MODFLOW-USG Case Study

Discussing Various Grid Geometries for MODFLOW-USG

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Outline

MODFLOW--USG Geometry Concepts
  - Layer Dependent Discretization
  - Pro/Cons of various UnStructured Grids
Creating UnStructured Grids: Methodology
Case Study: Numerical Experiments
  - MODFLOW-2005, -NWT
  - MODFLOW-USG
  - Using CLN for Wells
Results
Future Developments
Background: MODFLOW-USG

- MODFLOW-USG released May 2013
- **UnStructured Grids**
- Follows a Control Volume Finite Difference (CVFD) formulation; provides flexibility in grid types and cell shapes
- Overcomes limitations of finite-difference grids
- Includes MODFLOW processes/packages with finite element flexibility
UNSTRUCTURED GRID CONCEPTS
# MODFLOW Models: Structured vs. UnStructured

<table>
<thead>
<tr>
<th>Name</th>
<th>MODFLOW-2005, LGR, NWT, ...</th>
<th>MODFLOW-USG</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid Type</td>
<td>Structured</td>
<td>UnStructured</td>
</tr>
<tr>
<td>Grid Shapes</td>
<td>Rectilinear (Rectangular)</td>
<td>Varying geometries</td>
</tr>
</tbody>
</table>

- **Structured Grid Shapes**
  - Rectilinear (Rectangular)

- **UnStructured Grid Shapes**
  - Varying geometries
  - Voronoi Grids
  - Quad-Based Grids
MODFLOW-USG: Layer Dependent Discretization

- Each layer can have a different level of grid sizing/refinement
- Efficient gridding approach; ideal for complex geology
“Centroidal” Voronoi Polygon Grids (VGrid)

- Handle complicated geometries and boundaries with ease
- Closely honors CVFD constraints
  - line connecting the node generators is always perpendicular to the shared edges
  - bisector condition is “nearly met” when adjacent cell size is close
- Well and boundary nodes coincide exactly with the grid nodes
- Reduce the need to use GNC
  - higher accuracy
  - better convergence
- Layer-dependent discretization possible
  (but not used in the case study)
Quad-Based Grids (QGrids)

- Nested grids, Quadtree/Octree refined grids
- Shapes are similar to rectilinear (MF-2005) grids
- Smoothing the grids help to improve solver and accuracy
- Do not fully comply with CVFD criteria
  - Ghost Node Correction (GNC) can be used
- Well and boundary nodes may not coincide exactly with the grid nodes
  - GNC can be used to improve this
UnStructured Grid Generation around wells

Quad-Based Grid
- Well not located at cell center

Voronoï Grid
- Well located at grid node
Voronoi Grid

River at node generator (closer to cell center)

UnStructured Grid Generation around rivers

Quad-Based Grid

Cell center does not coincide with original river location

VGrid more closely honors original shape location
CREATING UNSTRUCTURED GRIDS: METHODOLOGY
## Grid Generation: Structured vs. UnStructured

<table>
<thead>
<tr>
<th>Structured MODFLOW-2005</th>
<th>MODFLOW-USG</th>
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<tbody>
<tr>
<td>1. Create uniform grid</td>
<td>1. Define grid “Add-ins”</td>
</tr>
<tr>
<td>2. Refine grid around <strong>areas</strong> of interest</td>
<td>2. Refine grid around <strong>individual</strong> wells/boundaries</td>
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</tbody>
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**Structured MODFLOW-2005**
- 1. Create uniform grid
- 2. Refine grid around **areas** of interest

**MODFLOW-USG**
- 1. Define grid “Add-ins”
- 2. Refine grid around **individual** wells/boundaries
Challenges of Creating UnStructured Grids

- MODFLOW-USG Manual:
  - “Unless grids are designed appropriately..., large errors in simulated heads and flows can result.”
  - These errors “may not be immediately apparent”
  - “It is important for MODFLOW–USG users to develop an understanding of these errors, what causes them, and how to reduce them through appropriate grid design strategies and flux correction approaches.”

- How to fully leverage all MODFLOW-USG capabilities?
- How to best represent discontinuous layers?
- Which grid type to use?
- Are the models working, do the results make sense?
Creating UnStructured Grids

- Start simple, add complexity later
  - Run USG model, check calibration, add further refinement
- Develop parallel MODFLOW-2005 model to ensure consistent results
- Evaluate several UnStructured Grids
  - Various shapes
  - Various levels of refinement

A conceptual modeling approach, with multi-model analysis, facilitates this!
Grid Generation: Conceptual Model Approach

- A conceptual model approximates the site geology; can account for discontinuous layers.
- Boundary Conditions are represented as shapes: points, polylines, polygons.
- These shapes are used as “seeds” (inputs) to the grid generator.
- VGrids are generated using “Triangle”:
  - Robust, quick 2D mesh generator (common in FEFLOW).
  - Smooth grid refinement; improves CVFD criteria.
- QGrids generated using a predicate approach:
  - Where a point, polyline, or polygon intersects a grid cell, refine x4 (horizontally and vertically).
  - Grids are smoothened to ensure no more than 2 connections along any cell edge.
MODFLOW-USG Workflow

Define Conceptual Model
- Geology: Coverage and Horizons
- Property Zones
- Boundary Conditions (rivers, wells, RCH...)

Define UnStructured Grid
- “Add in” points, polylines, polygons
- Define refinement options
- Total # cells

Numerical Model (USG)
- View/Edit Properties
- View/Edit Boundary Conditions
- Create input files for MODFLOW-USG

Convert to Numerical Model
- Calculate Pinchouts
- Calculate Properties and Boundary Conditions

Run Simulation & Analyze Results
- Heads/Drawdown: Qualitative
- Calibration Charts: Quantitative

Another Grid/Model?
CASE STUDY: REGIONAL WATERSHED
Conceptual Model

- A regional watershed model spanning 225 km² was generated.
- This model includes several meandering rivers, recharge, and 3 water supply wells.
- Objective: compare various numerical models/grids, with same refinement level around boundary features.
Case Study: Conceptual Model

- Properties: 6 layers, with layers 3 and 4 pinching out in the southern area of the model.
- Conductivity of the model ranges from 3.0E-7 m/s to 1.0E-5 m/s
- Boundary Conditions: rivers, pumping wells, and uniform recharge, (all steady-state)
Cross-section Properties, MODFLOW-USG
Note: Model Layers 3 and 4 are Discontinuous
Boundary Conditions in USG Numerical Models
Boundary Conditions in Numerical Models

MF-2005, 50m uniform cells

QGrid, 50m at wells/rivers

VGrid, 50m at wells/rivers
River Boundary Conditions: QGrid

Layer 3
Numerical Models: Methodology

- 4 Numerical models developed, with similar level of resolution around boundary features
  - MODFLOW-2005, globally refined
  - MODFLOW-NWT, globally refined
  - MODFLOW-USG VGrid
  - MODFLOW-USG QGrid

- The MF-2005/NWT grid used a uniform grid of 50 m spacing (290 rows * 306 cols). Model is 6 layers.

- The USG grids used 50 m refinement around the rivers and pumping wells.

- MF-NWT provided a better benchmark comparison due to the non dry cells (compare UPW to USG laytyp=4)

- Pinchout regions
  - Minimum layer thickness of 0.01 m used for Structured MODFLOW grids
  - USG QGrid/VGrid, these cells not counted
Methodology

- Numerical Models generated and run in Visual MODFLOW Flex
- xMD used for MODFLOW-USG Runs (with default settings)
- PCGN used for MODFLOW-2005 run; with hclose and rclose =1E-05.
- xMD used for MODFLOW-NWT (v.1.0.7) run, with Simple Solver settings (adjusted backtracking)
- All models run with x64 versions of MODFLOW
NUMERICAL EXPERIMENTS: RESULTS
Results: Calculated Heads

<table>
<thead>
<tr>
<th>MF-USG: QGrid</th>
<th>MF-USG: VGrid</th>
<th>MODFLOW-NWT</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="QGrid Image" /></td>
<td><img src="image2" alt="VGrid Image" /></td>
<td><img src="image3" alt="NWT Image" /></td>
</tr>
</tbody>
</table>

Heads

- 274.57
- 286.64
- 298.71
- 310.79
- 322.86
- 334.93
- 347.00
- 359.07
Results: Mass Balance Comparison

![Graph showing mass balance comparison for different models and grid types. The x-axis represents Total In and Total Out, while the y-axis represents Volumetric Budget (m³). The graph compares MODFLOW-2005, MODFLOW-NWT, USG-VGrid, BCF, USG-VGrid, LPF, USG-QGrid, BCF, and USG-QGrid, LPF.](image-url)
Results: Active Cell Count

<table>
<thead>
<tr>
<th>Engine</th>
<th># Active Cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>MF-2005</td>
<td>346,104</td>
</tr>
<tr>
<td>MF-NWT</td>
<td>346,104</td>
</tr>
<tr>
<td>VGrid</td>
<td>26,250</td>
</tr>
<tr>
<td>QGrid</td>
<td>22,236</td>
</tr>
</tbody>
</table>
Results: Runtimes

<table>
<thead>
<tr>
<th>Engine</th>
<th>Runtime (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MF-2005</td>
<td>52</td>
</tr>
<tr>
<td>MF-NWT</td>
<td>40</td>
</tr>
<tr>
<td>VGrid</td>
<td>6</td>
</tr>
<tr>
<td>QGrid</td>
<td>4</td>
</tr>
</tbody>
</table>

- MODFLOW-2005
- MODFLOW-NWT
- USG-VGrid, LPF
- USG-QGrid, LPF
Numerical Model Results

- MF-2005 exhibits some dry cells, which results in an unstable solution.
- MF-NWT run times a bit longer due to:
  - Nature of the solution
  - Solver settings
  - Non-parallelized
- LPF/BCF package was used for USG model runs. River leakage with LPF package slightly higher.
- It appears that QGrids tend to require higher level of refinement than VGrids in order to produce the same results.
- =>GNC may be more important on QGrids compared to VGrids (which is expected).
Additional Experiments: VGrid
Increased refinement at wells; WEL vs. CLN Package

Remarks:
- CLN node always located at grid node generator; thus head at the well is not affected by cell size
- Change in cell count is negligible; runtimes ~2.5 s
**Additional Experiments: QGrid**

Increased refinement at wells; WEL vs. CLN Package

**Remarks:**
- CLN well node not always located at cell center; thus head is affected by cell size/grading
- GNC was not used, would likely correct the CLN head value
- Change in total cell count is negligible;
- QGrid runs quicker than VGrids (fewer cells)

(CLN diam. 1 m)
Take Home Points

- MODFLOW-USG provides a great level of flexibility in designing the grid...similar to Finite Elements (and more!)
- UnStructured Grids allow you to...
  - ...focus grid resolution where it matters
    - Horizontally and vertically
    - Eliminate “min. layer thickness” for discontinuous layers
  - ...without sacrificing model accuracy and quality!
- MODFLOW-USG model runs with VGrids and QGrids show a nice match to MODFLOW-2005/NWT uniform grid benchmarks
- ...higher accuracy can be obtained with USG
- ...with minimal change in cell count, thus quicker run times
- CLN package is an efficient means for accurately representing wells
  - Detailed grid resolution around wells is not necessary
  - With QGrids, GNC package would likely be helpful to account for discrepancy between CLN well location and cell center
Future Developments

- Layer-dependent discretization
  - VGrids
  - QGrids (around well screens)
- GNC package for QGrids
- USG Transport model, using updated LMT package
Acknowledgements

- Serguei Chmakov, Schlumberger
  - Developing the grid generators
  - Review of benchmark results
- Sorab Panday, GSI
  - Technical review and guidance on MODFLOW-USG concepts and NWT model solver parameters
References

5. Lecture Slides, MODFLOW-USG, Sorab Panday, AMEC
Thank You.
Questions?