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Modifications to MODFLOW boundary conditions and an adaptive-damping scheme for Picard iterations for a highly nonlinear regional model

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ABSTRACT

Simulating ground-water flow in a regional-scale basin comprised of a system of bedrock aquifers and confining units unconformably overlain by alluvial aquifers presents challenges to a modeler. Simulation of the alluvial aquifers overlying alternating bedrock aquifers and confining units poses problems in formulation of boundary conditions representing recharge and evapotranspiration. Nonlinearities associated with head-dependent transmissivity and singularities in head-dependent boundary conditions create a problem that is resistant to efficient solution. This work describes modifications to MODFLOW-2000, including (1) new options for the Recharge and Evapotranspiration Packages for assigning the layer to which these boundary conditions apply, and (2) a revised adaptive-damping capability for the Geometric Multigrid Solver Package.

INTRODUCTION

Simulating ground-water flow in a regional-scale aquifer system that includes multiple unconfined aquifers presents challenges to a modeler. Simulation of alternating aquifers and confining units can pose problems in formulation of boundary conditions representing recharge and evapotranspiration. Numerous sources of nonlinearity can create a numerical problem that is difficult to solve to a satisfactory degree of precision with existing solvers. This work describes modifications to MODFLOW-2000 (Harbaugh and others, 2000) that make simulation of such a nonlinear system practical. Modifications include (1) enhancements to the Recharge (RCH) and Evapotranspiration (EVT) Packages to allow new options for assigning the layer to which these boundary conditions apply, and (2) addition of a new adaptive-damping capability to the Geometric Multigrid (GMG) Solver Package (Wilson and Naff, 2004).

PROBLEM DESCRIPTION

A complex, 12-layer model was constructed to represent a regional aquifer system using the Layer Property Flow (LPF) Package of MODFLOW-2000. The layers represent a sequence of six bedrock aquifers separated by five confining units and overlain by a discontinuous alluvial aquifer. The lowermost bedrock aquifer is the most geographically extensive of the bedrock aquifers; the uppermost bedrock aquifer is the least extensive. The alluvial aquifer unconformably overlies the uppermost bedrock aquifer in the central parts of the basin and progressively lower units toward the basin margins. The hydrologic role of each layer is described in Table 1. In the horizontal dimensions, the model has 124 rows and 84 columns. Each cell is a 1-mile square. Boundary conditions for the system were simulated using the RCH, EVT, General Head Boundary, River, and Drain Packages of MODFLOW-2000. Streams were simulated by the Streamflow-Routing Package (Prudic and others, 2004). Each model run consisted of a single steady-state stress period and started from the same initial head distribution.

Deactivation of cells underlying active cells where recharge was simulated produced unrealistic results. This problem arises where recharge is applied to a cell of small transmissivity that lacks vertical connection to another cell. In such a situation, large heads are needed to drive water out of the cell receiving recharge. Consider a case where NRCHOP is assigned as 3 in RCH input, so that recharge is applied to the uppermost active cell in a vertical stack of model cells. If the cell in a convertible layer goes dry, and it is overlain by a small-transmissivity cell in a confined layer, which also is the uppermost active cell, calculated head at the cell in the confined layer may be unrealistically high. This problem can be severe where cells in the confined layer are thin, as may be specified to simulate hydraulic connection across an unconformity.

Aspects of the simulated system that contributed to the nonlinearity of the model and instability of the solution process include (1) head-dependent transmissivity in 7 of the 12 model layers, and (2) singularities in the relations of flow rates to heads. The singularities are points of abrupt change in these relations: for example, at the extinction depth of the EVT Package. Attempts to use several of the solvers available in MODFLOW-2000 produced unsatisfactory results; either nonconvergence or excessively long execution times.

Model layer and layer type	Role in the aquifer system
1, convertible	Alluvial aquifer, unconfined. 2,210 cells are specified as active.
2, convertible	Aquifer, generally unconfined. 3,402 cells are specified as active.
3, confined	Confining unit, locally present. Where present, it forms a confining unit between layers 2 and 4. 3,402 cells are specified as active.
4, convertible	Aquifer, generally confined where overlying confining unit is present and generally unconfined where the confining unit is absent. 3,402 cells are specified as active.
5, confined	Confining unit. 3,492 cells are specified as active.
6, convertible	Aquifer, generally confined. 4,810 cells are specified as active.
7, confined	Confining unit. 4,972 cells are specified as active.
8, convertible	Aquifer, generally confined. 5,636 cells are specified as active.
9, confined	Confining unit, locally present. Where present, it forms a confining unit between layers 8 and 10. 5,636 cells are specified as active.
10, convertible	Aquifer, generally confined. 5,636 cells are specified as active.
11, confined	Confining unit. 6,285 cells are specified as active.
12, convertible	Aquifer, generally confined. 6,946 cells are specified as active.

Table 1. Role of model layers in the aquifer system.

MODIFICATIONS TO MODFLOW-2000

Modifications to the RCH and EVT Packages were made to address problems described in the previous sections. Modifications to the GMG Package were made to manage solver oscillation problems. The version of MODFLOW-2000 used for this work was documented by McAda and Barroll (2002). It eliminates the “vertical flow correction” (Harbaugh and others, 2000, p. 31) of the LPF Package, which is one source of solver oscillation that can arise as a result of cells being converted repeatedly between confined and unconfined conditions during the iterative solution procedure. The oscillation tends to be particularly problematic at locations in the model where a thin cell in a confined layer overlies a substantially thicker cell in a convertible layer.

Recharge and Evapotranspiration Packages

Simulation of convertible layers alternating with confined layers, in combination with deactivation (“drying”) of cells during the iterative solution procedure, creates a need for flexibility in assigning the layer to which recharge and evapotranspiration apply. This flexibility is needed to avoid unrealistically large calculated heads, as described in the Problem Description section. The new option is selected by specifying NRCHOP in RCH input as 4, which indicates that, for each vertical stack of cells, recharge should be applied to the highest active cell that is connected by active cells to the lowest active cell in the stack. For example, consider a stack of cells in the 12-layer problem (table 1) in which, at the beginning of the simulation, every cell is specified as active. Assume that, in the Formulate Procedure at a given iteration, the cells in layers 1, 2, and 4 have been converted to inactive status because all heads calculated for the stack at a previous iteration have dropped below the base of layer 4. In this situation, the cell in layer 3 would still be active because layer 3 has been specified as confined. Further assume that at this iteration the cells in layers 5 through 12 are active. With NRCHOP specified as 4, recharge would be applied to the cell in layer 5, because the cells in layers 5 through 12 are active; whereas, the

cell in layer 4 is inactive. This logic avoids the artificial buildup of calculated head that could result if recharge were applied to the uppermost active cell, which, in this case, is the cell in layer 3.

Simulation of evapotranspiration at the same cells where recharge is simulated may be needed to approximate real-world conditions and to help avoid artificial buildup of calculated head in areas of low transmissivity. A modification to the EVT Package was made to ensure that evapotranspiration is applied to the same cell in each stack of cells where recharge is applied. The new option is invoked by setting NEVTOP to 4, and the logic used to determine the cell in which evapotranspiration is simulated is the same as that described for the new option for NRCHOP of the RCH Package.

Geometric Multigrid Solver Package

Several of the solvers included with MODFLOW-2000 were evaluated in the course of modeling. The GMG Package was selected for its efficiency. To solve a nonlinear flow problem, MODFLOW reformulates the flow equation in Picard, or “outer,” iterations to account for nonlinearities. In each outer iteration, GMG executes one or more “inner” iterations to solve a linearized version of the flow equation. Wilson and Naff (2004) provide detailed documentation of GMG.

The GMG solver, unlike other packages of MODFLOW, uses source code written in the C programming language as well as Fortran. The actual solution algorithms are written in C. The Fortran parts of the code link the solver with the MODFLOW main program unit, which also is written in Fortran. Modifications were made only to the Fortran part of the code, including subroutines GMG1ALG and GMG1AP, and a new Fortran subroutine was added. No modifications were made to the C source code. The modifications do not affect the actual solution algorithm or the validity of the results of the solution process; their only effects are to allow the user more control over the number of inner iterations and over the degree to which the head-change vector is applied to the head array at each outer iteration.

When subroutine GMG1AP is called from the main program unit in an outer iteration, it calls a C function (MF2KGMG_ASSEMBLE) to assemble needed arrays, it sets a convergence criterion (variable DRCLOSE) to be used in determining how many inner iterations should be completed, and it calls another C function (MF2KGMG_EVAL) to execute the inner iterations and generate a vector of head changes. GMG1AP then calculates the maximum head change at any cell, checks for convergence, updates the head array, and returns. However, if user input specifies that damping should be applied and the (outer) convergence criteria have not been met, damping is applied to the head-change vector before the head array is updated by multiplying the head-change vector by a constant damping factor. A damping factor between 0 and 1 generally is used, although a value larger than 1 sometimes can be effective. A new subroutine was written to calculate a damping factor at this point in the code.

Another modification affects the convergence criterion for the inner iterations. GMG1AP sends the variable DRCLOSE to MF2KGMG_EVAL as the convergence criterion for the inner iterations. In the original version of GMG, GMG1AP calculates DRCLOSE as “DDAMP*RCLOSE+(1.0D0–DDAMP)*BIGR0”, where DDAMP initially is the user-input value of the damping parameter DAMP and is updated each outer iteration, RCLOSE is the user-input residual convergence criterion, and BIGR0 is the L2 norm of the residual vector prior to execution of the inner iterations. This method of calculating the inner closure criterion can reduce the number of inner iterations that are executed during early outer iterations, while allowing more inner iterations and a better approximation of the solution as convergence is approached. When DDAMP is a small fraction of 1, however, the calculated value of DRCLOSE is close to BIGR0. The effect of setting DRCLOSE nearly equal to BIGR0 is that the inner solution algorithm almost always reaches convergence in one inner iteration, because the L2 norm of the residual vector generated in the solution algorithm is being compared to DRCLOSE to determine if convergence has been reached. In contrast, John Wilson (U.S. Geological Survey, personal commun., 2005) and the author’s experience with the GMG solver indicate that the inner solution algorithm may need multiple inner iterations to obtain satisfactory head updates for each outer iteration. This problem is alleviated by a modification in the assignment of DRCLOSE, which takes effect when the new damping option is selected and DDAMP is less than 0.5. In this situation, DRCLOSE is assigned simply as RCLOSE. By monitoring the output generated when IOUTGMG is specified as 2 or 4, the user can adjust RCLOSE so

that an appropriate number of inner iterations are executed and so that the L2 norm of the residual vector is reduced to an acceptable magnitude during inner iterations.

The IADAMP input variable is used to select the new adaptive-damping capability. The meaning of IADAMP was modified so that:

If IADAMP = 0, then the value assigned to DAMP is used as a constant damping parameter.

If IADAMP = 1, then the value of DAMP is used for the first nonlinear iteration. The damping parameter is adaptively varied on the basis of the head change, using Cooley's method as described in Mehl and Hill (2001) for subsequent iterations.

If IADAMP = 2, then the adaptive-damping methodology documented in this article is used.

When IADAMP is 0 or 1, GMG works as originally documented. When IADAMP = 2, additional variables are read from the GMG input file to control the new adaptive-damping scheme. Values for the following REAL variables are read from the line containing ISM and ISC, following those values:

DUP is the maximum damping value that should be applied at any iteration when the solver is not oscillating; it is dimensionless. An appropriate value for DUP will be problem-dependent. For moderately nonlinear problems, reasonable values for DUP would be in the range 0.5 to 1.0.

For a highly nonlinear problem, a reasonable value for DUP could be as small as 0.1. When the solver is oscillating, a damping value as large as $2.0 \times \text{DUP}$ may be applied.

DLOW is the minimum damping value to be generated by the adaptive-damping procedure; it is dimensionless. An appropriate value for DLOW will be problem-dependent and will be smaller than the value specified for DUP. For a highly nonlinear problem, an appropriate value for DLOW might be as small as 0.001. Note that the value specified for the next variable, CHGLIMIT, could result in application of a damping value smaller than DLOW.

CHGLIMIT is the maximum allowed head change at any cell between outer iterations; it has units of length.

The new adaptive-damping scheme is similar to the relative reduced residual method of the Link-AMG (LMG) Package (Mehl and Hill, 2001) with the following differences:

- If the relative reduction in the L2 norm of the residual vector is negative, indicating solver divergence, the damping value is set to DLOW.
- A new test for oscillation, based on the behavior of the maximum head change over the most recent three outer iterations, is implemented in addition to the test for oscillation in LMG, which is based on the values of the L2 norm over two outer iterations.
- If either the original or the head-based test for oscillation indicates the solution is oscillating, the damping value is assigned as a random value between DLOW and $2.0 \times \text{DUP}$. In contrast, LMG assigns the damping value as a random value between 0.0001 and 1.5.
- The maximum head-change limitation is implemented by comparing the maximum head change calculated by MF2KGMG_EVAL against CHGLIMIT. If the absolute value of the maximum head change is larger than CHGLIMIT, a damping value calculated to make the maximum head change equal to CHGLIMIT is applied, overriding any previously assigned value. Appropriate values for CHGLIMIT are entirely problem-dependent.

Note that this adaptive-damping scheme could be implemented in any of the MODFLOW solvers.

RESULTS AND CONCLUSIONS

Results of four model runs, differing only in the assignment of variables in the GMG input file, are summarized in table 2. The graphs in figures 1 (IADAMP = 0 and DAMP = 0.02) and 2 (IADAMP = 2) have been truncated at the top and bottom to show the behavior of the solver as convergence is approached. The largest maximum head change (absolute value) for the run illustrated in figure 1 was about 3,500 ft. For the run illustrated in figure 2, the maximum was 20 feet, the CHGLIMIT limitation. The head-change values in the figures are those calculated after the head-change vector has been multiplied by the damping factor. The convergence decision, however, is based on the head-change vector before the damping factor is applied. After convergence is reached (figure 2, iteration 902), the damping factor is set to 1.0. The curve at this iteration has a value close to -1.0 and meets the head-change convergence criterion of ± 1.0 . For the run illustrated in figure 1, the L2 norm has a minimum value of about 50. Because the RCLOSE convergence criterion was specified as 0.01, the run with IADAMP = 0 was not as

close to convergence as figure 1 seems to indicate. For iteration 902 of the run with IADAMP = 2, the L2 norm has a value of 0.002, easily meeting the residual convergence criterion.

IADAMP	DAMP	Result
0	0.1	Convergence is not reached in 2,000 iterations. 1,812 cells convert to “dry.” Absolute value of maximum head change between iterations commonly exceeds 10^7 feet.
0	0.02	Convergence is not reached in 2,000 iterations. 1,012 cells convert to “dry.” See figure 1.
1	0.01	25,804 cells convert to dry in 10 iterations, at which point GMG fails due to “assembly error.” Absolute value of maximum head change between iterations exceeds 10^7 feet for 5 iterations.
2	0.1	With DUP=0.2, DLOW=0.02, and CHGLIMIT=20.0, convergence is reached in 902 iterations. 1,073 cells convert to “dry.” Volumetric budget discrepancy is 0.0003 percent. See figure 2.

Table 2. Results of model runs. For all runs, RCLOSE=0.01, IITER=10, HCLOSE=1.0, and MXITER=2000.

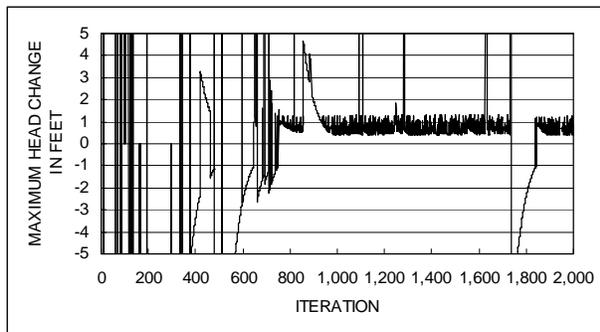


Figure 1. Results of run with IADAMP = 0 and DAMP = 0.02.

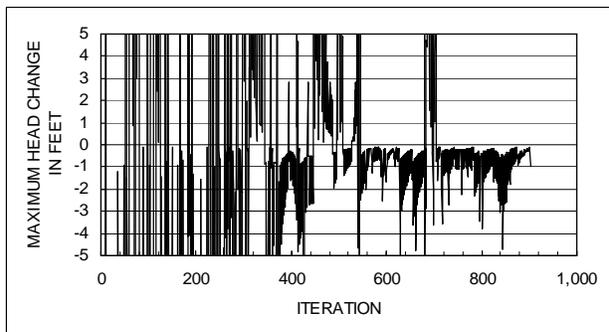


Figure 2. Results of run with IADAMP = 2

The modifications to MODFLOW-2000 described in this article, in combination with modifications described in McAda and Barroll (2002), provide options that may be advantageous when solving a highly nonlinear ground-water flow problem. The adaptive-damping approach described here has been shown to provide a valuable solution option. Of particular value is the ability to limit head change between solver iterations. The approach could be implemented in any of the MODFLOW solvers.

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