Exercise 5-1. “Ghost-node-like” correction on an unstructured, nested grid using XT3D

The standard, conductance-based formulation that MODFLOW 6 uses to compute the flow between two cells (flow is proportional to a conductance times the head difference between the cells) is accurate only if the model grid satisfies certain geometric “CVFD requirements” (Langevin and others, 2017). For grids that do not satisfy these requirements, as is often the case with unstructured grids, the Ghost-Node Correction (GNC) Package (Langevin and others, 2017) can be used to correct for the resulting error. Ghost nodes can work very well, but setting them up can be labor intensive and a bit of an art.

This exercise uses the “XT3D” option (Provost and others, 2017) to automatically effect a “ghost-node-like” correction on an unstructured, nested grid that does not conform to the CVFD requirements. The square model domain is discretized using square cells, except within a region in the center that contains a finer, unstructured grid of triangular cells (fig. 5-1).

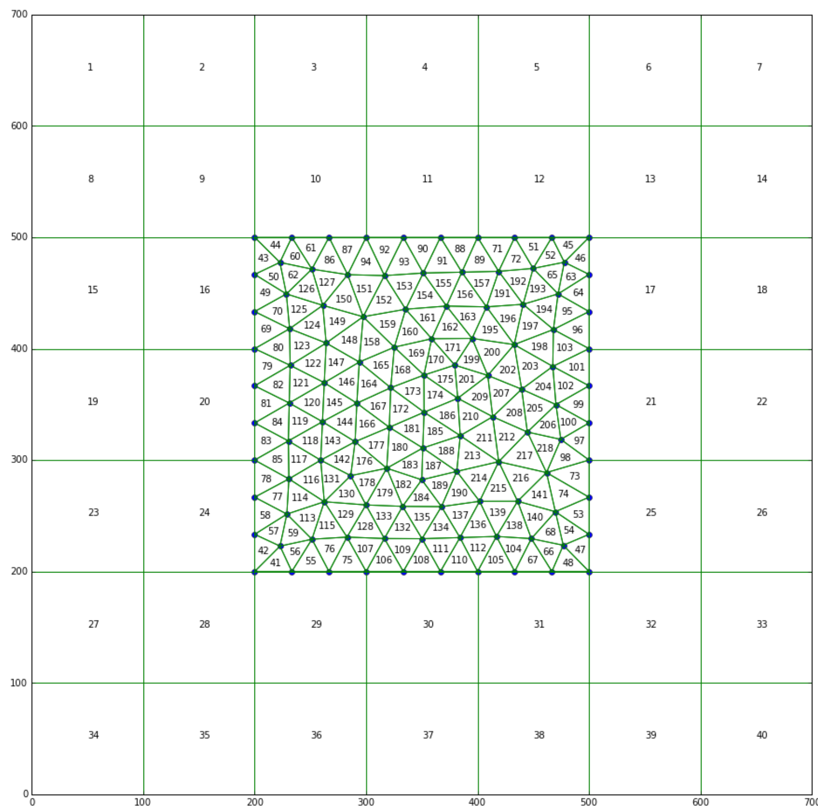

Figure 5-1. Nested grid used in Exercises 5-1 and 5-2.

Constant heads are imposed in cells along the left and right edges of the model, and the exact solution is a uniform head gradient and uniform flow across the box. The unstructured portion of the grid is what makes obtaining an accurate numerical solution to this seemingly simple problem a challenge.

The problem is first solved using the standard, conductance-based formulation (no correction) to observe the resulting error in the solution. It is then re-solved using the "XT3D" option to demonstrate how using this option improves the solution.

Step 1. Copy the MODFLOW 6 files from folder **`ex05-1_xt3d_nested_grid/original`** into the working folder (**`ex05-1_xt3d_nested_grid/work`**).

Step 2. The "XT3D" option is initially turned <u>off</u> by default.

Run the model "as is" and visualize the head results using HeadViewer.

Prepare a map of the difference (error) between the simulated heads and the exact solution stored in folder **`ex05-1_xt3d_nested_grid/data`**. What is the maximum error value?

Using Darcy's Law, calculate the expected total rate of groundwater flow through the model, i.e., the rate at which water enters through the left side, which equals the rate rate at which it exits through the right side. (The aquifer is confined, with a thickness of 10 m and a hydraulic conductivity 1 m/d. A head value of 1 m is assigned to the left column of cells [at x=50 m], and a head value of 0 m is assigned to the right column [at x=650 m].) How does the rate of groundwater flow computed by MODFLOW compare with the expected rate?

Step 3. Activate the "XT3D" option by adding the keyword "XT3D" on a new line within the "OPTIONS" block in file "flow.npf".

Run the model and visualize the head results.

As you did in Step 2, prepare a map of the difference (or error) between the simulated heads and the exact solution, noting the maximum error value.

Compare the new rate of groundwater flow computed by MODFLOW with the value from Darcy's Law you computed earlier.

Step 4. Hypothesize why the XT3D method performed as well as it did for this problem. (Hint: XT3D computes the flow between two cells based on an estimate of the head gradient at the cell interface. That estimate, in turn, is obtained by interpolating head-gradient information from other, nearby locations under the assumption that such information, while somewhat removed from the cell interface of interest, is still reasonably representative of conditions there. In this problem the head gradient is exactly the same everywhere.)

Speculate as to whether the XT3D method would perform as well in the vicinity of a strong source or sink.

Exercise 5-2. 2D anisotropy on an unstructured, nested grid using XT3D

Another advantage of the "XT3D" option is its ability to handle 2D or 3D anisotropic hydraulic conductivity on structured or unstructured grids. This exercise picks up where the previous one left off, adding (2D) anisotropy. The problem is first solved using the standard, conductance-based formulation, then re-solved using the "XT3D" option.

Step 1. Copy the MODFLOW 6 files from folder **`ex05-2_xt3d_anisotropy/original`** into the working folder (**`ex05-2_xt3d_anisotropy/work`**).

Step 2. Turn off the "XT3D" option. Introduce 10:1 anisotropy rotated 45° ccw from the x axis by adding a constant value of 0.1 for K22 (insert it after the entry for K) and a constant value of 45. for ANGLE1 (insert it after the entry for K33) in the "GRIDDATA" block.

Run the model.

Rename the head output file "flow.hds" to "flow_noxt3d.hds" to save it for comparison later.

Check and write down the simulated rate of flow through the model.

Step 3. Turn on the "XT3D" option.

Rerun the model.

Compare maps of the head distributions simulated with and without XT3D. How do they each compare with what you expected, considering the boundary conditions and anisotropy?

Compare the flow rates simulated with and without XT3D.

Step 4. What changes would you make to the constant-head boundary conditions to make the correct solution a uniform, left-to-right head gradient across the box? Look at the file "flow unif grad.chd" and convince yourself that the boundary conditions represented there will produce the desired gradient. Edit the file "flow.nam" to use constant heads from "flow unif grad.chd" (instead of "flow.chd").

Rerun the model (with the "XT3D" option still turned on).

Verify that the simulated head solution is now a uniform, left-to-right gradient across the box. The exact solution is available in folder **`ex05-2_xt3d_anisotropy/data`** for comparison.

Step 5. **(EXTRA CREDIT)** For constant-density flow through a 2D, anisotropic porous medium, the component of the groundwater flux in each coordinate direction depends on the head gradient in both coordinate directions, i.e., Darcy's Law generalizes to

$$q_x = -K_{xx}\frac{\partial h}{\partial x} - K_{xy}\frac{\partial h}{\partial y}$$

$$q_y = -K_{yx}\frac{\partial h}{\partial x} - K_{yy}\frac{\partial h}{\partial y}$$

The components of the conductivity tensor are given by

$$K_{xx} = K\,cos^2\{ANGLE1\} \, + \, K22\,sin^2\{ANGLE1\}$$

$$K_{yy} = K\,sin^2\{ANGLE1\} \, + \, K22\,cos^2\{ANGLE1\}$$

$$K_{xy} = K_{yx} = (K \, - \, K22)\,sin\{ANGLE1\}\,cos\{ANGLE1\}$$

where K and K22 are the principal conductivity values in the horizontal plane and ANGLE1 is the angle at which the principal conductivity directions are rotated ccw relative to the x axis. (K, K22, and ANGLE1 are the variable names used in the NPF's GRIDATA input block.)

Plug the numbers for the simulation in Step 4 in into the 2D, anisotropic version of Darcy's Law and show that you should get the same flow rate through the box as in Exercise 5-1.

Hints:

- If "north is up" in fig. 5-1, then flow enters the box along the western and southern boundaries and exits along the northern and eastern boundaries. To evaluate the flow into western boundary, calculate the x (eastward) component of the flux, q_x, and multiply it by the area of that boundary. To evaluate the flow into southern boundary, calculate the y (northward) component of the flux, q_y, and multiply it by the area of that boundary. Sum the western and southern boundary inflows.
- $sin\{45°\} = cos\{45°\} = \sqrt{2}/2 \approx 0.707107$; $sin^2\{45°\} = cos^2\{45°\} = 1/2$
- In this problem, the head gradient is in the x direction only, i.e., $\frac{\partial h}{\partial y} = 0$.

Step 6. **(EXTRA CREDIT)** Check the rate of inflow ("TOTAL IN") calculated by MODFLOW in Step 4. Why is it different than the flow rate you calculated in Step 5 using Darcy's Law? Convince yourself that this is not an error. [Hint: Look at the flows reported for individual constant-head cells in file "flow.lst". Why is the flow reported for cell "(1,1)", a.k.a. cell 1, different from the flows for other cells along the western boundary?]

Exercise 5-3. 3D anisotropy using XT3D: groundwater whirls

> "Numerical experiments with steady-state ground water flow models show that spiraling flow lines occur in layered aquifers that have different anisotropic horizontal hydraulic conductivities in adjacent layers. Bundles of such flow lines turning in the same direction can be referred to as ground water whirls." – Hemker and others (2004)

In this exercise, you will create groundwater whirls in the 3D problem pictured in figure 5-3a and visualize them using a particle tracking utility. Figure 5-3b shows the straight, boring tracks that result from the initial settings supplied for this problem. Your mission is to create much more interesting tracks by varying the 3D anisotropy.

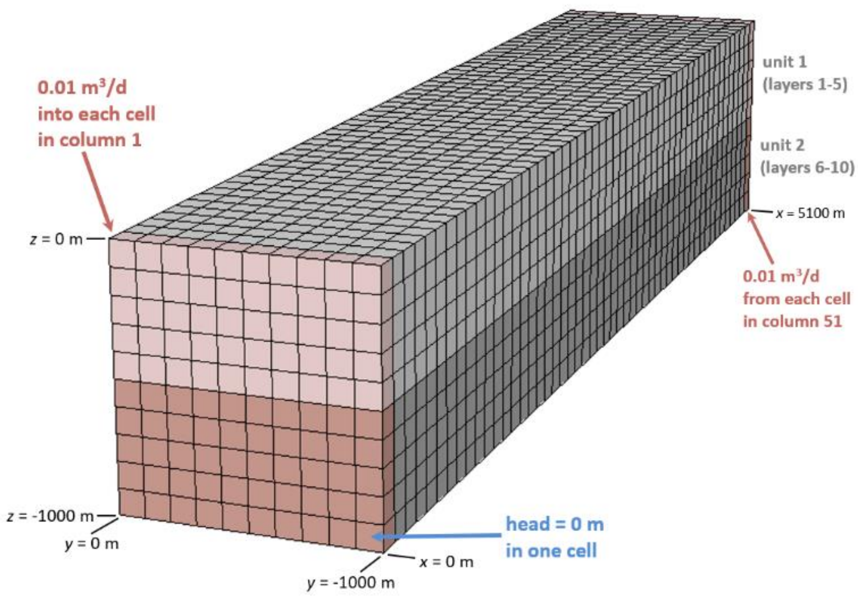

Figure 5-3a. Setup for Exercise 5-3. The model domain is a three-dimensional box with two hydrogeologic units (light and dark shading) identified for reference and constant heads (pink shading) specified at both ends. Coordinates and heads are in meters.

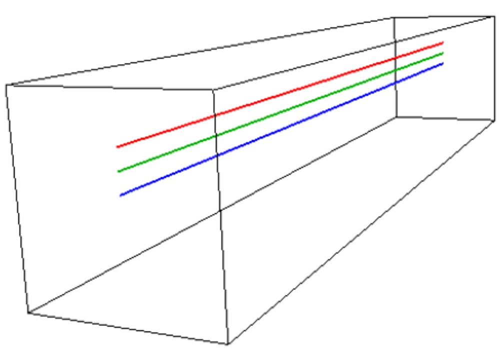

Figure 5-3b. Straight particle tracks obtained in Exercise 5-3 using the initial settings, which feature homogeneous, isotropic conductivity.

Step 1. Copy the MODFLOW 6 files from folder **`ex05-3_xt3d_gw_whirls/original`** into the working folder (**`ex05-3_xt3d_gw_whirls/work`**).

Step 2. The conductivity is initially set to be isotropic and homogeneous throughout the domain. Run the MODFLOW 6 problem without making any changes. Run the particle-tracking utility using the batch file “runtrack.bat”. Display the particle tracks using the batch file “showtrack.bat”. Verify that you get three straight particle tracks, as in figure 5-3b.

NOTE: In the visualization utility, the scene can be rotated by holding down the left mouse button and dragging, and zooming can be done by holding down the right mouse button and dragging. Maximize the window to full-screen if you prefer a larger image. Moving the cursor to the bottom of the window reveals additional controls. If you are interested, click on the “?” icon at the bottom of the window for a summary of what the various controls do.

Step 3. In the file “model.npf”, make the following changes:

- change K22 to 0.1 in all layers,
- change ANGLE1 in unit 1 (layers 1 - 5) to some non-zero value, and
- change ANGLE1 in unit 2 (layers 6 - 10) to the negative of ANGLE1 in unit 1.

Rerun the flow simulation, particle tracking, and track visualization. What happened to the particle tracks? Try other values of ANGLE1 to get the best-looking groundwater whirls you can.

Step 4. Add more particles or change existing ones by editing the file “track.in”. The first line specifies the number of particles (initially three). Each subsequent line specifies the initial coordinates and track color for a particle. The initial coordinates must be within the model domain: 0 < x < 5100 m, -1000 < y < 0 m, and -1000 < z < 0 m. Track color is indicated by specifying red, green, and blue values that each range from 0 to 1.

Step 5. Explore the effects of making other changes to the anisotropy in units 1 and 2. To vary a property separately in units 1 and 2, you will need to use the layered format used for ANGLE 1. The keyword “layered” after the property name indicates that the layered format is being used.

Can you get particles to move (part of the time) against the overall direction of flow, as pictured in figure 5-3c? (If you are stuck, see the bottom of the page for one set of parameter values that accomplishes this.) How does such retrograde motion not violate basic groundwater physics?

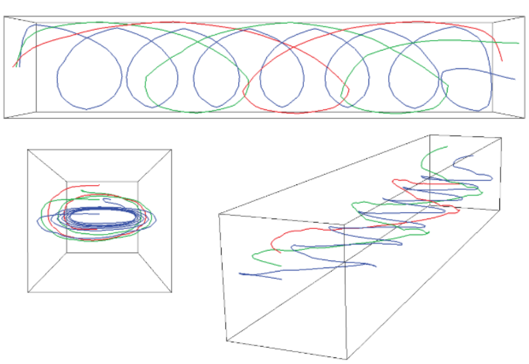

Figure 5-3c. Retrograde particle motion obtained in Exercise 5-3 using 3D anisotropy.

SPOILER ALERT!!!
Unit 1: K = K33 = 1, K22 = 0.001, ANGLE1 = 75, ANGLE2 = 0, ANGLE3 = 75
Unit 2: same as unit 1 except ANGLE1 = -75, ANGLE3 = -75

References cited

Langevin, C.D., Hughes, J.D., Banta, E.R., Niswonger, R.G., Panday, Sorab, and Provost, A.M., 2017, Documentation for the MODFLOW 6 Groundwater Flow Model: U.S. Geological Survey Techniques and Methods, book 6, chap. A55, 197 p., https://doi.org/10.3133/tm6A55.

Provost, A.M., Langevin, C.D., and Hughes, J.D., 2017, Documentation for the "XT3D" option in the Node Property Flow (NPF) Package of MODFLOW 6: U.S. Geological Survey Techniques and Methods, book 6, chap. A56, 40 p., https://doi.org/10.3133/tm6A56.

Hemker, Kick, van den Berg, Elmer, and Bakker, Mark, 2004, Ground water whirls: Ground Water, v. 42, no. 2, p. 234–242.