A Hybrid Approach for Building 2D and 3D *Conforming* Delaunay Meshes Suitable for Process and Device Simulation

G. Garretón, L. Villablanca, N. Strecker, W. Fichtner

Integrated Systems Laboratory, Swiss Federal Institute of Technology Zürich
Gloriastrasse 35, CH-8092, Switzerland

Abstract

We present the latest results of our research regarding meshes suitable for both process and device simulation. Two major results are discussed in this paper: a consistent multi-dimensional mesh quality definition and a new hybrid multi-dimensional mesh generation approach. The consistent definition achieved is based on the conditions imposed by the Box integration method applied for both semiconductor process and device equations. The hybrid approach developed reaches a consistent mesh quality in all dimensions and it overcomes the severe limitations of our former mesh generators. Finally, it has been experimentally demonstrated that both the unified conditions and the hybrid approach are suitable for stable discretization schemes for device simulations based on the Box method.

1 Mesh quality required for device simulation

When developing a multi-dimensional device simulation tool based on the Box method (e.g. DESSIS-ISE [1]), a consistent definition of the required mesh quality in all three spatial dimensions has a strong influence on the selection of the appropriate meshing techniques.

In the past, the 2D mesh quality requirements have been mainly expressed by non-obtuse angle conditions. These conditions have been regarded as necessary for a stable Box integration scheme. Different constraints on the maximum angle in the elements have been used as major arguments to justify different mesh generation tools and techniques for process and device simulation.

On the other hand, the mesh quality requirements mentioned in the literature for 3D device simulation do not correspond to their 2D counterparts [2]. In 2D, much stronger conditions have been imposed (not a single obtuse angle is allowed in the mesh), e.g in [3, 4]. Nevertheless, 3D device simulation has been successfully performed using weaker conditions, e.g. by using the Voronoi diagram of a Delaunay mesh.

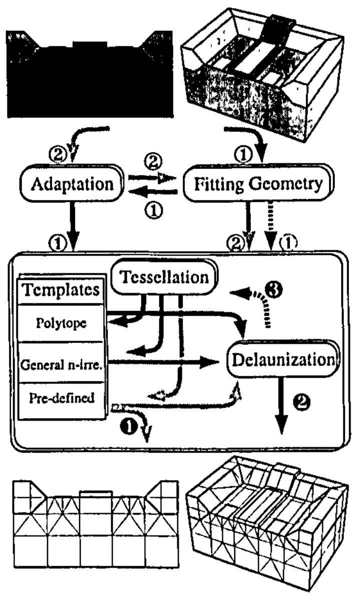

Figure 1: *The hybrid approach.*

It is rather difficult to express the 3D mesh quality criteria by constraints based only on angles. Instead, the corresponding 3D "Non-obtuse angle condition" can be easily expressed using the face and element Voronoi points, i.e. the centers of the circumscribed circle of the faces and the centers of the circumscribed sphere of the elements.

For 2D meshes with no obtuse angles, all Voronoi points (centers of circumscribed circles) of the elements are inside the elements. This condition can be extended into 3D as follows: all Voronoi points of the faces and all Voronoi points of the elements must be inside the elements. In this work, these meshes are referred to as *self-contained.*

However, 3D *self-contained* meshes are hard to build, and there is no 3D algorithm available in the current literature which guarantees this *self-contained* property for complex 3D devices without modifying the given geometrical description.

Therefore our research has been concentrated on two major issues:

- A consistent definition of the required mesh quality, based on the Voronoi diagram in d-dimensional space and its *dual,* the Delaunay meshes.
- The revision of the Box method applied in process and device simulation.

For a variety of difficult device simulation problems, we could demonstrate that our type of *conforming Delaunay tessellations* can be used together with a mildly modified version of the Box method [5, 6] to solve the tightly coupled system of semiconductor device equations. Following our analysis, the *self-contained* conditions are sufficient but not necessary for the simulation. *Self-contained* meshes define a narrower class of tessellations, which tolerates nearly arbitrary interpolation of physical quantities such as the mobility.

2 The hybrid approach proposed for mesh generation

The hybrid approach shown in Fig. 1 represents a revised version of the mesh generation scheme proposed in [7]. It is used as the meshing engine of both MDRAW-ISE and MESH-ISE [1]. The new mesh generation approach is based on a combination of two standard meshing techniques: (a) the modified quad-/oc-tree technique, and (b) the Delaunay technique.

The modified quad-/oc-tree technique is used for: (1) building a first conformal mixed-element tessellation for a set of complex general polygons/polyhedra, and (2) producing anisotropic refinement of the tree elements to ensure a proper resolution of the desired physical properties.

The final simulation mesh is constructed from the leaf elements of the refinement tree, using modified Delaunay algorithms. Standard Delaunay algorithms do not guarantee a proper tessellation at material interfaces [6]. Thus, our modified Delaunay algorithms have been tuned to ensure that all conditions imposed by the Box method for mixed-element meshes are satisfied.

For the comparison with our former mesh generators, device simulations have been performed using meshes generated by our new tools, MDRAW-ISE and MESH-ISE, and by our previous tools, MESHBUILD and OMEGA-ISE. All meshes have been successfully used in our device simulator DESSIS-ISE. The meshes constructed with the new tools are smaller in terms of mesh size (points and elements).

A key feature of the new scheme is the use of generic geometric classes to support the boundary handling, one of the most critical issues in the applied quad-/oc-tree techniques. These classes plus robust floating-point filters for geometric round-off error handling have been combined to solve two critical problems found in our previous meshing tools:

- Insufficient algorithms to build conformal tessellations in the quad-/oc-tree. The latest version of MESH-ISE includes extraction and tessellation algorithms for non-convex polyhedra.
- A fixed set of quad-/oc-tree elements, not capable of handling internal interfaces. This condition is especially critical in OMEGA-ISE, where geometries with faces of arbitrary orientation can not be meshed.

In Fig. 2, details of a rounded field oxide corner in a 3D transistor are shown.

On the top of the transistor, most of the faces are not aligned with any of the coordinate axes.

Using the new approach, this complex oxide region was meshed without excessive propagation of the refinement into the bulk of the transistor.

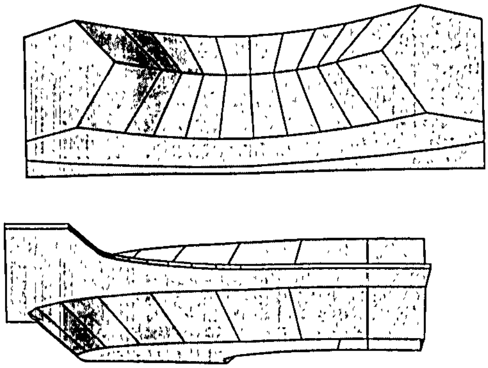

Figure 2: *Two snapshots of a rounded field oxide in a 3D transistor to be meshed.*

Acknowledgments

This work has been partially supported by the ESPRIT-8150 (PROMPT-I) Project and by the ESPRIT-24038 (PROMPT-II) Project.

References

[1] ISE Integrated Systems Engineering, Zürich, Switzerland, *ISE TCAD Software Manuals*, release 4.1 ed., 1997.

[2] P. Conti, M. Tomizawa, and A. Yoshi, "Generation of oriented three-dimensional delaunay grids suitable for the control volume integration method," *Int. J. Numer. Methods Eng.*, vol. 37, pp. 3211–3227, 1994.

[3] B. S. Baker, E. H. Grosse, and C. S. Rafferty, "Non-obtuse Triangulation of Polygons," *J. Disc. Comp. Geom.*, vol. 3, pp. 147–168, 1988.

[4] S. Müller, K. Kells, and W. Fichtner, "Automatic Rectangle-based Adaptive Mesh Generation without Obtuse Angles," *IEEE Trans. Computer Aided Design*, vol. 11, pp. 855–863, July 1992.

[5] G. Heiser, *Design and Implementation of a Three Dimensional General Purpose Semiconductor Device Simulator.* PhD thesis, Swiss Federal Institute of Technology, 1991.

[6] G. Garretón, *A hybrid approach for 2D and 3D mesh generation in semiconductors.* PhD thesis, Swiss Federal Institute of Technology, 1998. To be published.

[7] G. Garretón, L. Villablanca, N. Strecker, and W. Fichtner, "Unified grid generation and adaptation for device simulation," in *SISDEP*, (Erlangen, Germany), September 1995.