# Grid and Geometry Techniques for Multi-Layer Process Simulation

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#### Abstract

A robust grid generation and evolution technique for process simulation is presented. A quadtree approach is used to decimate the geometry and final triangulation is performed using templates. Warping is used to improve the grid quality near boundaries. The quadtree depends only on the structure's spatial extent and not on the specific vertices. This allows independent manipulation of the geometry and grid by various process simulation tools.

### 1. Introduction

The goal of our work is to insure a high quality computation grid at all times in multilayer process simulation. A grid module for process simulation should grid complex geometries, enable easy grid adaptation, and must be responsive to rapid topography changes due to etching, deposition, and oxidation simulations. An automatic quadtree based 2-D grid generator, called Forest, has been written to specifically address these issues. Forest stores and manipulates both geometry and grid data and can be used by grid based diffusion/oxidation simulators as well as string based etch/deposition simulators.

The geometry of the device is stored in a hierarchy of points, edges, boundaries and regions. This allows specification and manipulation of complex structures including those that contain voids. String based simulators use and update this data without directly manipulating the grid.

## 2. Quadtree Decimation

Initial grid generation (Figure 1) proceeds by surrounding the geometry with a root square and recursively decimating the root square until a final terminated lines quadrilateral mesh is obtained. Neither the root square nor the resulting quadtree depends on the specific vertices of the geometry; they only depend on the spatial extent of the structure. The level of decimation can be controlled by a number of factors including user specification, doping variation, or solution error.

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## 3. Triangulation

Triangulation of the terminated lines quadrilateral mesh is performed by using templates (Figure 2). The triangles are optimized for aspect ratio and the quality of the triangulation is measured by considering the ratio of the area of a triangle to the sum of square of its sides [1]. Normalizing this aspect ratio to be 1.0 for an equilateral triangle, the triangulation aims to produce triangles whose aspect ratios are at least 0.5.

Triangulation of interior quadrilaterals is easy and produces triangles of high quality all triangles are right or acute with high aspect ratios. Further treatment, however, is required for quadrilaterals with region boundaries. As shown in Figure 2b, boundary templates produce triangles of adequate aspect ratio if:

- The boundary does not intersect the quadrilateral very close to its corners.
- The boundary does not contain a vertex point that is very close to a quadrilateral corner or an edge.

Straightforward analysis yields a condition of closeness to be one third of the quadrilateral side length for producing triangles of aspect ratios greater than 0.5. Quadrilaterals that fail this criteria are preprocessed by a technique called warping (Figure 2c) [2]. The quadrilaterals are slightly deformed by moving the corner closest to an intersection point onto the intersection point. For vertex points close to a side, a similar concept is used to warp the side onto the vertex point. The resulting quadrilaterals are then triangulated, producing triangles with aspect ratios greater than 0.5. If obtuse triangles need to be eliminated or if the aspect ratio needs to be higher, then the quadrilaterals can be further divided and the whole process is repeated in a recursive fashion. This allows an user to trade-off grid quality with grid quantity. Another example of a Forest generated grid used in oxidation simulation is shown in Figure 3.

## 4. Advantages of Forest

One of the main advantages of this gridding technique for process simulation is illustrated in Figure 4 which shows a prototype interface between Forest and a string based etch/deposition simulator SPEEDIE [3]. The geometry of the structure is used to extract the top layer of the device and deposition simulation is performed. The grid is subsequently altered to conform to the new geometry. This entails only pruning or growth of the quadtree and triangulation locally over the regions where the boundary has changed. This results in minimal change to the existing grid. The technique can be applied to great advantage for coupled oxidation and diffusion simulation.

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## References

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- [2] M. Bern, et. al. Provably Good Mesh Generation. Proc. 31st IEEE Symp. Foundations of Computer Science (1990) 231-241.
- [3] J. McVittie, et. al. SPEEDIE User's Manual Version 2.0. Integrated Circuits Laboratory. Stanford University. Feb. 1992



Figure 1: Grid generation proceeds by enclosing a geometry (a) by a root square and decimating the square (b) resulting in a terminated lines mesh (c). The terminated lines mesh in then triangulated (d).



Figure 2: (a) Template used for triangulating interior quadrilaterals. (b) Template used for triangulating boundary quadrilaterals. (c) Warping used to improve triangle qualities of boundary quadrilaterals.



Figure 3: (a) Example of an initial grid generated by Forest for non-planar structures. (b) Geometry and grid after subsequent oxidation using SUPREM IV.



Figure 4: Prototype use of Forest and SPEEDIE to simulate deposition. (a) Grid and geometry in Forest. (b) Deposition simulation using SPEEDIE. (c) Conforming grid to new boundary.

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