# Grid Techniques for Multi-Layer Device and Process Simulation

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**Abstract**

A 2D numerical grid generation program suitable for device and process simulation is presented. The program meets the unique grid requirements encountered in multi-layer process simulation - rapidly changing topographies, and use of mesh based and string based TCAD tools.

Grids can be generated for the PISCES-II and SUPREM-IV device and process simulation programs. Adaptive gridding has been achieved for SUPREM-IV diffusion simulation and a prototype interface has been demonstrated for the etching/deposition simulator SPEEDIE.

**Introduction**

A grid module suitable for multi-layer device and process simulation must be capable of gridding complex geometries, adapting the grid based on various criteria, and being responsive to rapid topography changes. It must also be suitable for use with a wide variety of TCAD tools each with different internal data representations. *Forest*, a 2D automatic quadtree based grid program, provides grid functions with all these capabilities.

**Grid Generation**

Forest stores the device geometry as an hierarchy of points, edges, boundaries and regions. Each region can contain a number of boundaries allowing structures with voids. String based TCAD tools use and update this geometry data without directly manipulating the grid.

Grid generation (Figure 1) is performed by a quadtree decimation technique (2). The device geometry is surrounded with a root square which is recursively decimated resulting in a final terminated lines quadrilateral mesh. 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 doping variation, or solution error. For an initial grid, the user normally specifies the decimation level.

Templates are used to triangulate the terminated lines quadrilateral mesh as shown in Figure 2. Triangles are optimized for aspect ratio and the triangle quality 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.

Triangles of interior quadrilaterals are 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.

The condition of closeness is 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) whereby they 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 polygons are then triangulated producing triangles with aspect ratios greater than 0.5.

**Grid Adaptation**

Grid adaptation has been achieved for SUPREM-IV diffusion simulation. The SUPREM-IV program has been re-architectured such that each of the solvers is run as a client with no static data. At each time step, the grid data from Forest is used to create the data areas for diffusion. Upon completion of the time step, the newly computed solution values are updated in Forest. Grid adaptation is then performed based on the solution and the diffusion data areas created anew for the next time step.

Adaptation is performed by subdividing the triangular elements based on solution variation (3). Figure 3 shows a simple example of grid adaptation during diffusion simulation. Part of the device is masked during a thermal anneal in an impurity ambient. As the impurity front diffuses down the device, the grid keeps up with it - finer grid is allocated in areas where the concentration gradient is steepest. For the example presented in Figure 3, grid coarsening was not used.

### Interface with String Based Simulators

A prototype interface of Forest with the string based deposition simulator SPEEDIE (4) illustrates the power of the quadtree grid generation technique for process simulation. As illustrated in Figure 4, the structure's top layer is extracted from the geometry and a deposition simulation is performed using SPEEDIE. The grid is then subsequently altered to conform to the new boundary. This entails pruning or growth of the quadtree quadrilateral mesh and local triangulation. Minimal changes occur in the existing mesh - thereby reducing interpolation errors between meshes.

### User Interface

A graphical user interface (GUI) for specifying the initial geometry and initial impurity concentrations has also been developed. The GUI program is a modified version of the Interviews based drawing program *idraw* (5). The program allows the user to graphically draw the device using the mouse. Attributes like material, grid size, doping profiles and boundary conditions are set by mouse operations and by using pull down menus. Text can be used anywhere on the canvas for annotation. The structure is then gridded for device simulation (producing a PISCES mesh file) or for process simulation (producing a SUPREM IV structure file) using Forest. This provides a consistent interface for both types of simulations. Figure 5 shows a typical interface window.

### References


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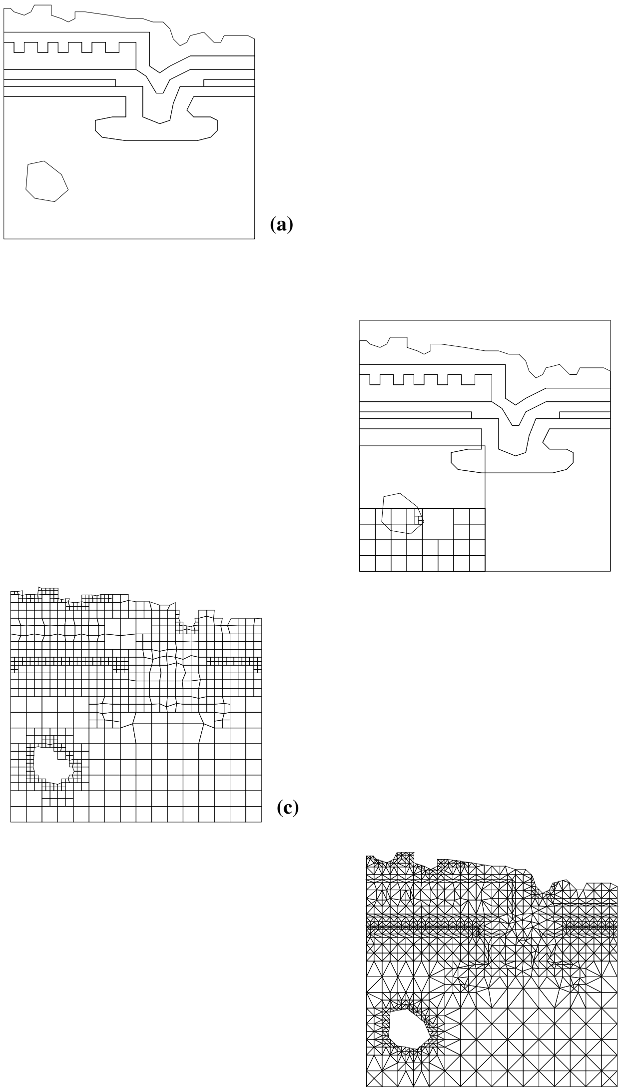


Figure 1: (a) Quadtree grid generation proceeds by enclosing the geometry by a root square. (b) The root square is decimated recursively. (c) The resulting terminated lines quadrilateral mesh. (d) The final triangulation.

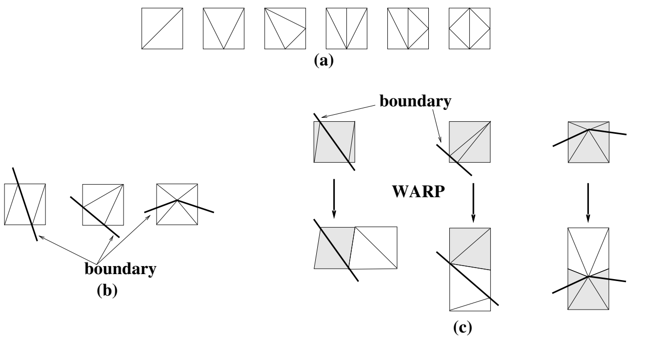


Figure 2: (a) Template used for triangulating interior quadrilaterals. (b) Template used for triangulating boundary quadrilaterals. (c) Warping used to improve triangle qualities of boundary quadrilaterals.

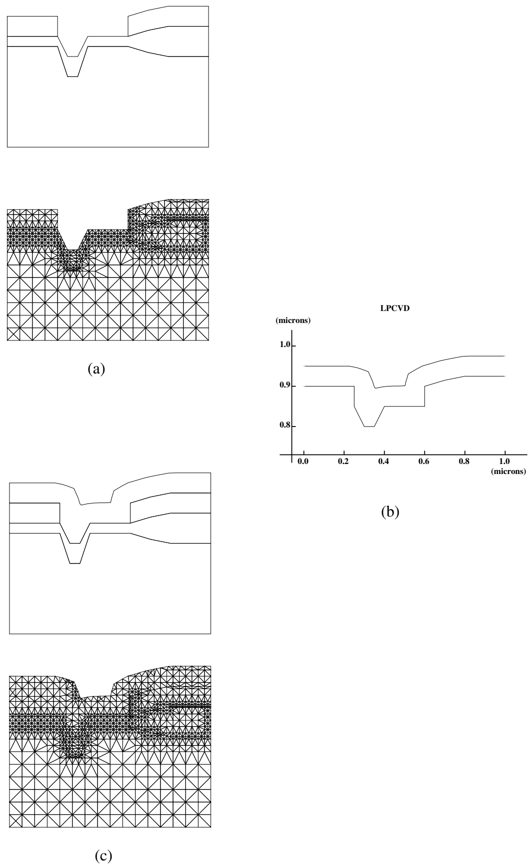


Figure 4: Prototype use of SPEEDIE and Forest for deposition simulation. (a) Grid and Geometry in Forest. (b) Deposition simulation using SPEEDIE. (c) Conforming grid to new boundary.

Figure 3: Illustration of grid adaptation during diffusion simulation. The grid is refined at each time step if the solution variation is greater than a threshold.

Figure 5: Graphical User Interface for device geometry specification.