

STAND-ALONE PROJECT - FINAL REPORT

Project number

P19532-N13

Project title

Mesh Generation, Error Estimation, and Adaptation

Project leader

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1. Summary for public relations work

English version:

The automation and coupling of a mesh generation and adaptation process driven by error estimation – considering the partial differential equations discretization technique used and the subsequent properties of the equation system – has been investigated.

A mesh with as small as possible a number of elements that captures all relevant features of the investigated geometry is desired in order to support methods for fast numerical analysis as well as an accurate description of the geometry. This in particular aids the discretization of partial differential equations used for the solution within areas on able amount of time, computer resources, and minimal manual interaction.

The technical problems we have solved in our project are mostly caused by finite numerics in the discrete scheme of computer-aided design. As a consequence algorithms based on geometrical predicates have been designed very carefully with respect to numerical issues.

From a software point of view the coupling of different software modules for modeling, generation, adaptation, and error estimation merit special consideration. This required new and more sophisticated methods of software design with special attention to robustness, orthogonality, modularity, and reusability.

The application of our approach is mostly focused on semiconductor device structures, but is not restricted to this field. Final results obtained from our meshing methodology have demonstrated with real-world examples, that the capabilities of previously used meshing techniques are now considerably surpassed.

German version:

Innerhalb dieses Forschungsprojektes wurden die Automation und Kopplung von Gittergenerierung und Gitteradaptierung untersucht. Die Automatisierung dieser Prozesse wird dabei von Fehlerabschätzungsalgorithmen gesteuert, die einerseits die zu lösende diskretisierte partielle Differentialgleichung und die Eigenschaften des Gleichungssystems berücksichtigen und andererseits die endgültige Lösung auf dem Gitter analysieren und gegebenenfalls das Gitter dahingehend anpassen, dass der jeweilige Fehler minimiert wird.

Das Ziel dieser Erzeugungs- und Adaptierungsprozesse war es, ein Gitter mit einer möglichst geringen Anzahl an Elementen zu erzeugen, welches jedoch alle wesentlichen Eigenschaften der zu untersuchenden Struktur enthält. Das Gitter muss für die Lösung der verwendeten Differentialgleichung geeignet sein und dabei die Zeit, Rechnerressourcen und die manuelle Interaktion des Benutzers minimieren.

Die zu lösenden technischen Probleme dieses Projektes lagen zum Großteil in der endlichen Abbildung der Numerik in den Bereich von Computersystemen. Die Notwendigkeit des sorgfältigen Entwurfs aller Algorithmen bezüglich geometrischer Eigenschaften ist dabei besonders hervorzuheben.

Die optimale Kopplung der einzelnen Module für Modellierung, Gittergenerierung, Fehlerabschätzung und Gitteradaptierung stellte dabei einen wesentlichen Teil dieses Projektes dar. Moderne Programmierparadigmen sowie aktuelle Programmier Techniken ermöglichten die Software-Entwicklung in Hinblick auf Robustheit, Orthogonalität, Modularität und Wiederverwendbarkeit.

Der Hauptanwendungsbereich unserer Forschung liegt im Bereich der Halbleiterbauelemente, ist aber nicht auf dieses Gebiet beschränkt. Resultate aus dieser Arbeit haben an praxisnahen Beispielen gezeigt, dass die Möglichkeiten von früheren Gittergenerierungstechniken nun weit übertroffen werden.

2. Brief project report

2.1 Report on the scientific work

2.1.1 Information on the development of the research work

Investigations of mesh generation and adaption related algorithms and data structures have been the basic aim of this research project in order to implement robust, orthogonal, and reusable software components. Due to the significant problems encountered in the available methodologies at the program start, a comprehensive numerical investigation, including the following issues has been part of our research:

- integer arithmetic
- adaptive floating point arithmetic
- exact arithmetic with arbitrary-length integer and rational data types
- high precision floating point data types

Compared with former approaches the developed approach is based on an orthogonal software library. Especially the numerical kernel has been designed to be exchangeable and therefore usable for many different software applications.

The influence of degenerated elements on the solving algorithms and their convergence has been investigated. Based on this research non-standard methods in the PDE discretization methodology coupled with spatial discretization techniques have been considered, e.g. partially non-Delaunay surfaces and Delaunay volume meshes. A possible shift to other mesh element criteria besides the Delaunay criterion has been investigated.

With regard to error estimation to control the mesh adaptation process, additional research has been carried out on the semiconductor equations with respect to a formal derivation of lower and upper error bounds. Robust and practical adaption algorithms have been achieved during this research.

The project aim includes insights into the quantitative analysis of robustness and efficiency improvements, which are accomplished with different types of numerical treatment. Special focus is placed on the coupling of all different sub-parts. A minimum of user interaction is strived for to reduce the complex task of manual point insertion.

Our investigations in the field of modern programming paradigms and techniques have shown the potential of new approaches for creating highly efficient and reusable software components - generic and multi-dimensional software components. Generic programming deals among other things with the separation of the actual data structure and the usable algorithms.

We have developed the software modules with a generic programming approach. Based on this data structural approach which is similar to the C++ STL, different algorithms can be investigated and compared very efficiently. It is possible to separate the geometrical predicates from the logical algorithm flow, which yields a high improvement in robustness, exchangeability, and speed.

There has not been any change of direction in the projected road at the start of the project to the very end.

2.1.2 Most important results and brief description of their significance

Results have been obtained in the following topical areas:

- Demonstration of increased robustness compared to currently used meshing methodologies
- Increased mesh capacity in terms of number of elements with different meshing techniques
- Decrease in the overall generation and adaptation run-time
- Reduction of the number of mesh elements
- Performance improvement in accuracy/convergence/run-time in numerical analysis

In addition to quantitative and qualitative analyses regarding currently used mesh generation approaches, a comprehensive comparison of mesh generation software has been performed. A rigorous investigation of relevant mesh generators has been carried out and gave fruitful hints on various details. Sophisticated examples have been used to test the different types of mesh generation approaches. It has been shown, that our proposed advancing front combined Delaunay approach performs best for all practically relevant structures.

A rigorous analysis and a comprehensive literature investigation of error estimation methods suitable for the semiconductor transport equations have been performed. Based on this information a new approach for an error estimation method for non-linear coupled PDE systems has been investigated. On the basis of linearized equations as local system matrix parts, a mesh adaptation algorithm has been developed to cope with drift-diffusion and higher-moment approximations of the Boltzmann equation. A new approach using a jet based error estimator has been analyzed and further developed. We started with the so-called ZZ estimators and residual error estimators to control an adaptive mesh generation process. We have investigated how to translate the results of the error estimator to the adaptive meshing kernel. For this purpose we have developed a rule-based graph algorithm to interactively control and adjust the threshold values for all adaptive meshing processes.

A particularly for our goals relevant topic we have researched on deals with numerical predicate libraries. Several currently available libraries have been analyzed, such as CGAL, MPFUN, or Triangle. We have developed software concepts to adapt the basic ideas of the investigated libraries to make them usable in an automatic, generic, and functional environment.

Due to the choice of programming paradigms we have been able to fully extend our meshing framework, which is now capable not only to create volume meshes in parallel but also to use additional meshing kernels. A unified programming interface, which governs the meshing kernel, enables us to exchange the underlying meshing kernels and to compare their results. Using this programming interface we have been able to investigate adaptive meshing approaches using different mesh generation and adaptation algorithms. During a supervised master thesis, programming techniques for algorithms for mesh element simplification and refinement have been investigated.

We have experienced that producing high quality volume meshes using an advancing front method is not possible without rigorously adapting and remeshing the input surface mesh as a whole. Therefore considerable effort has been spent on developing an adaptation algorithm also for the surface of multi-segmented and non-manifold structures using an advancing front approach. In particular the dissertation work has been focused on implementing these concepts into the mesh framework by enabling an extended advancing front algorithm which can deal with non-manifold input specification.

A comprehensive robustness and performance analysis of numerous examples regarding accuracy, convergence, and run-time has also been accomplished.

The final goal, namely the availability of chained modules for highly automated mesh generation, error estimation, and adaptation processes, has been achieved.

In order to visually highlight the progress in mesh adaptation, Fig.1 shows an initial mesh for a typical structure of modern microelectronics, an inverter designed with Complementary Metal-Oxide Semiconductor (CMOS) devices. Fig.2 shows the result of the adaptation to improve the mesh quality by simultaneously keeping the number of mesh elements minimal.

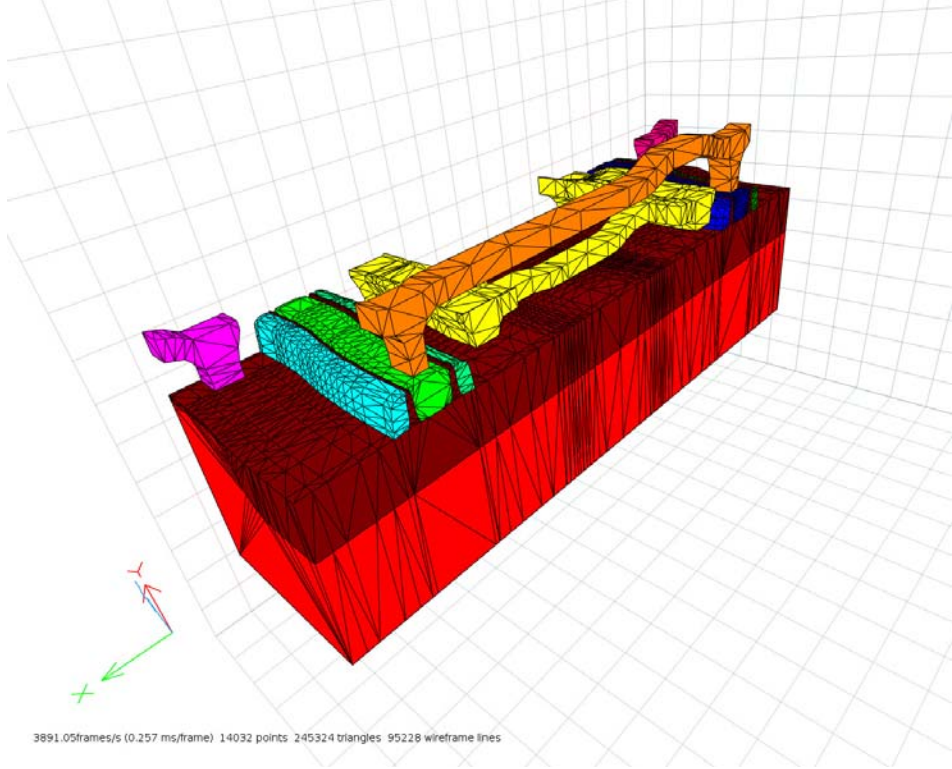


Fig.1. Initial CMOS structure mesh

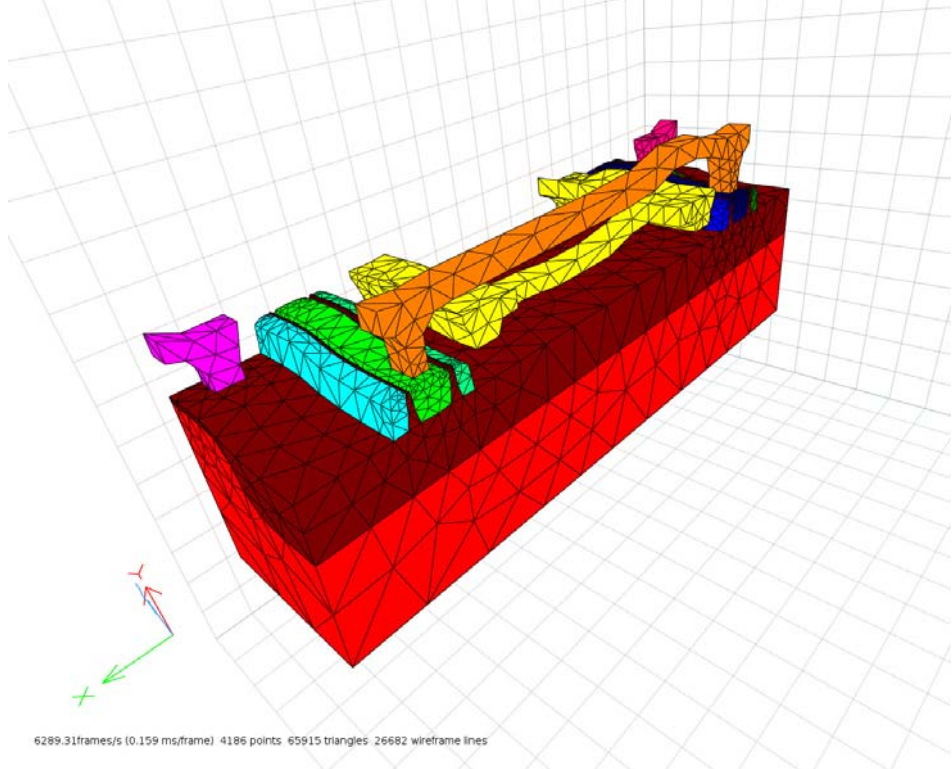


Fig.2. CMOS structure mesh after adaptation

2.1.3 Information on the running of the project, use of the available funding and where appropriate any changes to the original project plan relating to

The complete duration of the project was 39 months, 36 months were planned and an extension of 3 months without change in funding was granted. The project team consisted of Dr. René Heinzl and Dipl.-Ing Franz Stimpfl. The literature study was carried out by Dr. Heinzl. He also focused on the theoretical background for generic programming. Dipl.-Ing. Franz Stimpfl concentrated on the numerical details of particular relevance to the meshing modules. Dr. Heinzl took care of the implementation of the abstract algorithms in an as much as possible application independent manner. Tests were carried out by all members of the team and led to many fruitful discussions about the simulation results and various numerical algorithms and software design.

During the project all members regularly published and presented their results at international conferences and in scientific journals.

The available funding was entirely spent as planned in the proposal.

No changes to the original project plan were necessary.

2.2. Personnel development – importance of the project for the scientific careers of those involved (including the project leader)

The knowledge and experience gained during the FWF project serves as an excellent basis for further scientific work and personal development for all project members. Dr. René Heinzl had the opportunity to obtain valuable experience in organizing research work on the complex problem of generic programming. All members benefited from the great opportunity to develop and improve their strategies for publishing obtained results and from the communication with the scientific community. Dipl.-Ing. Franz Stimpfl, as a doctoral student during the project, had the opportunity to gain deeper understanding in the underlying software architectures and to improve his skills in solving the related programming problems.

2.3 Effects of the project outside the scientific field

With the knowledge gained during the project, Dr. René Heinzl and Dipl.-Ing. Franz Stimpfl advised the startup-company Shenteq, which is specialized on providing software and application support, training, management, and consulting in the three main areas

- mesh generation
- numerical simulation
- and scientific visualization

with generic software. After the project both researchers joined the company.

3. Information on project participants

not funded by the FWF			funded by the FWF (project)		
co-workers	number	Person-months	co-workers	number	Person - months
non-scientific co-workers			non-scientific co-workers		
diploma students	1	6	diploma students		
PhD students			PhD students	1	36
post-doctoral co-workers			post-doctoral co-workers	1	36
co-workers with "Habilitation" (professorial qualifications)			co-workers with "Habilitation" (professorial qualifications)		
professors	1	6	professors		

4. Attachments

List 1

1.a. Scientific publications¹

1.a.1. Peer-reviewed publications (journals, contribution to anthologies, working papers, proceedings etc.)

1) Schwaha P., Heinzl R., Stimpfl F., Selberherr S.,
“Synergies in Scientific Computing by Combining Multi-Paradigmatic Languages for High-Performance Applications”,
Intl.J.of Parallel, Emergent and Distributed Systems,
DOI: 10.1080/17445760902758552, Vol.24, No.6, pp.539-549, 2009.

2) Heinzl R., Schwaha P., Stimpfl F., Selberherr S.,
“GUIDE: Parallel Library-Centric Application Design by a Generic Scientific Simulation Environment”,
Intl.J.of Parallel, Emergent and Distributed Systems,
DOI: 10.1080/17445760902758545, Vol.24, No.6, pp.505-520, 2009.

1.a.2. Non peer-reviewed publications (journals, contribution to anthologies research reports, working papers, proceedings, etc.)

1.a.3. Stand-alone publications (monographies, anthologies)

1.b. Publications for the general public and other publications

¹ The publication list must mention for each work: all authors; full title; series/journal title; year; volume; and page numbers. Furthermore, if publications are freely available in the internet, please add the URL of the publication.

List 2 Project-related participation in international scientific conferences

2.1. Conference participations - invited lectures

2.2. Conference participations - lectures

- 1) Weinbub J., Schwaha P., Heinzl R., Stimpfl F., Selberherr S.,
"A Dispatched Covariant Type System for Numerical Applications in C++",
Proc. Intl. Conf. on Numerical Analysis and Applied Mathematics (ICNAAM)
(19.-25.Sept. 2010, Rhodos), ISBN 978-0-7354-0831-9, pp.1663-1666.
- 2) Stimpfl F., Weinbub J., Heinzl R., Schwaha P., Selberherr S.,
"A Unified Topology Layer for Finite Element Space Discretization",
Proc. Intl. Conf. on Numerical Analysis and Applied Mathematics (ICNAAM)
(19.-25.Sept. 2010, Rhodos), ISBN 978-0-7354-0831-9, pp.1655-1658.
- 3) Schwaha P., Heinzl R.,
"Marching Simplicies",
Proc. Intl. Conf. on Numerical Analysis and Applied Mathematics (ICNAAM)
(19.-25.Sept. 2010, Rhodos), ISBN 978-0-7354-0831-9, pp.1651-1654.
- 4) Sonderfeld R., Heinzl R.,
"A Generic and Self-Optimizing Polynomial Library",
Proc. Workshop on Parallel/High-Performance Object-Oriented Scientific
Computing (POOSC), (7.July 2009, Genova), 4 pages.
- 5) Schwaha P., Heinzl R., Nedjalkov M.,
"The Forced Evolution of Implementations: Using a Monte Carlo Algorithm as
Example",
Proc. Workshop on Parallel/High-Performance Object-Oriented Scientific
Computing (POOSC), (7.July 2009, Genova), 5 pages.
- 6) Heinzl R.,
"Data Structure Properties for Scientific Computing: An Algebraic Topology Library",
Proc. Workshop on Parallel/High-Performance Object-Oriented Scientific
Computing (POOSC), (7.July 2009, Genova), 6 pages.
- 7) Schwaha P., Baumgartner O., Heinzl R., Nedjalkov M., Selberherr S., Dimov I.,
"Classical Approximation of the Scattering Induced Wigner Correction Equation",
Proc. Intl. Workshop on Computational Electronics (IWCE), (27.-29.May 2009,
Beijing), ISBN 978-1-4244-3926-3, pp.177-180.
- 8) Stimpfl F., Heinzl R., Schwaha P., Selberherr S.,
"A Robust Parallel Delaunay Mesh Generation Approach Suitable for Three-
Dimensional TCAD",
Proc. Intl. Conf. on Simulation of Semiconductor Processes and Devices,
(9.-11.Sept. 2008, Hakone), ISBN 978-1-4244-1753-7, No.P-36, pp.265-268.
- 9) Heinzl R., Schwaha P., Stimpfl F., Selberherr S.,
"Parallel Library-Centric Application Design by a Generic Scientific Simulation
Environment",
Proc. Workshop on Parallel/High-Performance Object-Oriented Scientific Computing
(POOSC), (8.July 2008, Paphos), 5 pages.

10) Heinzl R., Schwaha P., Stimpfl F., Selberherr S.,
“A Parallel Generic Scientific Simulation Environment”,
Proc. Intl. Workshop on State-of-the-Art in Scientific and Parallel Computing
(PARA), (13.-16.May 2008, Trondheim), 8 pages.

11) Stimpfl F., Heinzl R., Schwaha P., Selberherr S.,
“High Performance Parallel Delaunay Mesh Generation and Adaptation”,
Proc. Intl. Workshop on State-of-the-Art in Scientific and Parallel Computing
(PARA), (13.-16.May 2008, Trondheim), 10 pages.

12) Stimpfl F., Heinzl R., Schwaha P., Selberherr S.,
“A Multi-Mode Mesh Generation Approach for Scientific Computing”,
Proc, European Simulation and Modeling Conf. (ESM), (22.-24.Oct. 2007, Malta),
ISBN 978-90-77381-36-3, pp.506-513.

2.3. Conference participations - posters

2.4. Conference participations - other

List 3 Development of collaborations

Indication of the most important collaborations (maximum 5), that took place (initiated or continued) in collaboration please give the name of the collaboration partner (name, title, institution) and a few words about the scientific content. Please also assign one of the following **categories** to each collaboration:

N			Nature	N (national); E (European); I (other international cooperation)
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	D within the discipline T transdisciplinary

N	E	D	Collaboration partner / content of the collaboration
			1) Name: _____ Title: _____ Institution: _____ Content: _____
			2) Name: _____ Title: _____ Institution: _____ Content: _____
			3) Name: _____ Title: _____ Institution: _____ Content: _____
			4) Name: _____ Title: _____ Institution: _____ Content: _____
			5) Name: _____ Title: _____ Institution: _____ Content: _____

Note: general scientific contacts and occasional meetings should not be considered as collaborations in the above sense.

List 4 “Habitations” (professorial qualifications) / PhD theses / diploma theses

4.1. Professorial Qualifications

4.2. PhD Theses

During the project period Franz Stimpfl almost completed his doctoral thesis with the tentative title “Mesh Generation based on Generic Programming”.

4.3. Diploma Theses

During the project period Josef Weinbub completed his diploma thesis “Adaptive Mesh Generation”.

List 5 Effects of the project outside the scientific field

5.1. Organization of scientific events

Dr. René Heinzl served on the Program Committee of the “Workshop on Parallel/High-Performance Object-Oriented Scientific Computing” (POOSC), (7.July 2009, Genova).

5.2. Particular honours, prizes etc.

5.3. Information on results relevant to commercial applications

5.4. Other effects beyond the scientific field

5.5. Relevance of the project in the organization of the relevant scientific discipline

List 6. Applications for follow-up projects

6.1 Applications for follow-up projects (FWF projects)

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

6.3 Applications for follow-up projects (International projects)