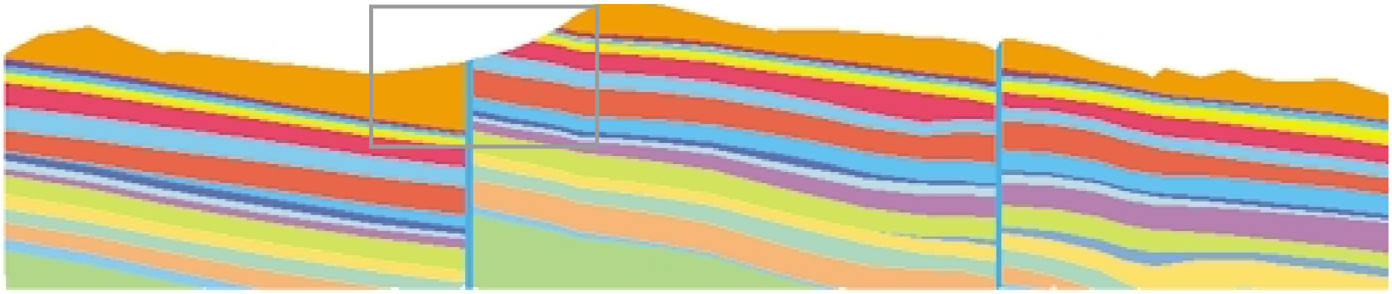


(a) Geological Model of a Cross Section at Yucca Mountain

Mesh Generation for Yucca Mountain

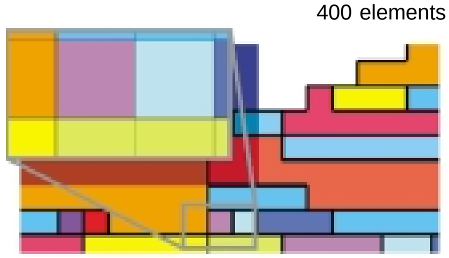
Carl W. Gable

To model the transport of waste radionuclides through Yucca Mountain, we must generate a grid, or mesh, on which our FEHM calculations can be run. Our primary tool for generating, optimizing, and maintaining computational meshes is LaGriT (for Los Alamos Grid Toolbox), a general-purpose software package. LaGriT is a spinoff of X3D, which was developed in the 1980s by Harold Trease.

Developed in the 1990s, LaGriT is a collaborative product of the Applied Physics, Theoretical, Earth and Environmental Science, and Computing, Information, and Communications Divisions at Los Alamos. It has been used to model such varied phenomena as shock physics, combustion, semiconductor devices and processes, biomechanics, the evolution of metallic microstructure, porous flow, and seismology.[1]

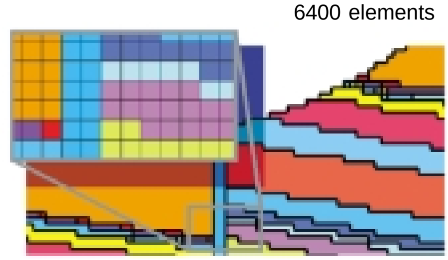
A mesh consists of nodes (points) at specific locations in space that are connected to form elements. These elements can be triangles or quadrilaterals in 2-D models and tetrahedra, hexahedra, prisms, or pyramids in 3-D models. The elements fit together like the pieces of a puzzle to represent physical systems such as the rock layers in Yucca Mountain, a human knee joint, or a semiconductor chip. Physical quantities such as pressure, temperature, or density, which are continuous in real materials, are usually represented by discrete values at the nodes or within the elements.

Mesh generation draws on both creativity and advanced mathematical algorithms. As Thompson et al. (1999) note, grid generation is "still something of an art, as well as a science. Mathematics provides the essential foundation for moving the grid generation process from a user-intensive craft to an automated system. But there is both art and science in the design of the mathematics for . . . grid generation systems, since there are no inherent laws (equations) of grid generation to be discovered. The grid generation process is not unique; rather it must be designed."[2]



(b) Low-Resolution Regular Mesh

Mesh generation can be automated but never becomes automatic. Although software like LaGriT helps automate complex "meshing" operations, generating successful meshes still rests on a series of judgment calls by an expert, who must weigh many tradeoffs. For example, imagine a calculation done on a $10 \times 10 \times 10$ grid of hexahedral elements. If we double the resolution to a $20 \times 20 \times 20$ grid, the total number of elements goes from 1000 to 8000. In addition, if the calculation involves modeling the change over time of a quantity such as saturation, doubling the resolution may require cutting the time steps in half, which doubles the computer time needed. Overall, then, doubling the calculation's resolution will increase calculation time by a factor of 16. Although high resolution best represents complex geometry and produces the most accurate physics solution, it requires more elements, which result in calculations that require more computer memory and cycles.



(c) High-Resolution Regular Mesh

The accompanying graphics illustrate various computational grids that could be generated for modeling Yucca Mountain. Our starting point is a geological model that represents the mountain as a sequence of sloping rock layers offset by two vertical faults (a). Focusing on the boxed area around the left-hand fault, we first create a simple mesh of square elements (b). The elements' colors correspond to those of the cross-section layers they represent

[1]More information on LaGriT is available from the software's Web site: http://www.t12.lanl.gov/~lagrit/.

[2]*Handbook of Grid Generation*. 1999. J. F. Thompson, B. K. Soni, and N. P. Weatherill, Eds. New York: CRC Press, p. iii.

and thus also to the layers' varying material properties (such as density and porosity).

The low-resolution squares in (b) do a poor job of representing the geology. The vertical fault is lost and individual rock layers are nearly lost because the mesh is so coarse. We can improve the mesh by increasing its resolution: the squares in (c) are one-quarter the size of those in (b). Now the geology is better represented, although the interfaces between rock layers are still represented by jagged stair steps. Also, only the thickest layers are represented by contiguous elements; thin layers and small features are still lost in the grid's coarseness.

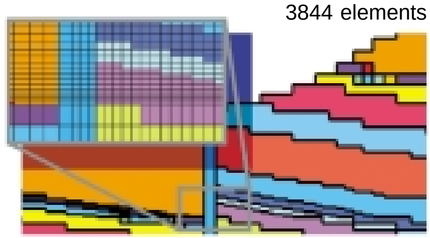
Another approach is to use variable mesh spacing, as shown in (d). Variable spacing allows us to "zoom in" with high resolution on some areas and maintain low resolution in others. However, variable spacing generally works well only for simple geometries in which the phenomena being modeled take place in a small portion of the entire computational domain and thus only a few areas require high resolution.

A more flexible approach is to adapt mesh resolution to the geometry of interest, as done in the quad-tree meshes shown in (e) and (f). These meshes allow cascading refinements: each element is subdivided into four elements, each of which is then subdivided into four still smaller elements, and so on.

In (e) and (f), we start with the mesh of (b) and then refine only selected elements. In (e), we refine along all material interfaces by a factor of 16 but leave regions far from these interfaces at low resolution. In (f), we refine only thin rock layers by a factor of 32, increasing their resolution while maintaining lower resolution in the thick layers. In both cases, however, the number of elements is much greater than in the previous meshes, which will slow down our calculations.

Our mesh examples so far are all structured: that is, they are made of quadrilateral elements whose positions are readily defined in terms of rows and columns and whose connectivity is

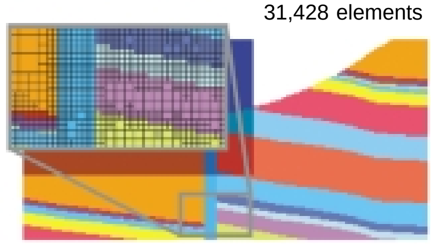
3844 elements



(d) Variably Spaced Regular Mesh

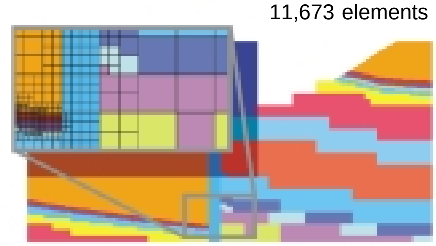
logical. Our last mesh examples are made of unstructured triangular elements whose connectivity is more arbitrary: for example, the nodes have varying numbers of triangles attached to them. This unstructured approach, however, allows us to create meshes that actually conform to the mountain's varied material interfaces.

31,428 elements



(e) Quad-Tree Mesh

11,673 elements



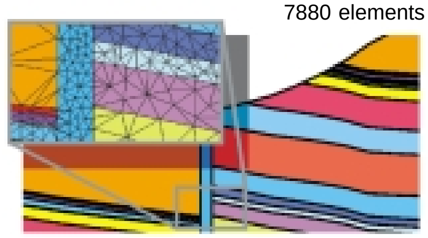
(f) Quad-Tree Mesh

Both low-resolution (g) and high-resolution (h) meshes do well in representing the geologic interfaces. The high-resolution mesh, however, will do a better job solving the physics of radionuclide transport because its smaller elements can more accurately represent variations that occur over short distances. In modeling Yucca Mountain, we must also contend with phenomena that lack symmetry, have a wide range of length scales, and involve very thin layers that must be preserved as continuous. As a result, triangles in 2-D modeling and tetrahedra in 3-D modeling have been our meshes of choice.

In addition to tradeoffs in how well they represent the mountain's geometry, meshes also pose tradeoffs in their suitability for different physics codes. Some codes can solve problems only on regular grids like those shown in (b)–(d). Others can use quad-tree meshes like those shown in (e) and (f) but not the unstructured meshes of (g) and (h). Thus the meshing approach must be compatible with the physics code that will be used.

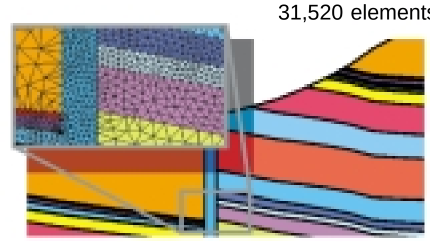
Developing flow and transport models for Yucca Mountain has pushed the limits of mesh generation technology. The models' size requires us to keep the number of elements as low as possible, their complex physics requires us to accurately represent the geology of the repository site, and the need for timely results requires us to automate mesh generation whenever possible. These often conflicting demands have been met by a collaborative effort in enhancing mesh generation capabilities to meet the challenges of modeling Yucca Mountain. ■

7880 elements



(g) Low-Resolution Triangular Mesh

31,520 elements



(h) High-Resolution Triangular Mesh