MODFLOW: A Finite-Difference Groundwater Flow Model or an Integrated Finite-Difference Groundwater Flow Model?

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ABSTRACT

The U.S. Geological Survey modular groundwater flow model (MODFLOW) by McDonald and Harbaugh is regarded as an implementation of a finite-difference numerical scheme applied to the governing groundwater flow equation. However, a comparison of MODFLOW's discretized form of the flow equation with that derived by an integrated finite-difference (IFD) technique reveals that MODFLOW implements an IFD numerical scheme within the confines of a finite-difference grid. An IFD numerical scheme inherent in MODFLOW enables minor modifications to be made to the method in which the model reads and prepares data to enable the construction of a grid with a more complicated geometry than that of a finite difference grid. Adapting MODFLOW in this fashion enables simulation of flow through a curvilinear grid constructed with trapezoidal shaped cells as well as rectangular finite difference grid cells. The modifications give MODFLOW the capacity to exploit the potential of its numerical scheme by adding versatility to the spatial discretization of the flow domain without compromising its modeling capability or introducing new solvers. The theory involved in illustrating MODFLOW's non-generalized IFD numerical scheme is outlined and a test problem is presented that verifies the method with an adapted version of MODFLOW.

INTRODUCTION

MODFLOW (McDonald and Harbaugh, 1988) is one of the most widely used groundwater flow models in the fields of consulting and research. The authors of MODFLOW designed it so that new capabilities could be added to the model structure. The Generalized Finite-Difference Package (Harbaugh, 1992) presents a method that removes some of the assumptions that are inherent in finite-difference grid construction. The discussion herein explains why removing these assumptions is possible and extends the generalization.

This paper illustrates that MODFLOW's numerical scheme is a non-generalized integrated finite-difference (IFD) method rather than a finite-difference method. This is demonstrated by outlining the discretization process involved when an integrated finite-difference method is used. The equation that results from the IFD discretization process is then compared with the equation solved by MODFLOW and found to be identical. A non-generalized IFD method is explained. Minor modifications to MODFLOW's source code are illustrated to enable flow simulations through a curvilinear grid. Finally, a test problem is presented that verifies the method with an adapted version of MODFLOW.

IFD NUMERICAL FORMULATION

The IFD numerical formulation, herein, follows that of Narasimhan (Narasimhan, 1976). Consider the governing partial differential equation for groundwater flow

$$\nabla \cdot \left(K \nabla h\right) + q = S_s \frac{\partial h}{\partial t}. \qquad (1)$$

Spatially integrating (1) over a small finite subregion V of the flow region gives

$$\int_V \nabla \cdot \left(K \nabla h\right) dV + qV = S_s V \frac{\partial h}{\partial t}. \qquad (2)$$

Now the divergence theorem is applied to the integral of the net outflux due to the head gradient in Equation 2. The divergence theorem states

$$\int_V \nabla \cdot F \, dV = \int_\Gamma F \cdot n \, d\Gamma \,. \tag{3}$$

Applying Equation 3 to the first term in Equation 2 yields

$$\int_\Gamma K \nabla h \cdot n \, d\Gamma + qV = S_s V \frac{\partial h}{\partial t} \,. \tag{4}$$

Equation 4 is the integral formulation of Equation 1, which can be discretized to obtain an IFD numerical approximation. Consider how Equation 4 can be discretized. Figure 1 shows a two-dimensional, five-sided cell in a generalized IFD grid. Assuming the cell in Figure 1 has a unit depth into the page and expressing the scalar projection of ∇h in the *n* direction as $\nabla h \cdot n = \partial h / \partial n$, then the two-dimensional discretized form of Equation 4 for node *m* = 6 is written as

$$\sum_{n=1}^{5} K_{mn} A_{mn} \frac{h_n - h_m}{L_{mn}} + q_m V_m = Ss_m V_m \frac{h_m^k - h_m^{k-1}}{\Delta t} \,, \tag{5}$$

where

K_{mn} = hydraulic conductivity between nodes *m* and *n* [LT^{-1}],
A_{mn} = area through which flow occurs [L^2],
L_{mn} = distance between nodes *m* and *n* [*L*],
q_m = source or sink external to aquifer at node *m* [T^{-1}],
V_m = volume of cell enclosing node *m* [L^3],
Ss_m = specific storage of cell enclosing node *m* [L^3],
h_m^k = head at node m at time step *k* [*L*],
Δt = time step chosen for iterative procedure [*T*].

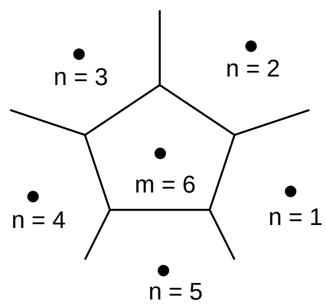

Figure 1. Five-sided cell in a generalized IFD grid

Node *m* = 6 has five sides resulting in a surface integral discretized into a sum with five terms. Likewise, for the general case, Equation 5 would be written for every cell (node) in the grid and the number of terms in each sum would correspond to the number of sides on the associated cell. This makes it possible to simulate flow through cells with varying numbers of sides in two dimensions. If conductance is expressed as the product of hydraulic conductivity and the area through which flow occurs divided by the length of flow, then it can be described as *C* = *KA/L* and Equation 5 can be written as

$$\sum_{n=1}^{c} C_{mn} \left(h_n - h_m\right) + q_m V_m = Ss_m V_m \frac{h_m^k - h_m^{k-1}}{\Delta t} \,, \tag{6}$$

where *c* = number of cell faces around node *m*. Conductance can also be described in terms of transmissivity. In this case, *C* = *Tw/L* where *w* is the width of the cell perpendicular to the direction of flow.

A notable feature of Equation 6 must be made clear. Since the divergence theorem converted the volume integral of the net outflux due to a head gradient in Equation 2 to a surface integral of the scalar projection of the head gradient normal to a surface enclosing a small finite subregion of the flow domain, a constraint was inherited that affects IFD grid construction. Ideally, the interfaces between elements should be perpendicular to the line joining any two nodal points and should intersect that line at its midpoint; although this ideal situation may be difficult to achieve in practice, it should be approximated as closely as possible (Narasimhan, 1976). This limitation is discussed below.

MODFLOW's DISCRETIZATION PROCESS

Rather than deriving a finite-difference analog to Equation 1, the authors of MODFLOW present an alternative approach simplifying the mathematics and explaining the computational procedure in terms of familiar physical concepts regarding the flow system (McDonald and Harbaugh, 1988). Essentially, the discretization process followed in MODFLOW is to discretize Darcy's law for flow through the six faces of a three-dimensional, block-centered cell. Then, for the same cell, a source/sink term which accounts for external flow rates is derived. Finally, the continuity equation that states the sum of all flows into and out of the cell must be equal to the rate of change in storage within the cell is applied. Using the same subscript notation as Equation 5, the resulting equation is expressed as

$$\sum_{n=1}^{6} C_{mn}(h_n^k - h_m^k) + P_m h_m^k + Q_m = Ss_m V_m \frac{h^k - h^{k-1}}{t_k - t_{k-1}} . \qquad (7)$$

For details on the actual discretization process, the reader is referred to the MODFLOW manual (McDonald and Harbaugh, 1988). The second and third terms in Equation 7 are the sum of a head dependent and a non-head dependent source or sink term external to the aquifer that can be expressed as

$$q_m V_m = P_m h_m^k + Q_m , \qquad (8)$$

where

q_m = source or sink external to aquifer at node m $[T^{-1}]$,
V_m = volume of cell enclosing node m $[L^3]$.

Combining Equation 8 with 7 produces Equation 6, hence, the discretized equation solved by MODFLOW implements an IFD numerical scheme. However, MODFLOW implements the scheme within cells that are limited to four sides in two dimensions which creates a non-generalized scheme.

It is apparent that MODFLOW utilizes an integrated finite-difference numerical scheme in that the discretized equation that MODFLOW solves is identical to the equation we arrive at when implementing the IFD discretization process. MODFLOW implements this scheme, however, through a flow domain represented with a finite-difference grid. Figure 1 illustrates the capacity of an IFD method to simulate flow through cells with shapes more complicated than rectangles. Hence, in its present form, MODFLOW has the potential to simulate flow through a domain comprised of shapes other than rectangles.

ENABLING MODFLOW TO UTILIZE ITS IFD METHOD

MODFLOW was designed to simulate flow through a finite-difference grid with intrinsically rectangular cells. The process of deriving a numerical solution is constrained by the shape of the grid cells in two areas: the calculation of area for each cell and the calculation of conductance between cells. Both of these calculations assume cell widths are constant along any row or column. MODFLOW's solvers are also equipped to solve for the head in a cell with only four sides in two dimensions. However, minor modifications to the source code of MODFLOW enable the cell areas and conductances between cells to be calculated within cells that form trapezoids in two dimensions. This enables MODFLOW to simulate flow through a curvilinear grid, since approximating the curvilinearity with straight-line segments results in a grid composed of trapezoidal cells as shown in Figure 2. Altering the grid in this fashion gives the code the capacity to exploit the benefits inherent in its numerical scheme. How MODFLOW's code would have to be adjusted to calculate the area of each cell and the conductance between cells is given below.

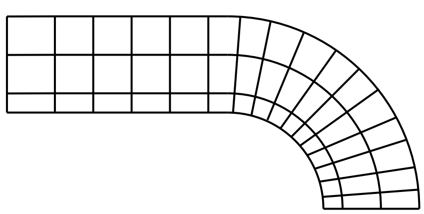

Figure 2. Example of curvilinear grid

With geographical information systems (GIS), obtaining the area for each cell within a grid is a routine process. A GIS can create or import a model grid, calculate the area of each cell, and return the cell areas in the form of a two-dimensional array that MODFLOW can be adapted to read. In this case, the area would be used in the calculation of storage capacity, vertical conductance, volumetric recharge and evapotranspiration rates within the model.

Modification of the conductance calculation entails using MODFLOW's existing equation in its unreduced form. Presently, MODFLOW calculates equivalent conductance between two cells as

$$C_{ij} = \frac{2T_i T_j w}{T_i L_j + T_j L_i}, \tag{9}$$

where

C_{ij} = equivalent conductance between cells *i* and *j* [L^2T^{-1}],
T_i = transmissivity of cell *i* [L^2T^{-1}],
L_i = length of flow within cell *i* [*L*],
w = width of cell normal to direction of flow in cell *i* or *j* [*L*].

However, Equation 9 was reduced by the assumption that the width of cells *i* and *j* is equal. If the widths were not equal, Equation 9 would take the form

$$C_{ij} = \frac{2T_i w_i T_j w_j}{T_i w_i L_j + T_j w_j L_i}. \tag{10}$$

Replacing Equation 9 with 10 is necessary to enable MODFLOW to calculate flow through a curvilinear grid. Finally, a method for calculating L_i and w_i must be developed. The simplest method is to adapt the model to read the *x* and *y* locations of grid vertices. The average length of flow within any cell in the row and column directions can then be calculated. Upon completion of these modifications, MODFLOW becomes capable of simulating flow through a curvilinear grid.

The interfaces between elements should be perpendicular to the line joining any two nodal points and should intersect that line at its midpoint. This ideal situation can only be achieved if actual curved lines were to be used in the grid constructed for simulating flow. If Equation 10 is used to calculate the equivalent conductance between nodes, then the way the ideal length is approximated is shown in Figure 3. It is also evident from Figure 3 that the sum of half the average length of flow in cell *i,j* and half the average length of flow in cell *i,j*+1 is an approximation of the actual curved length that improves as the spatial discretization is refined. Spatial discretization of a curve always implies such an approximation.

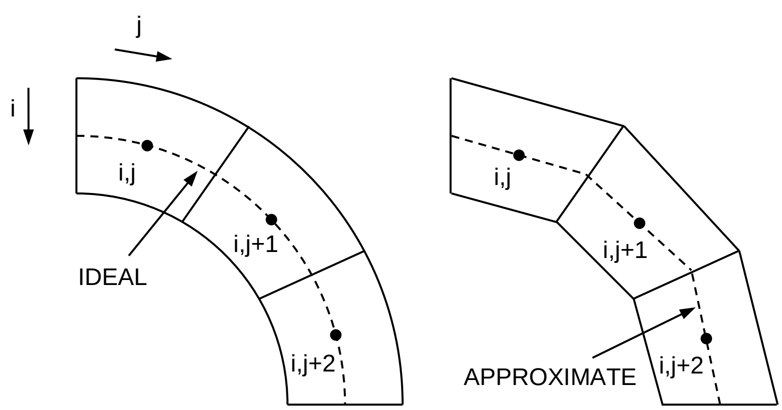

Figure 3. Approximated length of flow between cells

Source code containing the modifications described above is available free of charge from the author at www.balleau.com.

VERIFICATION OF MODEL MODIFICATIONS

A test problem is presented to check the validity of the model obtained from the aforementioned code modifications. A grid with radial symmetry is readily constructed with trapezoidal shaped cells. Figure 4 shows a plan view of the model grid for the problem. The problem is specified homogeneous and isotropic with a gradient of 0.667 over a radius of 15 feet. An analytical solution to the steady-state radial flow problem exists and is given as (Crank, 1967)

$$h = \frac{h_1 \log\left(\frac{r_2}{r}\right) + h_2 \log\left(\frac{r}{r_1}\right)}{\log\left(\frac{r_2}{r_1}\right)}; \quad r_1 \le r \le r_2, \tag{11}$$

where

h_1 = head at radius r_1,
h_2 = head at radius r_2.

Figure 5 illustrates a plot of dimensionless head vs. dimensionless radius solved over the flow domain and compares the result with the analytical solution.

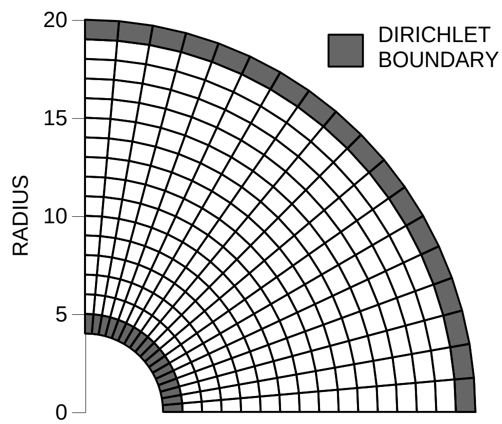

Figure 4. Curvilinear grid with radial symmetry

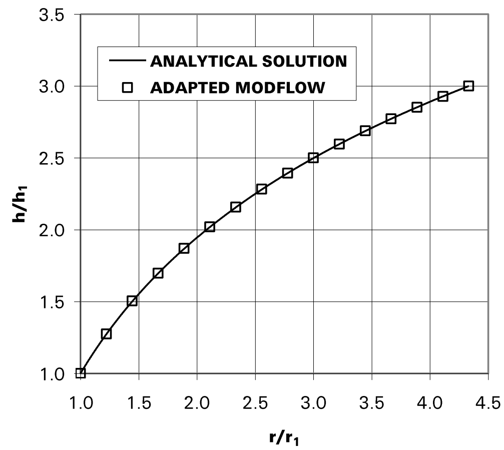

Figure 5. Comparison of analytical and numerical solutions

SUMMARY

MODFLOW is a widely used groundwater flow model that implements a non-generalized IFD numerical scheme within the confines of a finite-difference grid. One of the benefits associated with an IFD scheme is its ability to simulate flow through a grid with geometry more complicated than that of a finite-difference grid. Minor modifications can be made to MODFLOW's source code to enable flow simulations through a curvilinear grid constructed with trapezoidal shaped cells. The modifications maintain compatibility with MODFLOW's standard packages and increase the versatility of grid construction.

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