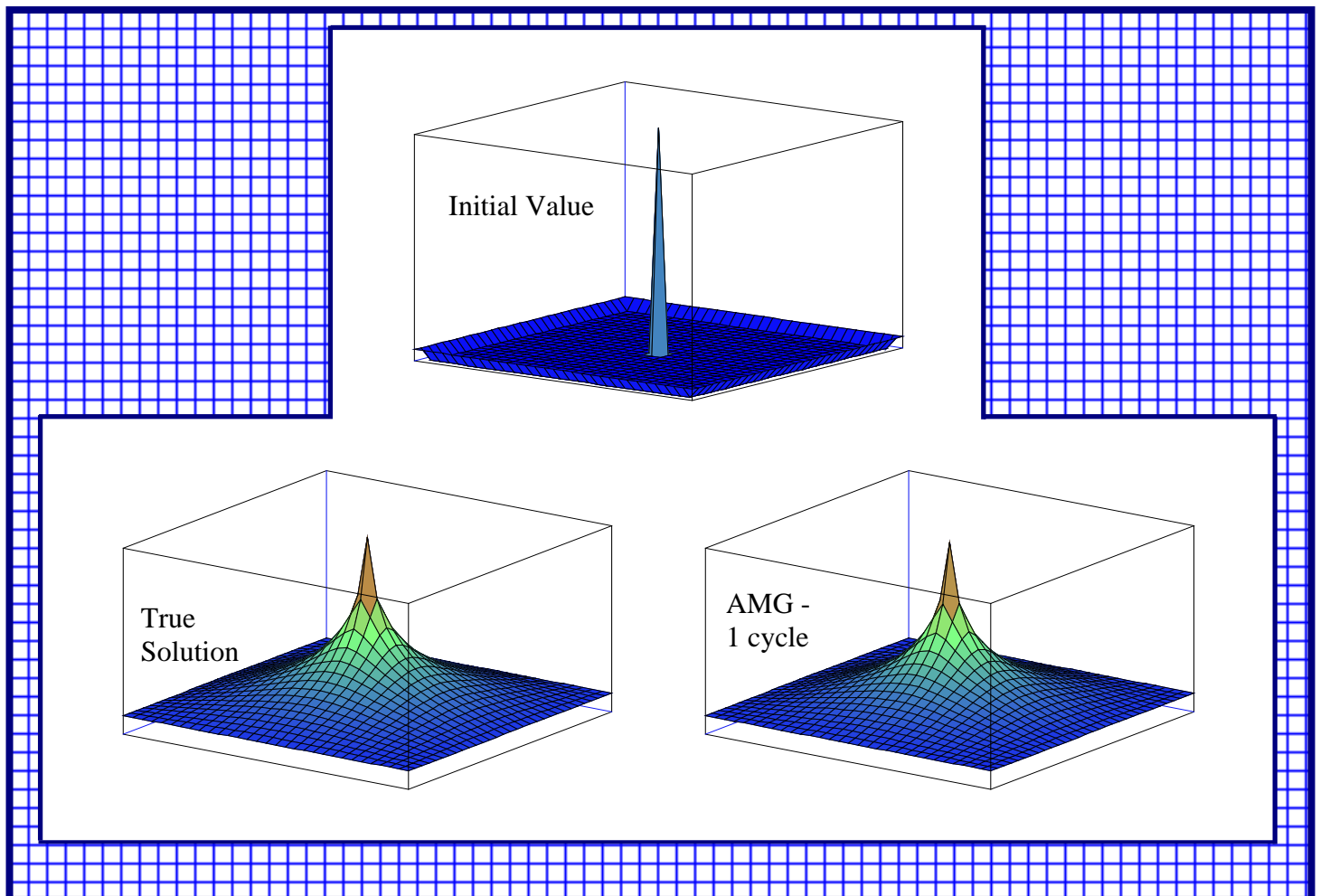# USGS
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U.S. Department of Energy**

MODFLOW-2000, THE U.S. GEOLOGICAL SURVEY MODULAR GROUND-WATER MODEL—USER GUIDE TO THE LINK-AMG (LMG) PACKAGE FOR SOLVING MATRIX EQUATIONS USING AN ALGEBRAIC MULTIGRID SOLVER

Open-File Report 01-177

Initial Value

True Solution

AMG - 1 cycle

MODFLOW-2000, THE U.S. GEOLOGICAL SURVEY MODULAR GROUND-WATER MODEL – USER GUIDE TO THE LINK-AMG (LMG) PACKAGE FOR SOLVING MATRIX EQUATIONS USING AN ALGEBRAIC MULTIGRID SOLVER

By STEFFEN W. MEHL *and* MARY C. HILL

U.S. GEOLOGICAL SURVEY

Open-File Report 01-177

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U.S. DEPARTMENT OF THE INTERIOR
GALE A. NORTON, *Secretary*

U.S. GEOLOGICAL SURVEY
Charles G. Groat, *Director*

PREFACE

This report describes a computer program that links MODFLOW-2000, the U.S Geological Survey modular three-dimensional finite-difference ground-water model, with an advanced technique for solving matrix equations, the freeware algebraic multigrid (AMG) solver produced by the GMD - German National Research Center for Information Technology. The AMG solver can be downloaded from the Internet URL at http://www.mgnet.org/mgnet/Codes/gmd/amg.tgz, where the version used in this report is identified as AMG1R5. For convenience it is also distributed with MODFLOW-2000. The AMG solver is, however, produced by GMD and, though freely distributed, is subject to restrictions defined by GMD. One of those restrictions is that GMD must be acknowledged in publications for which results were produced using the algebraic multigrid solver. The U.S. Geological Survey encourages users to respect this restriction. While this is the only restriction that will apply to most users, those using the algebraic multigrid solver in any other way should consult with GMD about additional restrictions.

More recent developments in AMG software not available for free may be available from a variety of vendors, and users may wish to consider these resources. These algorithms are more sophisticated and, as a result, are more efficient in their use of computer memory. In using such alternatives, the implementation provided by the Link-AMG (LMG) Package described in this report to make the AMG1R5 solver work with MODFLOW may be useful.

The performance of the program has been tested in a variety of applications. Future applications, however, might reveal errors that were not detected in the test simulations. Users are requested to notify the U.S. Geological Survey of any errors found in this document or the computer program using the email address available at the web address below. Updates might occasionally be made to both this document and to LMG. Users can check for updates on the Internet at URL http://water.usgs.gov/software/ground_water.html/.

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THE U.S. GEOLOGICAL SURVEY MODULAR
GROUND-WATER MODEL --

USER GUIDE TO THE LINK-AMG (LMG) PACKAGE FOR SOLVING MATRIX EQUATIONS USING AN ALGEBRAIC MULTIGRID SOVLER

By Steffen W. Mehl and Mary C. Hill

Abstract

This report documents the Link-AMG (LMG) Package that links MODFLOW-2000, the U.S. Geological Survey modular, transient, three-dimensional, finite-difference ground-water flow model, to an algebraic multigrid (AMG) solver for matrix equations. The LMG Package has some distinct advantages over other solvers available with MODFLOW-2000 for problems with large grids (more than about 40,000 cells) and (or) a highly variable hydraulic-conductivity field. Experience has indicated that, in such problems, execution times using the AMG solver are typically about 2 to 25 times faster than execution times using MODFLOW's PCG2 Package with the modified incomplete Cholesky preconditioner. The drawback to the AMG method used in LMG is the relatively large amount of computer memory required. In problems simulated for this work, the AMG solver used typically required 3 to 8 times more memory than PCG2. For one 465,600-node problem, for example, 151 megabytes (MB) of memory were required when the LMG package was used, whereas PCG2 required 47 MB of memory. The execution time, however, decreased from 942 seconds to 50 seconds, so there is a clear trade-off between execution time and memory requirements. On modern computers, such memory requirements are becoming increasingly attainable.

This report provides a brief description of the AMG method used, an explanation of the convergence criterion, a discussion of its memory requirements, some performance comparisons, and sample data inputs. In addition, detailed instructions on how the LMG Package links the AMG code to MODFLOW-2000 are provided.

Introduction

Ground-water modelers are constantly challenged by trying to represent realistically complicated natural systems using numerical models. Increased detail means larger model grids and longer execution times. In addition, increasingly complicated processes and methods for exploring model results, such as Monte-Carlo simulation and model calibration, make reduction of computer execution time extremely desirable. Reduction in computer execution time provides an opportunity for ground-water modelers to investigate their systems more thoroughly and in ways not previously possible. In recent decades, computer models of ground-water systems have taken advantage of improved processor speeds, but have not, in general, taken advantage as effectively of increased memory availability, other than increasing the number of grid nodes.

Algebraic multigrid solvers can attain significant reduction in computer execution time for many problems. Generally, the decrease in execution time is accompanied by the use of larger amounts of memory. The pioneering work that developed the theory behind algebraic multigrid methods took place in the early 1980s, and computer memory has evolved to where these methods can be used by a wide audience. The present report makes an algebraic multigrid (AMG) solver produced by GMD (German National Research Center for Information Technology) available for users of MODFLOW-2000, the U.S. Geological Survey modular, three-dimensional, finite-difference ground-water model.

The AMG solver is included in MODFLOW-2000 as distributed by the U.S. Geological Survey. When the Link-AMG (LMG) Package is activated through the Name file using file type LMG, the AMG solver is used to solve the equations produced by MODFLOW-2000s Ground-Water Flow Process for hydraulic head, and, if applicable, the equations produced by MODFLOW-2000s Sensitivity Process for sensitivities of hydraulic head throughout the grid. Linear or nonlinear flow conditions may be simulated.

Purpose and Scope

The purpose of this report is to document LMG, a program that links a freeware version of GMD's algebraic multigrid solver (AMG1R5), to MODFLOW-2000. This report provides a brief description of the AMG method used, an explanation of the convergence criterion, a discussion of its memory requirements, some performance comparisons, and sample data inputs. In addition, detailed instructions on how the LMG Package links the AMG code to MODFLOW-2000 are provided. This report was prepared in cooperation with the U.S. Department of Energy.

Acknowledgments

Brief Description of the Algebraic Multigrid (AMG) Solver

Ruge and others (1990) developed the AMG solver, AMG1R5, implemented by the LMG package. This USGS report highlights the general features of the AMG solver; for more detail refer to Stüben (1999, 2001) and Ruge and Stüben (1987). In addition, Briggs and others (2000) provide an excellent treatment of multigrid methods, and much of this overview is based on their discussion of the subject.

The characteristics of the AMG solver are described by considering its performance relative to alternative solvers using two small problems. The alternative solvers considered are successive over-relaxation (SOR), strongly implicit procedure (SIP), and the preconditioned conjugate-gradient method (PCG). The implementation of the SOR and SIP solvers is described by McDonald and Harbaugh (1988), the implementation of the PCG solver is described by Hill (1990), and the implementation of the AMG solver is described in this work. These implementations are all for MODFLOW. The performance of all the solvers is compared for both problems, and the differences are used to illustrate the characteristics of the AMG solver. While these small, simple problems can be solved quickly using the alternate solvers considered, for large, complicated problems the characteristics of the AMG solver illustrated can result in much faster execution times.

The performance of the SOR, SIP, and PCG2 solvers is heavily dependent on the initial head distribution. These solvers generally remove high frequency, highly oscillatory errors most effectively (particularly SOR). Thus, the convergence properties of these solvers depend on how oscillatory the error in the solution is. If the error is very oscillatory (such as the k=15 error in figure 1a), these solvers converge quickly. In contrast, if the error is relatively smooth (such as the k=1 error in figure 1a), these solvers will converge much more slowly. If the error contains components that are very oscillatory and other components that are smooth (such as the k=1+15 error in figure 1a), most of the oscillatory components will be removed after a few iterations, but the smooth error components will remain virtually unchanged. The slow reduction of smooth error components is what plagues the performance of these solvers. Thus, a good initial head distribution, which is equivalent to being void of smooth error components, is needed for rapid convergence.

The first problem was designed to illustrate the concept of reduction of error components. This problem represents one-dimensional flow with constant-head boundaries at both ends fixed at a value of zero. There is no gradient through the system, and the true solution is a value of zero throughout the domain (figure 1a). By using an initial head other than zero, one can examine how the solvers change this head to zero, the correct solution. To produce a problem that would emphasize the difference between the SOR, SIP, and PCG solvers and the AMG solver, the initial head for this problem was constructed by adding smooth and oscillatory error components, shown in figure 1a. The smooth component is the first wave number (k=1), while the oscillatory component is the fifteenth wave (k=15). Figures 1b and 1c show that the SOR and the SIP remove most of the high-frequency error after just two iterations, but the smooth error component is essentially unchanged. Figure 1d shows that the PCG solver with the modified incomplete Cholesky preconditioner makes much better progress reducing the error

components, but a smooth error component remains in the solution after three iterations. In contrast, the AMG solution shown in figure 1e reduces both the smooth and the oscillatory error in one cycle. The computation effort of one AMG cycle, however, is greater than one iteration of the other solvers, as explained later.
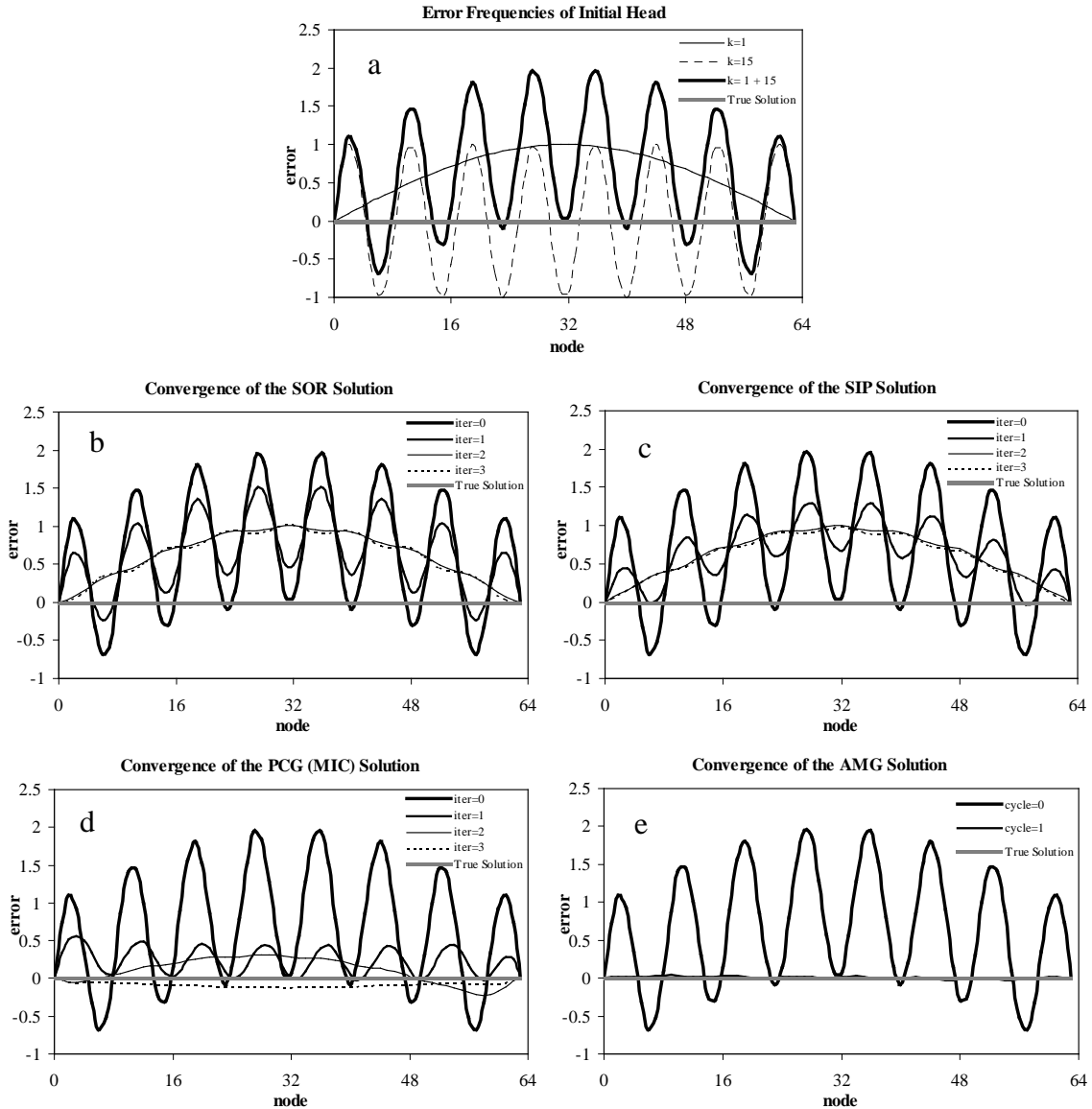

Figure 1. Errors in the solution to a one-dimensional flow problem with constant head boundaries of zero at both ends. (a) Components of initial head (errors), with smooth (k=1) and oscillatory (k=15) components. Reduction of error components for the (b) SOR, (c) SIP, (d) PCG2 with the modified incomplete Cholesky (MIC) preconditioner, and (e) AMG solvers.

There are two key ideas that result in multigrid methods being able to solve some problems so quickly. The first is that they exploit the rapid reduction of highly oscillatory error components by iterative solvers, such as the SOR. The second is that they solve the same problem on several different grids that are coarser than the initial grid. Errors that appear smooth on a finer grid will appear more oscillatory on a coarser grid and, thus, can be reduced more effectively on a coarser grid. The number of grids, the grid sizes, and the iterative solver used for each grid are selected such that the full range of error components are represented at a frequency that the particular solver eliminates quickly. Thus, by cycling between the different grids, all components of the error at all frequencies are reduced efficiently.

Another way to look at the solution characteristics is that the SOR, SIP, and PCG solvers calculate the updated head solution at a given node by various forms of averaging with the head solution at the neighboring nodes. This means that information is only propagated efficiently to close neighboring cells. Although solutions for each grid of a multigrid method are obtained using iterative solvers, multigrid methods propagate information more effectively throughout the system because some of the grids used are coarser. This has the effect of causing neighboring cell centers to be further away from each other in space, and the information is propagated a further distance.

The second problem illustrates how the solvers propagate information through the grid by examining the evolution of the head solution in a two-dimensional aquifer. The aquifer is homogenous with a single injection well at the center of a 31x31 grid and constant-head boundaries of 0.05 along the perimeter. The initial value is zero internally, except at the location of the well where it has a value of unity (figure 2a). By examining the true solution (figure 2b), one can see that the solvers need to increase the head throughout the interior of the domain, except at the injection well where the head needs to be decreased. Solutions after one and two iterations are shown for SOR, SIP, and PCG with the two preconditioners included in PCG2 (Hill, 1990). The AMG solution after one cycle also is shown. Figure 2 illustrates three characteristics of these solvers: (1) The SIP, SOR, and PCG solvers are limited in how much distant cells can be influenced at each iteration so that information is mostly propagated locally in space. (2) For PCG, the type of preconditioning is important as the modified incomplete Cholesky preconditioner allows the PCG to influence more distant cells and thus propagate information a farther distance. (3) The AMG solver is able to propagate information throughout the entire grid in one cycle.

initial value
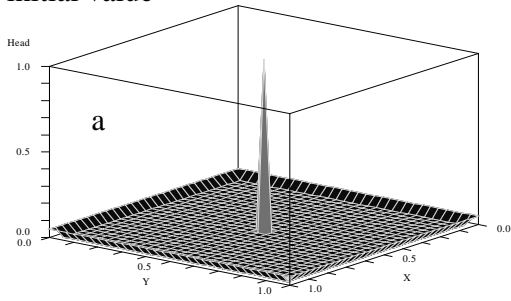
true solution
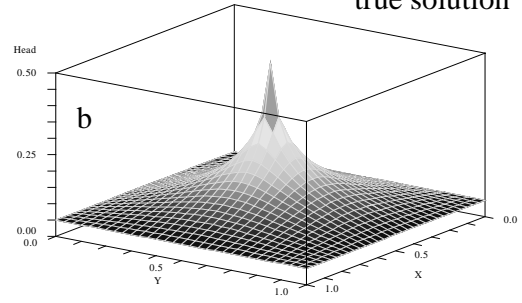
SOR   1 iteration
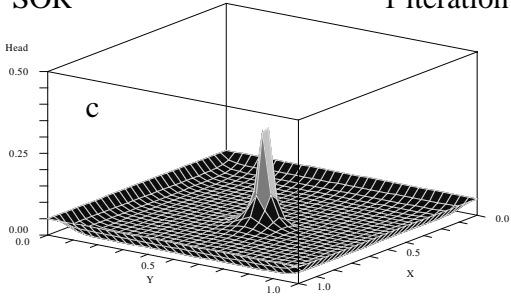
2 iterations
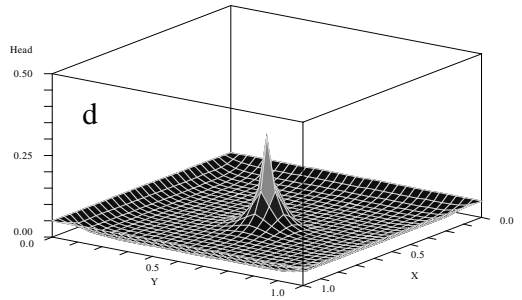
SIP   1 iteration
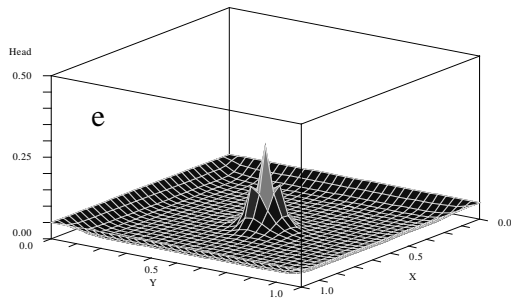
2 iterations
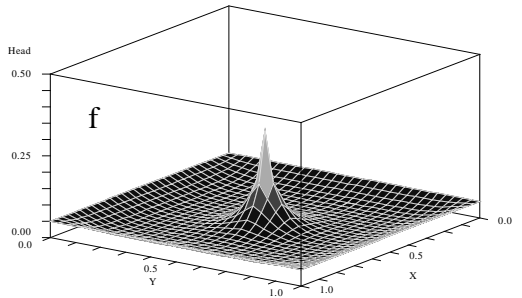
PCG (Polynomial)   1 iteration
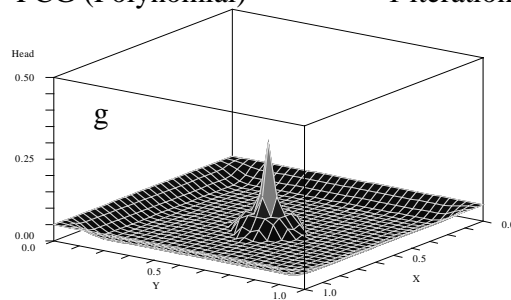
2 iterations
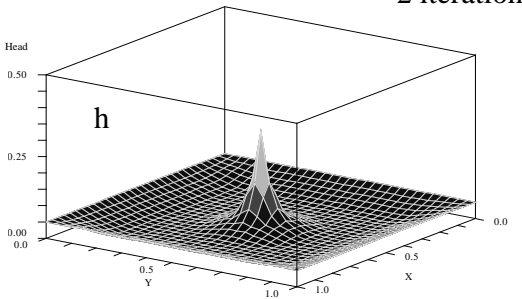
PCG (MIC)   1 iteration

2 iterations

7
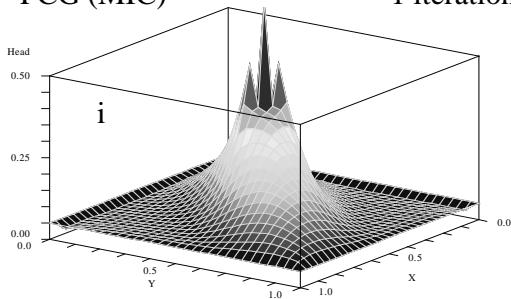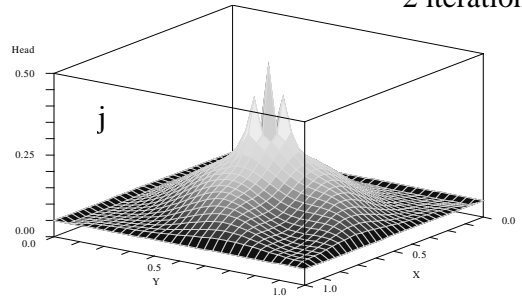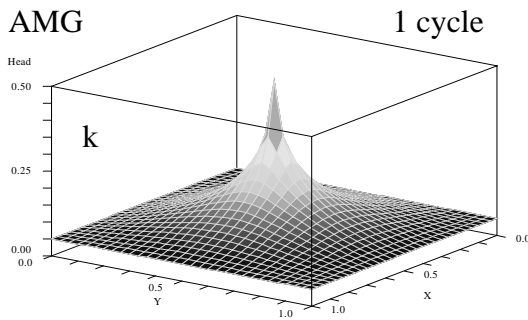
Figure 2. Head solution for a homogenous aquifer with a single injection well located at the center of 31x31 grid, with constant head boundaries of 0.05 along the perimeter. (a) initial value, (b) true solution, (c and d) SOR solution after 1 and 2 iterations, (e and f) SIP solution after 1 and 2 iterations, (g and h) PCG solution with the polynomial preconditioner after 1 and 2 iterations, (i and j) PCG solution with the MIC preconditioner after 1 and 2 iterations, (k) AMG solution after 1 cycle.

These small example problems were chosen for illustrative purposes; in these simple cases, the speed of the SOR, SIP, and PCG iterations relative to one AMG cycle means that the AMG is actually slower. This is because one multigrid cycle takes longer than one iteration of the SOR, SIP, or PCG, which is because one cycle involves multiple iterations on several different grids, as described below. However, examples shown later demonstrate that AMG attains smaller execution times for many large, complicated problems.

Geometric multigrid solvers work by taking the original problem and creating a series of associated, successively coarser grid representations. Approximate solutions are produced first for the finest grid considered, then on the next coarsest, on down to the coarsest grid representation. The solution on the coarsest grid is used to correct the solution at the next finest grid. This process is applied recursively such that corrections from a coarse grid to the next finest grid are applied until the finest grid is reached. Each of the cycles mentioned previously are composed of one such sequence. Convergence is checked and additional cycles are performed as needed.

The advantages of multigrid methods over the other iterative solvers mentioned are: (1) the effectiveness of the multigrid solver is not as dependent on the initial head distribution and (2) for many problems of interest, the rate of convergence scales approximately linearly with the size of the domain, unlike the other solvers where the rate of convergence increases nonlinearly (Demmel, 1997, p. 277). Thus, for many larger problems, multigrid methods can be extremely effective. One disadvantage of multigrid methods compared to the other iterative solvers mentioned is that information needs to be stored on more than a single grid so that the memory requirements for multigrid methods generally are greater than for other iterative solvers. This is probably one of the reasons why, historically, multigrid methods have not been popular for ground-water models, which tend to require considerable memory even when the alternative solvers are used. In addition, developing robust ways to interpolate values across several grids (especially in

8

three dimensions) when the discretization involves complex grid geometries has been difficult.

Geometric multigrid methods directly use information about the physical model grid to determine how to coarsen the grid and how to interpolate between the grids. These methods often fail given the complexity found in the broad range of ground-water flow problems that occur in practice. In contrast, algebraic multigrid (AMG) methods address this latter shortcoming and are not limited by complex grid geometries (Ruge and Stüben, 1987). The underlying idea of AMG is the same (fast reduction of smooth error components), but instead of coarsening the physical grid and applying a particular solver for that grid, AMG methods use a simple solver (typically Gauss-Seidel) and coarsen the matrix. That is, the coefficients of the matrix itself are used to determine where to coarsen and in which direction, such that the solver will be effective at each level of coarsening. Thus, no information about the grid or physical geometry is required beyond what is already contained in the coefficient matrix. Wagner and others (1997) used a similar approach, in which the multigrid solver incorporated algebraic information, to simulate ground-water flow and transport through several hydraulic-conductivity fields. They showed that their technique was able to solve problems where standard multigrid methods failed.

AMG methods generally use more memory and are not quite as efficient as geometric multigrid methods when the latter work, but the AMG methods successfully solve a broader class of problems, and this robust behavior makes them much more useful.

Implementation of AMG in MODFLOW-2000 Using the Link-AMG (LMG) Package

The AMG routine from the GMD (referred to by GMD as AMG1R5) was not modified. Instead, a package was written to interface MODFLOW-2000 with the AMG solver. This package is called Link-AMG (LMG) and is activated by including file type LMG in the name file as described by Harbaugh and others (2000, p. 7, 43-44). The actual equation solution is performed by calls from the LMG to the AMG1R5 routine. Nonlinear problems are solved using Picard iterations. A key difference between the LMG package and the other MODFLOW-2000 solver packages is how convergence is controlled. The implementation of Picard iterations and convergence control are discussed in the following sections.

Solution of Nonlinear Problems Using Picard Iterations

Nonlinear solutions for hydraulic head are produced by MODFLOW when model layers are simulated as being convertible and when some types of boundary conditions are used. For example, the River Package changes the calculation of flow to the ground-water system when the hydraulic head falls beneath the elevation defined as the bottom of the riverbed (McDonald and Harbaugh, 1988, ch. 6; Hill and others, 2000, p. 45). When the solution for hydraulic heads is nonlinear, the solver needs to solve a sequence of matrix equations, each using different, updated values of hydraulic heads to evaluate nonlinear terms. This continues until the updated hydraulic heads match the last set, using the convergence criterion as described below. The LMG Package solves nonlinear problems using Picard iterations, which is the same technique that the other MODFLOW solvers use. Picard iterations update the hydraulic heads for each solution in the sequence by simply using the hydraulic heads from the end of the last solution to calculate the equations for the subsequent solution.

Convergence Criterion

The AMG solver uses a scaled L_2 norm (the Euclidean norm) of the residual vector to measure how well a head distribution satisfies the matrix equations. To obtain a formulation for which the convergence criterion value has physical meaning and so that similar values can be used for most systems, scaling is needed. The scaling used in the LMG Package is described in this section.

Calculation of the scaled L_2 norm of the residual vector first requires the residual vector, which is calculated as

$$\{r\} = [A]\{h^k\} - \{f\}, \tag{1}$$

where

$\{r\}$ is the N x 1-dimensional residual vector [L^3/T if the solution is for hydraulic head];
N is the number of nodes in the finite-difference grid;

[*A*] is the N×N-dimensional coefficient matrix calculated as described by McDonald and Harbaugh (1988) and Harbaugh and others (2000) or, for sensitivities, as described by Hill and others (2000) [L^2/T if the solution is for hydraulic head];

{h^k} is an N-dimensional vector of hydraulic heads or sensitivities at the kth time step [L if the solution is for hydraulic head]; and

{*f*} is a vector of pumpage and terms related to other stresses and boundary conditions as defined by McDonald and Harbaugh (1988) and Harbaugh and others (2000) or, for sensitivities, as described by Hill and others (2000) [L^3/T if the solution is for hydraulic head].

The L_2 norm of the residual vector is calculated as:

$$\left\|\{r\}\right\|_2 = \left(\sum_{i=1}^{N} r_i^2\right)^{1/2}, \tag{2}$$

where r_i is the ith element of vector {*r*}. This norm is then scaled by dividing by the average value of the absolute value of the right hand side vector, $\overline{|\{f\}|}$. When

$$\frac{\left\|\{r\}\right\|_2}{\overline{|\{f\}|}} \le \varepsilon, \tag{3}$$

where ε [L^3/T] is the user specified tolerance BCLOSE, convergence is achieved. This criterion and scaling is similar to that used by Kipp and others (1998, eq. 25) to solve the matrix equations related to dispersive transport.

In the Picard iterations used to solve nonlinear problems, the coefficient matrix [*A*] and the right-hand-side vector {*f*} are updated after each iteration using the updated head solution. If the head solution continues to meet the convergence criterion after the equations are updated, convergence is achieved. If the criterion is no longer met, the solver is used to find a new head solution to the updated equations.

Tips for Achieving Convergence

There are a number of variables defined by the user that can affect the performance of the AMG solver. They are BCLOSE, the convergence criterion; MXITER, the maximum number of calls to the AMG routine; MAXCYC, the number of multigrid cycles performed per call to the AMG routine; ICG, a flag controlling the use of conjugate gradient iterations at the end of each multigrid cycle, and DAMP, which can be used to make the solution change more slowly and can be useful for nonlinear problems. Each of these variables is discussed below.

BCLOSE and MXITER

The AMG routine is called iteratively until the convergence criterion BCLOSE is met or the number of iterations has exceeded MXITER (equivalent to MXITER of PCG2; Hill, 1990). A convergence criterion value that is too large can be detected in

MODFLOW-2000 by unacceptably large global ground-water flow budget errors, sensitivity errors, or both. If such problems exist, BCLOSE should be decreased. Typically, decreasing BCLOSE by one order of magnitude will decrease the global budget error by about one order of magnitude.

A value of BCLOSE that is smaller than is needed will produce excessively long execution times. Such a situation probably exists if the global budget errors calculated for the solutions at all time steps and all parameters (if sensitivities are calculated) are less than 0.01 percent (0.00 will be printed by MODFLOW-2000 as the percent discrepancy for all budgets). If this occurs, BCLOSE can be increased incrementally by about an order of magnitude at each increment until the largest global budget error equals about 0.01 percent.

Another situation can occur where the solver fails to converge because BCLOSE is set too small. This can be detected by examining the residuals after each cycle (IOUTAMG=3) to see if the solver fails to lower the residuals any further after a certain number of cycles. When BCLOSE is too small, the closure criterion is below the limit of the round-off error in the calculations for this particular problem, and the solver cannot improve the solution any further. For this reason, the average value of the absolute value of the right hand side vector, $\overline{|\{f\}|}$, which is used to scale the L_2 norm, is also printed. The user has a reference point in that BCLOSE should not be chosen such that, when scaled, it is less than the limit of the solver for this problem.

MXITER is the maximum number of times that the AMG routines will be called to obtain a solution. MXITER is never less than 2 and rarely more than 50. MXITER often equals 2 when the problem is linear (all layers are confined, and no boundary conditions are nonlinear; the Evapotranspiration, Drain, and River Packages, for example, produce nonlinear boundary conditions). For nonlinear problems, MXITER generally is 50 or less; however values near 50 and sometimes even larger are needed for more severely nonlinear problems.

MXCYC

For each call to the solver, AMG cycles through one or more sequences of coarsening and refinement. The solver is limited to a maximum of MXCYC cycles per call to the solver (similar to ITER1 of PCG2; Hill, 1990). For most problems, convergence for each iteration is achieved in less than 50 cycles, so that generally MXCYC can be less than 50. For highly nonlinear problems, however, better performance may be achieved by limiting the solver to a small number of cycles and increasing the maximum number of iterations (MXITER). This prevents the solver from needlessly finding very accurate solutions at early iterations of these highly nonlinear problems.

ICG

In some cases, AMG can perform poorly as a result of a small number of error components that are not reduced during the AMG cycling. A few iterations of a conjugate gradient solver can often reduce these error components and thus help convergence (Cleary and others, 2000). In these cases, the parameter ICG can be set to 1 to perform

conjugate gradient iterations at the end of each multigrid cycle. Activating this option can decrease execution times for some problems, but it will also increase the amount of memory used by the solver.

DAMP

The damping parameter, DAMP, can be used to restrict the head change from one iteration to the next, which commonly is useful in very nonlinear problems. DAMP makes the solution change slowly, thus avoiding spurious deviations prompted by nonlinear effects at intermediate solutions. As implemented in the LMG Package, DAMP functions identically to ACCL in DE4 (Harbaugh, 1995, p. 12). Values of DAMP less than 1.0 restrict the head change (under relaxation), while values greater than 1.0 accelerate the head change (over relaxation). For linear problems, no damping is necessary, and DAMP should be set equal to 1.0. For nonlinear problems, restricting the head change (DAMP < 1.0) may be necessary to achieve convergence, and values of DAMP between 0.5 and 1.0 are generally sufficient. However, for nonlinear problems, the optimal value of DAMP cannot be determined beforehand.

For some nonlinear problems, imposing a fixed value of DAMP for every iteration can hinder convergence. One remedy for this condition is to adjust the amount of damping depending on how the head solution progresses. Cooley (1983) devised an empirical scheme for adjusting the level of damping when solving nonlinear, variably saturated flow equations using Picard iterations. His method was slightly modified by Huyakorn and others (1986) and compared to other nonlinear techniques by Paniconi and Putti (1994). They found that for some cases, the adaptive damping improved convergence compared to imposing a fixed level of damping. As part of this work, Cooley's method with Huyakorn's modification was investigated, and an empirical method that performed better in some circumstances was developed. For these reasons, two adaptive damping strategies are implemented in the LMG package: (1) Cooley's method with Huyakorn's modification, and (2) the relative reduced residual method developed for this work. Both schemes are described below.

In Cooley's method with Huyakorn's modification, the level of damping is adjusted based on a scaled measure of the maximum head change between successive Picard iterations. This scaled measure is calculated as:

$$S = \frac{\text{DHMAX}}{\text{DAMP} \cdot \text{DHOLD}}, \tag{4}$$

where

DHMAX is the change in head for all nodes in the grid that is maximum in absolute value; and

DHOLD is the value of DHMAX at the previous iteration.

If $S < -1$, the head change is greater in magnitude, and opposite in sign, than the previous iteration. This implies the solution is oscillating and diverging, so damping is applied according to equation 5a. If $-1 \leq S < 0$, the head change is still opposite in sign, but it is smaller in magnitude than the previous iteration. This implies the solution is still

oscillating, but not diverging, so damping is applied according to equation 5b, which will not be as restrictive as in the previous case. If $S \geq 0$, the head change is of the same sign as the previous iteration. This implies that the solution is probably converging to the correct solution, and the damping applied according to equation 5b results in a value of 1.0 regardless of the magnitude of S, which is equivalent to no damping.

$$DAMP = \frac{1}{2 \cdot |S|}, \qquad S < -1 \tag{5a}$$

$$DAMP = \frac{3 + S}{3 + |S|}, \qquad S \geq -1 \tag{5b}$$

In the relative reduced residual method developed for this work, the value of DAMP is adjusted at each iteration as the head solution progresses based on the relative reduction of the L_2 norm of the residuals scaled by the value of DAMP. The relative reduction in the residual (RRED) is calculated as:

$$RRED = \frac{\dfrac{RSQ2 - RSQ1}{RSQ2}}{DAMP}, \tag{6}$$

where

RSQ1 is the current L_2 norm of the residual; and

RSQ2 is the previous L_2 norm of the residual.

If RRED is greater than 0.5, the head solution is judged to be progressing adequately. In this case, the RRED is used as the value of DAMP for the next iteration. If this value exceeds DUP, the user input maximum allowable value of DAMP, then DUP is used instead. When the head solution progresses enough such that the problem behaves essentially linearly, the equation for RRED will produce values near 1.0, which is an appropriate level of damping. In contrast, if RRED is less than or equal to 0.5, the solution is not progressing adequately. In this case, the level of damping is calculated by:

$$DAMP = \frac{0.075}{0.75 - RRED} + DLOW, \tag{7}$$

where

DLOW is the minimum value of DAMP that will be applied as specified by the user.

Equation 7 will produce larger values of DAMP if RRED is close to 0.5, and smaller values of DAMP if RRED is much less than 0.5. In some circumstances, the nonlinearity can cause the head solution to oscillate, which in turn can cause oscillations in the values of DAMP produced by this scheme. In such cases, this scheme will apply a random value of DAMP between 0 and 1.5 in an effort to move the head solution away from this nonlinearity.

It is generally not possible to know beforehand if adaptive damping will be advantageous, and it is therefore recommended that the user start with a fixed level of

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damping. If the solution is making little progress and values of DAMP near or below 0.5 are required to achieve convergence, which can be an indicator of strong nonlinearities, adaptive damping should be considered. If the user specifies a value of DAMP that is –1 or -2, the first or second adaptive-damping strategy, respectively, will be used. Positive values of DAMP will be applied as a fixed value for all iterations. All other values of DAMP are automatically reset to 1.0.

Comparison of LMG with PCG2 for Ground-Water Flow Problems

This section shows how the LMG Package performed when solving five large ground-water problems. For comparison, the problems also were solved using the PCG2 Package (Hill, 1990) with the modified incomplete Cholesky preconditioner and those results also are shown. The closure criteria for the solvers were adjusted such that, for each comparison, the solutions had approximately the same accuracy as indicated by the MODFLOW-2000 budget summary.

Comparisons are made based on the execution time and memory required. The execution time and memory required depends on the size of the problem and the complexity of the hydraulic-conductivity field, which are described briefly. For each problem, table 1 shows the execution time in CPU seconds, the memory required, and the number of iterations or cycles needed for convergence. In addition, to demonstrate the effects of the DAMP and ICG options, some problems were simulated twice with the LMG using different values for DAMP and ICG.

Table 1. Comparison of computational differences between the PCG2 and LMG solvers for several different ground-water flow problems. Unless otherwise indicated, DAMP=1.0 and ICG=0 for all simulations. [SS, steady-state; TR, transient; L, linear; NL, nonlinear; #, number; MB, megabyte]

Prob-lem	Type	# of Nodes (# of layers, # of rows, # of columns)	PCG2			LMG		
			CPU Time (seconds)	Memory (Mb)	# of Iterations	CPU Time (seconds)	Memory (Mb)	# of Cycles
1	SS NL	1,728,000 (60, 240, 120)	3,082	121	565	1,761 [1]1,352	940 [1]966	40 [1]24
2	SS L	1,050,000 (1, 1500, 700)	5,243	50	2465	205	340	9
3	TR NL	147,440 (4, 190, 194)	852	14	4328	631	72	175
4	SS L	465,600 (15, 194, 160)	942	47	1864	50	151	9
5	SS NL	74,817 (3, 163, 153)	654	8	3718	[2]108 [3]54 [4]59	[2]29 [3]29 [4]29	[2]46 [3]25 [4]27

[1] ICG=1
[2] DAMP=0.50
[3] DAMP=-1 (Adaptive damping using Cooley's method)
[4] DAMP=-2 (Adaptive damping using the relative reduced residual method)

Problem 1 is a very large, three-dimensional model. The variance of the hydraulic conductivity field is approximately 2.0 (Sanford, W.E., U.S. Geological Survey, written communication, 2000). The LMG Package uses a large amount of memory to solve this problem, and the ICG option is helpful in reducing the CPU time.

Problem 2 is a large, two-dimensional model with a very complicated hydraulic conductivity field (Konikow, L., and Hornberger, G., U.S. Geological Survey, written communication, 2000). The LMG Package is very effective for this problem, reducing execution time by a factor of 25, while using substantially more memory.

Problem 3 is a moderately sized, transient model (Roberts, C.F., U.S. Geological Survey, written communication, 2001). The CPU time of both solvers is similar for this problem. This is primarily because the solution at the current time step is used as the initial head for the next time step, and in this case, the initial head approximation is very close to the converged solution, so both solvers perform well.

Problem 4 is a large, three-dimensional model with a complex heterogeneous hydraulic-conductivity field (O'Brien, G.M. and D'Agnese, F.A., U.S. Geological Survey, written communication, 2000). As with problem 2, which also had a complex heterogeneous field, the LMG Package performs very successfully for this problem.

Problem 5 is a moderately sized three-dimensional problem with very strong nonlinearites resulting from evaportranspiration and a hydraulic conductivity field that is also fairly complex (D'Agnese and others, 1998, and Tiedeman, C.R., U.S. Geological Survey, written communication, 2000). The adaptive damping strategies are very effective for this problem and reduce the number of cycles required for convergence.

The above results indicate that the LMG Package can substantially reduce the CPU time compared to the PCG2 Package, particularly for problems involving complex hydraulic-conductivity fields.

Compatibility, Portability and Memory Requirements

Compatibility and Portability

The LMG Package and the AMG solver are written in standard FORTRAN 77. Subroutine CTIME is machine independent as distributed but can be modified as needed for a given computer platform to calculate the computational times for various parts of the algorithm. As distributed, CTIME is simply a dummy routine, and the values for times printed when IOUTAMG = 2 or 3 (see Input Instructions) will always equal zero. Most users don't need internal timing information and will not need to change CTIME. For users interested in investigating internal execution times, CTIME is distributed with commented lines that correspond to the intrinsic timing functions for several platforms. To calculate the computational times, the user needs to "uncomment" the section that corresponds to the appropriate platform or use the intrinsic timing function for their compiler, and recompile the program. However CTIME is handled, it will not affect the performance of the AMG solver.

Memory Requirements

The LMG package uses a large amount of memory in the MODFLOW-2000 Z and IX arrays. The AMG1R5 code is written in FORTRAN 77 instead of FORTRAN 90, so three variables, STOR1, STOR2, and STOR3, are used to allocate memory for the arrays required by the AMG routine. The nature of the algebraic multigrid algorithm is such that the memory requirements cannot be determined beforehand. Nevertheless, reasonable estimates based on the number of nodes (NODES) and the number of non-zero elements in the coefficient matrix (NNA) can be used to allocate memory. The formulas for array dimensions shown in table 2 are based on recommendations from the authors of the AMG1R5 routine.

Table 2. Arrays used in AMG1R5, their dimensions, the user-defined variables that control the storage allocated for the arrays, values recommended by Ruge and others (1990), and the global storage arrays in MODFLOW-2000 in which the AMG1R5 arrays are stored. [NODES, number of nodes in the grid; NNA, number of non-zero elements in the coefficient matrix.]

Array name	Dimension	User-Defined Variable and Recommended Value	Global Storage Array
A	STOR1*NNA + 5*NODES	STOR1=3.0	Z
JA	STOR1*NNA + 5*NODES	STOR1=3.0	IX
IA	STOR2*NODES	STOR2=2.2	IX
U	STOR2*NODES	STOR2=2.2	Z
[1] FRHS	STOR2*NODES	STOR2=2.2	Z
IG	STOR3*NODES	STOR3=5.4	IX

[1] The array FHRS in the LMG package corresponds to the array F in the AMG1R5.

For most problems, the recommended values of STOR1, STOR2, and STOR3 are adequate. However, if memory usage is a problem, the user can adjust the storage values as necessary. The solver will stop and report an error if the storage space allocated for a array is insufficient. In such cases, the variable controlling the storage for that array needs to be increased.

Input Instructions and Sample Data Inputs

Input Instructions

The LMG Package reads its input data from the file indicated in the Name file as described by Harbaugh and others (2000, p. 7, 43) using File Type LMG. Input for the LMG Package is defined using two numbered items. Each item consists of several parameters that are specified in one record and are read free format.

```
1. STOR1    STOR2       STOR3        ICG
2. MXITER   MXCYC       BCLOSE       DAMP        IOUTAMG
      Item 3 is read if DAMP = -2
3. DUP      DLOW
```

STOR1 is a variable controlling the amount of storage allocated in the Z array for the array A and the amount of storage allocated in the IX array for the array JA. For most problems, a value of 3.0 should be adequate (table 2).

STOR2 is a variable controlling the amount of storage allocated in the Z array for the arrays U and FRHS, and the amount of storage allocated in the IX array for the array IA. For most problems, a value of 2.2 should be adequate (table 2).

STOR3 is a variable controlling the amount of storage allocated in the IX array for the array IG. For most problems, a value of 5.4 should be adequate (table 2).

ICG is a variable controlling whether or not conjugate gradient iterations are used at the end of each multigrid cycle. A value of 1 indicates that conjugate gradient iterations will be performed, while a value of 0 indicates no conjugate gradient iterations will be performed. All other values are automatically reset to 0. For some problems, using conjugate gradient iterations can improve convergence, but it will increase the memory used by the solver.

MXITER is the maximum number of iterations – that is, calls to the AMG solver. For linear problems, MXITER can be set equal to 2. For nonlinear problems, MXITER generally needs to be larger, but rarely more than 50.

MXCYC is the maximum number of cycles allowed per call to the solver. This is similar to the variable ITER1 in PCG2 (Hill, 1990, p. 13). A value of 50 is suggested. For some nonlinear problems, however, faster convergence may be achieved by reducing MXCYC and increasing MXITER.

BCLOSE is the budget closure criterion for the scaled L_2 norm of the matrix equations (eq. 3). A value similar to RCLOSE of PCG2 (Hill, 1990, p. 12-14) should be used. If the global budget error is too large, decrease BCLOSE by one order of magnitude to reduce the global budget error by about one order of magnitude. This approximation can be used to adjust BCLOSE until a satisfactory solution is attained. See the sections on Convergence Criterion and Tips for Achieving Convergence for more information.

DAMP is a damping/accelerating parameter identical to ACCL of the DE4 (Harbaugh, 1995, p. 12) solver. Generally, a value of 1.0 is sufficient for most problems. However, for nonlinear problems, values less than 1.0 may be necessary to achieve convergence (see problem 5, table 2, for example).

DAMP>0 This value of DAMP is applied for all iterations.
DAMP=-1 Cooley's method for adaptive damping is implemented.
DAMP=-2 The relative reduced residual method for adaptive damping is implemented.
All other values of DAMP are automatically reset to 1.0 (no damping).

IOUTAMG is a flag that controls the information printed each time step from the solver to the MODFLOW-2000 LIST output file (Harbaugh and others, 2000). Diagnostic messages from the solver are sent to a temporary file called "lmg_err.tmp" except if IOUTAMG=3, when they are printed along with the other iteration information. The "lmg_err.tmp" file is deleted upon successful termination of the solver. If the solver should fail, the output in this file may help to identify solver problems. The possible values of IOUTAMG and the information printed to the LIST file are as follows.

IOUTAMG=0 No printing from the solver to the LIST file.
IOUTAMG=1 Print scaling for residuals and residuals before and after cycling.
IOUTAMG=2 Print scaling for residuals, residuals before and after cycling, the computer storage used, and the computation times if the CTIME subroutine has been adapted to the computer operating system (see Compatibility and Portability).
IOUTAMG=3 Print solver messages, scaling for residuals, residuals after each cycle the computer storage used, and the computation times if the CTIME subroutine has been adapted to the computer operating system (see Compatibility and Portability).

DUP is the maximum value of DAMP that should be applied at any iteration. If the adaptive scheme calculates a value of DAMP that is greater than DUP, DAMP will be reset to DUP. A value of 1.0 is reasonable for most problems.

DLOW is the minimum value of DAMP that should be applied at any iteration. If the adaptive scheme determines that the value of DAMP should be decreased, it will calculate a new value of DAMP based on DLOW being the minimum (see eq. 7). A value of 0.2 is reasonable for most problems.

Sample Data Inputs

Sample data inputs as listed below are for typical linear and nonlinear problems. In these examples, the only differences are MXITER and DAMP. MXITER is typically 2 for linear problems. DAMP would generally be set to 1.0 for linear problems, but a value less than 1.0 might be advantageous for nonlinear problems.

Example data set for a linear problem:
```
  3.0        2.2        5.4          0
    2         50        .001        1.0              1
```

Example data set for a nonlinear problem:
```
  3.0        2.2        5.4          0
   20         50        .001        .75              1
```

Example data set for a nonlinear problem with Cooley's adaptive damping:
```
  3.0        2.2        5.4          0
   20         50        .001       -1.0              1
```

Example data set for a nonlinear problem with the relative reduced residual adaptive damping scheme:
```
  3.0        2.2        5.4          0
   20         50        .001       -2.0              1
  1.0        0.2
```

Brief Program Description

The LMG Package is composed of five modules, LMG1AL, LMG1RP, LMG1AP, ADAMP1, and ADAMP2. The function of each module and the names of the variables used are described in the following sections. Using the AMG solver also requires the AMG1R5 subroutine by Ruge and others (1990), which contains documentation within the source code, and the CTIME subroutine, which was discussed under in the section "Compatibility and Portability."

Narrative for Module LMG1AL

Module LMG1AP allocates space in the Z and IX arrays. This space is used by the other modules in the LMG package and in the AMG routine. Storage is allocated for the AMG arrays A, JA, IA, U, FRHS, and IG.

1. Print a message identifying the LMG Package.

2. Read values for STOR1, STOR2, STOR3, and ICG. Print values for STOR1, STOR2, and STOR3. Check value ICG and set to 0 if necessary.

3. Calculate storage allocation based on STOR1, STOR2, STOR3, (see Memory Requirements). Allocate space in the Z and IX arrays and set pointers for A, U, FHRS, IA, JA, and IG.

4. Calculate and print space used in the Z and IX arrays

5. Return

List of Variables for Module LMG1AL

IAMG	Module	Number of elements of the Z and IX arrays allocated for the AMG solver.
ICG	Package	Flag controlling the use of conjugate gradient iterations at the end of each multigrid cycle.
IFREFM	Global	A parameter used to indicate if free format is used.
IN	Package	Primary unit number from which input for this package will be read.
IOUT	Global	Primary unit number for all printed output.
ISIZ1	Package	STOR1*NNA+5*NODES
ISIZ2	Package	STOR2*NODES
ISIZ3	Package	STOR3*NODES
ISIZ4	Package	Same as ISIZ2, unless ICG=1, then ISIZ2+NODES.
ISOLD	Module	Value of ISUM upon entry into this module.
ISOLDI	Module	Value of ISUMI upon entry into this module.
ISUM	Global	Element number of the lowest element in the Z array that has

		not yet been allocated. When space is allocated to the Z array, the size of the allocation is added to ISUM.
ISUM1	Module	ISUM-1 or ISUMI-1
ISUMI	Global	Same as ISUM, but for the IX array
LCA	Package	Location in the Z array of the first element of the array A.
LCFRHS	Package	Location in the Z array of the first element of the array FRHS.
LCIA	Package	Location in the IX array of the first element of the array IA.
LCIG	Package	Location in the IX array of the first element of the array IG.
LCJA	Package	Location in the Z array of the first element of the array JA.
LCU1	Package	Location in the Z array of the first element of the array U.
LENIX	Global	Number of elements in the IX array (static storage).
LENZ	Global	Number of elements in the Z array (static storage).
LINE	Module	Character string used to read in data from the AMG input file.
NCL	Module	Number nodes per row of the grid (NCOL*NLAY).
NCOL	Global	Number of columns in the grid.
NLAY	Global	Number of layers in the grid.
NNA	Module	The number of non-zero elements in the coefficient matrix [A]. Calculated as NODES+2*(NCOL-1)*NRL+ 2*(NROW-1)*NCL+2*(NLAY-1)*NRC.
NODES	Global	Number of nodes in the grid (NCOL*NROW*NLAY).
NRC	Module	Number of nodes per layer of the grid (NROW*NCOL).
NRL	Module	Number nodes per column of the grid (NROW*NLAY).
NROW	Global	Number of rows in the grid.
STOR1	Module	Storage factor for arrays A and JA.
STOR2	Module	Storage factor for arrays FRHS, IA, and U.
STOR3	Module	Storage factor for array IG.

Narrative for Module LMG1RP

       Module LMG1RP reads and prepares data for the LMG package. Variables to control operation of the solver are read. MXITER is the number of calls to the solver, MXCYC is the maximum number of cycles per call to the solver, BCLOSE is a closure criterion, DAMP is a damping parameter, and IOUTAMG controls output from the solver.

1. Initialize HCLOSE so the sensitivity process, if used, executes without errors.

2. Read MXITER, MXCYC, BCLOSE, DAMP, and IOUTAMG. Check value of DAMP. If using adaptive damping, set IADAMP and read DUP and DLOW if necessary.

3. Print MXITER, MXCYC, BCLOSE, ICG, DAMP, and IOUTAMG. Print IADAMP, DUP, and DLOW if appropriate.

4. Set IOUTAMG to a value that AMG requires by adding 10 to the value specified in the LMG Package input file.

5. Return

List of Variables for Module LMG1RP

BCLOSE	Package	Budget closure criterion.
DAMP	Package	Damping/accelerating parameter for head change at each iteration.
DLOW	Package	Minimum value of damping.
DUP	Package	Maximum value of damping.
HCLOSE	Global	Dummy variable set to zero. Initialized here because if sensitivities are calculated, it requires HCLOSE to be initialized.
IADAMP	Package	Flag used to determine if adaptive damping is being used.
ICG	Package	Flag controlling the use of conjugate gradient iterations at the end of each multigrid cycle.
IFREFM	Global	A parameter used to indicate if free format is being used.
IN	Package	Primary unit number from which input for this package will be read.
IOUT	Global	Primary unit number for all printed output.
IOUTAMG	Package	Flag controlling the printing from the solver.
MXCYC	Package	Maximum number of AMG cycles per call to the solver.
MXITER	Package	Maximum number of calls to the solver.

Narrative for Module LMG1AP

Module LMG1AP sets up the matrix equations in a form that is compatible with the AMG solver provided by the GMD. This routine is called each time a head or sensitivity solution is needed.

1. Initialize variables and clear arrays.

2. Loop through all nodes in the grid and set up coefficients of the matrix equations and accumulate the L_2 norm of the current residual vector. This loop structure is identical to that of subroutine PCG2AP of the PCG2 (Hill, 1990, p. 31-32) solver.

3. Reset the coefficients of the matrix equations such that the diagonal elements are positive and the off-diagonal elements are negative. Set the diagonal to 1.0 and set FRHS to HNEW for inactive cells or constant-head cells. Accumulate the average absolute value of the FRHS vector for active cells and the maximum value of the FRHS vector for all cells.

4. Use a skyline type storage to store the coefficients of the conductance matrix in a single vector (A), with pointers to the diagonal (IA) and off diagonals (JA). For each row in the matrix, start at the diagonal, then pick up non-zero elements moving from left to right (but skipping the diagonal). Store initial value in vector U.

5. Set the dimensions for the variables used by the AMG solver. The extra storage is used by the solver as workspace. Set variables for solver control.

6. Control printing from the solver based on the value of IOUTAMG. A temporary file is opened for printing solver messages if IOUTAMG is < 13. The user inputs a value of 3 for IOUTAMG, but 10 was added to this value to maintain compatibility the AMG1R5 code.

7. Scale the L_2 norm closure criterion by the average absolute value and the maximum value of FRHS. Print scaled values. Check convergence. If converged, close temporary file (if necessary) and return.

8. Set up default values for the AMG solver. Call the AMG1R5 subroutine.

9. Check for solver errors. If there are errors, print identifying messages and stop. If the solver executed successfully, apply damping strategy, then close temporary output file (if necessary).

10. Return

List of Variables for Module LMG1AP

A	Module	DIMENSION(ISIZ1), double precision array containing the coefficient matrix [A].
BCLOSE	Package	Budget closure criterion.
CC	Global	Dimension(NCOL,NROW,NLAY), conductances along columns.
CR	Global	Dimension(NCOL,NROW,NLAY), conductances along rows.
CV	Global	Dimension(NCOL,NROW,NLAY), conductances between layers.
DAMP	Package	Damping/accelerating parameter for head change at each iteration.
DDAMP	Package	Double precision form of DAMP.
DHMAX	Package	Head change for current iteration that is maximum absolute value.
DLOW	Package	Minimum value of damping.
DONE	Module	Double precision variable containing a value of unity.
DUP	Package	Maximum value of damping.
DZERO	Module	Double precision variable containing a value of zero.
ECG1	Module	Double precision variable equal to 0.D0.
ECG2	Module	Double precision variable equal to 0.25D0.
EPS	Module	Double precision BCLOSE*FBAR/FMAX used for AMG scaled residual closure criterion.
EWT2	Module	Double precision variable equal to 0.35D0.
FBAR	Module	Double precision average of ABS(FRHS) for active nodes.
FMAX	Module	Double precision maximum ABS(FRHS) for active nodes.
FRHS	Module	DIMENSION(ISIZ2), double precision form of -RHS.
HCOF	Global	DIMENSION(NCOL,NROW,NLAY), coefficient of head in the finite-difference equations.
HNEW	Global	DIMENSION(NCOL,NROW,NLAY), most recent estimate of head in each cell.
IA	Module	DIMENSION(ISIZ2), array containing the location of the diagonal element in the coefficient matrix [A].
IADAMP	Package	Flag used to determine if adaptive damping is being used.
IBOUND	Global	DIMENSION(NCOL,NROW,NLAY), status of each cell: < 0 – constant-head cell $= 0$ – no-flow cell > 0 – variable head cell
ICG	Package	Flag controlling the use of conjugate gradient iterations at the end of each multigrid cycle.
ICNVG	Global	Flag that is set to one when convergence has occurred.
IFIRST	Package	Integer variable set equal to 10 which allows the current head to be used as the initial solution within the AMG1R5.
IG	Module	DIMENSION(ISIZ3), work array used by the AMG solver.
ILMGTMP	Module	Primary unit number to which messages from the solver will be printed if IOUTAMG = 0, 1, or 2.

IOUT	Global	Primary unit number for all printed output.
IOUTAMG	Package	Flag controlling the printing from the AMG solver.
ISIZ1	Package	STOR1*NNA+5*NODES
ISIZ2	Package	STOR2*NODES
ISIZ3	Package	STOR3*NODES
ISIZ4	Package	Same as ISIZ2, unless ICG=1, then ISIZ2+NODES.
ISWTCH	Package	Integer variable set equal to 4 so that all modules of the AMG1R5 are called.
IZERO	Module	Integer variable containing zero.
JA	Module	DIMENSION(ISIZ1), array containing the location of the off-diagonal elements of the coefficient matrix [A].
KITER	Global	Counts the number of calls to the solver.
LEVELX	Package	Integer variable set equal to 0 so that a standard value is used by the AMG1R5.
MADAPT	Package	Integer variable set equal to 0 so that a standard value is used by the AMG1R5.
MATRIX	Package	Integer variable set equal to 22 which defines properties of the matrix for the AMG1R5.
MXCYC	Package	Maximum number of AMG cycles per call to the solver.
MXITER	Package	Maximum number of calls to the solver.
N	Module	Cell index.
NA	Module	Index for array A.
NCD	Module	One-dimensional subscript of conductance to the adjacent cell, which is in the previous column.
NCF	Module	One-dimensional subscript of conductance to the adjacent cell, which is in the next column.
NCL	Module	One-dimensional subscript of the cell index of the adjacent cell which is in the previous column.
NCN	Module	One-dimensional subscript of the cell index of the adjacent cell which is in the next column.
NCOL	Global	Number of columns in the grid.
NCOUNT	Module	Number of active nodes.
NCYC	Package	Integer variable that controls the number and type of cycles used by the AMG1R5.
NDF	Package	Dimensioning for FRHS. Same as ISIZ4.
NDA	Package	Dimensioning for A. Same as ISIZ1.
NDIA	Package	Dimensioning for IA. Same as ISIZ2.
NDIG	Package	Dimensioning for IG. Same as ISIZ3.
NDJA	Package	Dimensioning for JA. Same as ISIZ1.
NDU	Package	Dimensioning for U. Same as ISIZ4.
NJ	Module	Index for array JA.
NLAY	Global	Number of layers in the grid.
NLL	Module	One-dimensional subscript of the cell index of the adjacent cell, which is in the previous layer.
NLN	Module	One-dimensional subscript of the cell index of the adjacent cell, which is in the next layer.

NLS	Module	One-dimensional subscript of conductance to the adjacent cell, which is in the next layer.
NLZ	Module	One-dimensional subscript of conductance to the adjacent cell, which is in the previous layer.
NNU	Package	Number of unknowns. Same as NODES.
NODES	Global	Number of nodes in the grid (NCOL*NROW*NLAY).
NRB	Module	One-dimensional subscript of conductance to the adjacent cell, which is in the previous row.
NRC	Module	Number of nodes per layer of the grid (NROW*NCOL).
NRD	Package	Integer variable set equal to 0 so that a standard value is used by the AMG1R5.
NRH	Module	One-dimensional subscript of conductance to the adjacent cell, which is in the next row.
NRL	Module	One-dimensional subscript of the cell index of the adjacent cell, which is in the previous row.
NRN	Module	One-dimensional subscript of the cell index of the adjacent cell, which is in the next row.
NROW	Global	Number of rows in the grid.
NRU	Package	Integer variable set equal to 0 so that a standard value is used by the AMG1R5.
NSOLCO	Package	Integer variable set equal to 2 so that the AMG1R5 uses a direct solver on the coarsest grid.
NTR	Package	Integer variable set equal to 0 so that a standard value is used by the AMG1R5.
NWT	Package	Integer variable set equal to 2 which is a standard value for the AMG1R5.
RHS	Global	DIMENSION(NCOL,NROW,NLAY) right-hand side of the finite-difference equations.
RSQ	Module	Double precision variable containing the current sum of squared residuals of the finite-difference equations.
TMP	Module	Temporary variable used when finding DHMAX.
U	Module	DIMENSION(ISIZ2) initial value upon entry to AMG solver and solution vector upon exit from AMG solver.

Narrative for Module ADAMP1

Module ADAMP1 changes the value of the damping parameter, DAMP, based on the maximum head change from the previous and current iterations. The strategy used is that proposed by Cooley (1983) and later modified by Huyakorn and others (1986).

1. Initialize S and calculate according to equation 4, if not on the first iteration.

2. Based on the value of S, apply damping according to equation 5. Values greater than or equal to -1 indicate the solution is progressing adequately and the damping is not very aggressive. The converse is true for values of S that are less than -1.

3. Return

List of Variables for Module ADAMP1

DHMAX	Package	Head change for current iteration that is maximum absolute value.
DHOLD	Module	Value of DHMAX at the previous iteration.
KITER	Global	Counts the number of calls to the solver.
S	Module	Fractional change in the maximum head change, scaled by the damping parameter. Calculated as DHMAX/DHOLD/WK.
WK	Package	Same as DDAMP.

Narrative for Module ADAMP2

Module ADAMP2 changes the value of the damping parameter, DAMP, based on the L_2 norm of the residuals from the current and two prior iterations. The strategy used is empirical and based on damping more aggressively if the residuals are not lowered sufficiently or if they are oscillating.

1. Calculate current residual and initialize variables for the first iteration.

2. Calculate the relative reduction in the L_2 norm scaled by the applied damping (RRED, see equation 6). If RRED is greater than 50 percent then moderate damping is applied with a value of DDAMP equal to RRED, but not greater than DUP. Thus, for larger RRED, the solution is progressing adequately and the value of DDAMP should approach 1.0 or DUP. The converse is true for RRED less than 50 percent. The damping is more aggressive for poorer reductions with a minimum value of DLOW. Note that the maximum value of DDAMP for this case will be DLOW + 0.3 (see equation 7).

3. Calculate the relative change in the L_2 norm between the current residual and the residual from two iterations ago (OSTERM). If they are within 10 percent of each other, then the solution is oscillating. Check to make sure DDAMP does not exceed DUP. If the solution is oscillating and the current value of DDAMP is within 1 percent of the damping that was applied two iterations ago (DAMP3), then the solution will continue to oscillate in this area. In this case, generate a random value of DDAMP between 0 and 1.5 to try and perturb the solution out of this area.

4. Store the values of the L_2 norm and damping for the next iteration.

5. Return.

List of Variables for Module ADAMP2

DAMP	Package	Damping/accelerating parameter for head change at each iteration. Current value of DAMP upon entry. Previous value of damping upon exit.
DAMP3	Module	Value of DDAMP two iterations ago.
DDAMP	Package	Double precision form of DAMP.
DLOW	Package	Minimum value of damping.
DUP	Package	Maximum value of damping.
RRED	Module	Relative reduction of the residuals scaled by the damping parameter. Calculated as (RSQ2-RSQ1)/RSQ2/DDAMP.
ICONST	Module	Integer used for random number generation. Equals 49297.
IMULT	Module	Integer used for random number generation. Equals 9301.
IPER	Module	Integer used for random number generation. Equals 233280.
KITER	Global	Counts the number of calls to the solver.
NRAN	Module	Integer used in generating a random number.
OSCIL	Module	Logical variable to flag if the solution is oscillating.
OSTERM	Module	Variable used to determine if the solution is oscillating by measuring relative difference in residuals. Calculated as (RSQ3-RSQ1)/RSQ3.
QRAND	Module	Quick random number generated uniformly between 0 and 1.
RSQ1	Package	Double precision variable containing the current sum of squared residuals of the finite-difference equations upon entry. Square root of the sum of squared residuals value upon exit.
RSQ2	Module	Double precision variable containing the value of RSQ1 at the previous iteration.
RSQ3	Module	Double precision variable containing the value of RSQ2 at the previous iteration (the same as RSQ1 two iterations ago).

References

Briggs, W.L., Henson, V.E., and McCormick, S.F., 2000, A multigrid tutorial: 2nd ed.: Philadelphia, Society for Industrial and Applied Mathematics, 193 p.

Cleary, A.J., Falgout, R.D., Henson, V.E., Jones, J.E., Manteuffel, T.A., McCormick, S.F., Miranda, G.N., and Ruge, J.W., 2000, Robustness and scalability of algebraic multigrid: SIAM Journal on Scientific Computing, v. 21, no. 5, p. 1886-1908.

Cooley, R. L., 1983, Some new procedures for numerical-solution of variably saturated flow problems: Water Resources Research, v. 19, no. 5, p. 1271-1285.

D'Angese, F.A., Faunt, C.C., Turner, A.K., and Hill, M.C., 1998, Hydrogeologic evaluation and numerical simulation of the Death Valley regional ground-water flow system, Nevada and California: U.S. Geological Survey Water-Resources Investigation Report 96-4300, 124 p.

Demmel, J.W., 1997, Applied Numerical linear algebra: Philadelphia, Society for Industrial and Applied Mathematics, 419 p.

Harbaugh, A.W., 1995, Direct Solution Package Based on Alternating Diagonal Ordering for the U.S. Geological Survey Modular Finite-Difference Ground-Water Flow Model: U.S. Geological Survey Open-File Report 95-288, 46 p.

Harbaugh, A.W., Banta, E.R., Hill, M.C., and McDonald, M.G., 2000, MODFLOW-2000, The U.S. Geological Survey modular ground-water model – User guide to modularization concepts and the ground-water flow process: U.S. Geological Survey Open-File Report 00-92, 121 p.

Hill, M.C., 1990, Preconditioned Conjugate-Gradient 2 (PCG2), A computer program for solving ground-water flow equations: U.S. Geological Survey Water-Resources Investigations Report 90-4048, 43 p.

Hill, M.C., Banta, E.R., Harbaugh, A.W., and Anderman, E.R., 2000, MODFLOW-2000, The U.S. Geological Survey modular ground-water model – User guide to the observation, sensitivity, and parameter-estimation processes and three post-processing programs: U.S. Geological Survey Open-File Report 00-184, 209 p.

Huyakorn, P.S., Springer, E.P., Guvanasen, V., and Wadsworth, T.D., 1986, A 3-dimensional finite-element model for simulating water-flow in variably saturated porous-media: Water Resources Research, v. 22, no. 13, p. 1790-1808.

Kipp, K.L., Konikow, L.F., and Hornberger, G.Z., 1998, An implicit dispersive transport algorithm for the U.S Geological Survey MOC3D solute-transport model: U.S. Geological Survey Water-Resources Investigations Report 98-4234, 54 p.

McDonald, M.G., and A.W. Harbaugh, 1988, A modular three-dimensional finite-difference ground-water flow model: U.S. Geological Survey Techniques of Water-Resources Investigations, Book 6, Chapter A1, 548 p.

Paniconi, C., and Putti, M., 1994, A comparison of Picard and Newton iteration in the numerical-solution of multidimensional variably saturated flow problems: Water Resources Research, v. 30, no. 12, p. 3357-3374.

Ruge, J, K., and Stüben, K., 1987, Algebraic Multigrid, *in* McCormick, S.F. ed., Multigrid Methods: Philadelphia, Society for Industrial and Applied Mathematics, p. 73-130.

Ruge, J., Stüben, K., and Hempel, R., 1990, AMG1R5, accessed March 12, 2001 at URL
http://www.mgnet.org/mgnet/Codes/gmd/amg.tgz.

Stüben, K., 1999, Algebraic multigrid (AMG) – An introduction with applications:
Gesellschaft für Mathematik und Datenverarbeitung mbH (GMD) Report 70, 127
p.

———2001, A review of algebraic multigrid: Journal of Computational and Applied
Mathematics, v. 128, no. 1-2, p. 281-309.

Wagner, C., Kinzelback, W., and Wittum, G., 1997, Schur-complement multigrid – A
robust method for groundwater flow and transport problems: Numerische
Mathematik, v. 75, no. 4, p. 523-545.