# Chapter 3 - Mesh Generation

## 3.1 Abstract

Computational mesh generation involves translating the Integrated Site Model, ISM (Zelinski and Clayton, 1996, Clayton et al., 1997), of geologic and hydrologic structure and stratigraphy to a finite element mesh. This process maintains the geometry defined by the ISM model while meeting additional geometric constrains on element size and geometry necessary for stable and accurate flow and transport solutions.

The GEOMESH/X3D grid generation toolkit, (Gable et al., 1995, Gable et al., 1996a and b, Trease et al., 1996), has been developed to provide an integrated software package for all grid generation steps including: import of initial ISM model, quality checking of input data, mesh optimization, mesh post processing and quality checking, mesh interfacing with the FEHM flow and transport code, and property interpolation from the mineralogy and petrology model (Chipera et al., 1997a and b). Chapter 3 describes the algorithms used for mesh generation and how the algorithms have been applied to the two- and three-dimensional meshes used for flow and transport computations.

## 3.2 QA Status of Software and Data

The GEOMESH/X3D grid generation toolkit, (Gable et al., 1995, Gable et al., 1996a and b, Trease et al., 1996) is non-Q with respect to YMP and Los Alamos quality assurance requirements. However, version control software tracking procedures identical to those used for the Q code FEHM are followed. GEOMESH/X3D utilizes well established procedures to insure robust mesh generation results and to insure traceability of changes to the software. A suite of test problems has been developed and all new releases are verified against the test suite.

| Table 3-1. QA Status of Data used in this Chapter | | | | |
|---|---|---|---|---|
| **REFERENCE** | **Q Status** | **DTN** | | **COMMENT** |
| **Buesch et. al., 1996**, "Revised Stratigraphic nomenclature and macroscopic identification of Lithostratigraphic units of the Paintbrush Group exposed at Yucca Mountain, Nevada", USGS Survey Open-File Report 94-496, 1996 | Q | GS941208314211.064 | | |
| **Clayton et. al., 1997**, "ISM2.0: A 3-D geological framework and integrated site model of Yucca Mountain: Version ISM1.0", Doc ID B00000000-01717-5700-00004 Rev 0, MOL. 19970122.0053, CRWMS M&O | Q | | | By agreement with DOE and NRC accepted as Q even though it utilizes some non-Q data |
| **Zelinski and Clayton, 1996**, "A 3-D geological framework and integrated site model of Yucca Mountain: Version ISM1.0", Doc ID B00000000-01717-5700-00002 Rev 1", CRWMS M&O | non-Q | | | |

## 3.3 Unsaturated Zone Computational Mesh from Stratigraphic Model

All grids are built from the detailed geologic framework model ISM (Zelinski and Clayton, 1996, Clayton et al., 1997) which is correlated to the Project's hydrologic units and nomenclature in Table 15-1. Faults are represented as vertical features. This is consistent with the model of Bodvarsson et al. (1997), that incorporates a subset of the faults used in this work as vertical features. An example of a two-dimensional cross section, within the framework of the three-dimensional mesh it is extracted from is, shown in Figure 3-1.

The primary criterion used in mesh construction is that the mesh will retain the original

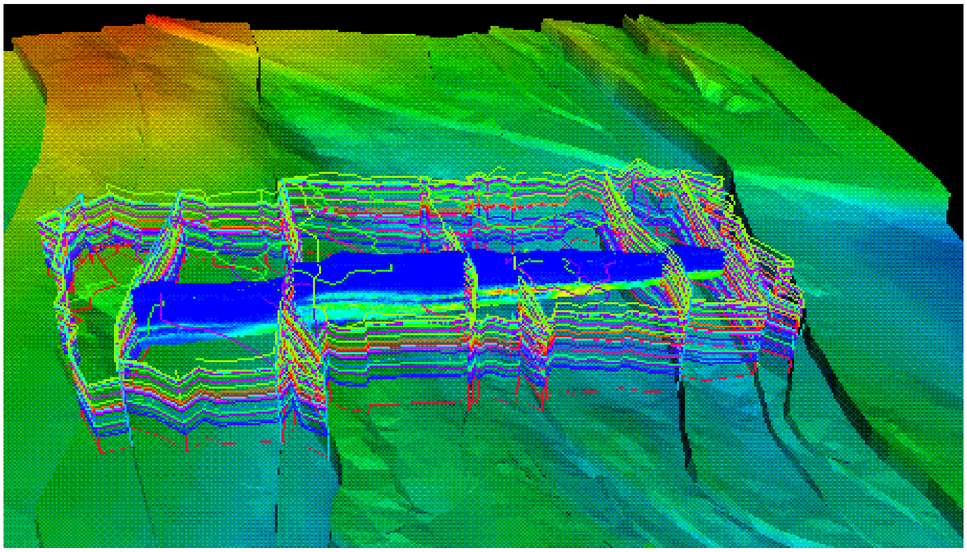

**Figure 3-1.** Layer 9 of ISM shown with colors representing elevation. The area in which a three-dimensional tetrahedral grid is build is shown by the wire frame in which each line represents a stratigraphic layer boundary. The two-dimensional grid used for computations is shown with zeolite abundance shown with red for high zeolite abundance and blue for low zeolite abundance.

geometry of the ISM model. In the grid generation process some smoothing, upscaling or reinterpretation of the ISM model is done. When approximations are necessary, they are carefully controlled and quantified to insure the final grid matches the ISM geometry.

### 3.3.1 Mesh Generation from ISM Input

The steps required to create a two or three-dimensional computable mesh from the Triangular Irregular Network (TIN) data are detailed below and include:

- Import ISM Triangular Irregular Network (TIN) data into GEOMESH/X3D
- Test and correct inconsistencies in TIN sheets
- Identify and tag the faults on the TIN surfaces
- Define polygonal subset of TIN surface
- Refine TIN surface grids in and adjacent to faults
- Define upper and lower boundary truncation surfaces
- Define minimum layer thickness
- Stack layers and build prism elements between surfaces
- Convert prism elements into tetrahedral elements
- If two-dimensional: Extract a two-dimensional hybrid grid from the three-dimensional tetrahedral mesh
- If two-dimensional: Convert the two-dimensional hybrid grid into a triangulated mesh
- If two-dimensional: Clip the mesh to area of interest
- Optimize the grid for computation using reconnection, smoothing, refinement and derefinement
- Interpolate attributes from geostatistics or Stratamodel representation of mineralogy
- Compute and output finite volume matrix coefficients
- Compute and output area coefficients of surface nodes
- Define node sets for setting initial conditions, boundary conditions and material properties
- Mesh quality checks

#### 3.3.1.1 Import ISM Data into GEOMESH/X3D

The first step required to integrate the ISM data is to import the ISM model. The ISM data is provided as 31 computer files that each contain a representation of the top surface of a geologic units. Each surface is represented by a TIN surface of 4976 x, y, z coordinates and the connectivity for 9823 triangles (Figure 3-2).

### 3.3.2 Quality Testing and Correcting of ISM TINs

To insure that the triangular sheets representing the ISM model form a valid triangulation, the tests that must be met are:

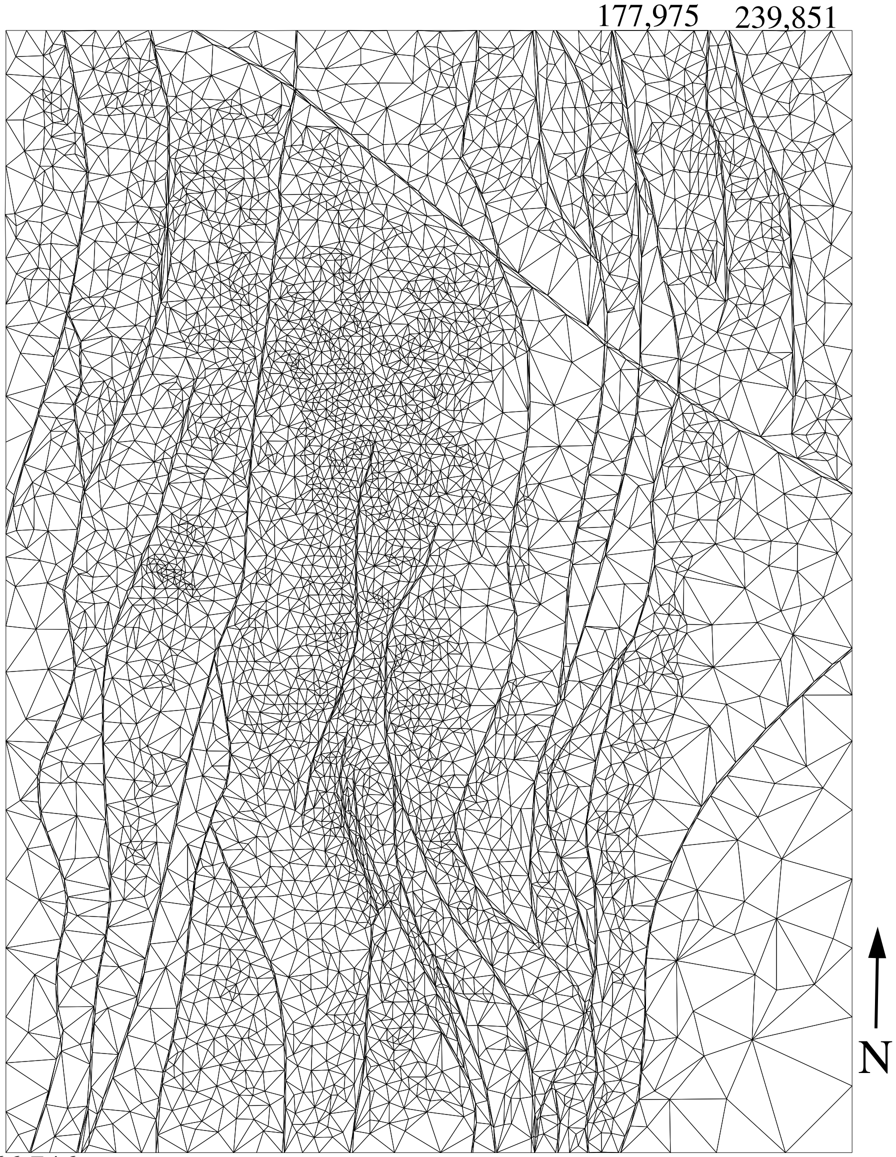


**Figure 3-2.** Top view of one TIN from ISM. TIN consists of 4976 nodes and 9823 triangles. Coordinates are Nevada State Plane in meters. Each triangle vertex is assigned an elevation, resulting in a piecewise linear representation of stratigraphic surfaces.

- TIN sheets have no holes
- No triangles overlap
- All triangles are ordered to have their normal vector on the same side of the TIN.

Examination of these data found that all the TIN sheets suffered from a small number of holes and overlaps. Although these holes and overlaps are inconsequential for creating computer visualizations of the data, these problems would make the subsequent mesh generation steps impossible if they are not first corrected. Thus software was developed to identify, characterize and repair the inconsistent TINs. This process resulted in the addition of 3 triangles to each of the 31 TINs and some minor to the connectivity to eliminate overlaps.

#### 3.3.2.1 Identify Faults

The triangular representation of each stratigraphic boundary in ISM does not have any attribute flags indicating which parts of the TINs represent faults and which parts of the TINs represent a stratigraphic boundary. It is essential for the flow and transport studies to identify which parts of the model are fault related so that hydrologic properties of faults can be included. An algorithm was developed to identify the portions of the TIN sheets that represent faults. The algorithm is based on the observation that faults can be identified in the TIN sheets by examination of the normal vector of each facet of the TIN. The algorithm is described as follows: The normal vector to each triangle is calculated. For these sheets, all normal vectors are within ninety degrees of vertical. If the normal vector is within 45 degrees of vertical, the triangle is taken to be a stratigraphic boundary. If the normal vector is greater than 45 degrees from vertical and less than 90 degrees, it is labeled as a fault triangle. The fault triangles are further identified by their tilt to the north, east, south or west. The result is that each triangle is identified as either a stratigraphic boundary or as one of four fault types (see Figure 3-3).

#### 3.3.2.2 Define polygonal subset of TIN surface

The area of interest for the current flow and solute transport modeling effort is smaller than the area defined in the geologic framework model ISM (Zelinski and Clayton, 1996). A polygonal subset of each TIN surface is created by removing any elements that fall outside a user defined area. Typically, this area is bounded by faults (Figure 3-4). Where no faults exist and a subset boundary is desired, elements are removed outside a straight line that connects natural fault boundaries. Since the element edges do not coincide exactly with the arbitrary bounding line, some unevenness of the boundary of the subset results. This unevenness does not effect the flow and solute transport modeling results because the boundaries are chosen to be sufficiently far from the model area of interest.

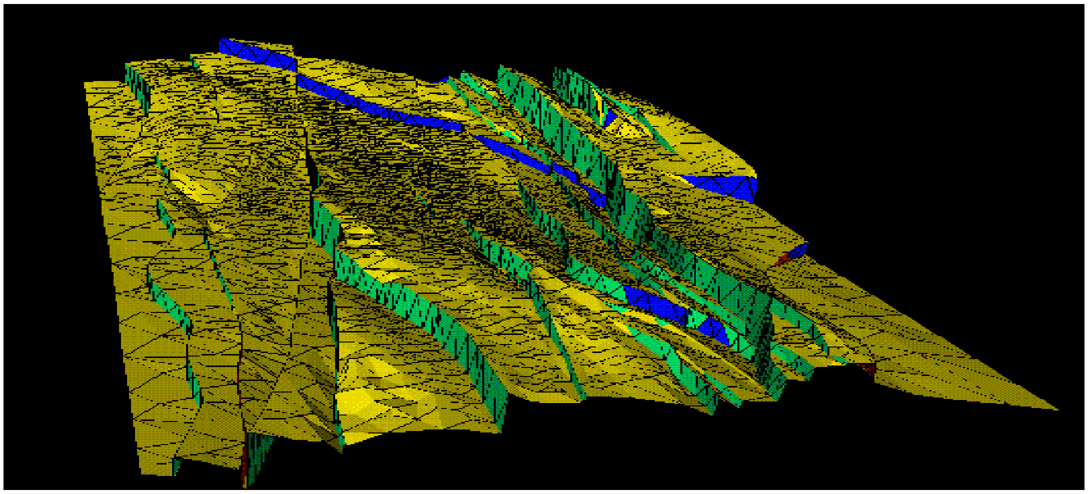

**Figure 3-3.** Layer 38 from ISM at 3X vertical exaggeration. Stratigraphic layer boundary is colored in yellow. West facing faults are green, south facing faults are blue.

#### 3.3.2.3 Refine TIN surface grids in and adjacent to faults

In order to more accurately model the effect of faults on the groundwater system, the element size in, and adjacent to, identified fault triangles on each surface is decreased by adding nodes to the center of element edges (refinement). To keep the horizontal element configuration of all layers identical, refinement is done to ISM layer 24 which is the base of TSW4. This layer has the most complete identification of fault triangles. The refinement is performed after a polygonal subset of TSW4 is extracted as described in Section 3.3.2.2. Refinement consists of adding a node to the center of any element edge containing at least one node that is identified as a fault when the edge is larger than 20.0 m. This refines the element size in, and immediately adjacent to, fault triangles. The new and old nodes are then reconnected into triangular elements. The resulting mesh of Layer 24 contains 4557 nodes and 6165 elements. The z coordinates of every other layer are then mapped onto the triangular element configuration of Layer 24 to create separate surfaces with the correct depth and identical element configurations.

#### 3.3.2.4 Define upper and lower boundary truncation surfaces

The ISM model defines stratigraphic layers much deeper than were needed for unsaturated zone calculations. Therefore, the ISM surfaces are truncated and no grids are generated below an

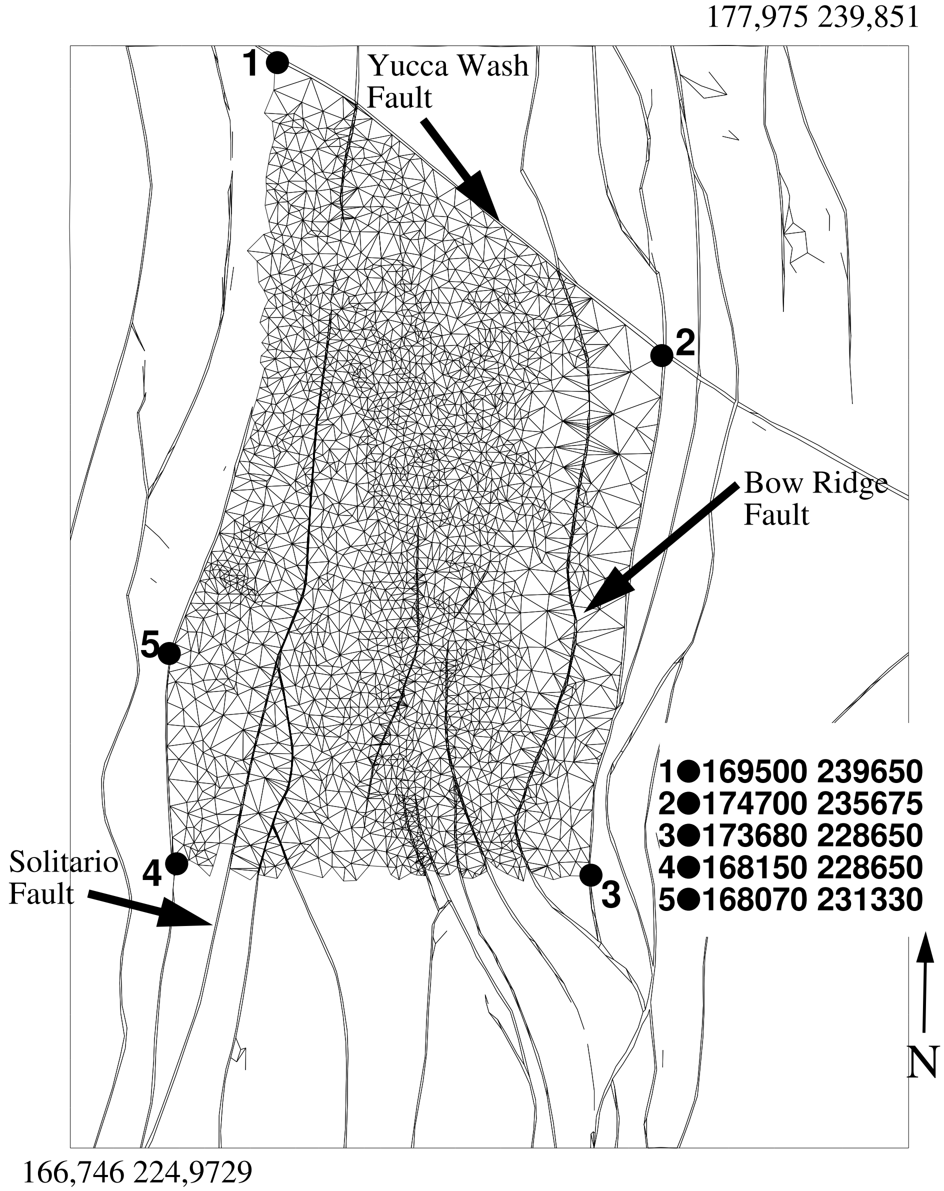


**Figure 3-4.** Top view of one TIN illustrating the subregion for the three-dimensional computational grid. TIN consists of 4557 nodes and 6165 triangles. Coordinates are Nevada State Plane in meters. Note the increased resolution near faults in comparison to the original TIN surface (see Figure 3-2).

elevation of 400 meters. This insures that 200 to 300 meters of the grid are available for calculations with different water table levels and also helps make grids smaller by not creating elements deep into the saturated zone.

The top surface of the grid must be truncated at the topographic surface. The ISM model defines stratigraphic surfaces above the topographic surface. The ISM model surfaces are filtered to check if the stratigraphic surface elevation is greater than the topographic elevation. If it is, it is reset to topographic elevation.

#### 3.3.2.5 Define minimum layer thickness

Practical and numerical considerations make it necessary to set a minimum layer thickness before producing volume grids between the stratigraphic surfaces. In areas where a particular unit pinches out to zero thickness or is truncated by faults or topography, there can be extremely thin layers. It was found that some layers in the ISM model were as small as 4 cm, an artifact of the model building process rather than an actual geological feature. In this work, if a layer thins to less than one meter, its thickness is set to zero. This insures that large aspect ratio tetrahedral and triangular elements are avoided.

#### 3.3.2.6 TIN Sheets Stacked and Converted to Prisms

The TIN sheets are stacked from lowest elevation to highest elevation, via a module from the GEOMESH/X3D system developed specifically for this application. The ISM model consists of a set of stacked triangle sheets that all share the same number of triangles and the same x and y coordinates for the triangle vertices. The only difference between sheets is the z elevation. The stacked sheet data structure is then converted to a finite element node and connectivity list. Now all elements are represented as prisms (6 nodes, 2 triangle faces, 4 quadrilateral faces) with vertical connections between adjacent layers. This module for the GEOMESH/X3D system was also developed specifically for this application.

Once stacked, we found that some sheets in the ISM model cross. Therefore, decisions were required for dealing with crossing TIN sheets. After consultation with William Zelinski, it was agreed that whenever a higher stratigraphic horizon crosses the layer below, the higher elevation sheet should be given an elevation equal to the lower layer. In this method layers pinch out to zero thickness if they cross. This approach exactly maintains the geometry of interfaces and faults except in the cases where the ISM model represented negative volumes, overlapping or very thin layers.

#### 3.3.2.7 Convert Prisms to Tetrahedra

Tetrahedral elements are fundamental to three-dimensional computations. Therefore, prism elements must be converted into tetrahedra. Another module had to be developed for the GEOMESH/X3D system to do this. Prism elements are converted to tetrahedral elements by one of two methods. The options are to create either eighteen or three tetrahedra from each prism. Eighteen tetrahedra are created by adding a node to the center of each face and a node the center of the prism element. Connections are then made to generate eighteen tetrahedra from each prism. Creating three tetrahedra does not require node addition, it is simply a change in the connectivity of the nodes representing each prism. In this work we chose to convert each prism to three tetrahedra. The resulting representation is now in the form of a tetrahedral mesh.

#### 3.3.2.8 Extract a Two-Dimensional Plane

For two-dimensional calculations, extraction of planes from the tetrahedral mesh follows. A plane through the tetrahedral mesh is defined, which can be at any orientation, and the intersections of the tetrahedral elements with the plane are calculated. The result of intersecting a tetrahedral mesh with a plane is a two-dimensional hybrid mesh consisting of triangles and quadrilaterals.

For this work, the plane chosen was an east-west cross section extracted at Nevada State Plane (NSP) coordinate 232,100 meters. The east and west boundaries of the plane are truncated at unnamed faults in ISM at NSP coordinates 168,274 meters on the west and 174,176 meters on the east (Figure 3-5).

#### 3.3.2.9 Convert Hybrid Grid to Triangles

The hybrid mesh of quadrilaterals and triangles must be converted to a triangular mesh. This requires that quadrilateral elements are split into 4 triangles, resulting in a fully triangular mesh.

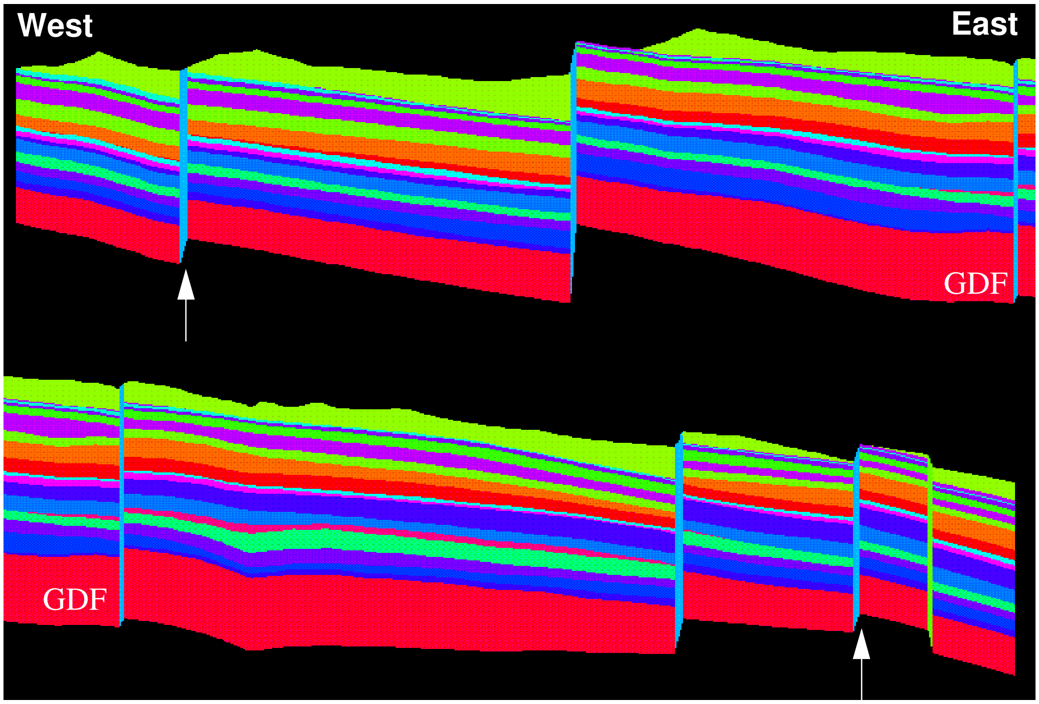


**Figure 3-5.** Cross section at NSP coordinate 232,100 meters extracted from ISM. In the figure, the cross section is split in two near the Ghost Dance Fault (GDF). The east and west extent of the computational model at NSP 168,274 meters and 174,176 meters are marked by arrows. Colors represent hydrogeologic units incorporated into the computational mesh.

### 3.3.2.10 Clip Mesh to Area of Interest

The two-dimensional computational mesh requires east, west and bottom boundaries different than those in the ISM model. The mesh is clipped at specified east and west boundaries immediately inside of the faults and at z=400 meter above sea level. This leaves 220 meters below the water table for applying a variable water table at the base of the model.

### 3.3.2.11 Optimize Mesh For Computation

Numerical solution techniques for flow and transport calculations with finite volume and integrated finite difference methods place geometric constraints on the quality of a mesh. To optimize the mesh, we use a combination of smoothing, refinement, derefinement and reconnection algorithms to enhance mesh quality while preserving geometry.

- Reconnection

Reconnection algorithms change the connectivity of a mesh without modification of node position or the number of nodes in the grid. Two-dimensional grids use a single reconnection algorithm which will flip the shared edge of two triangles. The result is a two-triangle to two-triangle transformation that can be used to improve the quality of the grid. In three dimensions, there are many more options. In addition to two tetrahedra flipped to two new tetrahedra (2to2), there are 2to3, 3to2 and 4to4 flips. These are used in an automated reconnection algorithm to improve grid quality.

- Smoothing

An elliptic smoothing algorithm is employed to smooth the two-dimensional grid. In this step, nodes on material boundaries are held fixed, while nodes in the interior are allowed to move. This produces a mesh with more equal aspect ratio triangles (Figure 3-7). The algorithm for moving nodes poses the problem of where to move nodes in terms of minimization of a function. An objective function is calculated based on the node positions and connections and a set of linear equations are solved to find which direction of motion each node should have to minimize the function. The smoothing used in this work attempts to smooth the grid so all triangle vertex angles are close to 60 degrees. In addition we must insure that the motion of nodes will not cause any overlapping or negative area/volume elements.

Reconnection can be done without adding points by allowing connections to flip. This is useful for keeping the grid from binding during repeated smoothing applications. For the final mesh, points are added as needed to create a Delaunay grid with positive coupling coefficients (Figure 3-6). This assures that the optimum computational mesh results.

- Refinement

There are many different options for grid refinement. The methods used most often are edge, face, and element refinement. Edge refinement adds a node to an element edge, face refinement adds a node to an element face center and element refinement adds a node to the

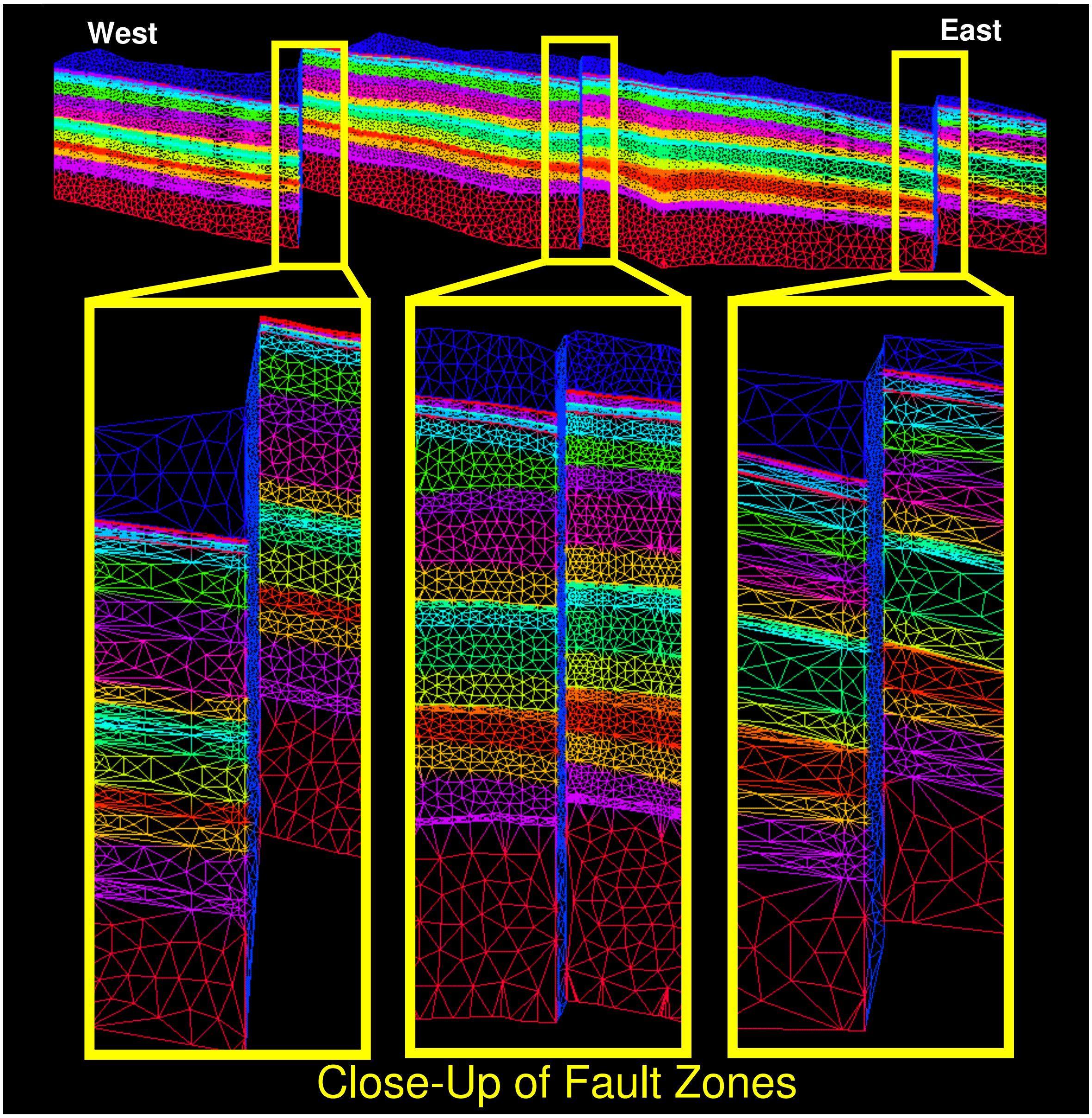


**Figure 3-6.** Two-dimensional mesh generated from YMP model ISM showing faults as part of the computational grid. The faults from west (left) to east (right) are Solitario Fault, Ghost Dance Fault and Bow Ridge Fault. The cross section is bounded on the west and east by unnamed faults in ISM. Colors represent different hydrogeologic units. Close-up views of the grid are shown at each of the faults.

centroid of an element. Nodes can also be added at any location the user desires and the code will figure out which type (edge, face, element) of refinement to use when adding the node.

The refinement algorithms are also closely coupled with grid refinement criteria algorithms. All the refinement methods also need criteria which trigger the grid refinement. Some

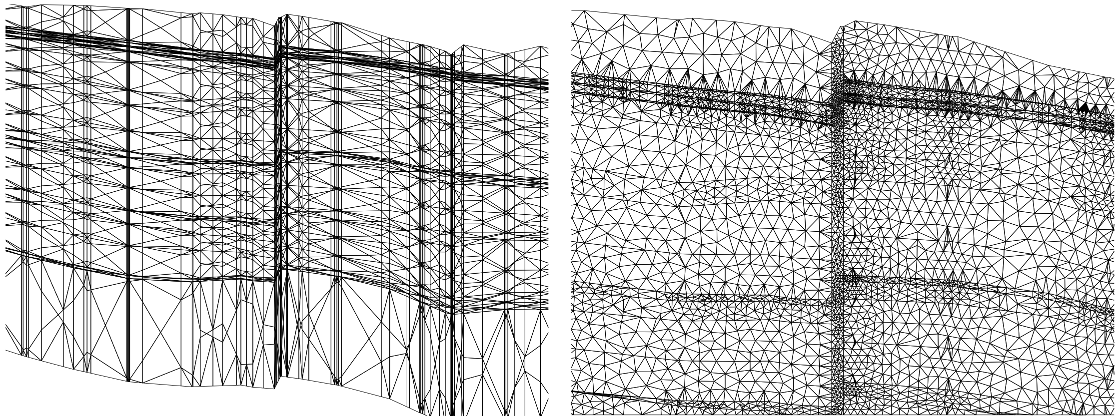

**Figure 3-7.** An example of how elliptic smoothing modifies the mesh. The mesh on the left has the topology that results from extracting a two-dimensional grid from a three-dimensional tetrahedral mesh. Material interfaces are maintained but the node distribution is very uneven. The mesh on the right has been smoothed by keeping interface nodes fixed but allowing nodes between material interfaces to move. The mesh on the right has a flat bottom by truncating the mesh at elevation 720 meters.

of the options for refinement criteria are geometric regions, element aspect ratio, element edge length, field value and field gradient. One or more of these criteria are set, and elements that meet the refinement criteria are refined by one of the above methods. Multiple uses of refinement can be performed on the same mesh.

- Derefinement

Derefinement is nearly the opposite of refinement. Derefinement removes nodes from the mesh based on a variety of criteria related to element optimization. The criteria can be specified as edge length, element aspect ratio, or element volume. An example would be to remove one node of every element edge in the mesh that is less than 20 m in length. If the criterion of element aspect ratio or element volume is used, one node is removed from the shortest edge of any elements matching the specified criterion. Material interfaces are preserved except when a geologic material layer has a vertical width less than a user specified tolerance. Then the nodes defining the layer at that point may be removed at the user's option, potentially leaving the geologic layer discontinuous.

After the removal of nodes using the derefinement option, the remaining nodes are reconnected leaving a mesh that contains no holes or overlapping elements. The refine, derefine, and smooth options can be used sequentially and can be repeated until the problem converges and no change would occur if the process were continued. When these steps have converged, we consider the grid to be optimal for our computations.

### 3.3.2.12 Mapping Properties From Three-Dimensional Mineral Distribution

Zeolite distributions from the three-dimensional mineralogy model (Chipera et al., 1997a and b) have been mapped onto the computational grids. Grid to grid mapping algorithms allow properties from one mesh, (the mineralogy model), to be mapped onto another mesh with a different node distribution, (the computational mesh) (see Figure 3-8).

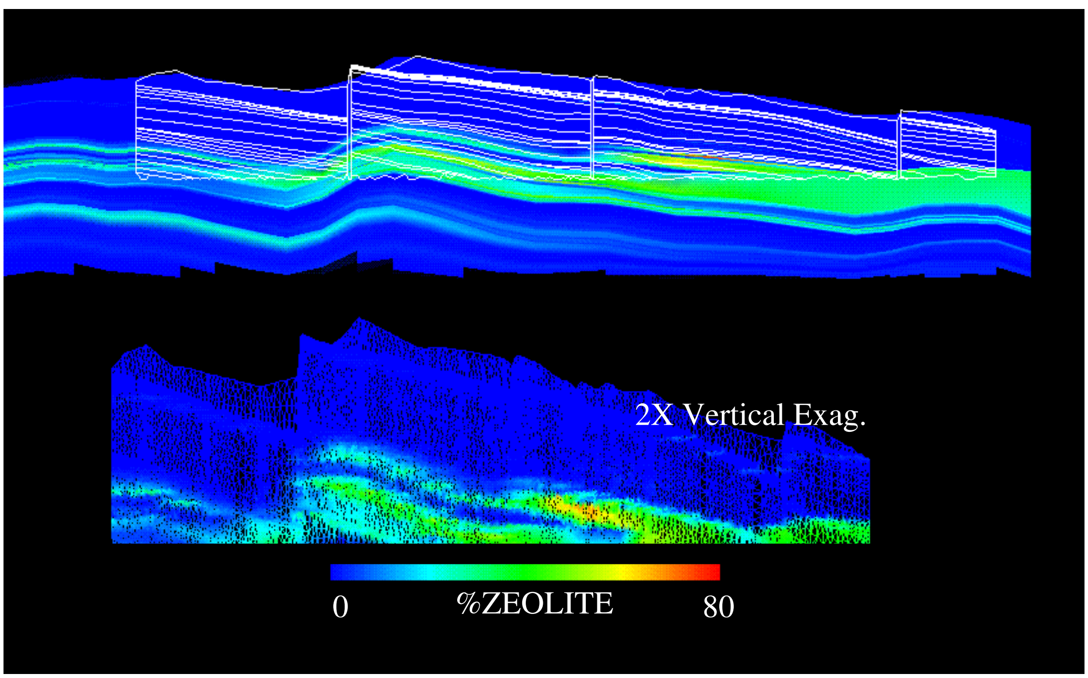


**Figure 3-8.** Zeolite distributions are mapped from a three-dimensional model onto the computational mesh. The upper figure show zeolite distributions on a grid extracted from the Stratamodel three-dimensional mineralogy model. The lower figure shows the zeolite distributions after being mapped onto the computational mesh.

The method requires a fully connected source mesh with interpolation onto the nodes of the sink mesh. The method is as follows. For each node in the sink mesh, find the corresponding element in the source mesh and interpolate a value for the sink node from all node values in source element. Interpolation options are linear, $\log_{10}$, $\log_e$ and hyperbolic sine. For mineral distributions, linear interpolation is used.

### 3.3.3 Generation of FEHM Input Files

#### 3.3.3.1 Compute Finite Volume Matrix Coefficients

The FEHM flow and transport code uses finite volume control volumes for solution of flow and transport equations. Part of the grid generation process is to calculate the Voronoi control volume associated with each node in the grid and the area of the polygonal faces of the Voronoi control volumes.

#### 3.3.3.2 Compute Area Coefficients of Surface

Each node on the surface of the grid has a an associated surface area. This is computed for use in scaling flux boundary conditions to infiltration maps.

#### 3.3.3.3 Output Information for Boundary Conditions and Material Properties

Lists of node sets are created and output. These lists are used by the FEHM code to set material properties and boundary conditions. The node set lists include outside, top and bottom nodes, stratigraphic unit number and fault number.

### 3.3.4 Mesh Quality Assurance Steps

The process of producing an optimized mesh for computation requires steps that alter the number of nodes and elements and move grid nodes. A number of tests are employed to ensure that the final grid meets the quality standards necessary for accurate and stable computations. These tests are:

- No holes in the mesh
- No overlapping triangles
- All elements have positive volume/area
- All material interfaces are maintained
- The mesh is a Delaunay triangulation
- All geometric coupling coefficients are positive

These tests were employed and passed for all meshes employed in this report.

## 3.4 Computational Grids Used in the Present Study

### 3.4.1 Three-Dimensional Unsaturated Zone Grid

The final grid used for three-dimensional calculations is shown in Figure 3-9. It contains 71,781 nodes and 414,313 tetrahedral elements. Faults represented in the ISM model are included as separate materials (Figure 3-10). Since the calculations are dual permeability, the number of grid point for FEHM calculations is 143,562.

### 3.4.2 Two-Dimensional Unsaturated Zone Grid

Two-dimensional cross section grids have been produced at two different resolutions. The grid shown in Figure 3-6 is a low resolution triangular mesh with 21,494 nodes and 42,086 triangular elements. The FEHM dual permeability grid has 42,988 nodes.

The mesh used for interpolation of geostatistical mineral distributions has much higher resolution between the Ghost Dance and Solitario faults at and below the potential repository, with 66,984 nodes and 78,312 triangular elements and 133,968 dual permeability grid points. A small portion of the high resolution grid is shown in Figure 3-12. In the high resolution area, the spacing between nodes is approximately 4-6 meters.

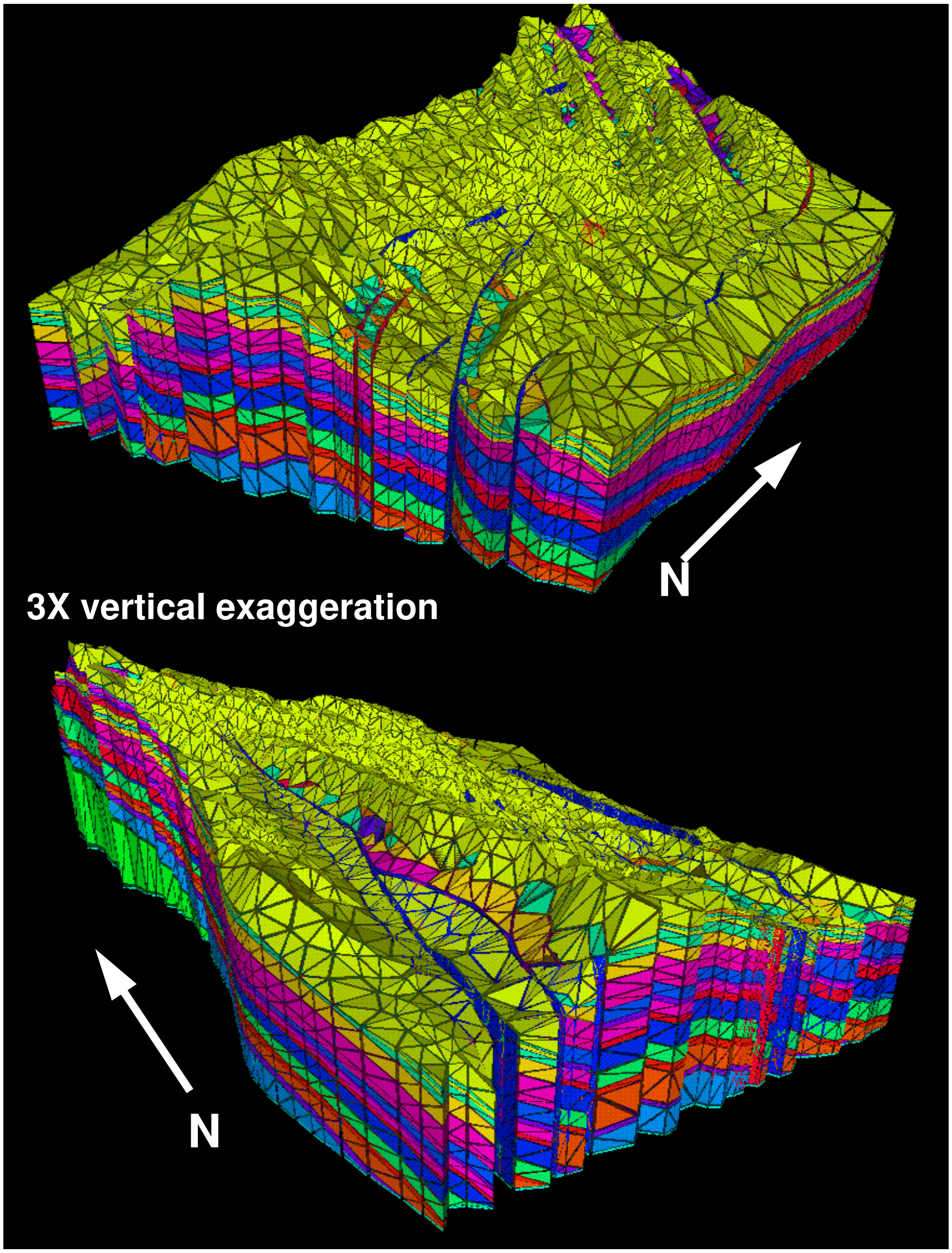


**Figure 3-9.** Three-dimensional unsaturated zone computational grid with 71,781 nodes, 143,562 dual permeability nodes and 414,313 tetrahedral elements.

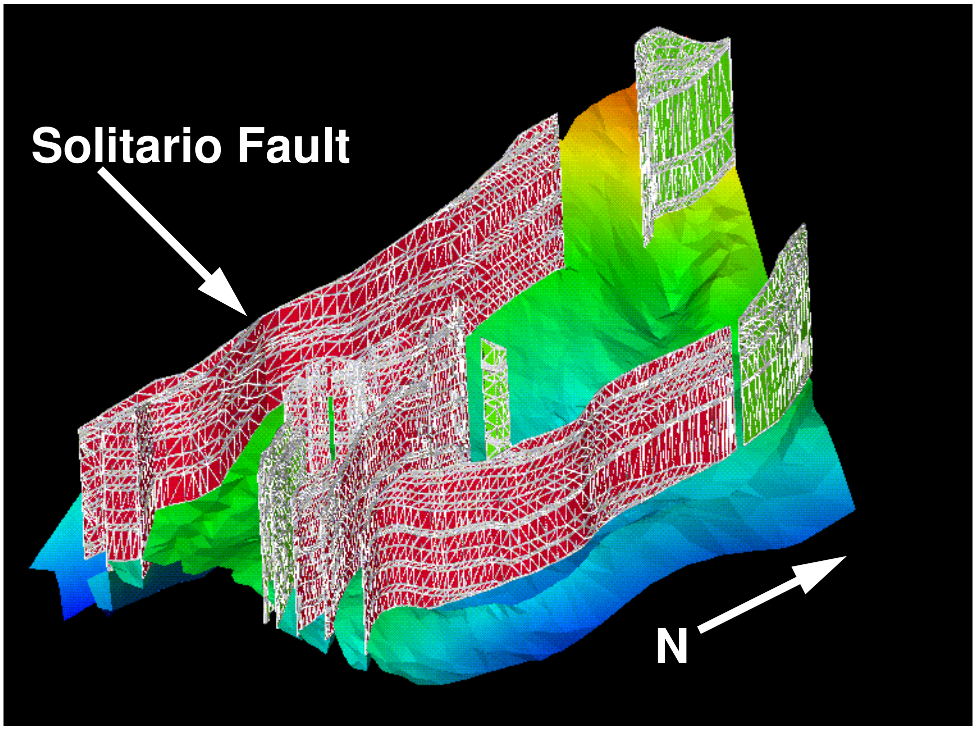


**Figure 3-10.**Faults are represented as distinct materials. Layer 9 from ISM is shown. There are 14,473 nodes and 45,386 tetrahedral elements used to represent the faults. Faults that dip to the west are filled in red, faults that dip to the east are filled with green.

## 3.5 Conclusions

Accurate simulation of flow and transport in the unsaturated zone at Yucca Mountain requires simulation tools capable of representing the complex stratigraphy which includes dipping, faulted geologic layers of varying thickness and extent. The GEOMESH/X3D toolkit was developed specifically to address such issues. Further, once the geometric constraints of the geologic system are resolved, the flow and transport simulations are only as accurate as the mesh upon which they are computed. GEOMESH automatically insures quality finite-element grids. Further, the GEOMESH/X3D toolkit is designed to accept electronic input directly from the geologic and mineralogic models, thus insuring nearly exact replication of the structure and attribute distributions in those models.

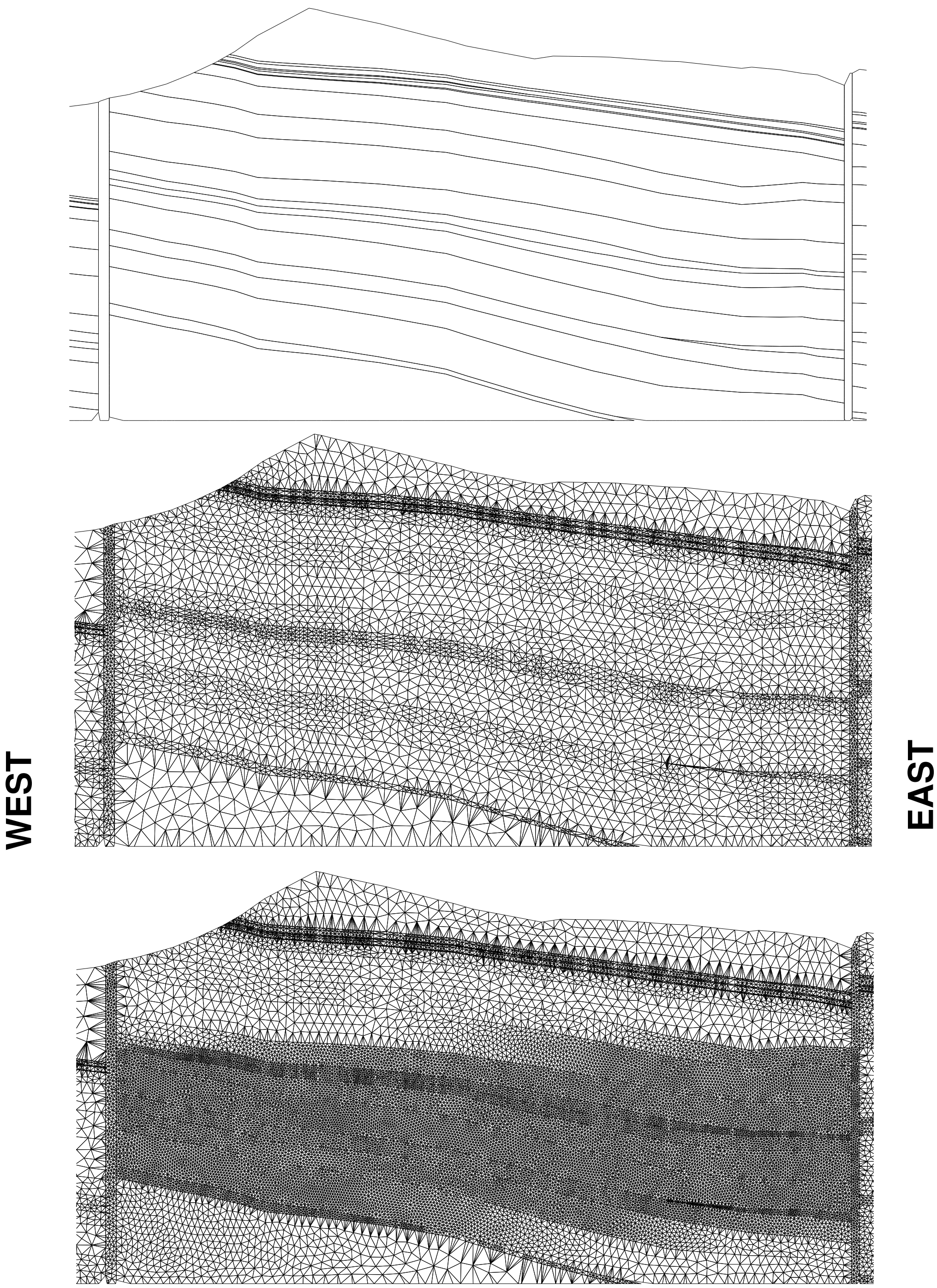


**Figure 3-11.** A portion of the two-dimensional cross section is shown bounded on the west by the Solitario fault and on the east by the Ghost Dance fault. a) Stratigraphic layer boundaries, b) low resolution computational grid, c) high resolution computational grid.

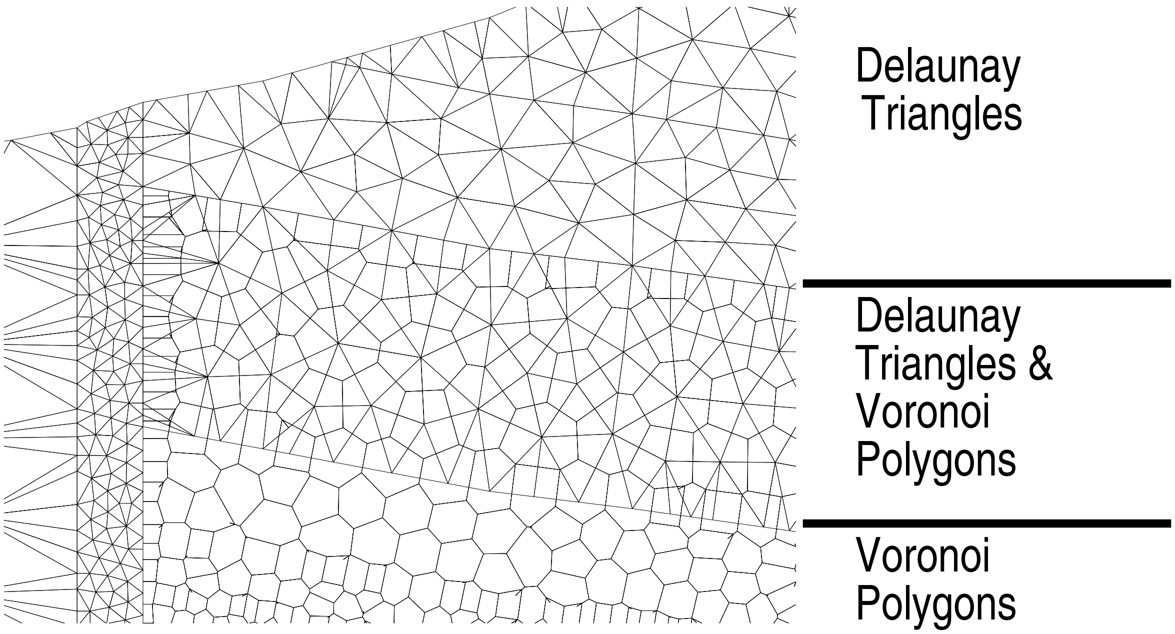


**Figure 3-12.** A small section of the high resolution two-dimensional grid near the Solitario fault showing the triangulation and the Voronoi cells associated with the triangles.