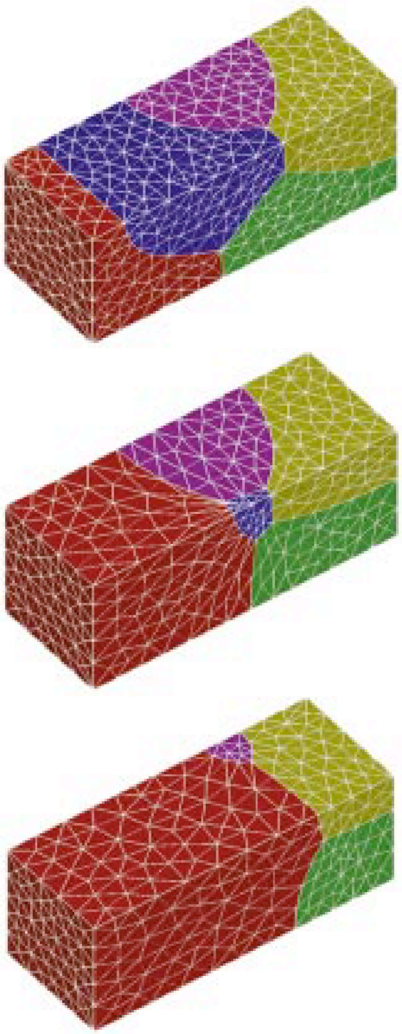
# LaGriT Grid Generation



*Three time-steps in a grain growth simulation in which interface motion by mean curvature leads to shrinkage and disappearance of "blue" grain. The grid connectivity is managed continuously to maintain approximately constant grid spacing.*

## Benefits

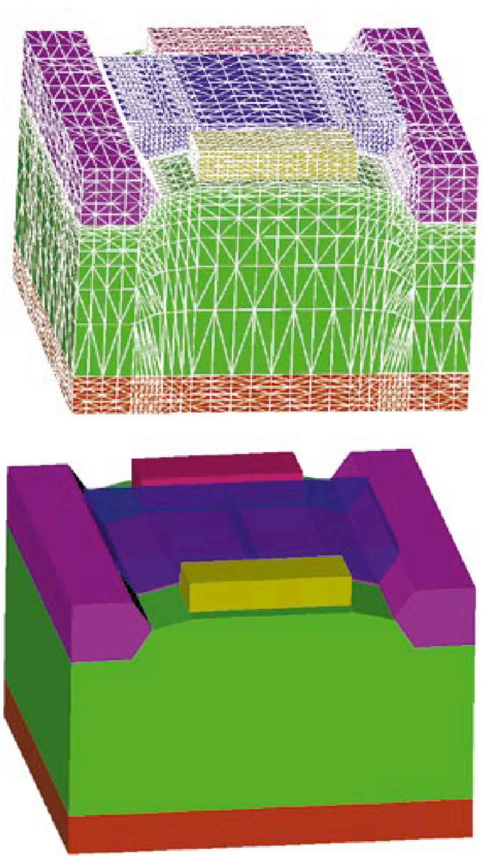
Three-dimensional, moving, adaptive, grid generation is an essential enabling technology allowing scientists and engineers to solve time-dependent, three-dimensional (3D) problems that use techniques such as finite-element methods. This newly developed software (LaGriT) provides a full set of grid generation and grid optimization tools for constructing and maintaining 3D unstructured grids.

In three dimensions, LaGriT's unstructured grid toolbox library minimizes required computer resources because grids created using LaGriT require a minimum number of grid nodes to resolve problem-specific properties such as moving boundaries and changes in field values, while still preserving material interface connectivity and curvature.

LaGriT was intentially designed to be easily applied to any 3D application through user-extensible data objects, user-defined commands, and easy to use interfaces for linking with existing application software. To date, the LaGriT software has been implemented and tested as a toolbox library on four different workstation platforms.

## How LaGriT Works

Modeling and simulation of static or dynamic, 3D processes require generation, optimization, and dynamic maintenance of high-quality 3D grids. The grid software produces grids that can be used by any numerical method for solving partial differential equations that supports unstructured elements. Grid generation creates a set of connected elements from a user-specified geometry. Elements are simple geometric objects such as tetrahedra or hexahedra; the vertices of the elements are called nodes. Grid optimization uses refinement and smoothing techniques to adjust the number of nodes and the node positions to provide optimal spatial resolution for the problem to be solved. In order to obtain accurate solutions in both time and space, the grids must be dynamically modified to follow moving region interfaces and time-dependent function changes. LaGriT provides a library of tools useful to both static and time-dependent applications over widely varying spatial scales ranging from microns for semiconductor device and process modeling to kilometers for geologic modeling. Realistic models usually require intricate geometries and multiple materials in order to capture the phenomena of interest. Grid generation algorithms must handle multiple materials and nonanalytic interfaces and must create well-shaped elements with carefully placed nodes. LaGriT generates grids meeting these requirements in the following three steps.



*Semiconductor device model-computational grid is generated from solid model. Note clean interfaces between materials, varied aspect ratios of elements, and use of proportional spacing in the green silicon region.*

*(Model contributed by Intel Corporation.)*

### Grid Generation

(1) LaGriT defines geometric regions as combinations of bounding surfaces, where the surfaces may be described analytically (e.g., planes, spheres, cylinders, or cones), or surfaces may be described as sheets (user-provided) which are collections of connected triangles or quadrilaterals. These sheets are topologically two dimensional but geometrically three dimensional as if one were to take a sheet of rubber and warp and stretch it to conform to an uneven surface. For example, to model an etch or deposition process over time in a semiconductor device, the interface between the silicon region and the silicon dioxide region is best represented as a dynamic sheet surface.

(2) Nodes are then distributed on the surfaces and within the volume of the geometry. In order to most accurately represent the actual spatial geometry, the user may choose among Cartesian, cylindrical, or spherical coordinate systems for each region and may choose even or proportional spacing to control node density.

(3) The last step connects the nodes into volume elements. LaGriT uses a modified Delaunay tetrahedralization algorithm which respects material interfaces by assuring that there are no multimaterial elements and which guarantees positive coupling coefficients in the volume, an essential requirement for solving the matrices used by modeling applications. Although primarily a 3D tetrahedral code, LaGriT supports hybrid grids which combine hexahedral and tetrahedral grid sections using pyramids and prisms as bridge elements and which provide the calculational advantage of fewer elements.

### Grid Optimization

Grid optimization combines refinement, smoothing, and reconnection tools which modify the grid to provide more spatial resolution where needed by the problem being solved. Grid refinement adds nodes based on geometric criteria such as edge length, or based on the value of a physical field. For example, in modeling boron diffusion in silicon, it is necessary to resolve very steep diffusion gradients where smaller elements are needed; the refinement tool creates more elements where the gradient is highest. Grid smoothing moves existing nodes to adapt the grid to a physical field and, at the same time, maintains quality element shape. Grid elements may become distorted or may become non-Delaunay as nodes are added as a result of refinement or moved as a result of smoothing operations. Grid reconnection then maintains the necessary element-shape quality and maintains the positive coupling coefficient criterion of the grid by interchanging the connections.

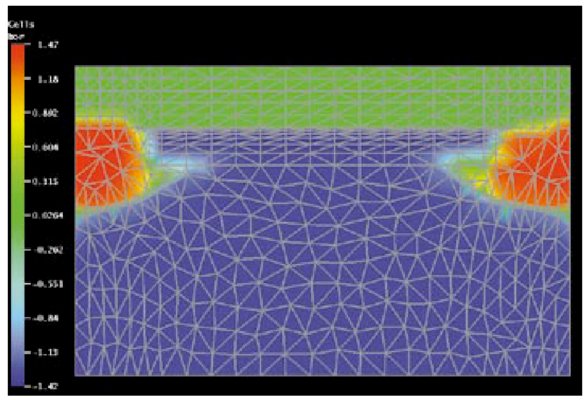
### Time-Dependent Grid Maintenance

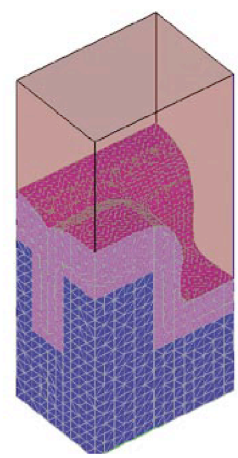
Grid maintenance in time-dependent simulations uses the refinement, smoothing, and reconnection tools to respond to function value changes and node movement. Additional requirements are imposed when tracking moving surfaces. For example in grain growth simulation, interface surfaces move and the regions touching these surfaces grow or shrink dynamically. As surfaces collide, the grid must respond by merging points and effectively squeezing out the material between the colliding surfaces. LaGriT provides these additional grid maintenance tools for time-dependent simulations.

### Grid Server Architecture

Because of the enormous variety of applications that need high-quality grids, the LaGritT data structures and libraries were designed as objects in order to be completely and easily user extendable. For example, if a diffusion simulation problem requires boron concentrations in silicon, the user will issue a command adding a boron field to the grid and to the data structure; LaGriT will assume all responsibility for maintaining that field as the grid evolves. User commands are also easily added to LaGriT. A user command might be as simple as reading a nonstandard interface file or as complex as solving a set of partial differential equations on the grid. To implement such a command the user would not have to change any lines of LaGriT code; the needed data are accessible through library functions, and the new command code module need only be linked with the LaGriT libraries. Finally, the LaGriT toolbox was designed to provide a direct and easy interface with user generated application codes. For example, a user-generated application can view the LaGriT toolbox as a grid server. The application will ask the server to create the initial grid and to

***2D grid extracted from a 3D grid during a semiconductor process simulation. The 2D grid was smoothed and refined to concentrate grid in areas of steepest gradient of the dopant concentration, while maintaining orthogonal grid orientation near the channel regions.***





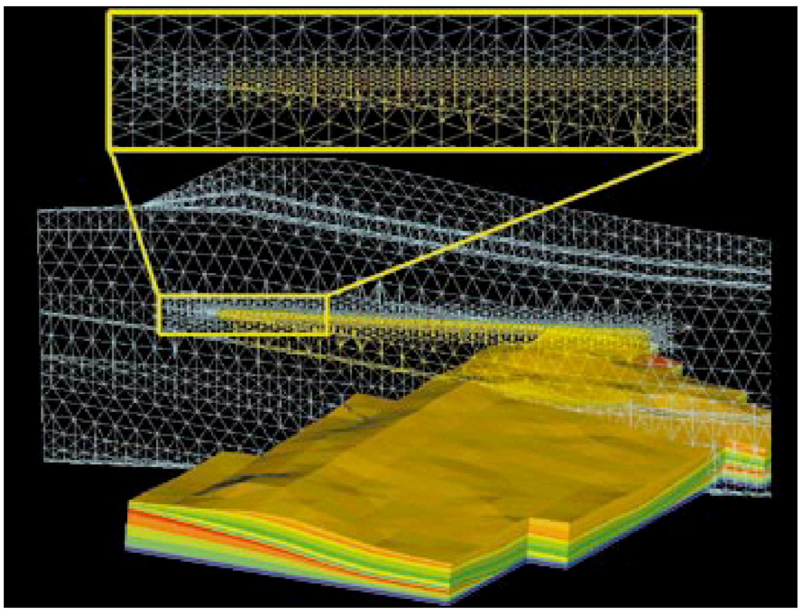
***Geometry defined using sheet surfaces as material interfaces. The top material is transparent so that the finely-gridded moving surface is visible. The history of a previous time step is visible in the surface trace in the "pink"material.***

***(Geometry contributed by Motorola.)***

perform user-specified operations on the grid. This design relieves the application from all grid chores.

**Geological Applications**

Geological applications require accurate representation of complex engineered systems (wells, tunnels, reservoirs) and geologic structure and stratigraphy (layering, folding, domes, faulting) in order to produce accurate numerical models of fluid flow and transport. Oil and gas reservoir production, ground water resource development, hazardous waste site characterization and remediation, and nuclear waste disposal in a geologic repository are some of the areas where modeling must be used to predict the long term behavior of a system. In all these systems, grid generation is the key to accurate and stable solutions. LaGriT is currently used for automated grid generation in geological applications to calculate fluid flow and reactive chemical transport by finite element and finite difference methods. Both coarse grids for preliminary calculations and refined grids for final, high-resolution calculations are used.



***Shown is a 3D model of geologic stratigraphy and a 2D computational mesh extracted from the 3D model. This is used for studying lateral flow resulting from stratigraphic and permeability contrasts.***

*Semiconductor applications are done in collaboration with the Semiconductor Research Corporation and the geologic application in collaboration with the Department of Energy's Yucca Mountain Site Characterization Project.*

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