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Geological Applications of Automatic Grid Generation Tools for Finite Elements Applied to Porous Flow Modeling

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Abstract

The construction of grids that accurately reflect geologic structure and stratigraphy for computational flow and transport models poses a formidable task. Even with a complete understanding of stratigraphy, material properties, boundary and initial conditions, the task of incorporating data into a numerical model can be difficult and time consuming. Furthermore, most tools available for representing complex geologic surfaces and volumes are not designed for producing optimal grids for flow and transport computation. We have developed a modeling tool, GEOMESH, for automating finite element grid generation that maintains the geometric integrity of geologic structure and stratigraphy. The method produces an optimal (Delaunay) tetrahedral grid that can be used for flow and transport computations.

The process of developing a flow and transport model can be divided into three parts: (1)Developing accurate conceptual models inclusive of geologic interpretation, material characterization and construction of a stratigraphic and hydrostratigraphic framework model, (2)Building and initializing computational frameworks; grid generation, boundary and initial conditions, (3)Computational physics models of flow and transport. Process (1) and (3) have received considerable attention whereas (2) has not. This work concentrates on grid generation and its connections to geologic characterization and process modeling.

Applications of GEOMESH illustrate grid generation for two dimensional cross sections, three dimensional regional models, and adaptive grid refinement in three dimensions. Examples of grid representation of wells and tunnels with GEOMESH can be found in Cherry *et al.* [1]. The resulting grid can be utilized by unstructured finite element or integrated finite difference models.

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Introduction

Automated grid generation has applications in a wide range of science and engineering. Each field has special needs due to the particular geometries that must be represented by grids or due to the physics equations that must be solved on the grid. Grid generation for geologic applications of fluid flow, heat transport and reactive chemical transport in porous media pose their own difficulties. The physical equations are highly non-linear, material properties of the media such as permeability may vary by orders of magnitude, geologic structures have none of the symmetry of engineered geometries and the domain of interest may span large volumes with phenomenon at small length scales having a substantial influence on the large scale solution. A major hurdle to grid generation is creating grids which maintain the complex material interfaces of a model with many different material types.

There are three steps in process modeling (1)Developing accurate conceptual models inclusive of geologic interpretation, material characterization and construction of a stratigraphic and hydrostratigraphic framework model, (2)Building and initializing computational frameworks; grid generation, boundary and initial conditions, (3)Computational physics models of flow and transport.

There a number of different approaches available for step (1) the geometry model construction phase[2]. Voxel based methods represent the geometry as a set of orthogonal or non-orthogonal hexahedral elements. Methods that utilize orthogonal elements are severely constrained in the complexity of geometries that can be represented. Non-orthogonal voxel methods, which are often still logically structured grids, also suffer some draw backs in their ability to model faulted structures and multi-valued surfaces such as the mushroom shape of a salt dome. They also often require the user to decide on a nominal grid resolution as part of the geometry model construction process. An alternative is to define a set of surfaces, either as analytic functions (NURBS) or two dimensional elements (triangles or quadrilaterals). These surfaces then define a closed volume. While volumes defined by surfaces are very general, exporting a large multi-material model can be very involved. This project is not restricted to any particular method of volume definition. Any description that uniquely defines volumes can be imported with minor code revision.

The focus of this work is step (2) grid generation. GEOMESH [3,4] is a grid generation application that imports various different forms of geologic geometry models and utilizes the many tools available in the X3D [5], grid generation system

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GEOMESH Grid Generation

GEOMESH is a software tool for importing and automatically producing unstructured finite element grids tuned to the special needs of geologic and geo-engineering applications. The application produces 2D and 3D grids of elements that are triangles and tetrahedra.

The core functions of GEOMESH utilize the X3D [5] grid generation tools developed at Los Alamos National Laboratory. GEOMESH developed out of a need for accurate and automated grid generation for 3D modeling of subsurface porous flow and transport. Since the grids represent the geology being modeled, the accuracy of the grid directly affects the accuracy of the model. It was also found that grid generation was tedious, time consuming, and prone to errors, especially for models with complex structures such as faults and stratigraphy such as pinch-outs and layer truncations.The grids produced by GEOMESH are widely applicable and can be used by any numerical algorithm that can utilize unstructured grids. They are not specific to any particular computational physics code

GEOMESH grid generation uses three criteria to insure grid quality. They are: (1) the final grid preserves the input geometry model, (2) the grid is Delaunay and (3) all coupling coefficients are positive to insure flux calculations do not have negative transmissibility. This insures that the coupling coefficients related to grid geometry produce a semi-positive definite matrix. The Delaunay criteria is met with the constraint that each material may not form a convex hull, however the connectivity within the bounding surface is Delaunay. In this constrained sense, the grid within each material is Delaunay.

GEOMESH Examples

Some of the grid generation utilities of the GEOMESH and X3D grid generation package are demonstrated by a series of examples. Some examples are 2D to make visualization easier however all of the utilities can be applied to 3D tetrahedral grids as well as 2D triangular grids. The examples demonstrate, (1) grid reconnection to insure a Delaunay grid with positive coupling coefficients while maintaining material interfaces, (2) grid smoothing to optimize grid quality by moving nodes and maintaining material interfaces, (3) grid refinement through point addition at arbitrary locations.

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Example 1: Grid Reconnection, Point Addition and Grid Refinement

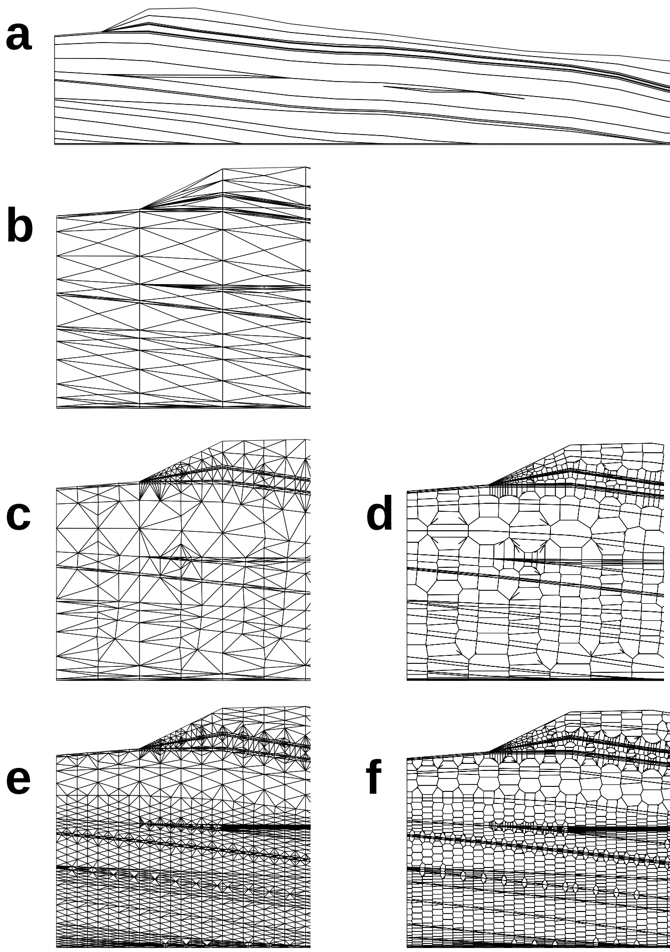

FIGURE 1. (a)A geometry model of a geologic cross section with 21 stratigraphic layers. (b)Non-delaunay triangular grid; (c)Delaunay grid, positive coupling coefficients; (d)Voronoi grid; (e)Delaunay grid with refinement; (f)Voronoi grid with refinement.

This examples shows grid generation from a geometry model, reconnection to form a Delaunay grid, point addition at material interfaces to insure positive coupling coefficients

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and grid refinement. Figure 1a shows the outline of a geologic cross section with 21 layers. The computational grid must not have any connections that cross these material interfaces. In Figure 1b a course grid is formed by placing nodes at regular intervals along the material interfaces and along the center line of each layer. The resulting grid is a good representation of the geometry however it is not Delaunay. In Figure 1c the grid is reconnected by edge flipping and nodes are added along material interfaces to insure a Delaunay grid with positive coupling coefficients. The Voronoi mesh of Figure 1c is shown in Figure 1d. The geometric coupling coefficients are computed as part of the grid generation process, and elements are subdivided and points are added on material interfaces to make the coupling coefficient matrix semi positive definite. For final calculations increased resolution is applied throughout the grid with double refinement in the lower nine materials, Figure 1e and 1f.

Example 2: 3D Tetrahedral Grid From Geologic Model

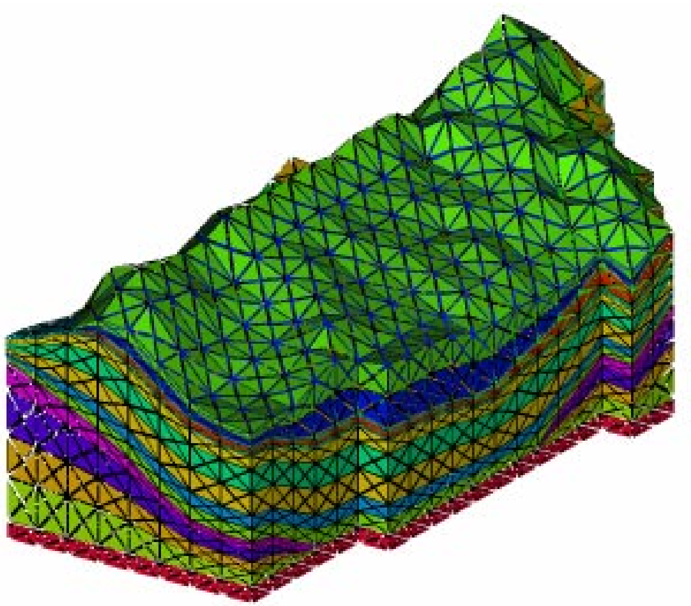

FIGURE 2. A 3D tetrahedral grid is produced from a hexahedral model of geologic layers. Each hexahedra is split into twenty-four tetrahedra and edge flipping and node addition at interfaces insures a computational grid with all positive coupling coefficients. The grid is shown at 5X vertical exaggeration.

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The grid generation process is separate from the geometry modeling. Geologic structure and stratigraphy is represented using a geoscientific information system (GSIS) for building 3D geologic models [6]. Figure 2 is a computational grid produced directly from a geologic modeling package. In this case the geometry model is exported as a hexahedral grid. The computational grid is produced by splitting each hexahedra into five or twenty four tetrahedra. In Figure 2 the twenty four option is used. Grid quality is insured by edge flipping and node addition at material interfaces.

Example 3: Interface Refinement and Grid Smoothing

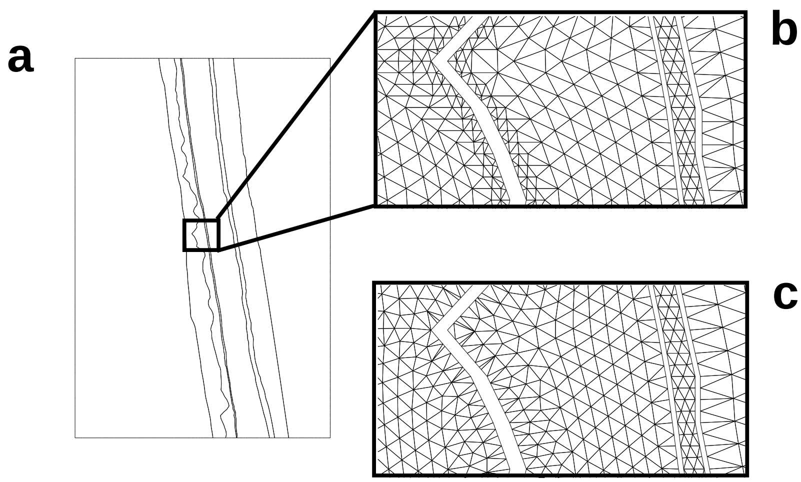

FIGURE 3. (a)Structure of geologic layers is represented by material interfaces. (b)A close-up of the grid shows increased resolution at some material interfaces. (c)Smoothing is applied to form a more isotropic grid while maintaining material interfaces. Grids are Delaunay with positive coupling coefficients. The grid is separated at material interfaces for visualization.

The cross section in Figure 3a is digitized from photographs of a tunnel wall. It is important to represent the fine scale undulations of the different materials and provide increased grid resolution near the interfaces where material properties change. Figure 3b is a small piece of the grid with increase grid resolution at the material interface. Because the grid is anisotropic a smoothing method [7] is applied that allows nodes to move within a material region while maintaining material interfaces. The smoothing combined with edge flipping results in the Delaunay grid shown in Figure 3c.

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Other applications of smoothing allow grid designs with node density pulled towards areas of high field gradient. This helps one construct grids with resolution concentrated in areas where the physical process is most difficult to resolve while not wasting computational resources in regions where resolution is not required.

Example 4: Grid Refinement With Point Addition

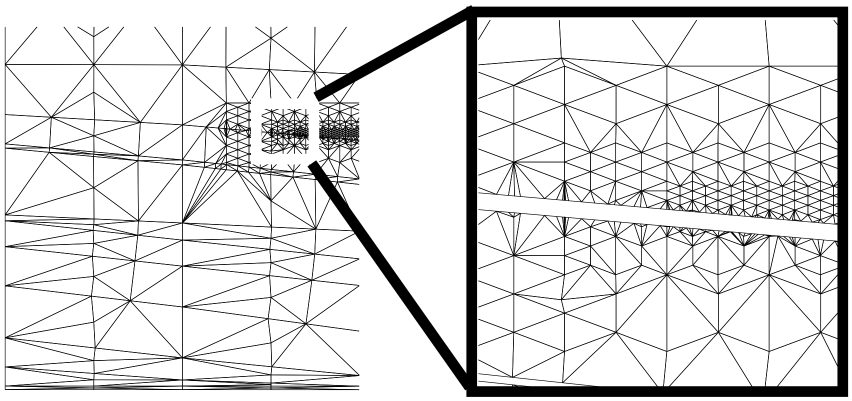

FIGURE 4. A small zone of the geometry model shown in Figure 1a required a high resolution grid. Resolution is increased by defining a high density of points in a particular region and inserting them into the grid shown previously in Figure 1b. The reconnection and point addition maintains the material interface that cuts through the high resolution region of the grid. The grid is split apart at the material interface to illustrate that no connections cross the interface.

For calculations of heat and vapor transport from an underground excavation, a very high resolution grid is required to model near field processes. The grid in Figure 4 is a close-up of the lower left side of a grid created from the geometry model of Figure 1a. This grid is created by inserting a high density point distribution in the area of the excavation. The points are added to the grid of Figure 1a one at a time with algorithms very similar to grid refinement algorithms. As each node is added we determine if the node falls in an element, on an element face, along an element edge or on a node. Depending upon where the node being added lands, a different refinement algorithm is used. The only difference from typical refinement is that the location of the added point is constrained by the input point distribution rather than being determined by the refinement algorithm. Note also that the high resolution grid crosses a material boundary but the grid connectivity never crosses the material interface.

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Another application of point addition is placing points at specific locations for comparison with data. For example, in a project to model ground water in a basin of over 1000 sq/km, the modeler had data on the location of the water table at 250 water wells. By placing a computational node at the three dimensional coordinates of each data point, it is was very easy to compare the water level of the model to actual data.

Conclusions

The GEOMESH grid generation application utilizes the X3D grid generation system to create unstructured finite element grids tuned to the special needs of geological applications (complex geometry, multi-material, positive coupling coefficients). Automated grid generation tools that directly access geologic modeling tools enable rapid construction and modification of computational grids. Grid quality tools insure that the final computational grid produced will perform well with the physics modeling algorithms the grid is constructed for. These tools allow more time to be spent on analysis of the physics being modeled and free the investigator to study situations that could not be approached without automatic grid generation tools.

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