A NOVEL TECHNIQUE FOR COUPLING THREE DIMENSIONAL MESH ADAPTATION WITH AN A POSTERIORI ERROR ESTIMATOR

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ABSTRACT

We present a novel error estimation driven three-dimensional unstructured mesh adaptation technique based on a posteriori error estimation techniques with upper and lower error bounds. In contrast to other work [1, 2] we present this approach in three dimensions using unstructured meshing techniques to potentiate an automatically adaptation of three-dimensional unstructured meshes without any user interaction. The motivation for this approach, the applicability and usability is presented with real-world examples.

1. INTRODUCTION

Most TCAD (Technology Computer Aided Design) problems can be formulated with partial differential equations and solved by numerical methods, usually finite difference, finite element and finite volume methods. They are used to model disparate phenomena such as dopant diffusion, mechanical deformation, heat transfer, fluid flow, electromagnetic wave propagation, and quantum effects. An essential step in these methods is to find a proper tessellation of a continuous domain with discrete elements, in our case tetrahedra.

This transition from the continous 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 we have no estimated or quantitative measurement of these errors. The general subject is referred to as *a posteriori error estimation*. It is an essential step to observe and bound the approximation error and to have a mesh adaptation strategy to guarantee the accuracy of the solution within a given range. In contrast to two dimensions where mesh generation and adaptation techniques are mostly based on hand crafted meshes or grids, it is almost impossible to design grids or meshes in three dimensions. On that account it is very important to generate and adapt meshes in three-dimensions automatically.

2. MESH GENERATION AND ADAPTATION

The first step in solving equations numerically is the discretization of the underlying computational domain. A widely used approach has been to divide the domain into a structured assembly of quadrilateral cells, with the topological information being apparent from the fact that each interior vertex is surrounded by exactly the same number of 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 elements produces a large number of points in the simulation domain. As a consequence the subsequent simulation and calculation steps are slowed down requiring a lot of computational resources.

The alternative approach is to divide the computational domain into an unstructured assembly of cells. The notable feature of an unstructured mesh is that the number of cells surrounding a typical interior vertex of the mesh is not necessarily 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 in 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 of the TCAD simulations are based on structured grids. But with the shift to real and complex input structures the grid approach with the involved refinement steps is no longer manageable. Here the unstructured mesh generation techniques come into play. In two dimensions most of the grid or mesh design procedure and adaptation steps are done by hand. With the step from two-dimensional to three-dimensional mesh generation and adaptation a hand crafted design and adaptation is impossible. First, the user interaction and visualization in three-dimensions is very difficult. Secondly the user can not be aware where the adaptation should be done. On this account three-dimensional mesh generation and adaptation must be coupled with error estimation techniques to ensure an automatic adjustment for a given problem without user interaction.

A difficulty in the field of mesh adaptation is that to this date the understanding of the relationship between the quality of mesh elements, numerical accuracy, and stiffness matrix condition remains incomplete, even for the simplest cases. Experience and mathematical results have shown that isotropic elements usually lead to good results while degenerated elements will negatively affect the computation. Therefore we derive an abstract quality criterion for elements which have to be refined so that automatic remeshing can be easily accomplished by locally removing tetrahedra patches and inserting points derived from the error estimator. Our novel technique of calculating an abstract quality criterion to control the mesh adaptation or remeshing step separates the mathematical error estimation step from the geometrical meshing step and can therefore be implemented with different error estimation models. Also the software components can be easily upgraded. In the field of unstructured mesh modification the following techniques are possible:

- H-method
  This method uses a geometrical parameter h for refinement (i.e. the height of a tetrahedron).
- 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.
- HP-method
  This method combines the p-method with the h-method.
- Adaptive remeshing method
  This method extracts a patch of marked elements which are accordingly remeshed.

For our technique we focus mainly on the adaptive remeshing method (some kind of advancing front method [3]) because of the maximum degree of freedom within mesh adaptation.

3. ERROR ESTIMATION

The numerical expression of a discretized problem results in a discrete distribution of quantities and ansatz functions of a certain function class (e.g. piecewise affine functions) to describe the behavior of the quantities. Apart from the quality of the underlying mesh the quality of the simulation essentially depends on the selection of the ansatz functions. Using piecewise affine or constant ansatz functions like finite volumes or finite elements we always obtain results with a certain error. In terms of function spaces we carry out a projection of the complete space of functions to the subspace of piecewise affine or constant functions. Usually the euclidian norm is used in order to measure the distance between two functions.

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

3.1 Residual based error estimation

On each triangle the solution function is interpolated piecewise (Figure 1) affinely so as to receive a globally continuous function. This function fulfills the Laplace equation in the interior of the triangle whereas the discontinuity of the interpolated solution function at the boundaries leads to an error which can be estimated locally by the following formula [4]:

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

where E_K denotes the edges of the triangle and E_{int} is the set of the interior edges. The local discontinuity of the gradient of the interpolated function at an edge is $\vec{J_E}$, where $J_{E,n}$ is the normal component and $J_{E,t}$ is the tangential component. The geometry factor h_K denotes a characteristic length of the triangle such as the mean edge length

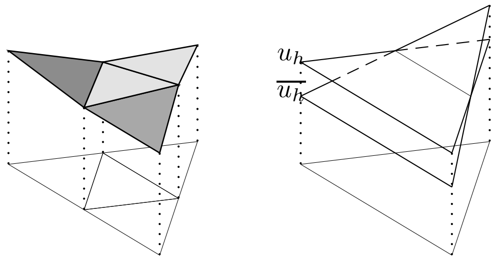


Figure 1: (left) Two-dimensional representation of the error estimator. The normal component of the error changes at the facet. (right) Discrete solution function u_h and the interpolation function $\overline{u_h}$ as function over the mesh triangle

or the circumference radius. An interpretation of the behavior of the error estimator is given in the following. A gradient in the potential causes a flux, which is free of sources in the case of the Laplace equation. If the flux is discontinuous through a facet of a tetrahedron there has to include source density on the facet. The Laplace equation states, however, that the source density vanishes. Therefore the estimated error is zero if the potential behaves smoothly when crossing a facet. As we use piecewise affine interpolation the function is continous and therefore the jump of the tangential field strength has to vanish. For this reason only the normal components of the field strength are relevant.

3.2 ZZ error estimation

The ZZ error estimator [5] measures how much the numerical solution u_h differs from a smoothed numerical solution $\overline{u_h}$ (Figure 1). For some types of differential equations such as the Laplace equation the ZZ estimator has been shown to have upper and lower 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 the norm (1) and yields,

$$\eta_k = \sum_i U_i^2 - \sum_{i \neq j} U_i U_j \qquad (3)$$

where the U_i are the result values in the vertices of the tetrahedron.

3.3 Evaluation of the error estimation

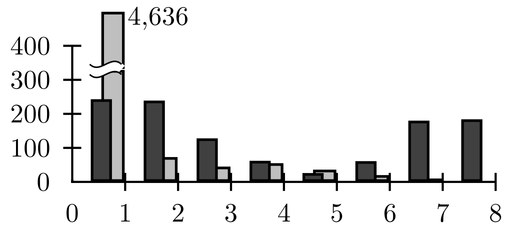
A quality statement regarding the calculation can be given counting the simplices within a certain error interval of error values. The range of errors (from zero to the maximum error) is divided into equidistant error classes, i.e. ten classes. With this separation different adaptation strategies can be used: *minimum number of elements*, *error in element*, or *maximum number of elements*. Here we use the *maximum number of elements* strategy, which is bound to 30% in each refinement step, and the *error in element* strategy, only to sort the elements.

4. RESULTS

In the following the results of the error estimation and mesh adaptation techniques are shown. We use two different examples to demonstrate the behavior of our novel technique of coupling the error estimation and mesh adaptation steps through an abstract interface. First, we use a non-planar capacitor structure and calculate the potential distribution between the contacts. Here we use the residual error estimation technique only to show the shift of the quality of the elements within each error class. The second example deals with a realistic interconnect line with tapered line elements (lines with angular side walls) and a pyramid element for the via, which connects the two lines. Here we compare the residual error and the ZZ error estimation technique. For the non-planar capacitor we give a comparison of the initial error and the error value after one remeshing step:

	Initial meshing	Remeshing
Tetrahedra	2,145	8,774
Minimum error	0.02	0.001
Maximum error	25.0	19.4

The next diagram shows the distribution of error values. The number of tetrahedra is plotted on the y-axis while the x-axis shows the error classes. The light gray boxes show the refined error values whereas the dark grey boxes show the initial error values:



As can be seen, the error values for the elements are shifted to the left side indicating that the local error values drop due to our refinement technique. Figure 2 depicts the error values without any refinement, whereas Figure 3 shows the distribution of error values after one adaptation step (zero stands for a lower error, and one denotes a higher error). As we have seen in the error value

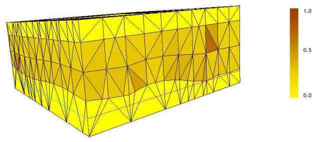


Figure 2: Initial local error values without refinement

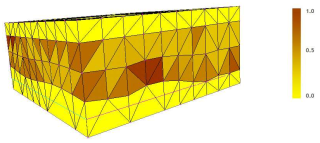


Figure 3: Local error values after one refinement step

diagrams the local error values are shifted to lower values.

To show the applicability and usability for a realistic example we solve the Laplace equation within an interconnect structure and show the successfully application of our technique. In Figure 4 we depict the structure, the contacts and the potential distribution. Figure 5 presents a three-dimensional visualization (not a cut through the structure) of the relative error based on the residual error estimation technique within each adaptation step. Compared to the residual error estimator, Figure 6 presents the adaptation steps based on the ZZ error estimation technique. The

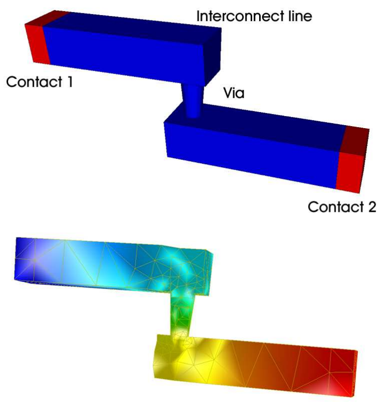


Figure 4: Initial interconnect structure (top) and potential distribution (bottom)

following table gives a comparison of the number of tetrahedra after each adaptation step within the two different error estimation techniques:

	Initial step	Step 1	Step 2
RS: Tetrahedra	1,720	2,052	2,334
ZZ: Tetrahedra	1,720	2,075	2,290

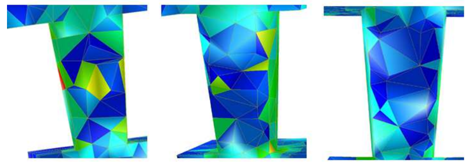


Figure 5: Residual based error estimator, zoomed into the important via: first three adaptation steps

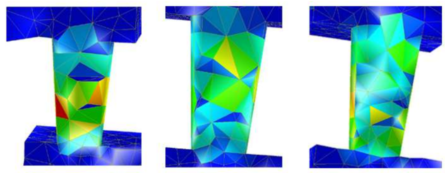


Figure 6: ZZ error estimator, zoomed into the important via: first three adaptation steps

5. CONCLUSION

Using the advantages of mesh refinement in combination with a posteriori error estimation leads to an enormous increase of simulation result quality. The benefits of adaptive mesh refinement allow us to locally improve the mesh quality without increasing the number of mesh points dramatically. For this reason the resolution of the critical simulation domain is much higher and the relevant processes can be better simulated whereas the regions of lower interest do not require much simulation time. In combination with a posteriori error estimation a measure was found which triggers the refinement and indicates if the quality of the solution is resolved adequately.

6. REFERENCES

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