Coupling Three-Dimensional Mesh Adaptation with an A Posteriori Error Estimator

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***Abstract*— A three-dimensional unstructured mesh adaptation technique coupled to a posteriori error estimation techniques is presented. In contrast to other work [1, 2] the adaptation in three dimensions is demonstrated using advanced unstructured meshing techniques to realize automatic adaptation. The applicability and usability of this complete automation are presented with a real-world example.**

I. INTRODUCTION

Several different methods are employed in TCAD to calculate the solutions of partial differential equations. The differential equations that need to be solved result from modeling a number of disparate physical phenomena such as dopant diffusion, mechanical deformation, heat transfer, fluid flow, electromagnetic wave propagation, and quantum effects. Every one of these methods, like finite differences, finite elements and, finite volumes, has its merits and shortcomings and so are more or less suited for different classes of equations. All of these methods have in common that they require a proper tessellation of the simulation domain. How suitable a given tessellation is, not only depends on the method employed to compute an approximate solution, but also only on the type of equation.

This transition from the continuous domain to a discretized domain will inherently produce errors in the computed results, no matter how sophisticated or how appropriate a mathematical model is. This approximation error can be enormous, and can completely invalidate numerical predictions if no estimated or quantitative measure of these errors is available. The general subject is referred to as *a posteriori error estimation*. When equipped with such a measure for the error resulting from the choice of a tessellation, the question arises how to change the tessellation in order to improve the accuracy of the calculated result. In order to meet most useful this has to be accomplished without user interaction, as the user usually does not have the necessary experience. The procedure of generating tessellations is commonly known as mesh generation, but in this work the focus is placed on mesh adaptation.

Attempts of error estimation and adaptive mesh generation have already been undertaken exhibiting a highly increased rate of convergence in two dimensions when using a mesh adaptation scheme [3]. The results for the three-dimensional case have not displayed this desirable trend. This is attributable in great part to the problems involved in mesh generation for the three-dimensional case. A novel, fuzzy classification scheme to characterize the quality of the adapted mesh has shown extremely promising results [4].

II. MESH GENERATION AND ADAPTATION

The discretization of the underlying computational domain is the first step in a numerical solution procedure. A widespread approach to spatial discretization is to divide the simulation domain into a structured assembly of quadrilateral cells, with the topological information being apparent from the fact that each interior vertex has exactly the same number of neighboring cells. This kind of discretization is called *structured grid* or simply *grid*. The major disadvantage of this approach is, that the discretization of highly non-planar geometries produces a large number of points in the simulation domain. As a result the following calculations are slowed down and require a lot of computational resources due to the great amount of excess points.

The alternative approach is to divide the computational domain into an unstructured assembly of more or less arbitrary formed cells. The shape of the cells is constrained by the needs of the following computations. The notable feature of an unstructured mesh is that the number of cells surrounding a typical interior vertex of the mesh is not constant. This kind of discretization is called *unstructured mesh* or simply *mesh*. The major disadvantage of this approach is that the element generation process is one of the most complicated procedures in the field of simulation. However the reduction of simulation time and the requirements on computational resources can be significant.

Based on the complex three-dimensional mesh generation process and the impracticality of using uniform refinement strategies most TCAD tools are based on grids. But with the shift to real-world input structures of almost arbitrary complexity the grid approach with the involved refinement steps is no longer viable and unstructured mesh generation techniques become increasingly attractive despite incurring several complications.

In two dimensions the user can supervise the generation of a mesh and even adjust its adaptation relatively easily. The move from two to three dimensions virtually eliminates this possibility, as both visualization and user interaction are by far more difficult. As a result the user has little knowledge where to best adapt the mesh. Because of this it is essential for three-dimensional mesh generation and adaptation to work in conjunction with some kind of error estimator to make automatic generation and adaptation without user intervention possible.

The relationship between numerical accuracy, the condition of the stiffness matrix, and the quality of the elements of the underlying mesh is still not completely understood, even for the simplest of cases. According to experience and mathematical results, isotropic elements usually lead to good overall results while degenerated elements will negatively affect the computation. An abstract quality criterion for elements which have to be refined had to be developed so that automatic remeshing can be accomplished easily by locally removing patches of tetrahedra and inserting points derived from the error estimator.

The calculation of the abstract quality criterion that controls the adaptation of the mesh is cleanly separated from the actual meshing procedure. This enables an easy exchange of the mathematical error estimator and also eases independent software development of the individual components.

In the field of unstructured mesh modification the following techniques are used: *the h-method*: this method uses a geometrical parameter h for refinement (i.e. the height of a tetrahedron), *the p-method*: this method varies the degree p in the approximation (i.e. quadratic ansatz functions within finite elements) while keeping the geometrical size h unchanged, *the hp-method*: this method combines the p-method with the h-method or *an adaptive remeshing method*: this method extracts a patch of marked elements which are accordingly remeshed. The adaptive remeshing method employing an advancing front meshing method [5] is the focus of the presented work because of its high degree of freedom.

III. ERROR ESTIMATION

Discretization of the equations describing the problem is needed to make numerical treatment possible. The discretized problem then results in a discrete distribution of quantities and ansatz functions. The accuracy of the simulation does not solely depend on the quality of the underlying mesh but also on the suitability of the ansatz functions that have been chosen. The use of piecewise affine or constant ansatz functions, as in the cases of finite elements or finite volumes, results in a certain characteristic of the error. In terms of function spaces a projection of the complete space of functions to the subspace of the chosen ansatz functions is performed. The euclidean norm can then be used to measure the distance of two functions.

$$\|f-g\|_2 = \sqrt{\int_{-\infty}^{+\infty} \big(f(x)-g(x)\big)^2 \mathrm{d}x} \tag{1}$$

A. Residual based error estimation

For a residual based error estimator (RS) a globally continuous function is constructed by piecewise affinely interpolating the computed numerical solution (Figure 1) for each triangle. The Laplace equation is satisfied exactly for the interior of the triangles but is discontinuous at the boundaries. This discontinuity of the interpolated function leads to an error that

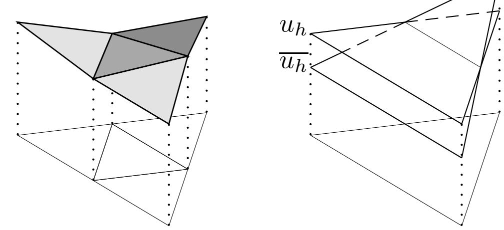


Figure 1: Left: Two-dimensional representation of the error estimator. The normal component of the error changes at the facet. Right: Discrete solution function u_h and the interpolation function $\overline{u_h}$ as function over the mesh triangle.

can be estimated locally by the following expression [6]:

$$\eta_K = h_K \Big(\sum_{E\in E_K \cap E_{\text{int}}} \| J_{E,n}(u_h) \|_E^2 + \sum_{E \in E_K} \| J_{E,t}(u_h) \|_E^2 \Big) \tag{2}$$

here E_K denotes the edges of the triangle and E_{int} is the set of the interior edges. The two components of the sum are the normal component $J_{E,n}$ and the tangential component $J_{E,t}$ of the gradient $\vec{J_E}$ of the local discontinuity of the interpolated function. The geometry factor h_K marks a characteristic length of the triangle such as the mean edge length or the circumference radius.

Due to the use of piecewise affine interpolation the resulting function is continuous and hence the tangential component of the jump vanishes and only the normal component has to be considered.

The behavior of this error estimator can be explained quite easily. A gradient of the potential leads to a flux that is assumed to be free of sources in the case of the Laplace equation. A discontinuity of the flux as it passes through a facet of a tetrahedron indicates a source of flux within the tetrahedron. This, however, is a contradiction to the assumption of vanishing source density associated with the Laplace equation. In case the potential behaves smoothly when crossing a facet the error thereby estimated approaches zero.

B. ZZ Error Estimator

The ZZ error estimator [7] assumes the smoothness of the correct solution. A smoothed solution $\overline{u_h}$ (Figure 1) is calculated form the numerical solution u_h and then compared to the numerical solution. The difference of u_h and $\overline{u_h}$ is interpreted as a measure for the error in the solution u_h. The ZZ error estimator has been shown to have both an upper and a lower bound for certain types of differential equations such as the Laplace equation [7]. Polynomial functions of degree one in each tetrahedron have been chosen to obtain the smoothed solution. The distance between the interpolated piecewise affine function and the piecewise constant function can be determined by the evaluation of the norm presented in (1) and yields:

$$\eta_K = \sum_i U_i^2 - \sum_{i\neq j} U_i U_j \tag{3}$$

where the U_i are the resulting potential values at the vertices of the tetrahedron.

IV. Results

In the following the results of the error estimation and mesh adaptation techniques are shown. We demonstrate the behavior of our mesh adaptation and error estimation coupling strategy with a realistic interconnect line with tapered line elements (lines with angular side walls) and pyramidal elements as the vias, which connect the two lines. The considered structure is presented in Figure 2. Afterwards we compare the residual and the ZZ error estimation techniques. The evolution of the quality of the tetrahedra during the mesh adaptation process is also presented.

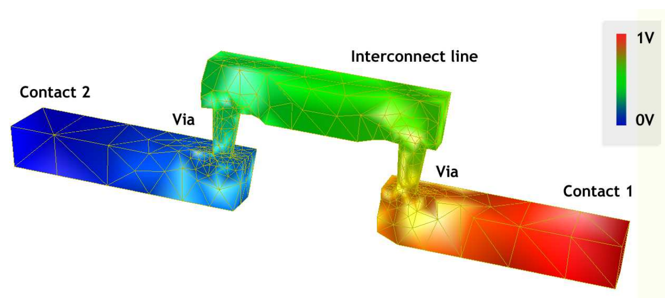
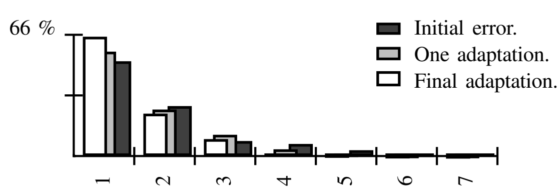


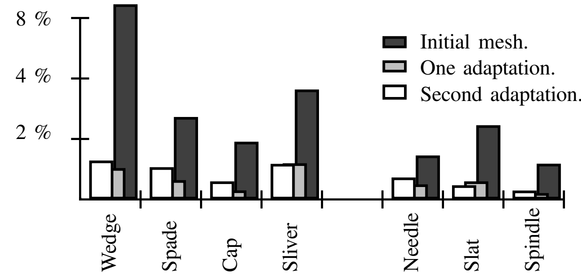
Figure 2: Initial interconnect structure with potential gradient

The next diagram presents the results from the residual error estimation technique. The residual of each element is calculated taking into account its neighboring elements, therefore the error estimates give an excellent indication where to adapt the mesh and the errors are quickly reduced. This comes at the expense of computation time, which is twice that of the ZZ error estimator.

With respect to mesh quality and the subsequent simulation steps, it is very important to bound the degree of degeneration to an upper limit. Therefore we use a fuzzy tetrahedra classification scheme [4] and separate the tetrahedra into seven categories. It is imperative for the following calculations that the *sliver* type is eliminated wherever possible.



The distribution of mesh elements indicating the mesh quality based on the fuzzy classification scheme is presented next. It can be seen that the error decreases due to the adaptation process, while keeping excellent overall mesh quality.



The visualization of the estimated error using the residual thechnique during three adaptation steps is shown in Figures 3, 4 and 5. Again the reduction of error is observed clearly.

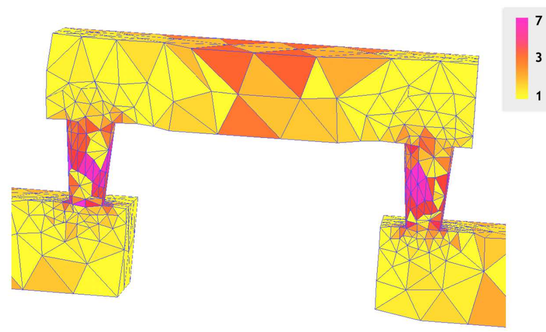


Figure 3: RS error estimation adaptive mesh refinement steps, initial error

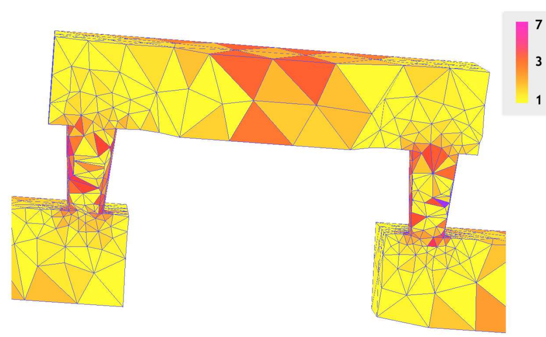
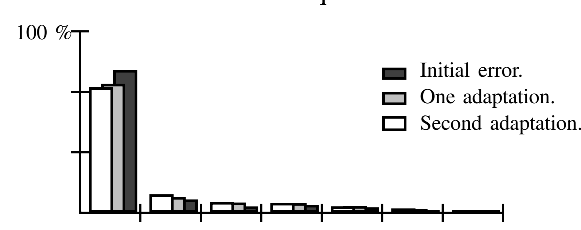


Figure 4: RS error estimation adaptive mesh refinement steps, first adaptation step

The next diagram presents the distribution of the ZZ estimated error classes within the first, second and last adaptation step. The ZZ error estimation technique is by its design very localized and therefore cannot include any information based on the neighboring tetrahedra. Because of this technique does not shift all elements to the lower error classes as quickly as the residual error estimation technique does.



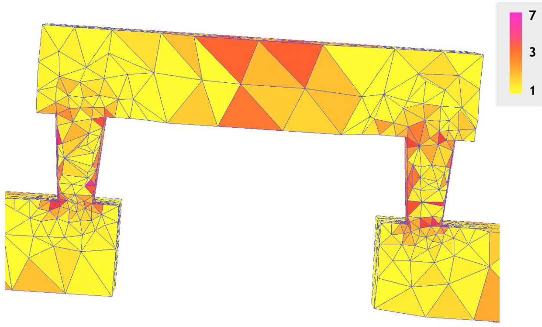
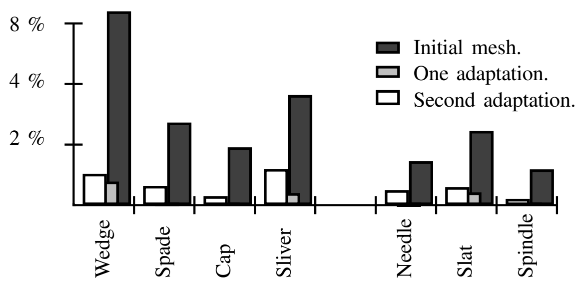


Figure 5: RS error estimation adaptive mesh refinement steps, last adaptation step



Finally, to give an impression of the estimated ZZ error we present a three-dimensional tetrahedra visualization of the error values in the next figures (Figures 6, 7, 8). All colors are mapped to the same range by a so-called transfer function.

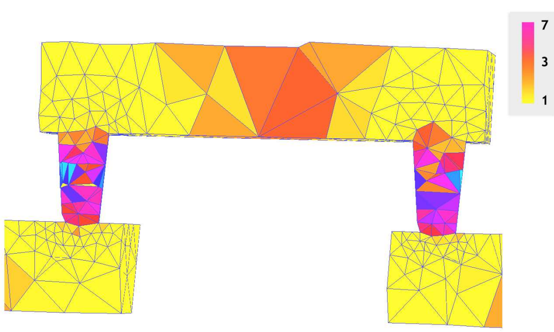


Figure 6: ZZ error estimation adaptive mesh refinement steps, initial error

V. CONCLUSION

The feasibility of coupling an a posteriori error estimator to adaptive meshing has been presented. Utilizing recent advances in mesh generation it has become possible to dramatically increase the quality of the simulation result while at the same time keeping the simulation time and required resources to a minimum. This is achieved by only refining areas corresponding to high error values using adaptive meshing leading to an automatic adjustment of mesh density in sensitive areas.

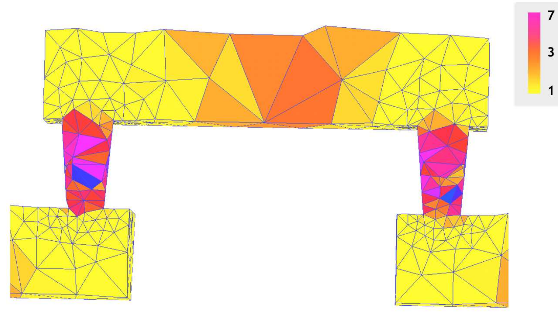


Figure 7: ZZ error estimation adaptive mesh refinement steps, after first adaptation step

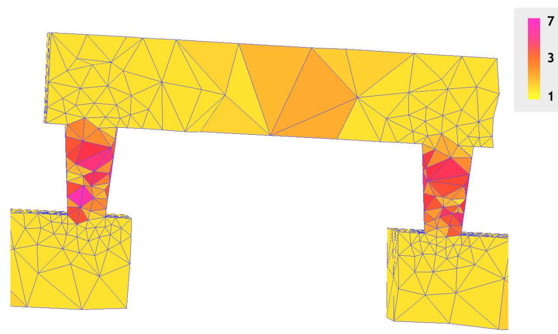


Figure 8: ZZ error estimation adaptive mesh refinement steps, last adaptation step

The ZZ error estimator is cheaper to compute compared to the residual error estimator, but also shows a lower rate of convergence.

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