STAND-ALONE PROJECT

FINAL REPORT

Project number: P23598

Project title[1] **Deterministische Lösung der Boltzmanngleichung für Bauteilzuverlässigkeitsanalysen**

Project leader **Tibor Grasser**______________________________________

I. Summary for public relations work

The project's most significant results (scientific advances) from the project leader's point of view should be presented on a single page (DIN A4, 11 pt font, line spacing 1.5) in a way that is comprehensible to the general public. In this text, it is important to use as few technical terms as possible in order to ensure that the text is interesting and understandable to people not familiar with the field. The main point should be mentioned at the very start of the summary. Please keep descriptions of the issues addressed and results obtained short and succinct. Possible applications to or implications for social, cultural, ecological, medical, economic or technological areas should also be mentioned briefly.

The summary should be submitted both in **German** and in **English**. The summaries will be made available via the FWF's project database. The FWF will not edit the summaries, meaning that the authors bear full responsibility for the content of these texts.

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1 Short title in English and German language

1. Zusammenfassung für die Öffentlichkeitsarbeit

Die stetig wachsenden Anforderungen an die Leistungsfähigkeit von Halbleiterbauelementen erfordern das Design schnellerer, kleinerer und energieeffizienter Bauteile. Die Annäherung an physikalische Grenzen bedingt somit ein zunehmend besseres Verständnis der zugrundeliegenden Prozesse. Ein solches Verständnis kann entweder durch teure und zeitaufwändige Versuche in Laboratorien erfolgen, oder durch Computersimulationen mit ungleich kürzerer Ablaufzeit und geringeren Kosten. Letztlich sind beide Zugänge notwendig, um Fortschritt sicherzustellen.

Im Rahmen dieses Projekts sind neue Algorithmen zur numerischen Lösung der Boltzmanngleichung entwickelt und implementiert worden. Da üblicherweise eine direkte Lösung der Boltzmanngleichung für realistische Bauteilgeometrien auf einem Computer als zu schwierig angesehen wird, werden in Produktivumgebungen oft einfachere Modelle basierend auf Momenten der Boltzmanngleichung verwendet. Dennoch werden Lösungen der Boltzmanngleichung als Referenz im Rahmen der semiklassischen Halbleitersimulation angesehen, bei der Quanteneffekte zwar nicht ignoriert werden, aber lediglich eine untergeordnete Rolle spielen. Die Forschungsergebnisse dieses Projekts erlauben numerische Lösungen der Boltzmanngleichung zu einem Bruchteil der Kosten konventioneller Zugänge, insbesondere der weit verbreiteten Monte-Carlo-Methode. Diese numerischen Fortschritte wurden im Numerikmodul dieses Projekts erzielt. Im zweiten Teil des Projekts, dem Physikmodul, wurden bessere physikalische Modelle in Hinblick auf realistische Bauteilgeometrien entwickelt.

Die Forschungsergebnisse im Numerikmodul ermöglichen detaillierte Simulationen komplizierter Bauteilgeometrien, wie etwa sogenannte Trigate-Transistoren. Derartige Bauelemente finden sich etwa in aktuellen Prozessoren wieder. Dazu entwickelten wir Diskretisierungsmethoden, die für allgemeine unstrukturierten Drahtgittermodellen in drei Raumdimensionen geeignet sind. Um den Speicherbedarf unter Kontrolle zu halten, haben wir Adaptierungstechniken entwickelt, die ein und dieselbe Simulation mit wenigen Dutzend Gigabytes anstelle von Hunderten Gigabytes ermöglicht.

Die Forschungsergebnisse des Physikmoduls ermöglicht die Berücksichtigung der Streuung von Ladungsträgern nicht nur am Kristallgitter, sondern auch an anderen Ladungsträgern. Weiters haben wir einen Formalismus entwickelt, der die als wichtig angesehene Generation und Rekombination von Elektron-Lochpaaren im Rahmen der direkten Lösung der Boltzmanngleichung erstmalig berücksichtigt.

2. Summary for public relations work

The ever-increasing demands on the performance of semiconductor devices mandates the design of faster, smaller, and more energy-efficient devices. As we get closer to fundamental physical limits, an increased insight into the underlying physical processes is mandatory. Such improved understanding can be obtained in an expensive and time-consuming trial-and-error approach in laboratories, or through computer simulations with much shorter turnaround time and much smaller cost. Either of these two approaches is vital for overall progress.

Within this project, new algorithms for the numerical solution of the Boltzmann transport equation have been developed and implemented. Typically, the Boltzmann transport equation is considered to be too hard to solve on a computer for realistic device geometries, hence simpler approaches based on moments of the Boltzmann transport equation are used in productive environments. Still, solutions of the Boltzmann transport equation are considered to be the golden standard of semiconductor device simulations for which certain quantum-mechanical effects are considered, but only play a secondary role for overall device operation („semiclassical" regime). With the results of this research project, solutions of the Boltzmann transport equation can now be computed at a fraction of the computational cost of other methods, most prominently the so-called Monte Carlo method. These numerical improvements were obtained in the 'numerics' module. The second part of this project, the physics module, focused on incorporating better physical models and to apply the new capabilities to modeling questions faced in real devices.

Our results in the numerics module enable highly detailed simulations of complicated device geometries such as recent three-dimensional trigate transistors, which are now state-of-the-art in modern processors. To do so, we developed a discretization able to deal with general unstructured grids in three spatial dimensions. Moreover, we developed adaptive schemes to dramatically reduce memory requirements, so that we can now run simulations requiring only tens of Gigabytes of main memory, whereas former techniques required hundreds of Gigabytes for the same simulation.

The results in the physics module enable the consideration of not only how charge carriers interact („scatter") with the crystal lattice, but also with each other. Also, we developed a model for considering the generation and recombination of electron-hole pairs, which, although generally considered important, has not been demonstrated for direct solutions of the Boltzmann transport equation before.

II. Brief project report

- **To be written in the language of the original application**
- Target group: **peer reviewers**
- **Length:** not to exceed 16,000 characters (without spaces, approx. 6 pages) in total; please mention each point (all together on 4 pages minimum, 11 pt font, line spacing 1.5, **no attachments apart from those mentioned in section III**)

1. Report on research work

1.1 Information on the development of the research project

The goal of the research project was to further develop the spherical harmonics expansion (SHE) method as a deterministic alternative to the stochastic Monte Carlo method for obtaining numerical solutions of the Boltzmann Transport Equation (BTE). In particular, the SHE method allows for addressing some of the major shortcomings of the Monte Carlo method: The inability to deal with small-signal analysis, large-signal analysis, and the resolution of rare events (e.g. small currents). The relatively large memory requirements of the SHE method has long been prohibitive for a successful application of the SHE method. However, as average personal computers are now equipped with Gigabytes of memory, sufficient main memory for running two-dimensional device simulations at high resolution was available. Still, at the start of the project, the SHE method was considered to be numerically too expensive for three-dimensional device simulation.

The introduction of non-planar trigate transistors in 2011 underlined the importance of fully three-dimensional device simulations. In order to enable such simulations, the project aimed at improvements in the discretization, ultimately demonstrating the first fully three-dimensional device simulations using the SHE method. These were achieved with two intermediate steps: First, the discretization was extended such that unstructured grids, as for example returned by process simulators, could be handled. This allowed for a high resolution in areas of interest, for example in the channel of a trigate transistor, and for a low resolution in areas of low significance, for example deep in the bulk. Second, an adaptive variable-order scheme was developed in order to improve the resolution of the momentum distribution of carries for a given spatial location. Similar in spirit to the use of unstructured grids for the spatial resolution, adaptive variable-order schemes enable a high resolution of the momentum space in areas of interest, while keeping compuational cost low in areas of the device where a low resolution of the momentum distribution suffices. With unstructured grids and adaptive variable order expansions at hand, we successfully reported the first fully three-dimensional semiconductor device simulations using the SHE method shortly after the project start at the renowned International Electron Device Meeting.

Although not explicitly stated as a explicit project goal, we also looked into parallelization opportunities in order to further reduce execution times (typically minutes to hours). We identified a block-structure of the resulting system matrices in each Newton step, which allows for a block-Jacobi preconditioner to be used within the iterative solver. This block-structure of the preconditioner is physically motivated by the free flight of carriers and resembles the collision-free motion of carriers. Our results showed savings in execution times of up to one order of magnitude when compared to conventional single-threaded implementations. This special-purpose preconditioner has since been refactored and general-purpose elements have been ported back to the free open source solver library ViennaCL. A second advancement, which was also not initially planned for this research project, was the development of a discretization scheme for unstructured grids which no longer requires the underlying mesh to fulfill the Delaunay property. This greatly simplifies the interfacing with external tools and simulators, as the requirements on the mesh are substantially relaxed.

The second module of this research project was focused on improving the accuracy of the physical models. The focus of our developments was on the needs of device reliability investigations, in particular hot carrier degradation. For these investigations, a good resolution of the so-called high-energy tails of the distribution function is essential. Carrier-carrier scattering is commonly considered to have a high influence on high-energy tails, but it is also computationally challenging because it introduces a nonlinearity in the scattering operator. We developed a methodology for considering carrier-carrier scattering in the context of the SHE method and found good agreement with Monte Carlo results for bulk silicon results published earlier. Unfortunately, a verification of our simulation results against measurement data, though desirable, is to-date impossible, because the distribution of carriers cannot be measured with the methods available. Nonetheless, we could demonstrate the applicability of our approach also for two-dimensional device simulation of a MOSFET. As it turned out, the extra cost of carrier-carrier scattering is too high for fully three-dimensional device simulation using the SHE method on conventional workstations, so future work will considering the use of supercomputers for that purpose.

The second major development in the physics module involved the simultaneous consideration of electrons and holes by solving the BTE for each carrier type. This second milestone was achieved in collaboration with Prof. Christoph Jungemann, RWTH Aachen, and enables new insights through the solution of the BTE for effects such as avalanche breakthrough.

The third milestone identified in the project proposal was the development of multi-band energy models. Shortly after the project start, however, a different group proposed a way to use full-band data with the SHE method. Our evaluation of their results turned out to fulfill our demands in terms of accuracy, hence we decided to look into quantum-correction schemes instead. Subsequently, we developed a density-gradient-like quantum correction model, which extends the quantum correction scheme from the drift-diffusion model to the SHE method for the BTE. The model was validated against a reference solution obtained from a Schrödinger-Poisson solver for an nMOS and a pMOS device.

Towards the end of the project, the techniques and methods developed during the project were also applied to the study of hot carrier degradation in semiconductor devices in collaboration with colleagues from the Institute for Microelectronics. This was a win-win situation: The results of this project acted as an enabler for their research, while the feedback received allowed us to further improve the simulator.

Overall, the initial project plan was followed and additional contributions beyond the initial project goals were made in both modules.

1.2 Most important results and brief description of their significance (main points) with regard to the following:

- Contribution to the advancement of the field (e.g. did the results contribute to increasing the importance of the field? In what way?);

Breaking of new scientific / scholarly ground (to what extent and in what respects?);

- Most important hypotheses / research questions developed (what relevance did the project have for the development of hypotheses / research questions, e.g. were new hypotheses / research questions developed or old hypotheses disproved?);
- Development of new methods;
- Relevance for other (related) areas of science (transdisciplinary issues and methods).

The results in this project sum up to making the SHE method an attractive choice for the next generation of technology computer aided design (TCAD) tools. Our contributions in the numerics module, in particular the support for unstructured grids and the availability of adaptive variable-order schemes, provide the foundations for successfully employing the SHE method for current state-of-the-art three-dimensional device geometries. At the same time, our contributions to the modeling, namely carrier-carrier scattering, simultaneous solution for electrons and holes, and quantum corrections, also enhance the attractiveness of the SHE method in terms of its already high accuracy due to full solutions of the BTE. Despite our contributions to the SHE method, the field has only grown moderately. We attribute this to the significant sophistication of the SHE method, which poses a high entry-barrier for a more wide-spread adoption. Regardless, the community is now aware of the SHE method as an attractive alternative to Monte Carlo. Also, commercial implementations of the SHE method became available during this project.

The new research questions developed in this project are mainly centered around further scaling the SHE method from the numerical standpoint. This is because a consideration of carrier-carrier scattering for fully three-dimensional devices is still too expensive for a single workstation. Also, the method's memory requirements still scale linearly with the applied voltage bias, hence becoming too expensive for high-power devices with voltages beyond 100 Volt. Hence, the new central research question is whether and how the SHE method can leverage supercomputers to run the desired simulations. Since the SHE method has been only been used on shared memory machines so far, the distributed memory nature of supercomputers requires a complete rethinking of the datastructures and solvers. A project proposal centered around how to use the SHE method was submitted by Karl Rupp in collaboration with the PIs of this project and a positive funding decision was made in May 2016.

1.3 Information on the execution of the project, use of available funds and (where appropriate) any changes to the original project plan relating to the following:

- Duration;
- Use of personnel;
- Major items of equipment purchased;
- Other significant deviations.[3]

The project started in November 2011 and ended in April 2016. The extended project duration is explained by a one-year postdoctoral stay of the postdoctoral researcher, Karl Rupp, at the Argonne National Laboratory, USA. The months November 2015 to April 2016 did not involve actively employed personnel, but were used to cover expenses smaller expenses related to this project.

The doctoral student initially considered for this project, Peter Lagger, decided to take a job in industry after obtaining his master's degree. Instead, Markus Bina worked on the project and completed his PhD thesis in mid 2014. Andreas Morhammer started as a new PhD student at the beginning of 2015, but moved on to a different project in May 2015 as funding was about to expire.

2. Personnel development – Importance of the project for the research careers of those involved (including the project leader)

- Brief comments on the project's effects on the research careers of all project members, including special qualifications and special possibilities / opportunities opened up by the project.

The project leaders' scientific track record was broadened through the research conducted in this project, strengthening the international standing of the group.

The main share of the project money was spent on the postdoctoral researcher Karl Rupp. His contributions allowed him to get better known in the semiconductor device simulation community, but also in the parallel computing community. As a result, his evolving interest in parallel computing resulted in a recently awarded FWF project on the 3D solution of the BTE on supercomputers, which will address the main new research question that emerged within this project.

3 The decision as to what should be regarded as a "significant deviation" is the responsibility of the project leader. As a guideline, any deviation of more than 25% from the original financial plan or work schedule should be accounted for.

Markus Bina accepted a job at Infineon Technologies in Munich, Germany, after the completion of his PhD studies, where he is again working on semiconductor devices.

All researchers funded from this project benefitted from the implementation-oriented nature of the project. The improved coding skills enables them to tackle new questions in computational science (Karl Rupp) and to apply these skills in industry (Markus Bina).

3. Effects of the project beyond the scientific field

- Brief comments on specific effects beyond the research field, including activities outside the sphere of academia.

All research codes developed in the course of this project are, in full alignment with the ideals of Open Research, available as free open source. The modular design of the code resulted in a library-centric architecture, enabling the reuse of components such as the parallel preconditioner or the unstructured grid management in other contexts. Overall, the project resulted in important software contributions to the software libraries ViennaCL (parallel solvers), ViennaGrid (grid management), and ViennaSHE (device simulator based on the SHE-method). These contributions overlapped with the work of colleagues carried out in other projects and resulted in several publications on the intersections of these activities: Mesh generation, mesh adaption, and the design of TCAD software in more general terms.

The open-source nature of our research codes also enabled us to participation at the Google Summer of Code in 2011, 2012, 2013, and 2014. This allowed students to contribute to and learn from our codes. Even though the Google Summer of Code projects were not directly tied to the research in this project, some of the students' work, for example in mesh generation, could be reused within this project.

4. Other important aspects (examples)

- Project-related participation in national and international scientific / scholarly conferences, list of most important lectures held;
- Organisation of symposiums and conferences;
- Prizes/awards;
- Any other aspects.

The results of our research activities were disseminated at several acknowledged international conferences, which include, but are not limited to, IEDM, the International Workshop on Computational Electronics (IWCE), and the International Conference on Simulation of Semiconductor Processes and Devices (SISPAD). A full list of talks at conferences is available in the next section; the most important for this project (including one best-paper award) are:

K. Rupp, T. Grasser, A. Jüngel: "On the Feasibility of Spherical Harmonics Expansions of the Boltzmann Transport Equation for Three-Dimensional Device Geometries"; International Electron Devices Meeting (IEDM), Washington DC, USA; 2011-12-05 - 2011-12-07;

K. Rupp, P. Lagger, T. Grasser: "Inclusion of Carrier-Carrier-Scattering Into Arbitrary-Order Spherical Harmonics Expansions of the Boltzmann Transport Equation"; International Workshop on Computational Electronics (IWCE), Madison, WI, USA; 2012-05-22 - 2012-05-25;

J. Weinbub, K. Rupp, S. Selberherr:
"A Generic Multi-Dimensional Run-Time Data Structure for High-Performance Scientific Computing"; World Congress on Engineering (WCE), London, UK; 2012-07-04 - 2012-07-06; **best paper**

K. Rupp, C. Jungemann, M. Bina, A. Jüngel, T. Grasser: "Bipolar Spherical Harmonics Expansions of the Boltzmann Transport Equation"; International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Denver, CO, USA; 2012-09-05 - 2012-09-07;

M. Bina, K. Rupp, S. E. Tyaginov, O. Triebl, T. Grasser: "Modeling of Hot Carrier Degradation Using a Spherical Harmonics Expansion of the Bipolar Boltzmann Transport Equation"; International Electron Devices Meeting (IEDM), San Francisco, CA, USA; 2012-12-10 - 2012-12-12;

K. Rupp, M. Bina, Y. Wimmer, A. Jungel, T. Grasser: "Cell-Centered Finite Volume Schemes for Semiconductor Device Simulation"; International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Yokohama, Japan; 2014-09-09 - 2014-09-11;

Y. Wimmer, S. E. Tyaginov, F. Rudolf, K. Rupp, M. Bina, H. Enichlmair, J.M. Park, R. Minixhofer, H. Ceric, T. Grasser: "Physical Modeling of Hot-Carrier Degradation in nLDMOS Transistors"; IEEE International Reliability Workshop (IIRW), South Lake Tahoe, CA, USA; 2014-10-12 - 2014-10-16;

P. Sharma, S. E. Tyaginov, Y. Wimmer, F. Rudolf, K. Rupp, H. Enichlmair, J.M. Park, H. Ceric, T. Grasser: "Comparison of Analytic Distribution Function Models for Hot-Carrier Degradation in nLDMOSFETs"; European Symposium on Reliability of Electron Devices, Failure Physics and Analysis (ESREF), Toulouse, France; 2015-10-05 - 2015-10-09;

III. Attachments

(lists may be as long as required)

1. Scholarly / scientific publications

Publications may only be listed if they relate directly to the project. **Up to three of the most important publications** should be highlighted as such (e.g. printed in bold letters).

Please note: In accordance with the guidelines of the FWF concerning Open Access, with the submission of the final report, **all peer-reviewed publications that resulted from the project have to be made openly accessible** (see: http://www.fwf.ac.at/en/research-funding/open-access-policy/). Exceptions to this rule, e.g., if a publication organ explicitly does not permit Open Access, must be proven. For projects funded after 1 January 2015, no exceptions are possible.

In the interest of the project continuation, it is requested to provide the activation within this period. For inquiries relating to the refund of publication costs please contact Katharina Rieck via: publikationskosten@fwf.ac.at. Please note that funding for publication costs can be requested (under the original project number) for up to three years following completion of a project.

Please indicate at the end of every peer-review publication (in brackets) the Open Access (OA) type as following:

- Gold OA = published in Open Access Journal, with or without an author fee (see register of all Open Access Journals http://www.doaj.org/)
- Hybrid OA = published in a subscription journal but Open Access by an author fee (see http://en.wikipedia.org/wiki/Hybrid_open_access_journal)
- Green OA = self-archived electronic copy of the final "accepted manuscript" which might include an embargo period (see: http://www.fwf.ac.at/en/research-funding/open-access-policy/)
- Other OA = any other type of Open Access
- No OA = not published Open Access

1.1 *Peer-reviewed publications / already published* (journals, monographs, anthologies, contributions to anthologies, proceedings, research data, etc.)

Citations should be provided in a **commonly used format.** For each work, the publication list **must mention the following**:

- Author(s)
- Title
- Journal
- Issue
- Year
- Pages
- DOI or ISBN (for books)
- If Open Access: URL
- Open Access (OA) Type

K. Rupp, C. Jungemann, S.-M. Hong, M. Bina, T. Grasser, A. Jüngel: "A Review of Recent Advances in the Spherical Harmonics Expansion Method for Semiconductor Device Simulation"; Journal of Computational Electronics (2016), 1-20. doi:10.1007/s10825-016-0828-z. [Gold OA]

P. Sharma, S. E. Tyaginov, Y. Wimmer, F. Rudolf, K. Rupp, H. Enichlmair, J.M. Park, H. Ceric, T. Grasser: "Comparison of Analytic Distribution Function Models for Hot-Carrier Degradation in nLDMOSFETs"; Abstracts of the 26th European Symposium on Reliability of Electron Devices, Failure Physics and Analysis, (2015), 60. doi:10.1016/j.microrel.2015.06.021. [no OA]

P. Sharma, S. E. Tyaginov, Y. Wimmer, F. Rudolf, K. Rupp, M. Bina, H. Enichlmair, J.M. Park, R. Minixhofer, H. Ceric, T. Grasser: "Modeling of Hot-Carrier Degradation in nLDMOS Devices: Different Approaches to the Solution of the Boltzmann Transport Equation"; IEEE Transactions on Electron Devices, 62, (2015), 1811 - 1818 doi:10.1109/TED.2015.2421282. [no OA]

P. Sharma, M. Jech, S. E. Tyaginov, F. Rudolf, K. Rupp, H. Enichlmair, J.M. Park, T. Grasser: "Modeling of Hot-Carrier Degradation in LDMOS Devices Using a Drift-Diffusion Based Approach"; Proceedings of the 20th International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), (2015), ISBN: 978-1-4673-7858-1, 60 - 63 doi:10.1109/SISPAD.2015.7292258. [no OA]

P. Sharma, S. E. Tyaginov, Y. Wimmer, F. Rudolf, K. Rupp, H. Enichlmair, J.M. Park, H. Ceric, T. Grasser: "Comparison of Analytic Distribution Function Models for Hot-Carrier Degradation in nLDMOSFETs"; Microelectronics Reliability, 55, (2015), 1427 - 1432 doi:10.1016/j.microrel.2015.06.021. [no OA]

P. Sharma, S. E. Tyaginov, Y. Wimmer, F. Rudolf, K. Rupp, M. Bina, H. Enichlmair, J.M. Park, H. Ceric, T. Grasser: "Predictive and Efficient Modeling of Hot-Carrier Degradation in nLDMOS Devices"; Proceedings of the 2015 IEEE 27th International Symposium on Power Semiconductor Devices & IC's (ISPSD), (2015), ISBN: 978-1-4799-6259-4, 389 - 392 doi:10.1109/ISPSD.2015.7123471. [no OA]

J. Weinbub, M. Wastl, K. Rupp, F. Rudolf, S. Selberherr: "ViennaMaterials - A Dedicated Material Library for Computational Science and Engineering"; Applied Mathematics and Computation, 267, (2015), 282 - 293 doi:10.1016/j.amc.2015.03.094. [no OA]

M. Bina, S. E. Tyaginov, J. Franco, K. Rupp, Y. Wimmer, D. Osintsev, B. Kaczer, T. Grasser: "Predictive Hot-Carrier Modeling of n-Channel MOSFETs"; IEEE Transactions on Electron Devices, 61, (2014), 3103 - 3110 doi:10.1109/TED.2014.2340575. [no OA]

Y. Wimmer, S. E. Tyaginov, F. Rudolf, K. Rupp, M. Bina, H. Enichlmair, J.M. Park, R. Minixhofer, H. Ceric, T. Grasser: "Physical Modeling of Hot-Carrier Degradation in nLDMOS Transistors"; 2014 IEEE International Integrated Reliability Workshop Final Report (IIRW), (2014), ISBN: 978-1-4799-7308-8, 58 - 62 doi:10.1109/IIRW.2014.7049511. [no OA]

F. Rudolf, J. Weinbub, K. Rupp, A. Morhammer, S. Selberherr: "Template-Based Mesh Generation for Semiconductor Devices"; Proceedings of the 19th International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), (2014), ISBN: 978-1-4799-5285-4, 217 - 220 doi:10.1109/SISPAD.2014.6931602. [no OA]

K. Rupp, M. Bina, Y. Wimmer, A. Jungel, T. Grasser: "Cell-Centered Finite Volume Schemes for Semiconductor Device Simulation"; Proceedings of the 19th International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), (2014), ISBN: 978-1-4799-5285-4, 365 - 368 doi:10.1109/SISPAD.2014.6931639. [no OA]

J. Weinbub, K. Rupp, S. Selberherr: "Highly Flexible and Reusable Finite Element Simulations with ViennaX"; Journal of Computational and Applied Mathematics, 270, (2014), 484 - 495 doi:10.1016/j.cam.2013.12.013. [no OA]

M. Bina, K. Rupp, S. E. Tyaginov, O. Triebl, T. Grasser: "Modeling of Hot Carrier Degradation Using a Spherical Harmonics Expansion of the Bipolar Boltzmann Transport Equation"; 2012 International

Electron Devices Meeting (IEDM) Technical Digest", (2012), 713 - 716 doi:10.1109/IEDM.2012.6479138. [no OA]

K. Rupp, C. Jungemann, M. Bina, A. Jüngel, T. Grasser: "Bipolar Spherical Harmonics Expansions of the Boltzmann Transport Equation"; Proceedings of the 17th International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), (2012), ISBN: 978-0-615-71756-2, 19 – 22. [no OA]

J. Weinbub, K. Rupp, S. Selberherr: "A Flexible Execution Framework for High-Performance TCAD Applications";Proceedings of the 17th International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), (2012), ISBN: 978-0-615-71756-2, 400 – 403. [no OA]

J. Weinbub, K. Rupp, S. Selberherr: "A Generic Multi-Dimensional Run-Time Data Structure for High-Performance Scientific Computing"; Proceedings of the World Congress on Engineering (WCE), (2012), ISBN: 978-988-19252-1-3, 1076 – 1081. [no OA]

K. Rupp, P. Lagger, T. Grasser: "Inclusion of Carrier-Carrier-Scattering Into Arbitrary-Order Spherical Harmonics Expansions of the Boltzmann Transport Equation"; Book of Abstracts of the 15th International Workshop on Computational Electronics (IWCE), (2012), 109 – 110. doi:10.1109/IWCE.2012.6242856. [no OA]

K. Rupp, A. Jüngel, T. Grasser: "A GPU-Accelerated Parallel Preconditioner for the Solution of the Boltzmann Transport Equation for Semiconductors"; Lecture Notes in Computer Science, Vol. 7174, R. Keller, D. Kramer, J.-Ph. Weiss (ed); Springer, 2012, ISBN: 978-3-642-30396-8, 147 - 157 doi:10.1007/978-3-642-30397-5. [no OA]

J. Weinbub, K. Rupp, L. Filipovic, A. Makarov, S. Selberherr: "Towards a Free Open Source Process and Device Simulation Framework"; Book of Abstracts of the 15th International Workshop on Computational Electronics (IWCE), (2012), 141 – 142. doi:10.1109/IWCE.2012.6242867. [no OA]

K. Rupp, T. Grasser, A. Jüngel: "On the Feasibility of Spherical Harmonics Expansions of the Boltzmann Transport Equation for Three-Dimensional Device Geometries"; International Electron Devices Meeting (IEDM), Washington DC, USA; 2011-12-05 - 2011-12-07; ISBN: 978-1-4577-0505-2, 4 page(s) doi:10.1109/IEDM.2011.6131667. [no OA]

1.2 Non peer-reviewed publications / already published (journals, monographs, anthologies, contributions to anthologies, research reports, working papers / preprints, proceedings, research data, etc.)

Citations should be provided in a **commonly used format.** For each work, the publication list **must mention the following**:

- Author(s)
- Title
- Journal
- Issue
- Year
- Pages
- DOI or ISBN or URL / if applicable
- Open Access / if applicable
- Open Access (OA) Type

F. Rudolf, J. Weinbub, K. Rupp, P. Resutik, S. Selberherr: "Mesh Healing for TCAD Simulations"; Abstracts International Conference on Large-Scale Scientific Computations (LSSC), (2015), 66. [no OA]

F. Rudolf, Y. Wimmer, J. Weinbub, K. Rupp, S. Selberherr: "Mesh Generation Using Dynamic Sizing Functions"; Proceedings of the 4th European Seminar on Computing, (2014), 191. [no OA]

K. Rupp, F. Rudolf, J. Weinbub, A. Jungel, T. Grasser: "Automatic Finite Volume Discretizations Through Symbolic Computations"; Proceedings of the 4th European Seminar on Computing, (2014), 192. [no OA]

J. Weinbub, K. Rupp, F. Rudolf: "A Flexible Material Database for Computational Science and Engineering"; Proceedings of the. 4th European Seminar on Computing, (2014), 226. [no OA]

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1.3 Planned publications

(journals, monographs, anthologies, contributions to anthologies, proceedings, research data, etc.)

Author(s)
Title
Sources
URL (if applicable)
Peer Review yes ☐ no ☐
Status in press/accepted ☐ submitted ☐ in preparation ☐

2. Most important academic awards

(Specific academic awards, honours, prizes, medals or other merits)

Name of award	n=national / i=international
Best paper award, World congress on Engineering	i

3. Information on results relevant to commercial applications

- Type of commercial application:

  1. Patent
  2. Licensing
  3. Copyrights (e.g. for software; no publications)
  4. Others

Type of commercial application		
Subject / title of the invention / discovery		
Short description of the invention / discovery		
Year		
Status	granted ☐	pending ☐
Application reference (or patent number)		

4. Publications for the general public and other publications

(Absolute figures, separate reporting of national / international publications)

- Type of dissemination activities:

  1. Self-authored publications on the World Wide Web
  2. Editorial contributions in the media (print, radio, TV, www, etc.)
  3. (Participatory) contributions within science communication
  4. Popular science contributions (books, lectures, exhibitions, films, etc.)

	national	**International**
Self-authored publications on the www		
Editorial contributions in the media		
(Participatory) contributions within science communication		
Popular science contributions		

5. Development of collaborations

Indication of the most important collaborations (no more than 5) that took place (i.e. were initiated or continued) in the course of the project. Please provide the name of the collaboration partner (name, title, institution) and a few words about the scientific content. Please **categorise** each collaboration arrangement as follows:

N				Nationality of collaboration partner (please use the ISO-3-letter country code)
	G			Gender **F (**female) **M** (male)

		E		Extent **E1** **low** (e.g. no joint publications, but mention in acknowledgements or similar); **E2** **medium** (collaboration e.g. with occasional joint publications, exchange of materials or similar, but no longer-term exchange of personnel); **E3** **high** (extensive collaboration with mutual hosting of group members for research stays, regular joint publications, etc.)
			D	Discipline **W** **within the discipline** (within the same scientific field) **I** **interdisciplinary** (involving two or more disciplines) **T** **transdisciplinary** (collaborations outside the sciences)

N	G	E	D	Name	Institution
GER	M	E2	W	Prof. Christoph Jungemann	RWTH Aachen
KOR	M	E2	W	Dr. Sun-Ming Hong	Gwangju Institute of Science and Technology

Note: General scientific contact and occasional meetings should not be considered collaborations for the purposes of this report.

6. Development of human resources in the course of the project

(Absolute figures with an indication of status (in progress / completed)

Note: It is not possible to assign a *venia* thesis / work (*Habilitation*) to a single project; here it is necessary to mention those *venia* theses for which the project was important. A similar caveat applies to Ph.D. and diploma theses: The FWF does not support thesis work, but instead funds the scientific work that forms the basis for such theses.

	In progress	Completed	Gender f	Gender m
Full professorship				
Venia thesis (*Habilitation*) / Equivalent senior scientist qualification				
Postdoc	1			1
Ph.D. theses		1		1
Master's theses				
Diploma theses				
Bachelor's theses				

7. Applications for follow-up projects

(Please indicate the status of each project and the funding organisation)

7.1 Applications for follow-up projects (FWF projects)

Please indicate the project type (e.g. stand-alone project, SFB, DK, etc.)

Project number (if applicable)	P29119		
Project type	Stand-alone Project		
Title / subject	3D Solution of the Boltzmann Equation on Supercomputers		
Status	granted ☒	pending ☐	in preparation ☐
Application reference (if a patent is applied)			

7.2 Applications for follow-up projects (Other national projects)

(e.g. FFG, CD Laboratory, K-plus centres, funding from the Austrian central bank [OeNB], Austrian federal government, provincial agencies, provincial government or similar sources)

Funding agency	Please choose an item: Wählen Sie ein Element aus.		
Other national funding agencies			
Project number (if applicable)			
Project type			
Title / subject			
Status	granted ☐	pending ☐	in preparation ☐
Total costs (granted)			

7.3 Applications for follow-up projects (international projects) (e.g. EU, ERC or other international funding agencies)

Country			
Funding agency	Please choose an item: Wählen Sie ein Element aus.		
Project number (if applicable)			
Project type			
Title / subject			
Status	granted ☐	pending ☐	in preparation ☐
Total costs (granted)			

IV. Cooperation with the FWF

Please rate the following aspects with regard to your interaction with the FWF. Please provide any **additional comments (explanations)** on the supplementary sheet with a reference to the corresponding question/aspect.

Scale:	
-2	highly unsatisfactory
-1	unsatisfactory
0	appropriate
+1	satisfactory
+2	highly satisfactory
X	not used

Rules
(i.e. guidelines for: funding programme, application, use of resources, reports)

Rating

Application guidelines	Length	+1
	Clarity	+1
	Intelligibility	+1

Procedures (submission, review, decision)

Advising	+1
Duration of procedure	0
Transparency	0

Project support

Advising	Availability	+1
	Level of detail	+1
	Intelligibility	+1

Financial transactions (credit transfers, equipment purchases, personnel management)	+1

Reporting / review / exploitation

Effort	+1
Transparency	+1
Support in PR work / exploitation	0

Comments on cooperation/interaction with the FWF:

The FWF is the ***only*** funding source which allows us to focus on science rather than on writing reports and being entangled in lengthy book-keeping activities.