Three-Dimensional Adaptive Mesh Relaxation

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Abstract

In numerical calculations based on partial differential equations the kind of discretization, in particular the kind of mesh that can be used is of atmost importance. Unfortunately, meshing is a rather unsolved discipline, especially in three dimensions. Although some occasional solutions exists there is hardly a tool that has integrated possibilities to handle this problem. This paper presents a numerical method for adaptive mesh relaxation, applicable in three dimensions, where with little effort a big benefit can be reached by adaptive mesh relaxation for a numerical simulation.

1. Introduction

A numerical method is presented for optimizing the placement of element nodes used in numerical calculations based on finite elements or finite-boxes. The problem that is addressed is as follows: Starting from a given mesh with a fixed connectivity structure we seek a numerical model to adjust the position of the nodes in a way so that a minimum error of a given analytical criterion can be achieved. A new triangulation with the same topology but adapted to a given criterion is computed.

The presented method is a mixture of an adaptive local mesh refinement and coarsement using an error estimation and a moving mesh based on artificial imprinted forces into a elasto-mechanical model depending on the element geometry. With AMIGOS [1] as a rapid prototyping system it was possible to reduce the rather complex elasto-mechanical differential equations used for relaxation to a very simple equation system that stays linear even in case of big movements of nodes.

2. Adaptive Mesh Relaxation Based on Element Geometry

The first approach was, to optimize the angles of a single element by using linear elasticity and internal forces which were proportional to the angles of the belonging element (Fig. 1). For the elasto-mechanical equations the displacement vector

$$\varepsilon = \begin{pmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_{xy} \end{pmatrix} = \begin{pmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial v}{\partial y} \\ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial y} \\ \frac{\partial u}{\partial x} & \frac{\partial v}{\partial y} \end{pmatrix} \cdot \begin{pmatrix} u \\ v \end{pmatrix} \tag{1}$$

has to be calculated in dependence of the stress tensor σ. In case of general linear elastic behavior, the relationship between stresses and strains are of the form

$$\sigma = D \cdot (\varepsilon - \varepsilon_0) + \sigma_0 \tag{2}$$

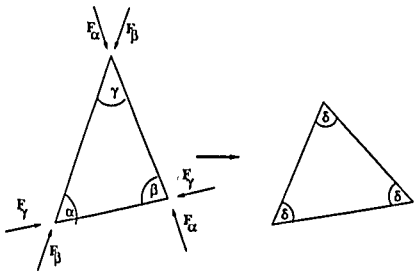

Figure 1: Imprinted forces depending on element angles.

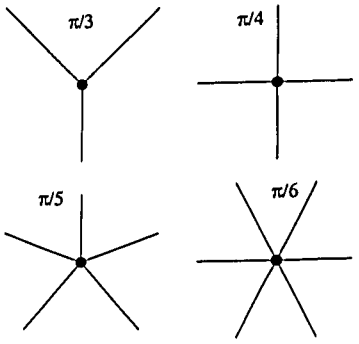

Figure 2: Resulting optimum angles due to given connectivity.

The nodal forces are calculated in dependence of the elements angle corresponding to the directions of displacement at node i

$$F_i = k \cdot (\frac{\pi}{3} - \varphi_{jk})^3 \tag{3}$$

under the condition that $\sum_{i=1}^{j} F_i = 0$. Unfortunately this attempt results in a non-linear formulation depending on the actual state of the angles of a single element and therefore calculation time increases significantly. Furthermore, the parameter k of (3) is essential for convergence and can not be set to a satisfying general value usable for any grid. Nevertheless, the results were very promising and due to the dualism of mechanics (on the one hand high nodal stresses where displacement is not possible, e.g. boundary corners, and on the other hand total relaxation where the system has enough freedom to move) the expected effect of grid relaxation was clearly recognizable. To increase the freedom of the system even at the boundaries the only restriction required is to preserve the geometry as can be seen in (Fig. 3).

Due to the fact that the relaxation should be material independent, and even shear stress is not important the mechanical equations can be reduced drastically. All we are looking for is an energetical minimum of the whole system which is equivalent to the vanishing of all inner forces artificially imprinted into the system but preserving the geometry. It turned out that this can simply be satisfied by forces compressing a single element, which minimize the volume. The forces have to be oriented along each elements edges with the condition $\sum_{i=1}^{n} F_i = 0$ per element like in the first attempt. Because of pinned boundary conditions (geometry preservation) the triangles do not collapse. Due to the imprinted forces each point moves towards its local optimum depending on the connectivity to other element points (Fig. 2). Furthermore this condition is now independent of the mechanical equations, because the minimum volume does not depend on the mechanical behavior since the compressment always tends to zero volume. The resulting degenerated equation system can now be written as

$$\vec{F_i} = k \cdot \vec{v_{ij}} \tag{4}$$

where F_i are the imprinted forces at the element nodes and v_{ij} denotes the orientation of the force along the element edge from point i to point j.

As a global result a stiffness matrix can be found where the total internal forces have to be minimized $\sum_{i=1}^{n} F_i^j = 0$. The simplified model is now linear and independent of the parameter k, since the optimum is always the same no matter how strong the

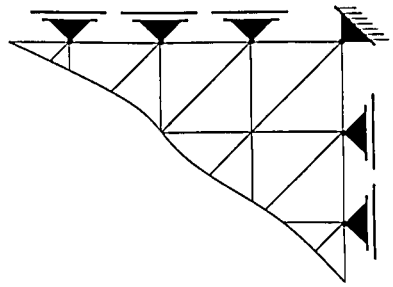

Figure 3: Moving boundaries for minimum restriction of freedom but preserving the geometry.

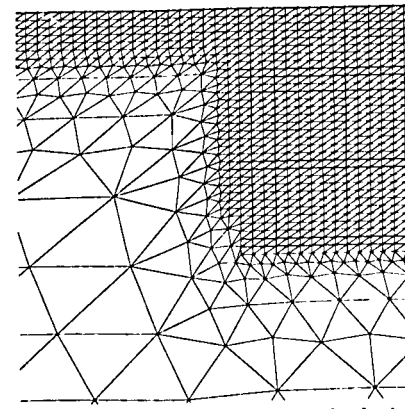

Figure 4: Mesh adaptation calculating a change in grid orientation along an internal topology change.

artificial forces are compressing. Unfortunately, there are some external influences to be considered. On the one hand, the boundary itself has less freedom in movement. This represents a massive bad influence on the optimum, which leads to the fact that sometimes a surface retriangulation might be necessary. But in most cases boundary conditions where surface points are allowed to move along the edge are enough to reach high quality grids (Fig. 5). On other hand internal connectivities of elements can not be changed and therefore it sometimes leads to a deviation of the optimum. A local retriangulation seems to be the only solution for this problem.

3. Examples

Since the influence mechanisms are quite simple, a mesh can also be extracted from an ortho-grid by splitting each rectangle into two triangles. As first example the interface between oxide and silicon of an oxidizing block is calculated using a level set method to distinguish between the two materials [2]. The corresponding grid is adapted to the moving interface (Fig 5). During recalculation of the grid, an adaptive hierarchical split method [3] is used and due to relaxation the resulting grid degradation is minimized by implicit smoothing. Even changing orientations can be achieved by a suitable grid-criterion (Fig. 4). The fact that a hierarchical adaptation is used which supports both, refinement and coarsement, is essential, otherwise due to grid movement the adaptation of a quantity would result in a miss-fitted adaptation.

The advantage of this method is, that it can immediately be used for three dimensions without any modifications. The example in (Fig. 6) shows an interface of oxygen and silicon adapted with the mesh relaxation method where the accuracy can be preserved but the number of mesh-points can be reduced in comparison to non-relaxation methods.

4. Conclusion

The presented method for adaptive mesh relaxation was the first attempt to use a general solver such as AMIGOS for grid adaptation purposes. The ability to combine this approach together with a physical model offers an attractive possibility for future simulations. To get rid of boundary and connectivity problems a powerful grid algorithm has to be combined together with the presented model to get a general usable grid adaptation without obvious restrictions.

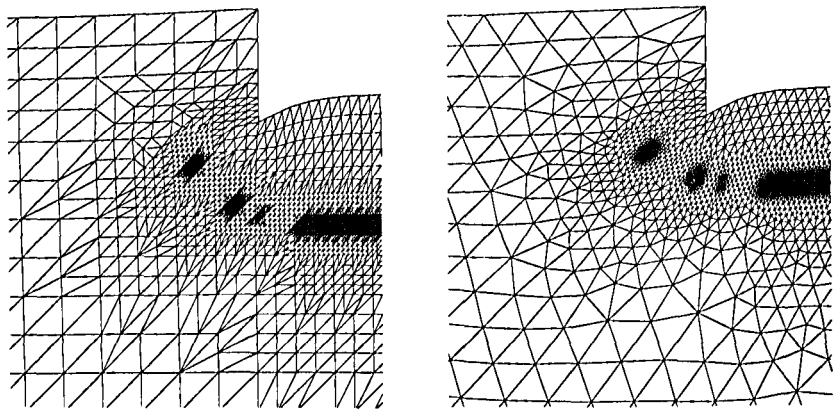

Figure 5: Adaptive hierarchical adaptation without and with relaxation.

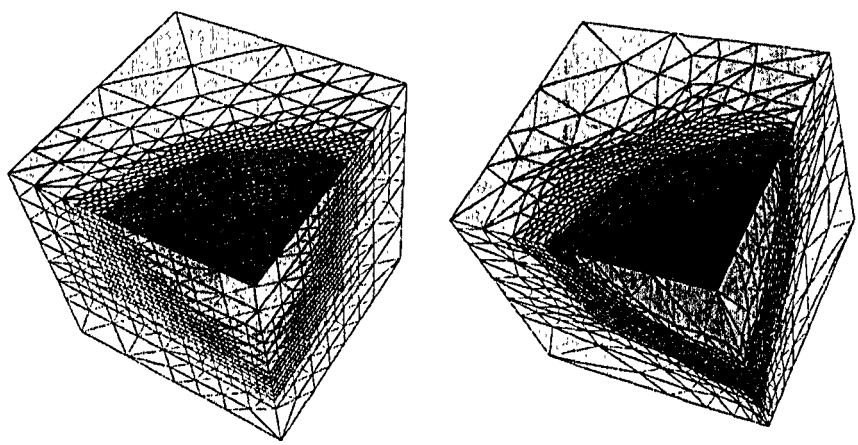

Figure 6: Hierarchical adaptation of a sphere calculated without (10742 points, 37482 tetraheadrons) and with (7588 points, 24901 tetraheadrons) relaxation to a maximum error of 10^{-5}.

References

[1] M. Radi, E. Leitner, E. Hollensteiner, and S. Selberherr, "AMIGOS: Analytical Model Interface & General Object-Oriented Solver," in *International Conference on Simulation of Semiconductor Processes and Devices*, (Cambridge, Massachusetts), pp. 331–334, 1997.

[2] M. Radi, E. Leitner, E. Hollensteiner, and S.Selberherr, "A Novel Diffusion Coupled Oxidation Model,"in *27th European Solid-State Device Research Conference* (Stuttgart, Germany), pp. 472–475.

[3] E. Leitner and S. Selberherr, "Three-Dimensional Grid Adaptation Using a Mixed-Element Decomposition Method," in *Simulation of Semiconductor Devices and Processes* (H. Ryssel and P. Pichler, eds.), vol. 6, (Wien), pp. 464–467, Springer, 1995.