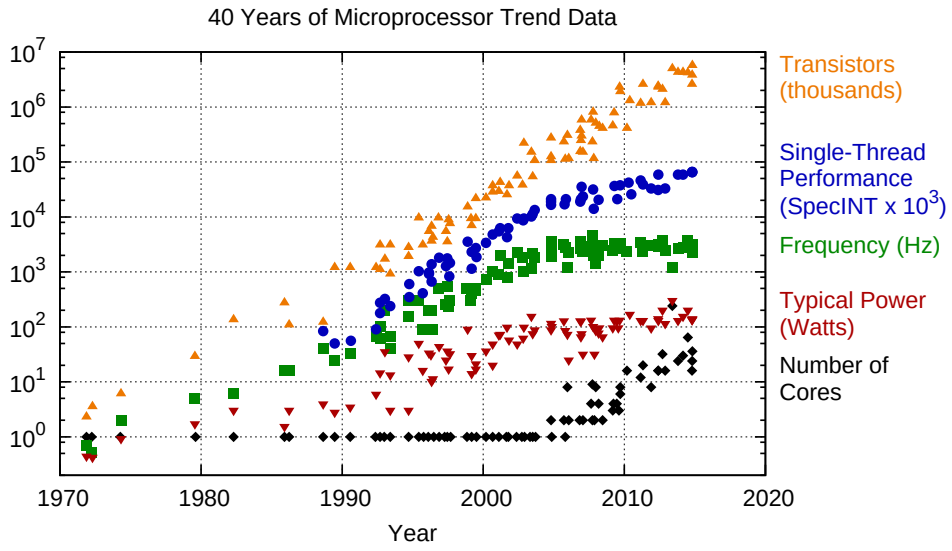

Figure 1

Microprocessor trend data reflecting the last 40 years. A kink in power consumption, frequency, single-threaded performance, and the number of cores around the year 2005 is clearly visible. Original data up to the year 2010 was collected by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond and C. Batten.

components are resolved by spherical harmonics. Consequently, only a nonlinear system of partial differential equations in four dimensions (three spatial dimensions and one energy dimension) needs to be solved instead of six dimensions for a direct solution of the BTE. Simulation results using the SHE method with 80 Gigabytes of main memory for highly accurate two-dimensional device simulations (i.e. a three-dimensional simulation space due to the additional energy coordinate) at high accuracy have been reported recently in the literature [3]. In light of the previous example of increasing the computational effort by two orders of magnitude when transitioning from two-dimensional to three-dimensional device simulation, we estimate main memory requirements of about 8 Terabytes for fully three-dimensional device simulations (using a four-dimensional computational domain due to the additional energy coordinate) at high accuracy using the SHE method. These requirements can only be met through a distributed solution on supercomputers. With a typical memory configuration of 64 Gigabytes per compute node (cf. Vienna Scientific Cluster, third generation), 125 compute nodes (out of 2020 provided on the Vienna Scientific Cluster) are required to provide the necessary 8 Terabytes for fully three-dimensional device simulations.

Let us now consider a single compute node in detail. The cubic increase in power consumption with the clock frequency has finally resulted in a stagnation of clock frequencies

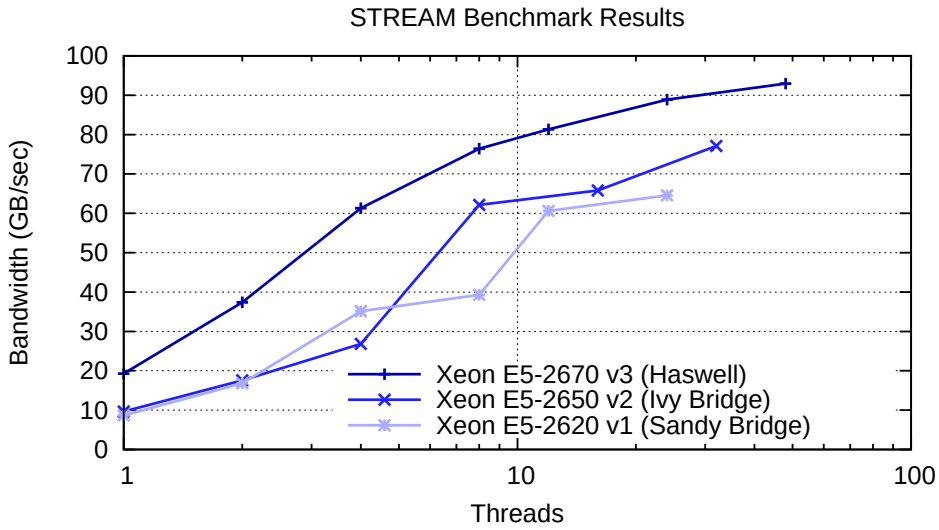

Figure 2

STREAM benchmark results on a single compute node equipped with dual socket Intel Xeon CPUs. About 10 threads are necessary to use the memory channels well.

of processors around the year 2005, forcing vendors to provide multiple cores to further increase the computational power. Even though the number of transistors kept increasing in accordance to Moore's Law, only parallel implementations can leverage the full computational power available today, cf. Figure 1. While the total number of floating point operations per second continues to increase at an unchanged rate, memory bandwidth between the processor and the main memory increases at a much smaller rate. This disparity of processing power and memory bandwidth, known as *memory wall*, results in applications with a low arithmetic intensity, i.e. the ratio of floating point operations per byte transferred from main memory, to be bound by memory bandwidth. In particular, the numerical solution of partial differential equations using conventional low-order finite element or finite volume methods with iterative solvers are bound by memory bandwidth. Unfortunately, a single thread is unable to transfer data using the full memory bandwidth, but instead about 10 threads (or MPI processes) are needed on typical two-socket configurations to use the memory channels sufficiently well, cf. Figure 2. When using coprocessors such as the Intel Xeon Phi or graphics processing units, even higher thread counts are necessary, for which fine-grained parallelism at the computational hot-spots needs to be exposed. Overall, highly efficient and accurate three-dimensional semiconductor device simulation using the SHE method on 125 compute nodes are estimated to run with at least 1250 processes or threads.

Status of Research

In this section we will first review the state-of-the art for the SHE method. After that, the current status of research for large-scale solvers for partial differential equations, not restricting the discussion to semiconductor device simulation, is outlined.

The SHE Method

The SHE method relies on a truncated expansion of the unknown distribution function $f(\boldsymbol{x}, \boldsymbol{p}, t)$ into spherical harmonics $Y_{l,m}(\theta, \varphi)$ at the spatial location $\boldsymbol{x}$, momentum $\boldsymbol{p}$, and time t:

$$f(\boldsymbol{x}, \boldsymbol{p}, t) = f(\boldsymbol{x}, \mathcal{E}, \theta, \varphi, t) \approx \sum_{l=0}^{L} \sum_{m=-l}^{l} f_{l,m}(\boldsymbol{x}, \mathcal{E}, t) Y_{l,m}(\theta, \varphi) \ , \tag{1}$$

where $\mathcal{E}$ denotes energy (either total energy or kinetic energy), and θ and φ are the polar angles in momentum space. Plugging this ansatz into the BTE and projecting the resulting equation onto the spherical harmonics, one finally obtains a system of partial differential equations for the unknown coefficients $f_{l,m}(\boldsymbol{x}, \mathcal{E}, t)$.

Spherical Harmonics Expansion Order

From the approximation quality point of view, a larger expansion order L leads to a better approximation of the unknown distribution function [4]. However, larger expansion orders considerably increase the complexity of the problem. Consequently, the lowest expansion order $L = 1$ was used in first publications on the SHE for the BTE [5, 6]. Already two years later, arbitrary order expansions were proposed and results for expansions up to fourth order were presented [7]. Since then, expansion orders of three to seven were demonstrated to be necessary for certain applications in order to compute accurate numerical approximations of the distribution function [8].

To reduce the computational cost of higher-order expansions, an adaptive variable-order scheme has been developed by the PI, allowing for a two- to three-fold reduction in the number of unknowns [9]. Furthermore, our investigation of the resulting system of partial differential equations for the SHE method has shown that the equations are weakly coupled [10]. As a consequence, a reduction of memory requirements for higher-order SHE proportional to $(L+1)^4$ down to $(L+1)^2$ was possible.

Discretization of the Simulation Domain

The SHE method requires numerical approximations of the unknown expansion coefficients $f_{l,m}(\boldsymbol{x}, \mathcal{E})$ in (1). In analogy to the drift-diffusion system, stabilization schemes are required, otherwise spurious numerical oscillations will occur. One stabilization scheme is based on the so-called H-transform, where the energy variable is transformed from kinetic energy to total energy [11], cf. Figure 3. Further important contributions with respect to stabilizations and discretization schemes preserving and reflecting conservation properties of the continuous model were provided by Ringhofer [12–14] and refined by Jungemann *et al.* [15].

At the discrete level, a discretization of the energy coordinate has been preferred in recent publications (see [8] and references therein) and we plan to follow this approach within this project. The only use of unstructured grids dates back to Gnudi *et al.* [11], who used a prismatic mesh for first-order SHE expansions. To enable the first fully three-dimensional device simulations using the SHE method, the PI developed a discretization for the higher-order SHE method on unstructured grids [16]. The initial requirement of Delaunay meshes was recently resolved by the PI by proposing a cell-centered scheme [17]. This pioneering work also emphasized the need for large-scale simulations: Despite of several techniques for minimizing memory footprint, merely a tetrahedral mesh consisting of only $27\,456$ vertices could be simulated on a single workstation, which is by at least an order of magnitude too small in order to properly account for corner singularities or steep doping gradients.

Solution of the Linear System

First publications on the SHE method successfully used a direct solver due to the small number of unknowns encountered at that time [5, 6]. Meanwhile, the linear systems have become to large for a direct solution, hence iterative methods from the family of Krylov methods are typically employed [18]. Among iterative solvers, the use of a stabilized conjugate gradient method has been reported in [11]. Later, Jungemann *et al.* used a generalized minimum residual method [18] for the solution of the linear equations and also discussed the importance of preconditioning [15]. The preconditioner used in [15] was a sequential incomplete LU (ILU) factorization preconditioner, which did not use additional structural information already available at the continuous level.

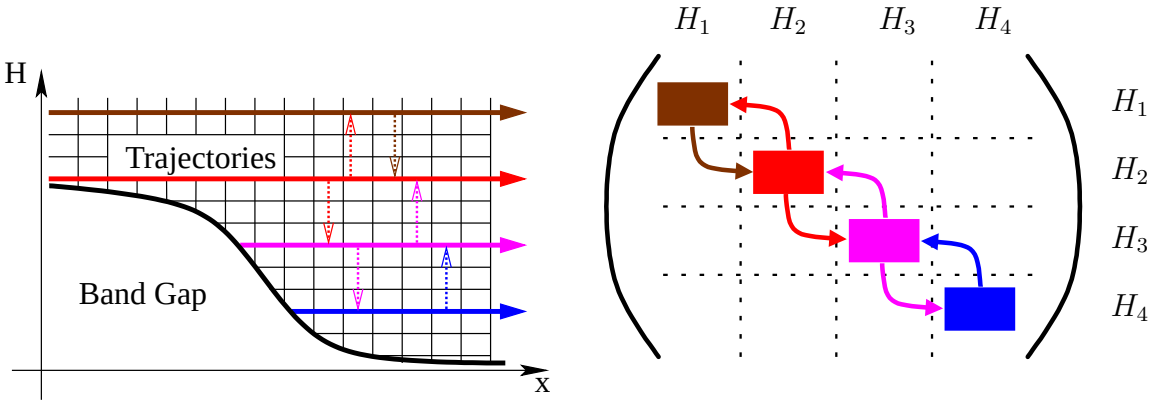

Figure 3

***Left**: Trajectories of carriers in free flight are given by constant total energy H. This is exploited by the H-transform for stabilization purposes, but also brings the disadvantage of changes to the computational domain with each update of the electrostatic potential.*

***Right**: Schematic of the system matrix structure for four discrete energies $H_1, \ldots, H_4$. The different trajectories lead to block matrices, which are coupled by contributions from inelastic scattering processes.*

We have developed a block-ILU preconditioner based on properties of the underlying physical processes for the SHE method [19], cf. Figure 3. This preconditioner is based on the observation that a good approximation of the full linear system is obtained if inelastic scattering processes are ignored, resulting in a block-diagonal system for which preconditioners per block can be computed in parallel. The high degree of parallelism enabled the successful use of graphics processing units (GPUs) in the solver cycle stage, whereas the setup stage was run on the CPU. However, the block-ILU preconditioner exhibits similar non-optimal asymptotic behavior than other ILU-based preconditioners, thus the number of solver iterations required for convergence grows with the system size. Other preconditioners for the SHE method based on advanced techniques, especially multigrid techniques, have not been investigated yet, but appear promising and will be considered in this project.

Physics in the SHE Model

Substantial improvements of the accuracy of the SHE method have been made since its introduction in the early 1990s, making the method comparable to the stochastic Monte Carlo method at a fraction of the computational cost [20]. Most importantly, full-band effects are captured for arbitrary order expansions based on extensions of an approach initially proposed by Vecchi *et al.* [8, 21]. Available charge carrier scattering mechanisms include phonon scat-

tering, alloy scattering, impurity scattering, impact ionization, and surface roughness scattering (see [8] and references therein). To capture carrier generation and recombination, the PI developed a bipolar SHE method [22] as well as a scheme for carrier-carrier scattering [23] to more accurately model highly energetic carriers.

While it is easier to include accurate physics in the Monte Carlo method, the SHE method is applicable to scenarios for which the Monte Carlo method is not suitable. Successful applications reported in the literature include small signal analysis, small currents, noise, and more recently the simulation of avalanche breakdown in pn-junctions [8, 24]. Also, the ability of computing the distribution function over virtually unlimited orders of magnitude has stimulated important contributions in modeling hot carrier degradation of both short- and long-channel devices [25, 26].

Large-Scale Solvers for Partial Differential Equations

A finite volume method is used for the discretization within the SHE method, hence a broad set of developments in areas such as computational solid and fluid dynamics may be adopted. Therefore, we subsequently summarize the main architectural features of large-scale solvers for partial differential equations encountered in the these areas.

Domain Setup and Decomposition

When using a structured grid, the computational domain of size $N_\mathrm{x} \times N_\mathrm{y} \times N_\mathrm{z}$ is usually decomposed into subdomains of size $n_\mathrm{x} \times n_\mathrm{y} \times n_\mathrm{z}$ for each process. Additional overlap regions (*halo* or *ghost* layers) are added to facilitate an efficient exchange of information across subdomains. As reflected by recent research on minimizing communication across processes [27], best performance is obtained when minimizing the surface-to-volume ratio of all subdomains [28].

Complicated geometries mandate the use of unstructured grids, which no longer allow for a direct decomposition merely based on index calculations. Instead, graph partitioner packages such as ParMETIS [29] or Pt-Scotch [30] are used for a decomposition, minimizing subdomain surfaces [31]. A graph partitioner may also be run on a coarse mesh followed by a refinement of the subdomains on each process until the desired resolution is obtained [32].

Even if subdomain surface areas are minimized, communication ultimately remains a bottleneck in the strong scaling limit because of the inherent latency of the communication network. Also, non-blocking communication needs to be used on very large clusters with up to millions of cores in order to overlap data exchange and computations [33]. Although we do not aim at simulations at such an extreme scale in this project, awareness for these kinds of bottlenecks is crucial for the design of efficient algorithms and implementations.

Krylov Solvers and Preconditioners

Because direct solvers become prohibitively expensive for large-scale numerical solutions of partial differential equations, in particular the systems obtained via the SHE method, iterative solvers equipped with advanced preconditioning techniques are the methods of choice [34]. Frequently used Krylov solvers are the conjugate gradient method for symmetric positive definite system matrices and the generalized minimum residual (GMRES) method for indefinite systems. Domain decomposition preconditioners and multigrid methods are both examples of the divide and conquer paradigm and therefore particularly attractive for large-scale solvers due to their superior asymptotic behavior when compared to other methods [35]. These favorable properties are also reflected in the emerging high performance conjugate gradient (HPCG) benchmark[1], which is based on locally symmetric Gauss-Seidel smoothers driven by a multigrid approach on a set of nested coarse grids. Similarly, the high performance geometric multigrid (HPGMG) benchmark[2] aims at providing a representative, large-scale workload for finite element and finite volume methods.

The setup of a coarse grid hierarchy for multigrid approaches is particularly challenging for unstructured grids, especially if the geometry is very complex such as it is the case for transistors with thin oxide layers. If a geometric grid hierarchy cannot be provided, algebraic multigrid preconditioners can be still be used as black-box preconditioners, since they are solely based on information in the system matrix. The favorable black-box nature has led to the development of many flavors of algebraic multigrid techniques over the years [36]. Still, the injection of additional domain-specific knowledge into algebraic multigrid preconditioners can pay off in order to achieve optimal performance [37].

[1] http://hpcg-benchmark.org/
[2] https://hpgmg.org/

Many-Core Architectures

A lot of research has recently been conducted on exposing fine-grained parallelism in iterative solvers and preconditioners in order to efficiently use many-core architectures such as graphics processing units (GPUs) and Intel's many integrated core (MIC) architecture. This includes contributions by the PI, both in the form of publications [38–41] and via the free open source linear algebra and solver library ViennaCL[3]. The dominant factor for overall performance in the context of the SHE method are the linear solvers. Fortunately, significant progress has been made in recent years: Fast kernels for sparse matrix-vector products are available [42, 43], which constitute essential building blocks for smoothing operators in multigrid methods. Several components for preconditioners, e.g. multi-coloring and level scheduling techniques [44, 45], are available. Results on algebraic multigrid preconditioners on GPUs [46, 47] are promising for a successful application to the SHE method.

Despite the availability of efficient building blocks, the high cost of data transfers often mandates custom compute kernels in order to avoid unnecessary communication to and from main memory, or across the PCI-Express bus [38]. Furthermore, GPUs only exhibit a fairly narrow sweet spot: On the one hand, system sizes needs to be large enough to hide PCI-express latencies, but also small enough to fit into the available GPU main memory.

Large-Scale Semiconductor Device Simulation

Because one- and two-dimensional semiconductor device simulations have long been sufficient, research efforts for semiconductor device simulation on distributed memory machines were focused on quantum mechanical simulations. As a result, very few publications deal with semiclassical device simulations on distributed memory machines: Early results for a three-dimensional parallel Monte Carlo simulator on up to 10 processors were reported by Kepkep *et al.* in 2001 [48]. In 2009, a three-dimensional parallel Monte Carlo simulator with results for up to 64 cores was presented by Zhang *et al.* [49]. Lin *et al.* demonstrated simulations based on the drift-diffusion system using an algebraic multigrid preconditioner on up to 4096 cores [50]. Gong *et al.* reported the solution of the drift-diffusion system for a circuit of 24 transistors using of up to 48 cores in 2012 [51]. However, no results using the SHE method on distributed memory machines have been reported yet.

[3] http://viennacl.sourceforge.net/

Aims of the Project

Industrially relevant state-of-the-art devices for both logic as well as memory are fundamentally three-dimensional [52]. A fully quantum-mechanical treatment is computationally too expensive if complex geometries including process variability effects are to be considered, which also rule out simpler mode-space approaches. On the other hand, macroscopic transport models such as the drift-diffusion model are no longer valid in the deca-nanometer regime [1], hence results obtained after extensive fitting to data no longer reflect the underlying physical processes properly. A good compromise are solutions of the semiclassical BTE, particularly when using the SHE method, providing the necessary accuracy for predictive device simulation at manageable computational expense. Important fields of application include the modeling of flash cell programming by hot electrons, for which a truly-3D bipolar SHE solver is of high interest in the community [52]. Therefore, the aim of this research project is to conduct the first large-scale, highly accurate 3D semiconductor device simulations based on deterministic solutions of the BTE. This will be achieved through a parallel solution on supercomputers such as the Vienna Scientific Cluster, for which the necessary parallel algorithms will be developed in this project. Although the focus of this project is on the SHE method, our results may also be applicable to other deterministic solution approaches such as Discontinuous Galerkin methods [53] or multigroup equations [54] as well.

The Institute for Microelectronics and the Institute for Analysis and Scientific Computing will join their expertise to achieve the project aim and successfully overcome the challenges from the mathematics, computer science, and physics point of view. Thereby, this project will further strengthen the already existing successful collaboration [10, 16, 17, 19, 22, 23]. Furthermore, the results of this project will provide important stimuli for ongoing research activities at both institutes: Research on semiconductor device reliability lead by T. Grasser will benefit from highly resolved high energy tails for an improved modeling of hot carrier degradation. Similarly, full solutions of the BTE constitute an important baseline for the development of spin-based macroscopic models at the group of A. Jüngel. The ongoing Christian Doppler Laboratory for Reliability Issues in Microelectronics at the Institute for Microelectronics also provides access to valuable input for state-of-the-art technology by industrial partners. This ensures early and frequent feedback from users of the parallel SHE method throughout the project, which will add to the quality of the conducted research.

The individual subjects of research on the SHE method within this project are as follows:

Discretization	Fast Linear Solvers	Efficient Nonlinear Solvers
Logarithmic SHE	Parallel Preconditioners	Fast Newton-like Schemes
Sparse Energy Grid	Tensor Structure	Multimodel Corrections

The PI and the PhD student will jointly work on all three modules. A. Jüngel will contribute his experience in the discretization module, T. Grasser will share his experiences with macroscopic transport models in the nonlinear solver section. Since a large fraction of each of the three modules can be addressed in isolation, unexpected delay in one module will not block progress in others. More details on the individual modules are given in the following.

Advances in the Discretization

As depicted in Figure 3 earlier, the SHE method requires an embedding of a spatial device mesh into an augmented $(\boldsymbol{x}, H)$-space, where $\boldsymbol{x}$ denotes the spatial coordinates and H the total energy coordinate. With the employed tensor-construction using an energy spacing of about 10meV, there are several hundred discrete energies H_n necessary to span an the typical energy range of several electron Volts. However, two problems are encountered with this scheme, which have not been addressed yet: First, the exponential decay of the distribution function with energy leads to a numerical range of solution values spanning ten to fifty orders of magnitude, which complicates the solution process. Second, the dependence of the computational domain on the electrostatic potential may result in a large fraction of the simulation domain to be unused at high bias voltages. We plan to address both issues.

Logarithmic SHE Method

The carrier distribution function f is known to be nonnegative and discrete approximations of the distribution function can safely be assumed positive within the conduction and valence bands. Also, f asymptotically decays exponentially to zero with respect to energy, hence an expansion of the energy-dependence of f into higher-order polynomials is a poor approximation, but instead f needs to be approximated by low-order polynomials in sufficiently small intervals. Consequently, the energy-dependence of f is approximated by piecewise constant basisfunctions with tiny (about 10meV) intervals using the SHE method.

We will address the problems induced by the exponential decay of f with energy via an expansion of the logarithm of f into spherical harmonics at a given spatial location, i.e.

$$\log f(\boldsymbol{x}, \mathcal{E}, \theta, \varphi, t) =: g(\boldsymbol{x}, \mathcal{E}, \theta, \varphi, t) \approx \sum_{l=0}^{L} \sum_{m=-l}^{l} g_{l,m}(\boldsymbol{x}, \mathcal{E}, t) Y_{l,m}(\theta, \varphi) \,, \tag{2}$$

which transforms the asymptotically exponential decay into a linear function due to the Fermi-Dirac distribution attained in equilibrium. Such an expansion of the logarithmic distribution function is in analogy to Slotboom variables for the drift-diffusion system and has the following important benefits:

- The function g also fulfills a BTE where the linear free streaming operator is unchanged, only the collision operator becomes (weakly) nonlinear. However, since the Boltzmann-Poisson system is nonlinear anyway, this additional nonlinearity does not complicate the solution process.
- f and g share the same discrete conservation properties when using the established finite-volume discretization.
- The energy dependence of g can be approximated well by low-order polynomials over larger energy intervals, particularly in the thermal tail of the distribution function. We expect that this will considerably enhance the smoothing properties of relaxation methods for use in multigrid methods (cf. subsection on preconditioners). Also, we expect that a discretization using higher-order polynomials with respect to energy can provide higher accuracy for fixed computational cost.

Sparse Energy Grid

In recent work we have applied the SHE method for the first time to power devices [17], for which bias voltages are substantially higher than for transistors used for logic circuits in conventional complementary MOS-technology. While the H-transform ensured stability at the applied bias of 16 Volt, it also required a proportionally larger total energy range to be considered for the simulation. The larger total energy range, however, resulted in a much higher number of elements in the augmented mesh, which was obtained from a tensor-construction based on the spatial mesh using N discrete energies for the extension into the

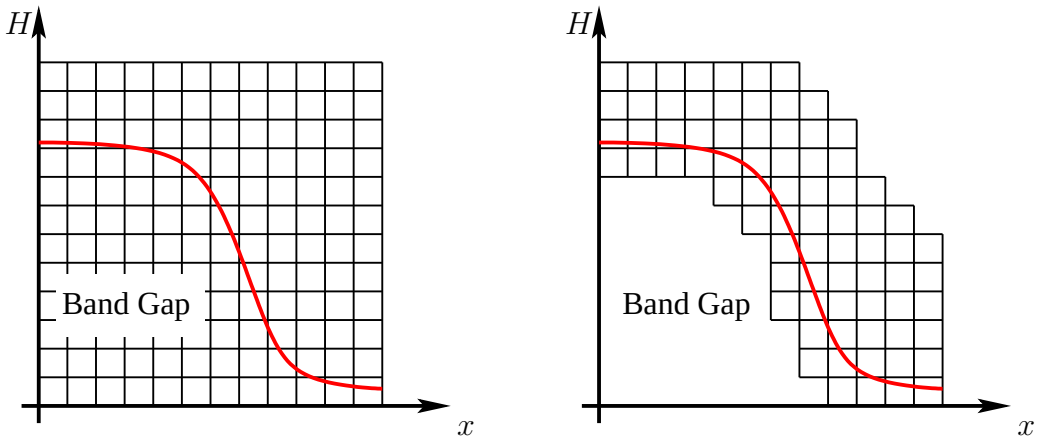

Figure 4

Left: *Schematic view of a tensor-mesh in $(\boldsymbol{x}, H)$-space for one-dimensional device simulation with exemplary band edge depicted in red. Many unneeded boxes are stored in the band gap and at high kinetic energies when using the conventional scheme.*

Right: *We will develop a datastructure such that only boxes essential for the simulation at relevant kinetic energies are stored in memory.*

$(\boldsymbol{x}, H)$-space. With the typical energy spacing of 10meV as mandated by phonon energies and a bias of 16 Volt, N is on the order of $1\,600$, resulting in memory requirements for the mesh in $(\boldsymbol{x}, H)$-space being about $1\,600$ times higher than for the original spatial device mesh. However, most elements in the augmented mesh in $(\boldsymbol{x}, H)$-space do not contribute to the simulation at such high bias, because they either represent negative kinetic energies in the band gap, or extremely high kinetic energies where the distribution function is not of interest, cf. Figure 4.

In order to enable successful applications of the SHE method to power devices with an applied bias of up to 100 Volt, we will develop a datastructure to store only those elements in $(\boldsymbol{x}, H)$-space which represent relevant kinetic energies. This will be achieved by only storing elements right on or above the band edge up to a user-defined kinetic energy. In the background, index shifts determined by the discrete energy will be employed to access the correct element and data, so that each of the stencil operations for the system matrix assembly can still be carried out at constant cost. Overall, the proposed datastructure will result in memory requirements independent of the applied bias. The price to pay is an additional index calculation when accessing data for each element, which, however, is a minor price to pay for the huge savings in memory requirements at high bias voltages.

Fast Linear Solvers

The sparse linear systems obtained via the SHE method are too large to be solved efficiently with direct solvers. Iterative solvers, on the other hand, require good preconditioners when used for the SHE method [15]. Unfortunately, efficient parallel black-box preconditioners do not exist in general. Consequently, the aim of this module is to develop specialized parallel preconditioners for the SHE method to obtain fast convergence on supercomputers.

Parallel Preconditioners

All preconditioners employed for the SHE method so far are based on incomplete LU factorizations. However, the sequential nature of incomplete LU factorization preconditioners is not suitable for a direct application on distributed memory machines. Some parallelism can be achieved by concurrently applying incomplete LU factorizations to suitably chosen, independent blocks on the matrix diagonal. The PI demonstrated such a block preconditioner for the SHE method using incomplete LU factorizations on shared memory machines [19], where physical properties of the SHE method were exploited to specify the individual blocks based on discrete total energies, cf. Figure 3. Because the number of discrete energies N is at least 100 even if only low voltages are applied, the resulting preconditioner exposed enough parallelism so that good performance could even be obtained GPUs. In this project we will extend the described block decomposition to a parallel domain decomposition preconditioner for distributed memory machines. This first step will be accomplished using the software package PETSc[4] and serve as the starting pointer for further investigations. The number of discrete energies N will suffice to scale simulations up to the 125 compute nodes set as a target in the introduction.

Our second step is to increase the parallelism for each subdomain by considering a parallel version of incomplete LU factorization preconditioners as recently proposed by Chow and Patel [55]. Their variant replaces the sequential factorization stage with a parallel nonlinear relaxation scheme and has been demonstrated to run efficiently on Intel's MIC architecture. We will extend their preconditioner to GPUs using our previous experience [38–41], extensively document its efficiency for the SHE method, and ensure that our implementation is freely available to the computational science community through ViennaCL and PETSc.

[4] http://www.mcs.anl.gov/petsc/

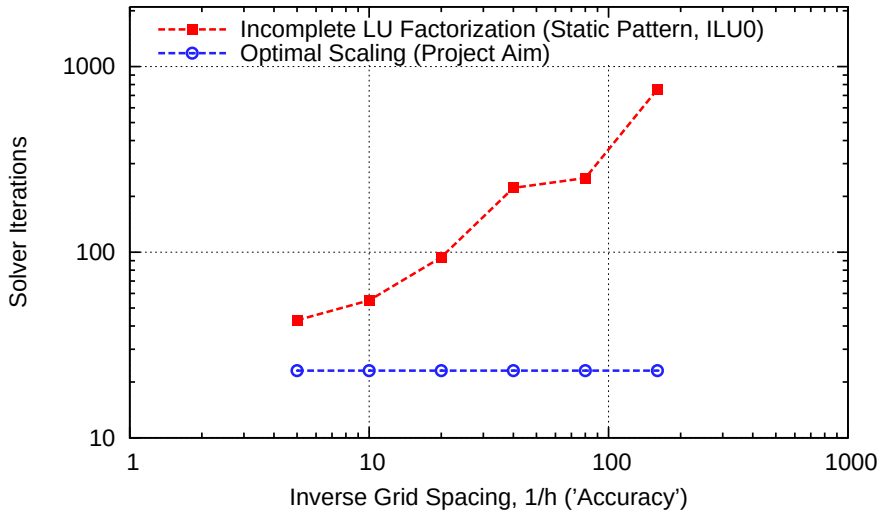

Figure 5

Iterative solver iterations required for the SHE method as a function of the inverse grid spacing $1/h$ when using an incomplete LU factorization preconditioner for the simulation of an nin-diode. The exemplary data for preconditioners with optimal scaling illustrate our project aim of finding optimal parallel preconditioners for the SHE method, where the number of solver iterations remains constant or grows only very mildly as the grid is refined.

In a third step, we will investigate the use of multigrid preconditioners for the SHE method. We will start with existing methods available via PETSc, which also includes the preconditioners implemented in the packages Hypre[5] and ML[6]. Earlier work on multigrid preconditioners for the drift-diffusion model [50] suggests that these methods may also be an effective preconditioner for the SHE method. However, the additional energy coordinate required for the SHE method with the exponential decay of the distribution function with increasing kinetic energy may destroy the necessary smoothing properties of conventional relaxations. We will experiment with relaxation methods taking the exponential decay of the distribution function into account, both by developing relaxation routines explicitly tailored to the SHE method, and by employing the logarithmic SHE method discussed earlier. If no satisfactory results can be obtained using these algebraic multigrid variants, we will fall back to the investigation of geometric multigrid preconditioners, even though these may not be applicable for complicated device geometries. In either case, our efforts in finding a preconditioner for the SHE method with optimal scaling as depicted in Figure 5 will finally be summarized in a taxonomy similar to that of Elman *et al.* for the incompressible Navier-Stokes equations [56].

[5] http://acts.nersc.gov/hypre/

[6] http://trilinos.org/packages/ml/

Exploiting the Tensor-Structure of Higher-Order SHE

Spherical and elliptical symmetries in the underlying physical processes allow for a decoupling of the angular component of the phase space from the $(\boldsymbol{x}, H)$-space when using the SHE method [8, 10]. As a consequence, the resulting system matrix $\boldsymbol{A}$ exhibits a tensor-product structure [10]:

$$\boldsymbol{A} = \sum_{i=1}^{9} \boldsymbol{X}_i \otimes \boldsymbol{Y}_i \,, \tag{3}$$

where the matrices $\boldsymbol{X}_i$ describes the couplings in $(\boldsymbol{x}, H)$-space, the matrices $\boldsymbol{Y}_i$ denote the angular couplings of the spherical harmonics, and $\otimes$ denotes the Kronecker product.

We plan to exploit the Kronecker-product structure (3) in a novel fashion as follows:

- Develop fast matrix-vector product routines for CPUs as well as accelerators by inlining the a-priori known matrices $\boldsymbol{Y}_i$ directly in the kernel sources rather than holding the values in main memory. This allows for the full memory bandwidth to be available for loading the matrices $\boldsymbol{X}_i$ and also maximizes the cache available for the vectors.
- Develop preconditioners for higher-order SHE based on a much smaller system matrix for lowest-order SHE. The preconditioner will then also be a tensor product $\boldsymbol{W} \otimes \boldsymbol{V}$, where the dimensions of $\boldsymbol{W}$ and $\boldsymbol{V}$ match those of $\boldsymbol{X}_i$ and $\boldsymbol{Y}_i$. For lowest-order SHE, $\boldsymbol{V}$ degenerates to a one-by-one matrix.

These two steps will give rise to a “dual-order” solver scheme, from which we expect substantial savings in memory and memory bandwidth when compared to an explicit storage of the system matrix, ultimately also reducing execution time. The proposed scheme extends a related strategy originally proposed for nodal finite elements [57] to the SHE method.

Efficient Nonlinear Solvers

The aim of this module is to accelerate the existing nonlinear solution scheme of the SHE method, which is a Newton-scheme supplemented by Picard iterations for additional robustness with respect to the initial guess provided [8]. Details on how we plan to reduce the average cost of each nonlinear iteration and also the overall number of nonlinear iterations are given in the following.

Fast Newton-like Schemes

A common optimization for Newton-like schemes is to reuse the preconditioner for inverting the Jacobi matrix for several iterations and only recompute the preconditioner if convergence rates have degraded. Unfortunately, the H-transform prevents a direct application of such a strategy, because the dimensions of the linear systems change in response to a modification of the band edge induced by updates of the electrostatic potential.

We plan to enable a preconditioner reuse by augmenting the computational domain slightly to consider also energies in the band gap close to the band edge. In the first nonlinear iteration, the SHE coefficients for these forbidden states will already be part of the linear system, but forced to zero (*trivial unknowns*). If these initially forbidden states become part of the computational domain in the second or a later nonlinear iteration, the system matrix does not change its dimensions, but only its values. Therefore, the preconditioner from the first iteration can be reused and is only recomputed if the convergence rate degrades. We expect savings in execution time by up to a factor of two.

Multimodel Corrections

About 20 to 100 Picard iterations (also referred to as Gummel iterations) are usually performed first to improve the quality of the initial guess for Newton's method [8]. We plan to substitute about half of these expensive numerical solutions of the SHE equations by far less expensive solutions of suitably modified drift-diffusion equations to reduce the overall numerical cost. Because the drift-diffusion system can be derived from the SHE equations in the scaling limit of dominant phonon and electron-electron scattering [58], we refer to our proposed approach as *multimodel scheme*.

In order for the drift-diffusion model to reproduce the SHE method for a given potential profile, we will fit the free parameter in the drift-diffusion model, namely the carrier mobility, to numerically reproduce the carrier densities computed by the SHE method in the respective nonlinear step. This modified drift-diffusion system will then be solved together with the Poisson equation at much lower cost, and the updated electrostatic potential will be fed back to the full SHE model. We emphasize the novelty and innovative character of this multimodel approach, which is enabled by the availability of a model hierarchy for solving the BTE.

Infrastructure of the Research Institutes

The proposed project fits well into the research activities of the Institute for Microelectronics and the Institute for Analysis and Scientific Computing. The former has a substantial amount of experience in the area of device simulation and will benefit considerably from the results obtained in this project for ongoing research on device reliability. The latter institute has a strong reputation in the development of new numerical methods in quantum mechanics, semiclassical device models, and finite element methods.

Tight collaborations with industrial partners (austriamicrosystems, Infineon) have been set up at the Institute for Microelectronics within two generations of Christian Doppler Laboratories (for TCAD in microelectronics and for reliability issues in microelectronics) as well as in European projects (ATHENIS, MODERN, MORDRED). A. Jüngel has well established contacts with Infineon Munich due to a former project on modeling hot electrons. Ongoing fruitful cooperations with TU Eindhoven have led to the development of efficient schemes for the solution of nonlinear discrete systems. A joint application with Global TCAD Solutions for the Marie Curie International Training Networks is currently under preparation.

The close cooperation of the Institute for Microelectronics and the Institute for Analysis and Scientific Computing is a long tradition and dates back to the 1980s. In particular, the fruitful collaboration of the PI with Prof. Grasser and Prof. Jüngel has resulted in over 20 publications within the last five years.

The available infrastructure at the two institutes makes us well prepared for developing the proposed algorithms and their implementations. High-end GPUs from NVIDIA and AMD as well as Xeon Phi (Knight's Corner) coprocessors are available in powerful work stations at both institutes. Moreover, the Institute for Microelectronics hosts a cluster consisting of 13 nodes, each equipped with four AMD Opteron CPUs and 32 to 128 gigabytes of main memory. To test scalability in a realistic environment, we ask for appropriate allocations on the Vienna Scientific Cluster, including access to the next-generation Xeon Phi (Knight's Landing) processors.

Time Schedule

The project is scheduled for 36 months. In the first year, the PI and the PhD student will work on the MPI-based parallelization of the existing simulator. First results on the effectiveness of different parallel preconditioners are expected towards the end of the first year. The second year is devoted to intensive work on the discretization module by the PI and further linear solver improvements by the PhD student by investigating multigrid approaches and exploiting the tensor structure for higher-order SHE methods. In the third year, the PI will optimize the most efficient preconditioners identified by the PhD student for accelerators, while the PhD student will work on the nonlinear solver module.

Dissemination

As part of their scientific curriculum, both the PI and the PhD student will publish significant results obtained during the course of the project using the usual channels (journal papers, conferences, etc.) in agreement to the Open Access policy of the FWF. Newly implemented algorithms are thoroughly tested and integrated into our free open source SHE simulator ViennaSHE[7]. Any general purpose solver components developed as necessary by-products will be made available through ViennaCL and subsequently PETSc. We consider this additional free open source code dissemination effort vital for promoting Open Science in order to give other groups the ability to build their work on top of ours and in turn provide feedback and valuable suggestions on further improvements. At the end of the project, all project achievements will also be documented in detail in the dissertation of the PhD student.

Human Resources

The PI has accumulated valuable experience with the SHE method in a previous project funded by the Austrian Science Fund (P23598). With the proposed project he aims to prove early in his academic career that he is able to successfully lead a research project. His one-year stay as a postdoctoral researcher with the PETSc team at the Argonne National Laboratory, USA, makes him well prepared for the computational challenges in this project.

The PhD student will become acquainted with practical aspects of the state-of-the-art in parallel computing and the efficient use of modern computing architecture. This complements his former education in technical mathematics with a focus on computer science perfectly.

[7] http://viennashe.sourceforge.net/

Requested Funding

To conduct the proposed research, funding for the PI (senior post-doctoral level) and one doctoral student (candidate: A. Morhammer) for a period of 36 month is required.

Name	First Year	Second Year	Third Year	Total
K. Rupp	69 810 €	69 810 €	69 810 €	209 430 €
A. Morhammer	36 340 €	36 340 €	36 340 €	109 020 €
Total	106 150 €	106 150 €	106 150 €	**318 450** €

The coverage of travel costs is requested for research visits at the institutions of our scientific collaborators: In the first year, a visit at the PETSc group at Argonne National Laboratory, USA, will be vital for setting up an effective MPI-based device simulator. A visit at Prof. Gundolf Haase, University of Graz, Austria, at the end of the second year will refine further directions on optimizing the best preconditioners identified for the SHE method for graphics processors. Finally, a stay at Prof. Christoph Jungemann at RWTH Aachen, Germany, towards the end of the project will explore possible future directions in device modeling based on the higher accuracy of the fully parallel simulator.

Name	Destination	Duration	Travel Cost	Hotel Cost	Sum
First Year					
K. Rupp	Argonne, USA	12 days	1 000 €	600 €	1 600 €
A. Morhammer	Argonne, USA	12 days	1 000 €	600 €	1 600 €
Sum					3 200 €
Second Year					
K. Rupp	Graz, Austria	12 days	50 €	600 €	650 €
A. Morhammer	Graz, Austria	12 days	50 €	600 €	650 €
Sum					1 300 €
Third Year					
K. Rupp	Aachen, Germany	12 days	200 €	600 €	800 €
A. Morhammer	Aachen, Germany	12 days	200 €	600 €	800 €
Sum					1 600 €
Total					**6 100** €

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Abbreviations

BTE	Boltzmann transport equation
GPU	graphics processing unit
MIC	many integrated cores
MOS	metal-oxide-semiconductor
MPI	message passing interface
SHE	spherical harmonics expansion

Curriculum Vitae

Karl Rupp (Project Leader)

(CV is not part of the public version of this proposal to protect the privacy of all partners involved in the project)

10 Most Relevant Publications of K. Rupp

[1] M. Bina, S. E. Tyaginov, J. Franco, K. Rupp, Y. Wimmer, D. Osintsev, B. Kaczer, and T. Grasser, "Predictive Hot-Carrier Modeling of n-Channel MOSFETs," *IEEE Transactions on Electron Devices*, vol. 61, no. 9, pp. 3103–3110, 2014.

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All Publications of K. Rupp since 2010

For a complete and up-to-date list please refer to `http://www.iue.tuwien.ac.at/`

[1] M. Bina, S. E. Tyaginov, J. Franco, K. Rupp, Y. Wimmer, D. Osintsev, B. Kaczer, and T. Grasser, "Predictive Hot-Carrier Modeling of n-Channel MOSFETs," *IEEE Transactions on Electron Devices*, vol. 61, no. 9, pp. 3103–3110, 2014.

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(CV is not part of the public version of this proposal to protect the privacy of all partners involved in the project)

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Ansgar Jüngel (Scientific Partner)

(CV is not part of the public version of this proposal to protect the privacy of all partners involved in the project)

Peer-Reviewed Publications of A. Jüngel since 2010

For a complete and up-to-date list please refer to `http://juengel.at.vu/`

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