

Moving Adaptive Unstructured 3-D Meshes in Semiconductor Process Modeling Applications *

Andrew Kuprat, Denise George, Eldon Linnebur, Harold Trease
Los Alamos National Laboratory

R. Kent Smith
AT&T Bell Laboratories

Abstract

The next generation of semiconductor process and device modeling codes will require 3-D mesh capabilities including moving volume and surface grids, adaptive mesh refinement and adaptive mesh smoothing. To illustrate the value of these techniques, a time dependent process simulation model was constructed using analytic functions to return time dependent dopant concentration and time dependent SiO₂ volume and surface velocities. Adaptive mesh refinement and adaptive mesh smoothing techniques were used to resolve the moving boron dopant diffusion front in the Si substrate. The adaptive mesh smoothing technique involves minimizing the L_2 norm of the gradient of the error between the true dopant concentration and the piecewise linear approximation over the tetrahedral mesh thus assuring that the mesh is optimal for representing evolving solution gradients. Also implemented is constrained boundary smoothing, wherein the moving SiO₂/Si interface is represented by moving nodes that correctly track the interface motion, and which use their remaining degrees of freedom to minimize the aforementioned error norm. Thus, optimal tetrahedral shape and alignment is obtained even in the neighborhood of a moving boundary. If desired, a topological "reconnection" step maintains a Delaunay mesh at all times. The combination of adaptive refinement, adaptive smoothing, and mesh reconnection gives excellent front tracking, feature resolution, and grid quality for finite volume/finite element computation.

Key Words: adaptive mesh refinement, adaptive mesh smoothing, mesh reconnection, multimaterial grids, moving grids, moving surfaces, unstructured grids.

The Multimaterial Grid Code X3D

X3D, the Los Alamos grid code^{1,2}, is a toolbox of multimaterial grid generation, adaptive mesh refinement, adaptive mesh smoothing, mesh reconnection, and mesh manipulation operations that are well suited to semiconductor process and device modeling. The toolbox commands operate on mesh objects that are user extensible and automatically sized; information stored within the mesh objects assures the correct attribute values are assigned to new nodes and elements as created and allow for time dependent geometric

* Work supported by the U.S. Department of Energy.

reconfiguration that can result from moving grid and moving surface applications.

To illustrate the capabilities of X3D, a time dependent process simulation model was constructed using analytic functions to return dopant concentrations and SiO₂ surface velocities. The model consists of layers of silicon, SiO₂, polysilicon, and nitride: a T-shaped mask is centered in the nitride. As the model is symmetric, only half the model was calculated. Initially all interfaces are planar (Fig. 1) and the dopant isosurfaces are highly curved (Fig. 2). Over time as the polysilicon is converted to SiO₂, the nitride region is pushed up; eventually the lower oxide surface penetrates the silicon at which time the dopant diffusion is effectively stopped at the silicon/oxide interface (Figs. 3, 4). X3D models the nitride region as a moving volume mesh, and models the lower oxide surface as a moving surface. At each time step the X3D tool, **extract**, is invoked to create a two dimensional mesh object, which is moved and then reinserted into the main three dimensional mesh object. By reinvoking the geometry definition, nodes and elements are assigned correct attributes.

Simultaneous Grid Adaption to Diffusion and Oxidation

In the lower Si portion of the model, an implanted boron dopant diffuses while at the same time a moving oxide boundary shrinks the Si. Complete grid adaption is accomplished by (1) refining the mesh based on the dopant concentration field, (2) smoothing the mesh to minimize the error in representing the concentration field, and (3) reconnecting the mesh to allow necessary topological changes to occur as the dopant field and problem domain deform.

The X3D **smooth** option invokes Minimum Error Gradient Adaption (MEGA) which is a 3D generalization of a 2D adaptive smoothing scheme of Bank and Smith³, combined with the *gradient weighting* concept of Carlson and Miller⁴. The idea is to adjust the positions of the vertices so as to minimize the functional

$$F = \int_{\Omega} \|\nabla(u - u_L)\|^2 w dx. \tag{1}$$

That is, the weighted \mathcal{L}_2 norm of the gradient of the error between the true solution u

and its piecewise linear approximation u_L on each tetrahedron. Minimizing the gradient of the error leads to optimal resolution of solution gradients which can be crucial for correct calculation of diffusion profiles. A secondary benefit of minimizing the error gradient is that it works to prevent “tet collapse” as the mesh moves. This is because solution gradients are poorly represented on wafer-thin tetrahedra, and are thus avoided when minimizing this functional. For sufficiently large grids, the gradient weighting factor w can be omitted, and the grids produced become independent of the scale of u , thus eliminating fiddling with parameters.

Since the exact solution u in (1) is generally unknown, the method is to approximate the error by the six quadratic “bump” functions associated with the edges of each tetrahedron. (The “bump” functions are the pairwise products of the four linear “hat” functions associated with the four vertices of each tetrahedron.) To use the **smooth** command, all that is needed is an estimate of the error at each edge midpoint in the mesh. In our analytical model of boron diffusion, this data is exactly known, but this data can also be obtained as *a posteriori* error estimates which are routinely computed when numerically solving differential equations.⁵

In Fig. 5, we show the initial Silicon grid with boron contours of greatly exaggerated width. In Fig. 6 we show this grid after adaptive refinement; contour widths have been corrected but are highly irregular. A call to **recon** has been issued—the **recon** command is a novel 3D algorithm for re-establishing a Delaunay triangulation after mesh movement. **Recon** performs internal face swaps and boundary edge swaps in the mesh which typically modify a small proportion of the mesh connectivity during any given time step. As is well known, maintaining a Delaunay grid at all times is a crucial requirement for many finite volume PDE solvers. In Fig. 7, we show the effect of smoothing the grid via Minimum Error Gradient Adaption; the grid has now contracted and realigned to accurately resolve the boron contours.

In Fig. 8, we show the grid at $t = 4000$ when the oxide interface has partially collapsed the solution domain. Note how the front surface grid distribution has shown the remarkable

ability to “deconcentrate” (through the repeated use of **smooth** and **recon**) as the boron diffuses.

In Figs. 9-11, we show a workstation run with 9765 nodes where we have chosen not to refine or reconnect the mesh, but to adapt the mesh solely with MEGA. Note the “tri-band” structure at $t = 0$ which indicates locations of large second derivative in the dopant function. Fig. 11 is a close-up of the front face of the smoothed $t = 0$ mesh and shows boron contours in a region of very high curvature. In contrast, Fig. 12 shows the same close-up on a much larger uniform hexahedral grid of 206,500 nodes. (The full hexahedral grid is not pictured.) The contours are more accurately resolved on the smaller MEGA smoothed mesh.

References

1. D.C. George, X3D User’s Manual, Los Alamos National Lab Report LA-UR-95-3608 (1995).
2. H.E. Trease, *Three-Dimensional Free Lagrangian Hydrodynamics*, Proceedings of the first Free-Lagrange Conference, Lecture Notes in Physics, Springer-Verlag, Vol. 238 (1985), pp. 145-157.
3. R.E. Bank and R.K. Smith, *Mesh smoothing using a posteriori error estimates*, SIAM J. Sci. Comp., to appear.
4. N. Carlson and K. Miller, *Gradient weighted moving finite elements in two dimensions*, in “Finite Elements Theory and Application”, D.L. Dwoyer, M.Y. Hussaini and R.G. Voigt, editors, pp. 151-164, Springer Verlag, 1988.
5. R.E. Bank and R.K. Smith, *Some a posteriori error estimates based on hierarchical bases*, SIAM J. Numerical Analysis, 30 (1993), pp. 921-935.

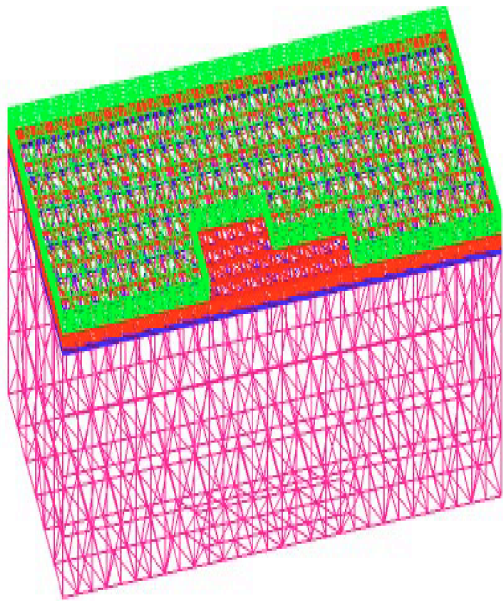


Figure 1: Initial planar surface and interface grids with T-mask.

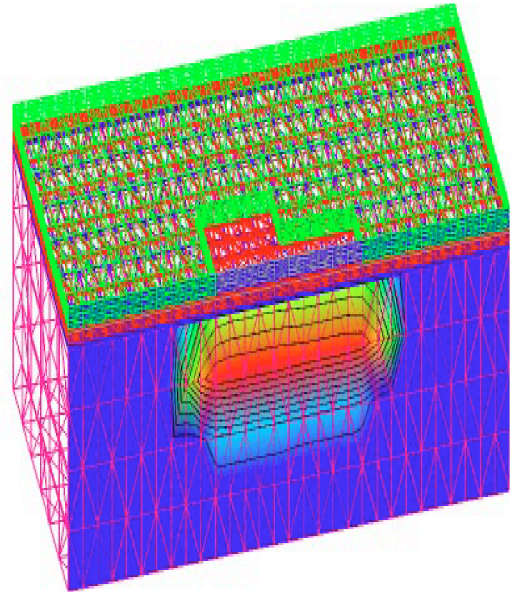


Figure 2: Boron concentration contours at $t = 0$.

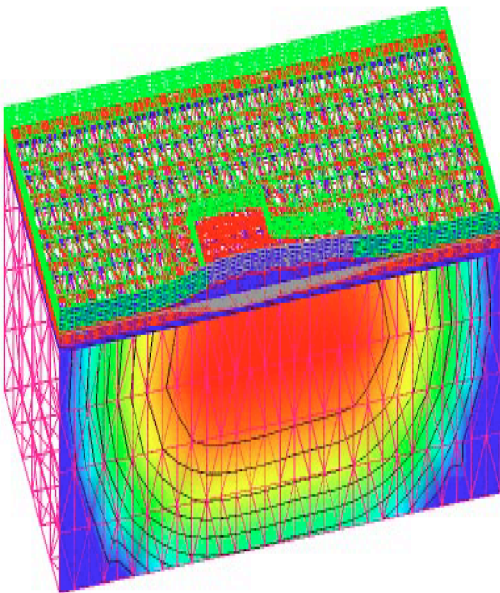


Figure 3: Boron concentration contours and moving surfaces at $t = 800$.

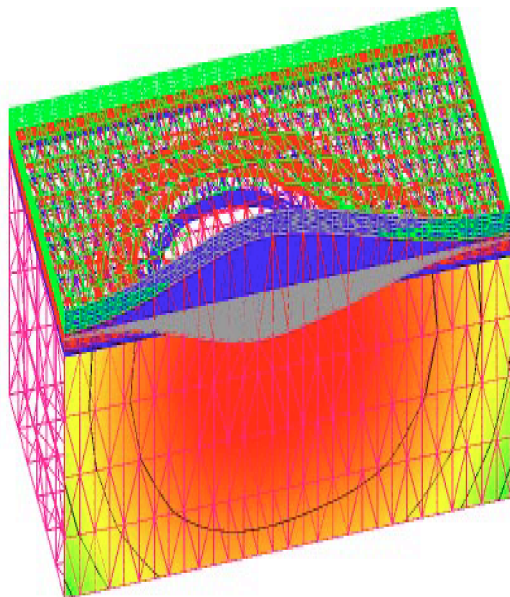


Figure 4: Boron concentration contours and surfaces at $t = 3600$.

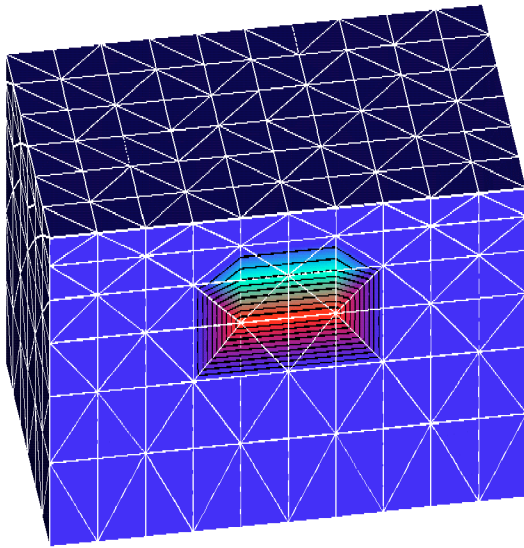


Figure 5: Initial unrefined, unsmoothed regular grid with boron contours.

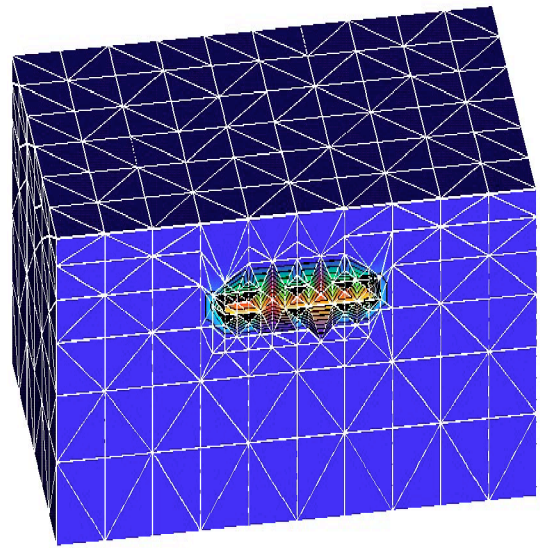


Figure 6: Refined, reconnected initial grid.

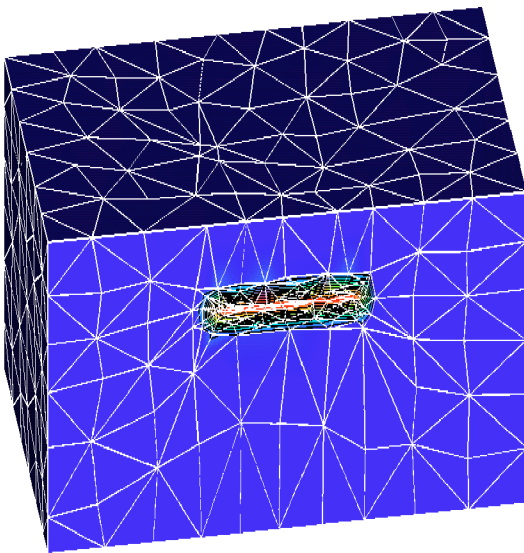


Figure 7: Refined, reconnected and smoothed initial grid.

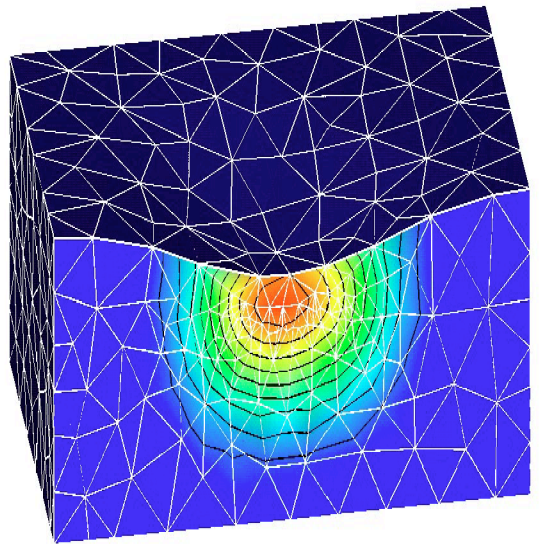


Figure 8: MEGA smoothed grid at $t = 4000$.

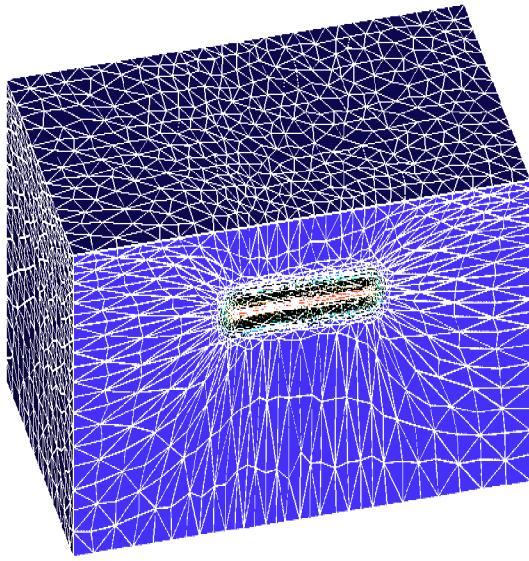


Figure 9: MEGA smoothed grid with 9765 nodes at $t=0$.

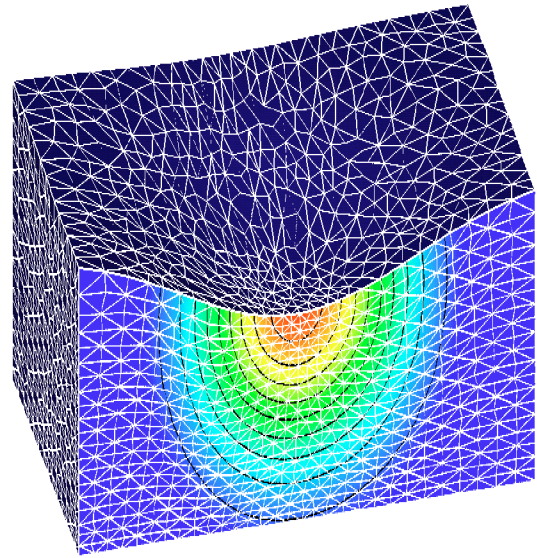


Figure 10: Grid at $t=8000$ showing boron contours.

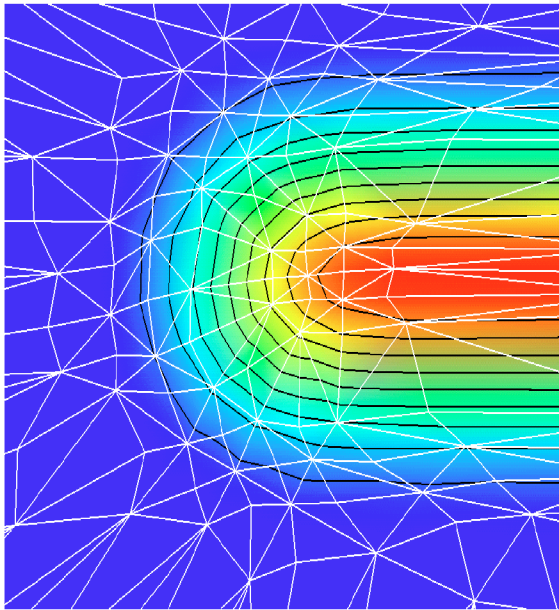


Figure 11: MEGA smoothed grid with 9765 nodes at $t=0$. (Close-up showing boron contours.)

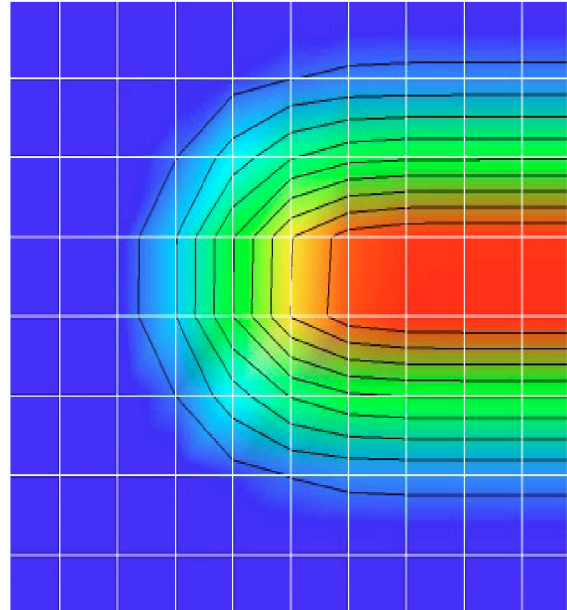


Figure 12: Same close-up as Fig. 11, but using 206,500 node uniform hexahedral grid.