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Three-Dimensional Grid Adaptation Using a Mixed-Element Decomposition Method

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Abstract

A new method for adaptive refinement of unstructured grids has been developed. This method ensures preservation of the element quality and the structural anisotropies of the initial grid. The flexibility of unstructured grids in combination with the implemented error estimation provides a powerful basis for three-dimensional simulation of time dependent processes.

1. Introduction

Efficient and accurate simulation of transient three-dimensional redistribution processes requires adaptive gridding methods. The computational grid is responsible for both the accuracy of the solution as well as for the simulation efficiency. In order to meet with these requirements throughout a transient simulation, the grid has to be adapted as the distribution of the solution changes.

One approach to solve this problem is to start with a coarse initial grid and to adapt the local grid density by means of recursive element refinement. On one hand the low required density of the initial grid allows a fast generation and, on the other hand, the recursive refinement can also be carried out efficiently. Thus, the overall computational effort for the grid handling is kept low.

2. The mixed-element decomposition method

Our adaptation algorithm starts from a coarse unstructured grid, which resolves the computational domain and may consist of tetrahedrons and octahedrons. In contrast to octree based methods (e.g. [1]) the alignment of the grid elements is not restricted to a rectangular bounding box. Thus, also oblique interfaces and boundaries can be resolved optimally. The elements of this initial grid are refined recursively until the desired accuracy is reached. As the diffusion advances further adaptation steps may be required. Then already refined elements are either refined again or replaced by their parent element to achieve the required grid density.

For a recursive refinement algorithm it is important to preserve the essential grid properties, i.e., the grid quality and the structural anisotropies. Therefore we developed the mixed element decomposition method:

We divide a tetrahedron into four tetrahedra of the same shape and one octahedron. The four tetrahedra are located at the parent's corners and the octahedron is placed in the center (Fig. 1). An octahedron is divided into six octahedra of the same shape and eight tetrahedra. The six octahedra are located at the parent's corners and the remaining tetrahedral parts have a common node in the center (Fig. 2). In order to discretize an octahedron, we split it into eight tetrahedron, each of which has one face of the octahedron as ground plane and the octahedral center as opposite node.

To evaluate the effectivity of the method, it is of interest, how much the grid quality is decreased by the refinement. In order to compare the element quality of the elements generated by the refinement with the element quality of the parent element, we use (1) as a measure for the element quality, where V is the volume and h_{max} is the maximum size of the element (see [2]).

$$Q_e = \frac{V}{h_{max}^3} \tag{1}$$

The first refinement step introduces elements with a new aspect ratio. The elements generated by all following refinement steps have either the shape of the tetrahedra or the shape of the octahedra which exist after the first refinement step (see Fig. 3). Thus, the element quality is affected only by the first refinement step.

Taking into account the discretization of the octahedron permits a reasonable comparison of the octahedron and the tetrahedron: we compare the element quality of the tetrahedral parent with the element quality of the tetrahedra used for discretization of the octahedron. It can be shown, that the degradation of the element quality after (1) is limited to a factor of 1/2 for the tetrahedron and 1/4 for the octahedron.

As the refinement is always done locally, unrefined elements may be adjacent to refined ones. These neighbouring elements are called incompatible elements, and we define the order of incompatibility as the difference of the refinement levels of two adjacent elements. In our algorithm the order of incompatibility is restricted to one. A two dimensional example of such an incompatible situation is shown in Fig. 4. In order to estimate the grid quality at a compatible node between incompatible elements, we use $Q_n = \min(V_i)/\max(V_i)$, where V_i are the volumes of all elements incident to this node (see [2]). It can be shown, that the degradation of this nodal grid quality is limited to a factor of 1/4 for the tetrahedron and 1/8 for the octahedron.

3. Error Estimation

For the practical use of the mixed element decomposition method, an error estimation was implemented, which is based on a gradient smoothing of a finite element solution (see [3]). It allows to compute the gradient error as well as the local dose error. We use a linear combination of both as grid density criterion, where the weights can be chosen independently. All elements which are not reaching the desired accuracy are refined. On the other hand, elements with a very small discretization error are replaced by their parent elements (coarsening).

A proper discretization of the incompatible elements within one parent has to account for the C_0-continuity condition, which is a common requirement for the standard finite-element method. The function values for the incompatible node are determined by the interpolation equation which is the shape function of the parent element. For consistency reasons the matrices for the elements which are incident to the incompatible node are preassembled locally, and the equations for the incompatible nodes are replaced using the interpolation function. This results in a reduced matrix which we assemble to the global system matrix.

4. Example

We applied our algorithm to the silicon block of a conventional LOCOS-structure (Fig. 5). Firstly, we performed a Boron channel-implant, which we computed by a Monte-Carlo ion implantation simulation module[4] with an energy of 20keV and a dose of 1e14cm^{-2}. Then we adapted the initial grid according to the Boron profile, where the discretization error limit was set to 3% for the dose error and to 10% for the gradient error. Fig. 6 shows the resulting grid which consists of 9146 elements and 4285 nodes.

5. Conclusion

The mixed-element decomposition method combines the high flexibility of fully unstructured grids and the fast adaptation capability through recursive element refinement. From the shape preserving property it follows, that our algorithm preserves the boundaries and interfaces, and the structural anisotropy of the grid. Additionally, the quality degradation caused by the algorithm is limited to a constant factor. Thus, our grid adaptation method provides a powerful basis for three-dimensional process simulation.

Acknowledgement

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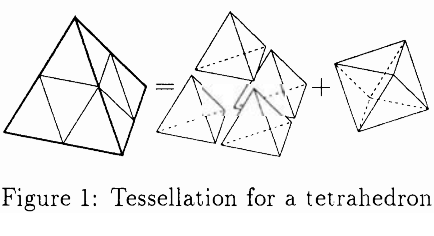

Figure 1: Tessellation for a tetrahedron

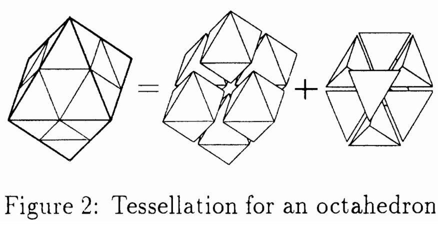

Figure 2: Tessellation for an octahedron

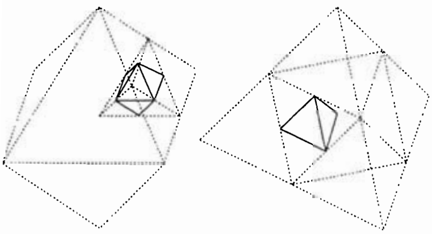

Figure 3: Shape preservation for recursive refinement

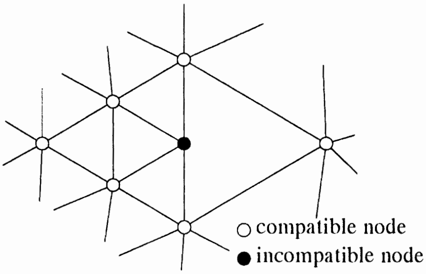

Figure 4: Incompatible elements

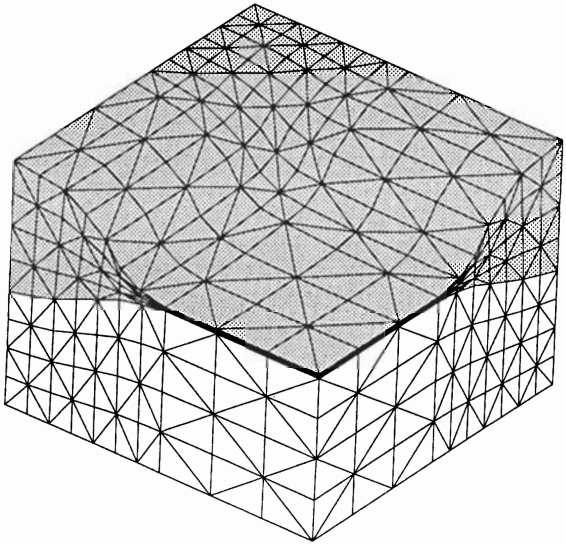

Figure 5: Initial grid for corner of the LOCOS structure

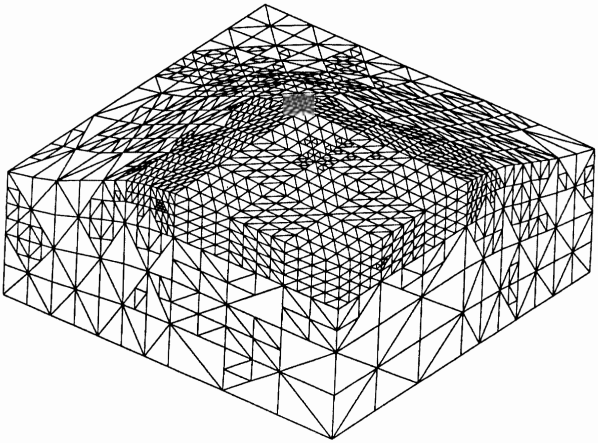

Figure 6: Grid of the silicon block adapted to the implanted Boron profile