WinGridder—
AN INTERACTIVE GRID GENERATOR FOR TOUGH2

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ABSTRACT

The TOUGH (Transport Of Unsaturated Groundwater and Heat) family of codes has great flexibility in handling the variety of grid information required to describe a complex subsurface system. However, designing and generating such a grid can be a tedious and error-prone process. This is especially true when the number of cells and connections is very large. As a user-friendly, efficient, and effective grid generating software, WinGridder has been developed for designing, generating, and visualizing (at various spatial scales) numerical grids used in reservoir simulations and groundwater modeling studies. It can save mesh files for TOUGH family codes. It can also output additional grid information for various purposes in either graphic format or plain text format. It has user-friendly graphical user interfaces, along with an easy-to-use interactive design and plot tools. Many important features, such as inclined faults and offset, layering structure, local refinements, and embedded engineering structures, can be represented in the grid.

INTRODUCTION

WinGridder is a Windows-based software package for designing, generating, and visualizing at various spatial scales numerical grids used in reservoir simulations and groundwater modeling studies. Development of this software was motivated by the requirements of the TOUGH (Transport of Unsaturated Groundwater and Heat) family of codes (Pruess 1987, 1991) for simulating subsurface processes related to high-level nuclear waste isolation in partially saturated geological media. Although the TOUGH family of codes has great flexibility in handling the variety of grid information required to describe complex objects, designing and generating a suitable irregular grid can be a tedious and error-prone process, even with the help of existing grid generating programs. This is especially true when the number of cells and connections is very large. The processes of inspecting the quality of the grid or extracting sub-grids or other specific grid information are also complex. The mesh maker embedded within TOUGH2 generates only uniform numerical grids and handles only one set of uniform fracture and matrix properties throughout the model domain. This is not suitable for grid generation in complex flow and transport simulations (such as those of Yucca Mountain, which have heterogeneity in both fracture and matrix media).

The objective of WinGridder is to provide an efficient, user-friendly, integrated gridding software tool with graphical interfaces and visual inspection capabilities. With WinGridder, the user can easily design and generate complex grid that properly represents the stratigraphic features, inclined faults, engineering structures, and fractured media.

MODELS AND APPROACHES

Single-continuum Grid

A single-continuum grid generated by WinGridder is commonly used for TOUGH2 modules to simulate fluid flow and transport in regular porous media. Such a grid discretizes the simulation domain into a collection of cells (i.e., the ELEME block in a TOUGH2 input file) connected by the interfaces between them (i.e., the CONNE block in a TOUGH2 input file). The cell is a control volume over which the governing equations will be integrated, while the closed surface of the cell is discretized into several interfaces (i.e., surface segments) corresponding to its neighboring cells.

Dual-continuum Grid

A dual-continuum grid generated by WinGridder can enable TOUGH2 modules to simulate fluid flow and transport in fractured porous media. Such dual-continuum grids can be generated for three types of fractured media:

(1)   A single set of parallel, infinite fractures (Type #1) with uniform spacing within each hydrogeologic unit;

(2)   Two orthogonal sets of parallel, infinite fractures (Type #2) with uniform spacing within each hydrogeologic unit;

(3)   Three orthogonal sets of parallel, infinite fractures (Type #3) with uniform spacing within each hydrogeologic unit.

To generate a dual-continuum grid, WinGridder duplicates a primary single-continuum grid and adds inner connections between the corresponding fracture cells and matrix cells, with modified cell volumes and connection areas based on the fracture properties of each hydrogeologic unit. It uses the following formulas to calculate the volumes of the fracture and the matrix cells:

$$V_f = \phi_f \, V_n \qquad (1)$$

and

$$V_m = \left(1 - \phi_f\right) V_n \qquad (2)$$

where V_f and V_m are volumes of fracture and matrix elements, respectively, for the dual-permeability grid, and V_n is the volume of cell n of the primary mesh from which the dual-permeability grid is being generated. The porosity or volume fraction of fractures within the bulk rock is represented by ϕ_f.

The connection information for the dual-continuum grid is determined as follows:

Global fracture-fracture and matrix-matrix connection data are kept the same as those of the connections in the single-continuum grid for the same/corresponding grid cell. This implies that permeabilities used for both fracture and matrix systems are the "continuum" values for both, relative to the bulk connecting areas. Inner connection distances between fractures and matrix within a primary grid cell are calculated as (Pruess, 1983):

$$D_f = 0 \qquad (3)$$

$$D_m = \frac{D}{6} \qquad \text{for Type \#1 fractures} \qquad (4)$$

$$D_m = \frac{D}{8} \qquad \text{for Type \#2 fractures} \qquad (5)$$

$$D_m = \frac{D}{10} \qquad \text{for Type \#3 fractures} \qquad (6)$$

and

$$D = \frac{1}{F} \qquad (7)$$

where D_f is the distance between the fracture center to the surface of matrix cells; D_m is the distance between the surface and an inner point of matrix cells, based on the quasi-steady state assumption (Warren and Root 1963); D is the fracture spacing; and F is the fracture frequency with the unit.

The interface area (A) between fractures and matrix cells is estimated by

$$A = A_{fm} \, V_n \qquad (8)$$

where A_{fm} is the volume-area factor, standing for total fracture-matrix interface areas per unit volume of rock, determined from the site fracture characterization studies.

Multiple-continuum (MINC) Grid

The MINC grid generated by WinGridder is based on a similar principle to that of the dual-continuum grid. The difference is that the matrix cell in a dual-continuum grid is split into N connected subcells in the corresponding MINC grid. N is a number specified by the user.

MAIN FEATURES

WinGridder is a Windows-based software. Detailed descriptions of the software are provided in the WinGridder manuals (Pan et al., 2001a; Pan, 2002). The following is a brief description of its main features.

Graphic user interface

Graphic user interfaces are major communication platforms between the user and WinGridder, occurring in the form of windows. The main window has many components that display information for the user or in response to the user's actions (Figure 1). A caption bar located at the top of the main window shows the name of the current project (or a greeting message if no project open). A status bar located at the bottom of the main window shows the action status of WinGridder. The progress bar may tell the user how much of a current job has been done. Menu bars enable access to all the functionality groups that the user can select.
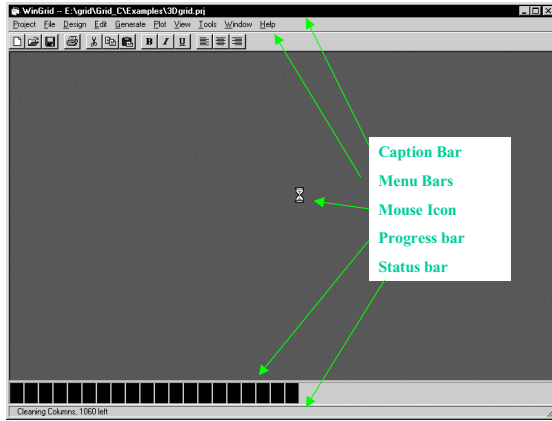
Figure 1. Main window of WinGridder

WinGridder also responds to certain keystrokes, mouse actions, or some combination thereof in certain contexts. Within the main window, child windows are used to plot the grid or facilitate interactive grid design. Other dialog boxes, including the file selection box, the input box, and the printer setting box, automatically or manually engage to aid the user in various tasks. Through graphic user interfaces, WinGridder provides a user-friendly platform to generate variably complex 3-D grids.

Design 2-D (map view) grid

Design 2-D (map view) grid is the first step in grid development. It starts with the assignment of nodes in map view. Based on the location of these nodes, a primary 2-D grid is generated with Voronoi tessellation techniques. The polygon surrounding a node in the map view represents a column of cells in the 3-D grid. Figure 2 shows an example of such grid design using WinGridder.

WinGridder provides capabilities for a user to add, delete, move, and edit any node (or segment) interactively on screen, besides the normal systematic way of assigning nodes for objects (e.g., subregions, faults, drifts, and boreholes) with user-specific parameters. The 2-D grid (map view) acts as a base for generating the third dimension of the grid.
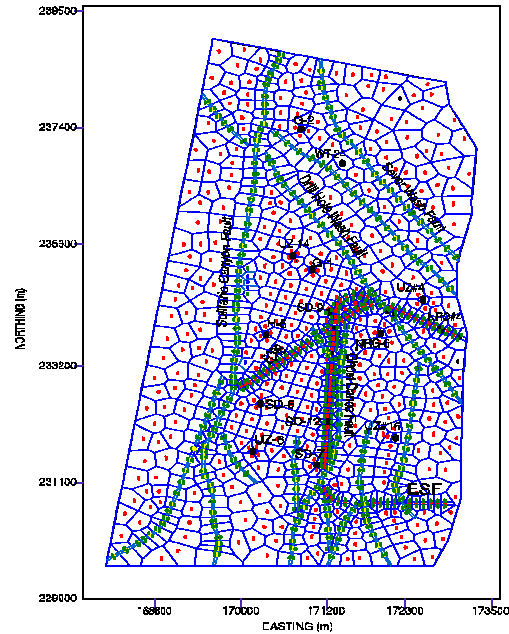

Figure 2. A map view of the 3-D grid of the Yucca Mountain site

Conservation of stratigraphic features

Conservation of stratigraphic features in a 3-D grid is realized in generating the third dimension of a grid. All 3-D cells are created column by column (cutting a column into cells), based on the geometry of each hydrogeologic unit (layer). Then, the lateral connections are built between adjacent columns on a cell-by-cell basis according to their stratigraphic similarity (i.e., belonging to the same layer), unless one of the columns is a fault column or other special columns. In this way, all layer contact interfaces are conserved as interfaces between cells in the 3-D grid, and all adjacent cells within the same layer are connected laterally, unless interrupted by a fault (Figure 3).
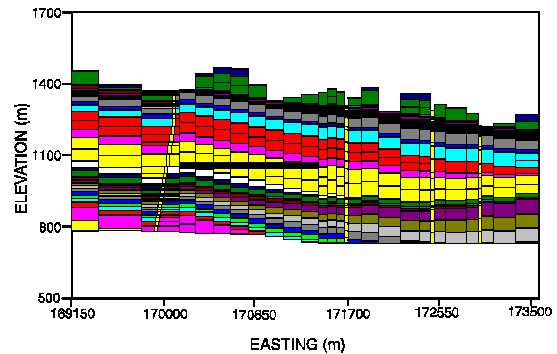

Figure 3. An E-W cross section of the 3-D grid of the Yucca Mountain site

The geometry of each layer is represented by a set of data (either thickness or elevation) with regular spacing. Within these data sets, three major horizons must be in elevation: (1) a top boundary (e.g., the topographic or bedrock surface), (2) a structural reference horizon (i.e., a typical layer contact interface), and (3) a bottom boundary (e.g., the water table). The reference horizon is the surface from which elevations of all hydrogeologic-unit interfaces are calculated by stacking layer thicknesses above or below it based on their stratigraphic position. All offsets resulting from faulting are described by the reference horizon data. Any portions of hydrogeologic units lying above the top boundary or below the bottom boundary after stacking are removed (clipped).

For simple layering structure (i.e., flat layering), a user can easily create the vertical structures of geological units using on-screen.editing functionnality provided by WinGridder.

In general, material properties are assigned to cells depending on the hydrogeologic layer to which the cell corresponds. For layers with multiple rock types, assignment of material properties to grid cells is confined to the appropriate rock zones. These rock zones are defined by material polygons in the aerial extent.

Representation of Faults

Conceptually, three important features of a fault are conserved in the numerical gridding formulation of WinGridder. First, a fault is a separator that causes discontinuity of geological layers and may serve as a structural barrier to lateral flow. Second, a fault zone is continuous and may serve as a fast path for flow depending on its hydraulic properties. Third, a fault may or may not be vertical, and its angle of inclination may vary spatially. To implement these features in a grid, three parallel rows of fault-related columns are built for each fault. Each section of a fault in map view consists of three connected columns, with the fault column located in the middle (Figure 2). Each fault column is connected to two side columns and two neighboring fault columns only. Adjacent fault columns belonging to the same fault will always be connected to each other. Two columns on opposite sides of a fault are always separated by a fault column.

The three fault-related columns (the fault column and its two side columns) are processed together to generate 3-D cells representing the fault and layer offset. Additional vertical resolution is added to facilitate the representation of an inclined fault, based on the location of stratigraphic boundaries on both sides of the fault. Therefore, vertical grid discretization in each set of three fault-related

columns is identical, and often much greater than non fault-related columns. Interfaces between stratigraphic units in both side columns correspond to the interfaces between grid cells (Figure 3). Consequently, the x-y location of fault cells can shift according to the elevation and dip of the fault. Similarly, the volumes and the center (nodal point) location of the corresponding side cells are adjusted accordingly. As a result, the inclination of the fault is described by a series of connected fault cells whose x-y locations vary with elevation. The fault-related cells are vertically connected if they belong to the same column, regardless of the fault angle. Columns of side cells are connected in a similar fashion regardless of the horizontal shifting of position and change in volume.

The layer identification and rock properties of fault cells are then assigned according to the hydrostratigraphic position.

The assignment of lateral connections that involve fault-related cells is different from the way lateral connections are assigned to normal (nonfault-related) cells. Fault-related lateral connections are of two types, fault-fault cell connections and fault-side cell connections. In these two cases, lateral connections occur between cells that share the same interface, no matter what layers they belong to. The interface area is the contact area between the two cells.

For convenience in numerical gridding, contour lines (traces) of each fault at three user-specified elevations are used to define its 3-D orientation. Usually, the highest elevation is the projected elevation of the fault just above the top boundary of the modeled domain, while the lowest elevation is taken at some value just below the bottom boundary. The middle elevation is taken at some arbitrary horizon, preferably near the middle (vertically) of the model domain.

Local Refinement

Local refinement is often necessary for many applications to apply computing resources more effectively. In WinGridder, local refinement of a grid can be realized in three ways (or their combination). First, the user can define many polygons in input files to split the domain into subregions (in map view) with various node spacing and patterns (e.g., a repository area, areas along faults and drifts, and boreholes [see Figure 2]). Second, the user can specify different vertical resolutions for the different layers. Third, for some important 3-D engineering structures (e.g., the potential repository in Yucca Mountain), the user can define the geometry in the input files. The 3-D structure will be represented by a special set of grid cells with the user-specified resolution in the grid (Figure 3). Note that the so-

called repository can have optional multiple subregions (polygons) and multiple drifts. This provides great flexibility in describing complex engineering structures.

Input files

All files described below are user-specified except those noted. Input files are described below.

Table 1. Summary of the input files

Name	Optional/ Required	Format
Domain boundary	Required	Text, free
Repository	Optional	
Geological layers	Required	Text, free, except the individual layer files (binary)
Rock properties	Required	Text, free
Faults	Optional	
Drifts		
Boreholes		
Fractures		

Table 2. Functional description of the input files

Name	Description
Domain boundary	Define the aerial extent (as a polygon), the top and the bottom elevations of the modeling domain in x-y-z coordinates
Repository	(single region) Define the aerial extent (as a polygon) and the parameters of the elevation equation of the repository (multiple region) Define the aerial extent (as a polygon) of each sub-region and coordinates of all individual drifts
Geological layers	Define the geometry relationships between hydraulic units and the thickness (or elevation) of these units
Faults	Define the 3-D layout of faults with x-y-z coordinates and the width of fault zones
Fractures	Define the fracture properties of each hydraulic unit
Boreholes	Define x-y coordinates of each boreholes
Drifts	Define the 3-D layout of drifts with x-y-z coordinates and the size of drifts

Output options

WinGridder provides various output files to facilitate an easy process to design, check, and use complex 3-D grid besides a convenient graphic user interface. Table 3 summarized these output files.

Table 3. Output files

Type	Format	Content
For TOUGH2	TOUGH2 compatible	Entire grid, a selected subset of the grid (e.g., several boreholes, a cross section, or a subregion)
For DCPT	DCPT compatible	
For Checking	Free text	
Informational	Free text	List of cells of a specified layer, List of fault columns, list of borehole columns, list of repository cells, segment file
Graphic	Electronic (user specified on the virtual printer, e.g., EPS)	Map view of the grid (nodes, segments, or connections) Cross section view of the grid

Mesh files for TOUGH2 are standard mesh files used by TOUGH2 family codes. Mesh files for DCPT are standard mesh files used by DCPT (Pan and Bodvarsson, 2002, Pan et al., 2001).

SUMMARY AND CONCLUSIONS

WinGridder is designed for generating 3-D grids that conserve the physical relationships between objects with a finite number of cells. It can save mesh files that can be used as part of the input to the TOUGH2 family of codes. WinGridder can also output additional grid information for various purposes, such as grid inspection and visualization. It has user-friendly graphical interfaces. Moreover, with its interactive editing functions, a user can easily check and modify a layout of columns.

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