Simulation of Microelectronic Structures using A Posteriori Error Estimation and Mesh Optimization

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Introduction

Problems occurring in microelectronic device design and TCAD (Technology Computer Aided Design) are often modeled by means of partial differential equations (PDEs). An essential step in all of these methods is to find a proper tessellation of a continuous domain with discrete elements, either based on ortho-product grids or unstructured meshes.

The major advantages of the unstructured mesh approach is that tetrahedral or triangular meshes are locally adaptable and surfaces can be modeled with arbitrary precision. While in two dimensions mesh generation and adaptation techniques are mostly based on hand crafted meshes, it is almost impossible to design and adapt meshes in three dimensions. On that account it is very important to automatically generate and optimize meshes in three-dimensions.

Error Estimation Techniques and Mesh Optimization

As a first step we estimate the error caused by the discretization we have chosen. This may either be a finite volume or finite element discretization. First we will introduce residual error estimators. Due to the discretization the numerical solution does not fulfill the differential equation exactly and therefore the residuum is used as a measure of the discretization error [1]. The ZZ error estimator [2] measures how much the numerical solution u_h differs from a smoothed numerical solution $\overline{u_h}$. For some types of differential equations, such as the Laplace equation, the ZZ estimator has been shown to have upper and lower error bounds [2].

After calculating a local measure for the error we have to adapt the mesh in order to improve the quality of the solution if this measure exceeds an upper limit. On the other hand, we have to coarsen the mesh if the error is smaller than a lower error limit in order not to use unnecessarily fine meshes in regions of low error. The process of inserting more tetrahedra into the mesh is called mesh refinement, removal of elements from the mesh is called coarsement. In the following the complete processes is referred to as mesh adaptation.

There are different techniques of mesh control. The easiest method is to introduce an upper and a lower bound for refinement and coarsement as mentioned before. Second the upper error bound can be set to a level so that a certain number of cells (e.g. the worst 20 per cent) is refined.

Examples and Conclusion

To illustrate the applicability we analyze an interconnect structure by solving the Laplace equation in the SiO_2 layer around the contacts. The main aim of this simulation is to determine the capacitance between the two electrodes both very precisely and efficiently.

Using the advantages of mesh adaptation in combination with a posteriori error estimation leads to an enormous speed up of the calculations while the accuracy of the simulation result is comparable to the uniformly refined and highly resolved solution. For this reason mesh adaptation allows us to improve the mesh quality locally without increasing the number of mesh points dramatically.

[1] T. Barth. A Posteriori Error Estimation and Mesh Adaptivity for Finite Volume and Finite Element Methods, Springer series Lecture Notes in Computational Sciene and Enginerring (LNCSE), volume 41, 183–203. volume 41, page 183, 2004.

[2] O.C. Zienkiewicz and J.Z. Zhu. *A Simple Error Estimator and Adaptive Procedure for Practical Engineering Analysis, Int. J. Numer. Meth. Engrg. 24 (1987) 337–357. MR 87m:73055.* 1987.