A New Approach to Mesh Generation for Complex 3D Semiconductor Device Structures

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1 Introduction

In order to avoid numerical instability in solution of the large linear system derived from discretization by control volume method, the discretization mesh must satisfy the following two conditions. First, it should be the Delaunay partitioning defined by the mesh points. Second, it should be a "well-fitted" mesh to the boundary of the simulation domain, i.e. not only no mesh element intersects the boundary, but also the circumcenter of the mesh element lies in the same domain that the element belongs to. For instance, the tetrahedral element shown in Fig. 1 is not allowed in "well-fitted" 3D mesh. Although several 3D mesh generators have been developed that can handle complex device structures [1-3], general requirements for "well-fitted" mesh have not been investigated deeply. This paper presents a new approach to generate "well-fitted" tetrahedral mesh based on the consideration of such requirements.

2 Basic Procedure for Tetrahedral Mesh Generation

The flow of the new mesh generation procedure is given in Fig. 2 (a), which begins with triangulation of the domain boundary. Once the triangular mesh upon the boundary is given, "forbidden region" (hatched region in Fig. 2 (b)) can be determined around the boundary where any internal mesh point should not be placed so that circumcenters of the mesh elements lie within the domain. For example, the "forbidden region" given by a non-obtuse triangular element consists of one hemispherical region associated with the triangle (Fig. 3 (a)) and three hemispherical regions associated with each edge of the triangle (Fig. 3 (b)). Since the "forbidden region" is already known, an internal mesh in the simulation domain can be generated whose vertices lie out of "forbidden region," and this condition ensures the mesh to be "well-fitted." The final discretization mesh is obtained by constructing the Delaunay partitioning defined by the triangular mesh points on the boundary and the internal mesh points. This strategy does not put any restriction on the way of internal mesh generation nor the way of Delaunay partitioning. Therefore, any method that is considered as efficient or useful can be combined.

3 Implementation of Prototype 3D Mesh Generator

A prototype of 3D mesh generator based on this strategy is developed to investigate its practicality. Actual procedure is illustrated in Fig. 4. At present, triangulation of the domain boundary (1st step) is not implemented yet, and it is assumed that the triangular mesh is given. In order to allocate the internal mesh points in the domain, finite box mesh which roughly fits the boundary is generated through recursive box subdivision into 8 boxes starting from the bounding box of the domain. Since the mesh point close to the boundary will be eliminated in the next step, it is no use fitting to the boundary too fine. The box is divided if it includes more than 1 triangular mesh points, which is used as a heuristic domain approximation rule. These boxes are controlled by octree data structure which makes it easy to adapt box size according to certain quantity (impurity concentration, for instance) as shown in Fig. 5, except for the region near the boundary.

In the 3rd step, finite box mesh points that lie out of the domain or lie within the "forbidden region" are eliminated. Such points can be detected efficiently since each triangular mesh point keeps the box including it, which is an another advantage in utilizing octree. Finally, Delaunay partitioning is constructed by making tetrahedral element one by one, that does not include any other mesh point within its circumsphere. In order to make this process stable and fast, the last step is achieved by two separate steps. Firstly, such box elements that lie enough inside the domain are picked out and Delaunay partitioning for each box is constructed one by one. And then the intermediate region between the boundary and already tessellated boxes is divided into tetrahedra.

Fig. 6 shows the tetrahedral mesh generated for the domain with curved boundary approximated by faces with various slopes. Since tetrahedral mesh generation is possible as long as the triangular mesh on the boundary is maintained properly, this method will be able to cope with moving boundary. Mesh adaption near the boundary requires the ability to modify the triangular mesh flexibly, since the size of tetrahedral element around the boundary is mostly determined by the point density of the triangular mesh. This should be realized in future by, for instance, incorporating some 2D mesh adaption scheme proposed so far.

4 Summary

A new approach to mesh generation for general 3D domain is proposed. A prototype mesh generator which utilize octree for easy manipulation of 3D structures, is developed. It shows that "well-fitted" tetrahedral mesh can be constructed assuming that an appropriate triangular mesh upon the boundary is given. There is a good chance that adaptive meshing and moving boundary will be managed well in this mesh generation method.

References

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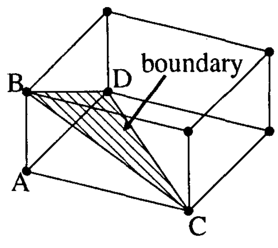
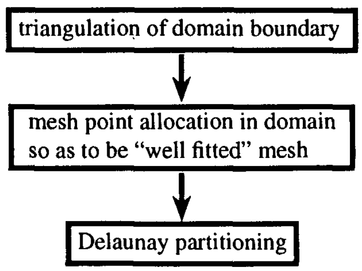
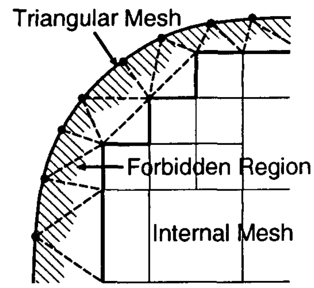


Fig. 1: A bad tetrahedral element (ABCD). Since its apexes locate on box corner point, the circumcenter of the tetrahedron lies in the other side of the boundary (BCD).

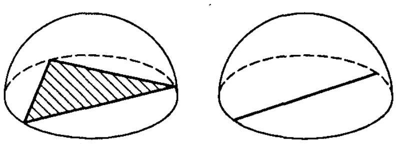


(a) Basic process flow



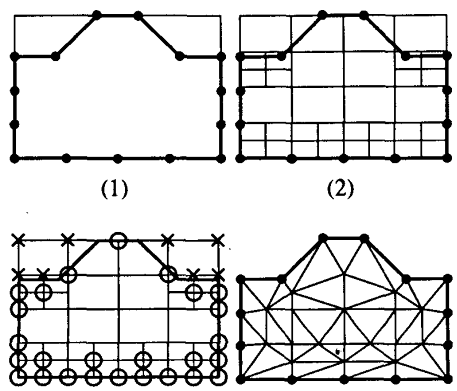
(b) Schematic view

Fig. 2: New meshing procedure.



(a) (b)

Fig. 3: Forbidden region for non-obtuse triangle upon the boundary. It is formed by a union of two kinds of hemispheres on domain side. (a) A circumsphere whose center locates at circumcenter of the triangle. (b) A sphere whose diameter is one of the edges of the triangle.



(1) (2) (3) (4)

Fig. 4: Mesh generation procedure realized in the prototype. (1) Triangulation of the domain boundary (not implemented yet). (2) Finite box mesh generation based on octree. (3) Elimination of the points out of the domain (×) and the points within the "forbidden region" (○). (4) Construction of Delaunay partitioning from the remaining mesh points. Internal boxes are divided first. These boxes should not have any eliminated points, and in addition, "forbidden region" formed by the box surface should not include any mesh point on the boundary.

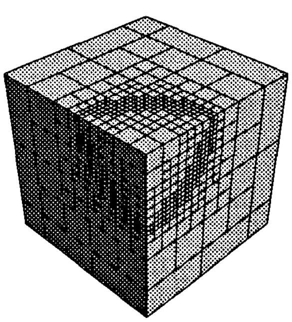
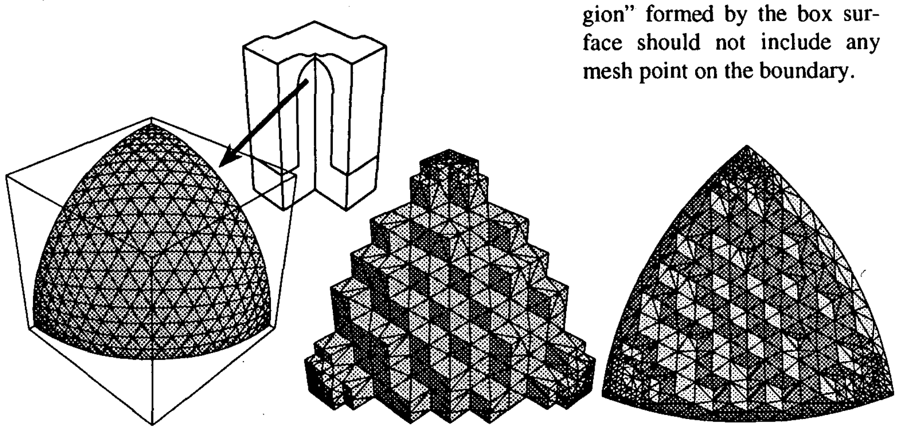


Fig. 5: Finite box mesh adapted to a virtual profile (spherical *pn* junction around one corner of box domain).



(a) (b) (c)

Fig. 6: An example of tetrahedral mesh generation. (a) Triangular mesh (~200 points) upon an artificial boundary. Hidden side of the boundary is considered as a simulation domain. (b) Tessellated internal boxes. (c) Tessellated intermediate region (reverse side).