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

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Abstract. We present an error estimation driven three-dimensional unstructured mesh optimization technique based on a posteriori error estimation techniques. We briefly summarize error estimation techniques as well as mesh quality estimations and apply them to problems of semiconductor device and process simulation. We then optimize the tessellation of the simulation domain with different strategies.

In contrast to other work [1, 2] our approach also covers three-dimensional domains with unstructured tetrahedral meshes. The major advantages of this approach is that tetrahedral meshes are locally adaptable and surfaces can be modeled with arbitrary precision.

Maximum error criteria trigger the refinement procedure and increase the accuracy of the solution. The simulation domain is refined in regions of high error without any user interaction or hand crafted mesh generation which makes it applicable for real world problems.

Introduction

Problems occurring in microelectronic device design and TCAD (Technology Computer Aided Design) are often modeled by means of partial differential equations (PDEs). For the solution numerical methods such as the finite element method or the finite volume method are used. An essential step in all of these methods is to find a proper tessellation of a continuous domain with discrete elements.

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 provide automatically generated and optimized meshing capabilities.

Mesh adaption and optimization has to meet various requirements from very different kinds of TCAD:

- On the one hand, process simulation requires boundary integrity, has to handle all kinds of degeneration in topography simulation [3], and has to generate surface and interface aligned elements for ion implantation and diffusion simulation [4]. The finite-element [5] method needs well shaped elements but up to now it is not clear, how to measure this criterion.
- Device simulation, on the other hand, is mostly based on the finite-volume method [6], which means that the elements must be Delaunay conforming [7]. In addition highly non-linear models require a direction dependent mesh density.
- At last we will have to consider the discretization error and the influence of the mesh on the error. As discretization procedures do not lead to exact results the mesh has to be properly defined in order to resolve the simulation domain accurately. Due to the dimension reduction of the discretization we have to make sure that the solution can be resolved accurately with the ansatz functions within the simulation domain. This can be archieved either by a finer meshes (h-refinement) or a bigger variety of ansatz functions (p-refinement). As we are more interested in the influence of the spatial discretization, namely meshing, we will restrict ourselves to h-refinement.
- Furthermore we have to consider that different differential equations result in discretization errors which behave completely different on the same mesh. For this reason it is necessary to tailor the mesh to the respective differential equation.

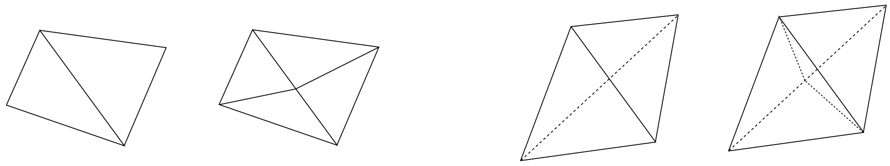

Figure 1: Simple refinement procedure. The maximum face/longest edge are split and connected to the opposite vertex.

Error Estimation Techniques

As a first step we estimate the error caused by the discretization. First we will introduce residual error estimators. The main idea of residual error estimation is to re-insert the solution into the original differential equation. Due to the discretization of the differential equation the equation is of course not exactly fulfilled and the residuum is used as a measure of the error. For the derivation of residual error estimators we refer to [8, 9].

If we assume the solution of our problem to be smooth we can estimate the error by measuring the distance between the numerical solution u_h and a smoothed solution $\overline{u_h}$. Even though this difference is not a residuum in the usual sense its value can be used for error estimation. For some types of differential equations, such as the Laplace equation, these estimators have been shown to have upper and lower error bounds [5]. For the interpolation function of the discrete numeric solution u_h we use polynomial functions of degree one in each tetrahedron. The distance between the interpolated piecewise affine function and the piecewise constant function can be determined by the evaluation of a suitable norm.

Mesh Quality Estimation

Apart from the estimation of the quality of the solution it has been shown that the geometry of the mesh has also a strong influence on the resulting equation system and on the solution. In the following we will specify geometrical criteria which state if an element of the tesselation, in our case triangles and tetrahedra, will produce an accurate tesselation. These statements however can only be valid for a class of model problems because each problem places different requirements on the mesh.

For finite volumina [6] we always need meshes which fulfill the Delauney criterion. This means that a single degenerated element can cause a useless mesh. Moreover it has been shown that in three dimensions flipping algorithms fail to produce Delaunay triangulations [7].

Finite elements [5] however can implicitly handle sliver elements and in some anisotripic cases the use of problem adapted anisotropic elements is more accurate and less time consuming than isotropic elements.

Mesh Adaptation

In the following we will introduce basic termini for the mesh adaption process. Most numeric errors are caused by meshes which are too coarse. In this case the exact function can not be approximated by the ansatz functions of the element in an accurate way. This, however, can lead to enormous numerical errors, oscillatory behavior or other numerical artefacts which have to be eliminated by a finer resolution of the mesh. Methods which increase the resolution of the mesh are called mesh refinement methods. In the following we will show a simple refinement procedure. A common and simple method (Fig. 1) to refine cells is to chose its longest edge (in 3D its largest facet) and split it. Then we connect both parts to the opposite vertex and thus we have two new cells. This procedure implies that the refinement of a cell causes the refinement of neighbor cells.

If time stepping in combination with fine resolution is needed in different locations of the simulation domain at different times it might be necessary to re-coarse a once refined mesh element. This is even more necessary if we consider the huge amount of calculation time which is caused by equations which are placed unnecessarily in regions of the mesh where the high resolution is not required any more. For these cases mesh-coarsement is crucial and we will introduce a combined coarsement-refinement technique named hierarchical mesh as well as coarsement-only techniques.

Even though coarsement (Fig. 2) of a mesh is a method of reducing numerical effort the geometrical coarsement procedure is not as easy as could be expected. General mesh coarsement methods provide a loss of geometrical as well as topological information and therefore have to be treated carefully. There are many constellations where coarsement leads to regions of covering triangles and tetrahedra.

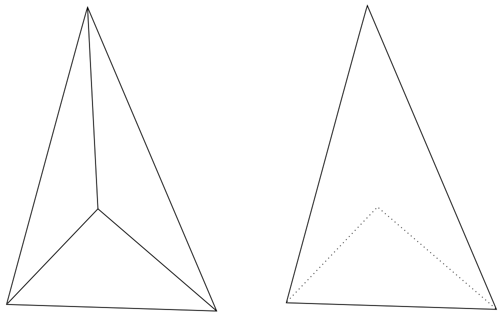

Figure 2: If the union of two cells is not convex, coarsement by cell collapsing causes covering cells.

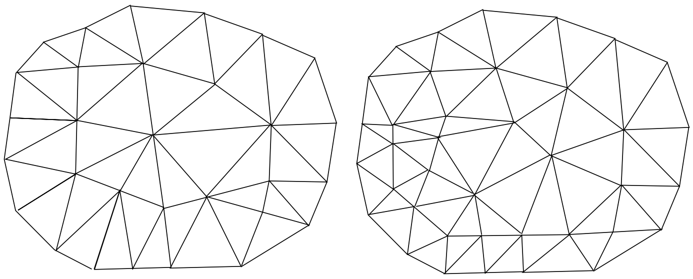

Figure 3: Within a local region the complete mesh is reorganized in order to obtain a finer resolution. The rest of the mesh is not affected.

A method which allows mesh refinement as well as mesh coarsement is the hierarchical mesh method [7]. The main idea of this method is that an element which originates from a mesh refinement step knows the original element it originated from. From a base tesselation we can refine an element using a certain refinement method. The newly created cells know the old (eliminated) cell they originate from. If the region has to be coarsed we can fall back on the original tesselation. The main problem with this method is that local refinements and coarsements always cause refinements of cells within the local patch. As this procedure is recursive there can be a global effect when refining a local cell.

In some cases it can be necessary to reconstruct a complete mesh (Fig. 3). Even though this can be time consuming we have the possibility to specify the local element or vertex density or even insert new vertices at certain points. This allows us to handle the mesh adaptation process as meshing with certain constraints. As the whole remeshing process is quite time consuming we can select the regions of interest and remesh only locally. As the initial boudary for meshing we chose the boundary of the region where refinement is needed.

In general we refer to methods which change the mesh as mesh adaptation methods. These cover mesh refinement, coarsement as well as point relocation. All these methods can be used by mesh control methods which evaluate error estimates or geometrical quality measures.

Mesh Optimization

In the following we point out some kind of overall control mechanism which brings together the error estimation methods as well as geometrial quality measures with the methods of mesh adaptation. We will introduce some control heuristics (Fig. 4) which reduce the global error to a given limit by adapting the mesh.

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 too fine meshes in regions of low error. In some cases points have to be relocated in order to obtain a better fit to the continous problem.

There are different techniques of mesh control. First, one can 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%) is refined.

The solution quantities are very sensitive to the mesh so that it is possible that local remeshing changes the

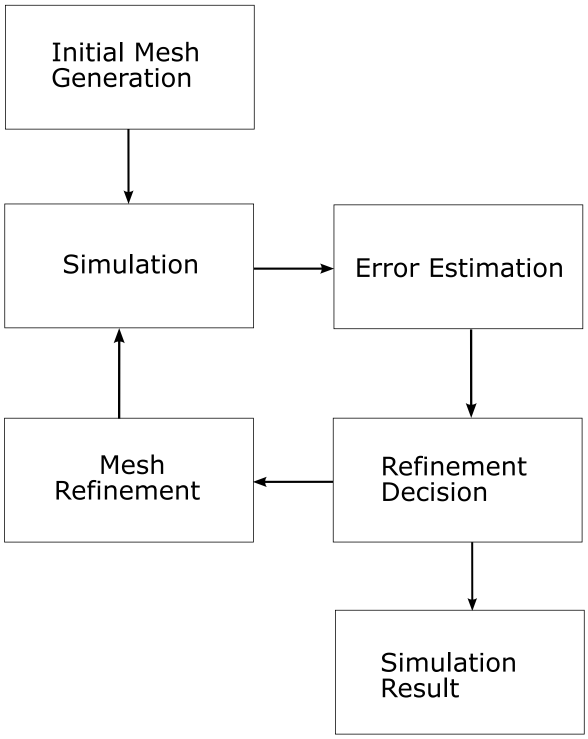

Figure 4: Mesh controlling loop. This loop is run through while the mesh is adapted to the model problem.

integral quantities by some ten per cent. Therefore stepping quantities is problematic because changes of the mesh result in discontinuities in the resulting characteristics which are artefacts of the mesh adaption.

Examples and Results

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. In the following we will compare the accuracy of the solution as well as the complete time for the iterative mesh optimization process to the uniform refinement.

We start with an initial mesh (Fig. 5) and increase the point density in regions where the error estimator returns very high values (Fig. 7). Then we solve the Laplace equation again and re-estimate the error on the new structure (Fig. 8). We do this iteratively until we have only elements with an error below a certain error bound.

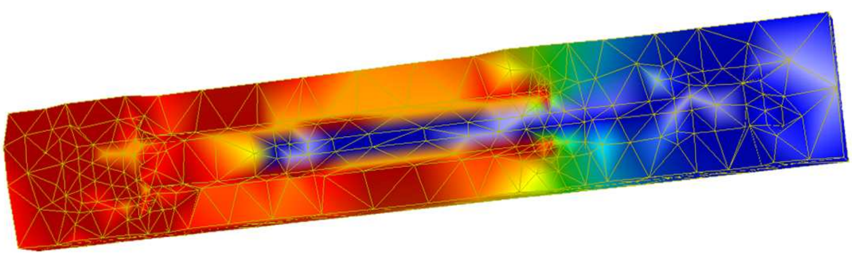

Figure 5: The structure with initial mesh (about 1000 points).

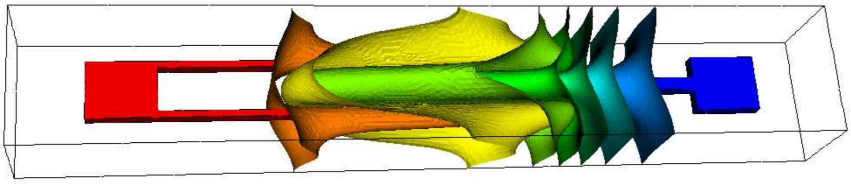

Figure 6: (left) Iso-potential surfaces of a referenc estructure with uniform refinement (53 million points).

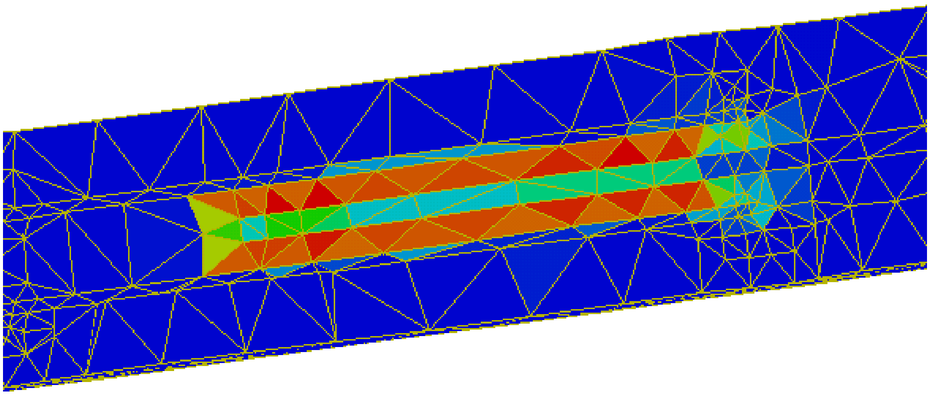

Figure 7: Adaptively refined structures. The error after the initial calculation (1000 points).

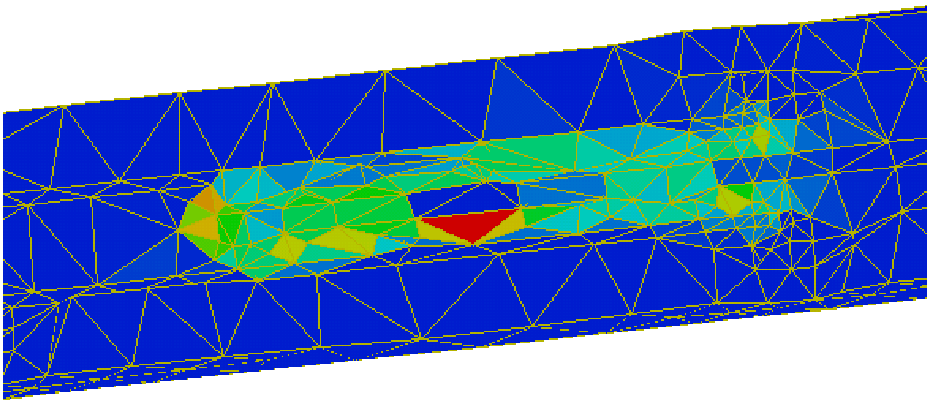

Figure 8: Adaptively refined structures. Error after two steps calculation(1500 points).

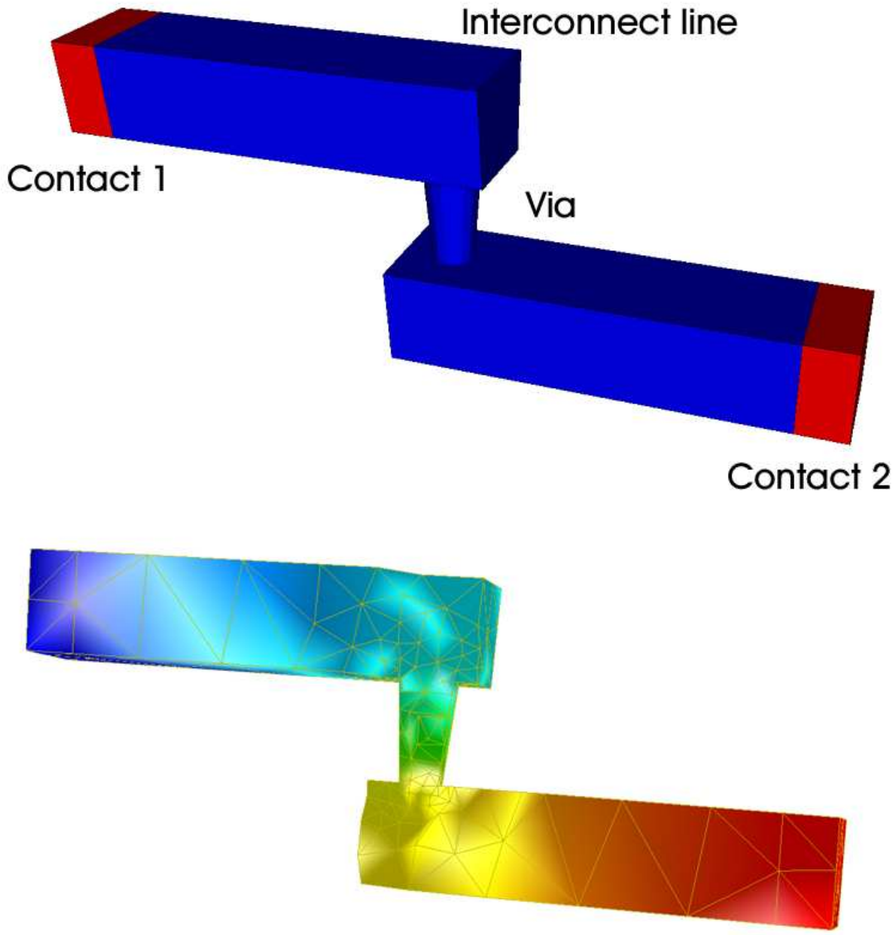

Figure 9: The initial structure: (top) At the red ends of the interconnect structure Dirichlet boundary conditions are applied. In the interior of the structure we assemble the Laplace equation with finite elements. At the blue boundary of the structure we use zero Neumann boundary conditions. (bottom) The initial mesh as well as the solution of the first calulation step.

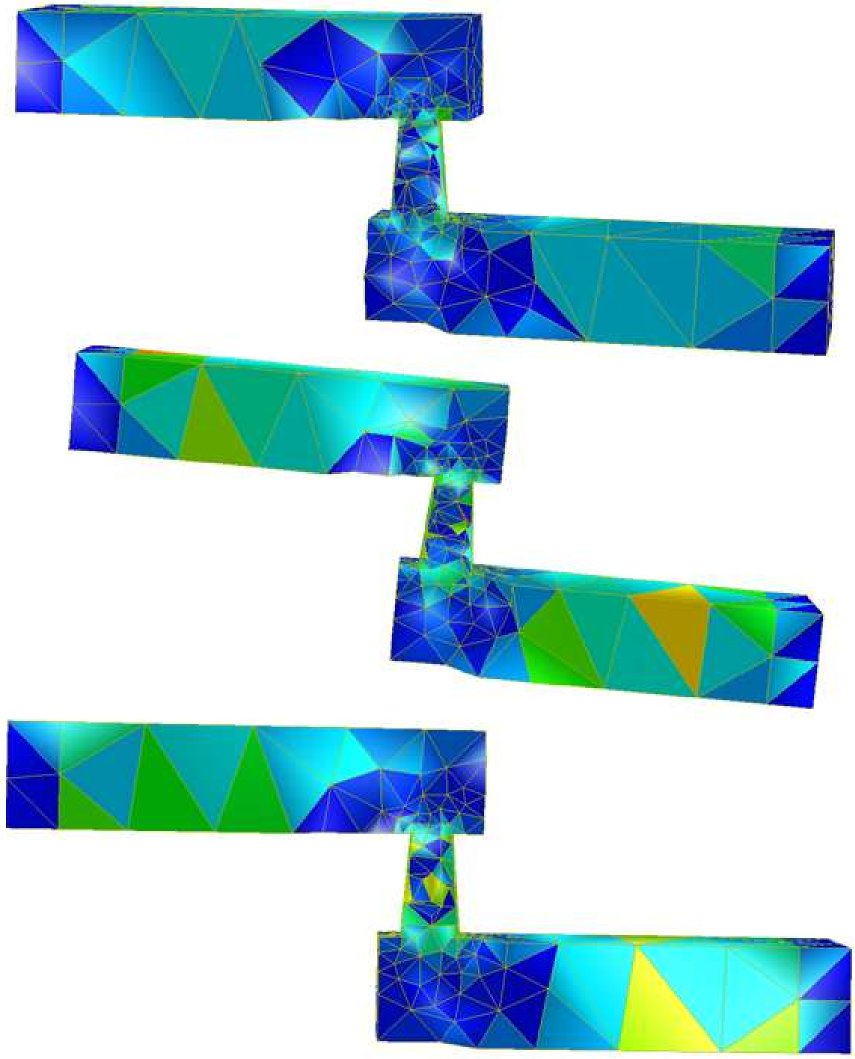

Figure 10: As we could expect the error estimator indicates that a greater resolution is required in the interior of the region. The blue regions indicate low error whereas the red regions indicate higher error. As we can see the via regions have to be resolved much finer than the line regions.

As we can see from these figures the local errors could be decreased by inserting 500 points. In contrast to uniform refinement which would increase the number of vertices and cells by a factor of 8 when we chose half of the aspect ratio. In both cases we can show that the adaptive meshes lead to solutions of high precision without the drawbacks of high numerical effort.

Conclusion

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. Mesh adaptation allows us to improve the mesh quality locally without increasing the number of mesh points dramatically. For this reason the mesh of the critical simulation domain is much finer whereas the regions of lower interest do not increase the simulation time without any relevant loss of accuracy. In combination with a posteriori error estimation a measure was found which triggers the refinement and indicates whether the mesh was adapted accurately.

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