FACHGUTACHTEN
PROJEKTNUMMER: P28364-N35

Reviewer A

1.) Scientific/scholarly quality (including innovative aspects and originality) with special attention to strengths and weaknesses:

Strengths:
Dr. Rupp proposes to develop a 3-D devices simulator, based on the Boltzmann equation as the underlying physical model and a spherical harmonic expansion (SHE model) as a numerical approach. While the SHE model in itself is nothing new, the challenge here is the size of the system for an actual 3-D solver, leading to a large system of 4-dimensional partial differential equations (3 space dimensions and energy as independent variables.) The result would be a practical device solver which goes beyond the currently commercially and academically available drift - diffusion solvers and avoids the non-locality problems of quantum mechanical models. Given the increased available computing power, this is feasible and, to my knowledge, has never been done so far.

Weakness:
The proposal could be a little bit more explicit about the architectures that will be used. How portable will the code be?

Summary:
So, in summary, this is a nice project which will result in an important contribution to the device modeling field. The resulting linear algebra work on massively parallel architectures would have applications beyond the field.

EXCELLENT

2.) Approaches/methods and feasibility of the proposal with special attention to strengths and weaknesses:

The project is certainly doable. The key feature is the development of data structures on parallel architectures which allow for non - rectangular arrays (avoiding the 'forbidden' energy zones). This will be a valuable contribution beyond the device modeling field.

VERY GOOD

3.) Qualifications of the researchers involved (based on their academic age) with special attention to strengths and weaknesses:

Dr. Rupp has an impressive record. He has world class experts (Grasser for SHE models, Selberherr for numerical linear algebra and Juengel for numerics and mathematical analysis) in the same building. So it would be hard to imagine a better infrastructure for such a project.

EXCELLENT

4. Ethical issues:

Not applicable

5. Overall evaluation with regard to key strengths and weaknesses and final funding recommendation:

This is a well thought out proposal with excellent chances for success. The results will make a valuable contribution to and beyond the field.

Overall rating: EXCELLENT

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Reviewer B

1.) Scientific/scholarly quality (including innovative aspects and originality) with special attention to strengths and weaknesses:

The proposal aims at building a deterministic solver for the spatially 3D BTE governing charges transport in semiconductor devices. The solver will be designed for execution in an HPC environment. The scientific part of the proposal seems to have been well written, with attention to the fundamental aspect of the problem.
However, I think that it also presents some weaknesses, in the present formulation. More precisely:

1. Although not directly addressed to the BTE for semiconductors, a considerable amount of work on deterministic methods for the solution of the 3D Boltzmann equation for rarefied gases has been done. In particular, highly parallel implementations of deterministic and semi-deterministic schemes have been developed and studied by the "Russian school"" (F. Tcheremissine, V. Aristov, V. Titarev...)[1]. Is such experience of any use for the present project? This aspect should be touched, since the structure of the governing equation and the difficulties met on the way of efficient parallelization are very similar.
2. I would have appreciated a greater effort to imagine and present the (still hypothetical but foreseen) performances of the code to be developed. The Proposer gives a rough estimate of huge memory requirement, but no estimate of the computing time of a typical run (one hour? One year?) I think it would be very useful if the Proposer were able to imagine a significant benchmark problem for which the proposed technique would be competitive in comparison to others and provide even crude, but motivated, estimates of computational resources.

[1] V. Titarev, M. Dumbser, S. Utyuzhnikov „Construction and comparison of parallel implicit kinetic solvers in three spatial dimensions", Journal of Computational Physics 256 (2014) 17–33.

☐ excellent	☐ very good	☒ good	☐ average	☐ poor

2.) Approaches/methods and feasibility of the proposal with special attention to strengths and weaknesses:

The approaches and methods seem to represent the state of the art for the very particular problem addressed by the Proposer

☐ excellent	☒ very good	☒ good	☐ average	☐ poor

3.) Qualifications of the researchers involved (based on their academic age) with special attention to strengths and weaknesses:

The proposer seems to be highly qualified to bring the project to conclusion within the allotted time window. The scientific production appears to be of good quality, considering the age of the Proposer. Perhaps, too many publications are in the form of conference proceedings which seem to limit their impact on the reference community. However, their number and content show the very good capabilities of the Proposer in the field the proposal refers to.

☐ excellent	☒ very good	☐ good	☐ average	☐ poor

4. Ethical issues:

no

5. Overall evaluation with regard to key strengths and weaknesses and final funding recommendation:

I think the Proposer did a good job. However, he should put more effort to compare his methodology with similar works already done in nearby fields. Moreover, he should try to figure out the final capabilities of the solver at the best of his knowledge.
I am sure that the requested changes will turn the proposal into one worth funding.

☐	Excellent - funding with highest priority
☐	Very Good - funding with high priority
☒	Good - resubmission with some revisions
☐	Average - resubmission with major revisions
☐	Poor - rejection

FACHGUTACHTEN
PROJEKTNUMMER: P28364-N35

Reviewer C

1.) Scientific/scholarly quality (including innovative aspects and originality) with special attention to strengths and weaknesses:

This proposal addresses an important and updodate topic of classical simulation semiconductor devices. The novel aspect is that PI challenges the precise numerical simulation of 3d system by solving the Boltzmann transport equation (BTE). Already for 2d system, it poses a significant computational problem, since the BTE is effectively 4d in phase space which make the memory and requirements very high. In order to obtain numerically accessible model, authors use new method called SHE, which allow to solve a system of (n+1) equation for ndimensional system. This method has already demonstrated its usefulness in solving 1,2d system. It turned out, however, that the latter case practically requires up to ~80GB of memory. The transition 2d3d would then reach scale of Terabytes. This however requires distributed computing of a HPC cluster. This is the way proposed in this grant.

The strengths of this proposal are definitely coming from facts that it addresses current, unsolved and complex problem, uses stateoftheart approach (SHE) and proposes effective tools to solve it (which I will comment below). Additionally, results of this project can have immediate applications in technology.

At this point I will not point any weaknesses as they might belong to next section. It mean that claim of solving 3d BTE at this scale cannot have weaknesses by itself, as long as authors of this claim are really able to accomplish it.

☒ excellent	☐ very good	☐ good	☐ average	☐ poor

2.) Approaches/methods and feasibility of the proposal with special attention to strengths and weaknesses:

The main question to such large scale project is in fact can authors accomplish the goal. Based on thorough inspection of their previous works, as well as the proposal text think they can do it.

The proposed methods of solution are solely focused on modern, but already proven, SHE approach to BTE. This is a solid ground for the start. PI also include prof. Tibor Grasser as a scientific partner and advisor of the PhD student involved which will significantly improve amount of available expertise in the working team.
The work is split into three independent packages: Discretization, Fast Linear Solvers and Efficient Nonlinear Solvers, which can improve overall performance of the work. Each of those work packages addresses a particular problem in numerical analysis. The detailed discussion in the proposal text as well as the reading of the previous publication of PI clearly indicates that the some methods developed during the project will be deeply specialized for a given problem. For example, the team will make use of the properties of the sparse energy grid to eliminate unused nodes, take into account the form of coupling between different energies, implement specialized parallel block iterative solvers etc. The spectrum of those planned tasks is impressive, and one might doubt in its feasibility, however PI has already proven to be proficient enough in all those aspects (as described below).

One weak point of this work could come from the fact that PI plans to proceed along single path solving of BTE with SHE on unstructured grid using clusters of CPU based solvers. Using GPU is mentioned by itis suggested that it has limited application in this case. However, structured grid approach on multi GPU architecture might be also an option.

Strengths: creation of deep specialized numerics, instead of relying on black box solutions, use of state of the art numerical approach

Weaknesses: only one approach, but considering the fact that this is not a large cooperation but "Stand alone Project" with two financed researchers, this should not diminish the value of this project at all.

☒ excellent	☐ very good	☐ good	☐ average	☐ poor

3.) Qualifications of the researchers involved (based on their academic age) with special attention to strengths and weaknesses:

The scaling problem from a single workstation (or 1 GPU) to a cluster is not an obvious process. It might fail in many points, e.g. due to bad scaling of the solver. The interdisciplinary qualifications of researchers play in such challenge important role.

The publication record of PI is impressively long almost 60 papers in last 5 year and indicated extraordinary involvement in research. The closer inspection, however show that they are mostly conference proceeding or abstracts and 11 are regular journal articles. Majority of them cover the field of this proposal. Some of them deal with indepth analysis of programming GPU processors. This clearly indicated that PI has required interdisciplinary skills.
Scientific papers of PI do not have impressive citation numbers, one could conclude that his area of interest is highly specialized.

There is also another aspect of PI activity. He is an active author and contributor to the open software. His largest project is ViennaCL, which is basically many core linear algebra library. This software consist of 107397 line code C++ code and is developed with a community (https://github.com/viennacl/viennacldev), where PI is a major contributor. This is a modern and for now perhaps the only efficient way to develop of large software within a framework of scientific research. First, the software is opensource, which makes huge positive impact on potential reproducibility of the scientific results. Secondly, the source is developed in a process of public collaboration, which makes it better maintainable code and give much better forecast for its continuation. In this case, since, the project aim is to develop a software solution for rather big computational problem, the "github" record of the PI is at least equally important as his publication list. The design of the software (viennacl) is novel and ambitious it tries to reconcile easy of use (by pyviennacl), performance and flexibility (independence on particular computational backend). It must be stressed that PI develops also another pieces of software which together make a framework for BTE simulation. The planned development in this project is promised to be published as ViennaSHE library, which will be based on ViennaCL and PETS (PI is a contributor) packages.
Therefore I would like to emphasise that based on published code, the qualifications of the PI are excellent.

PhD candidate specified in the proposal seems to have required qualifications based on the proposal one could describe his profile as "applied mathematician proficient in programming" which fits perfectly into this project. He is already involved in the project field as one might conclude from his website information and his employment at the Institute of Microelectronics.

Scientific Partner, and PhD advisor CV and publication record are excellent and thus do not require further comments. His involvement will certainly improve the scientific recognition of the project results and assure scientific quality of the project as a whole.

Strengths: PI has very good publication record, excellent record of open software development, building and contributing to the open community and experience and deep knowledge of numerical methods

Weaknesses: One could point out the small recognition of journal publications of PI, but it is more than compensated by his "github" record.

☒ excellent	☐ very good	☐ good	☐ average	☐ poor

4. Ethical issues:

no

5. Overall evaluation with regard to key strengths and weaknesses and final funding recommendation:

Strenghts:
This project tackles a big computational challenge of the simulation 3d semiconductor device using Boltzmann device. PI as well scientific partner have excellent record in this field, in particular PI has proven his excellence in creating and maintaining large and open software projects. Importantly, the results of the project will be disseminated not only as journal publications but also as open source code, which is a key factor in both reproducibility of the simulation results as well as reusability of the efforts for other research groups, which might use ViennaSHE library.

Weaknesses:

Basically I do not see any major weaknesses, few has been addressed in the previous point but they do not change my opinion on the project on overall.

☒	Excellent - funding with highest priority
☐	Very Good - funding with high priority
☐	Good - resubmission with some revisions
☐	Average - resubmission with major revisions
☐	Poor - rejection