ground water

Methods Note/

Adaptive Underrelaxation of Picard Iterations in Ground Water Models

by Timothy Durbin[1] and David Delemos[2]

Abstract

This methods note examines the use of adaptive underrelaxation of Picard iterations to accelerate the solution convergence for nonlinear ground water flow problems. Ground water problems are nonlinear when drains, phreatophytes, stream aquifer, and similar features are simulated. Typically, simple Picard iterations are used to address such nonlinear problems. Nevertheless, the convergence rate can be slow, or convergence cannot be obtained. However, convergence often can be accelerated using Picard iterations with adaptive underrelaxation, and convergence often can be obtained where it otherwise would not occur.

Introduction

Most practical ground water simulation problems are nonlinear, which requires solving a system of nonlinear algebraic equations at each time step. Nonlinearities arise from the water table conditions, nonlinear head-dependent sources and sinks, and similar conditions. Such nonlinearities are handled in ground water modeling software using iterative schemes. Typically, either Picard (Harbaugh et al. 2000) or Newton (Hydrogeologic Inc. 1996) iterative schemes are used. The Picard scheme involves successive updating of the coefficient matrix based on the previously calculated heads (Huyakorn and Pinder 1983; Huyakorn et al. 1986; Paniconi and Putti 1994; Mehl and Hill 2001; Banta 2006; Mehl 2006), while the Newton scheme is a gradient method that involves successive updating of the Jacobian matrix (Huyakorn and Pinder 1983). Mehl (2006) indicates that the Picard scheme is a simple and effective method for the solution of nonlinear, saturated, ground water flow problems, but the effectiveness of the Picard scheme can be improved for solving more nonlinear problems by underrelaxing the heads used to update the coefficient matrix. Cooley (1983), Huyakorn et al. (1986), and Mehl (2006) indicate that the effectiveness can be improved further by adapting the underrelaxation to the iterative progress. This note describes the implementation of adaptive underrelaxation within the ground water modeling program FEMFLOW3D (Durbin and Berenbrock 1985; Durbin and Bond 1998; Southern Nevada Water Authority 2006).

Underrelaxation Approach

FEMFLOW3D (Durbin and Bond 1998) is a program for the simulation of three-dimensional (3D) ground water systems using the finite-element method. Nonlinearities occur due to the deformation of the finite-element mesh to track the water table position (Durbin and Berenbrock 1985). They occur also due to the representations of stream-aquifer interactions, phreatophyte discharges, and springs. These simulation elements result in a coefficient matrix that is dependent on the computed heads at each time step. Picard iterations are used to solve the nonlinear system of equations. However, FEMFLOW3D has been updated (Southern Nevada Water Authority 2006) to implement adaptive Picard iterations.

Using this modification of the Picard scheme, the coefficient matrix is updated based on the heads computed from the relation:

$$\tilde{H}_{i,t}^{(k+1)} = H_{i,t}^{(k)} + \gamma\left(H_{i,t}^{(k+1)} - H_{i,t}^{(k)}\right) \tag{1}$$

where k is the iteration counter, i is the node, t is the time step, $\tilde{H}$ is the head at node i and time step t used to update

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the coefficient matrix, H is the computed head at node i and time step t, and γ is the underrelaxation factor.

The underrelaxation factor γ depends on the progress of the iterations as shown on Figure 1. As the iterations converge, γ approaches unity. The relation between γ and the convergence is given by the function:

$$\gamma = \gamma_{\min} + (1 - \gamma_{\min}) \exp(-\alpha(\delta - \varepsilon)) \quad \text{for } \delta > \varepsilon \quad (2a)$$

and

$$\gamma = 1 \quad \text{for } \delta \leq \varepsilon, \quad (2b)$$

where

$$\delta = \max_i \left| H_{i,t}^{(k+1)} - H_{i,t}^{(k)} \right| \quad (3)$$

and where $\gamma_{\min}$ is the minimum value of the underrelaxation function, α is the shape factor for underrelaxation function, δ is the maximum change in head between two iterations, and ε is the convergence or closure criterion.

The parameters $\gamma_{\min}$, α, and ε are specified inputs to the iterative procedure.

If the Picard iterations diverge between two iterations, which means the maximum head change increases, the underrelaxation function is scaled downward as shown on Figure 2. The function is scaled based on the relations:

$$\gamma_{\min}^{(k+1)} = \gamma_{\min}^{(k)} \rho \quad (4)$$

and

$$\alpha^{(k+1)} = -\frac{\ln\left(\dfrac{\gamma^{(k)}\rho - \gamma_{\min}^{(k+1)}}{1 - \gamma_{\min}^{(k+1)}}\right)}{\delta - \varepsilon}, \quad (5)$$

where ρ is the scaling factor such that $0 < \rho < 1$.

This scaling produces the result that $\gamma^{(k+1)}$ equals $\gamma^{(k)}\rho$ after the scaling. The parameter ρ is a specified input to the iteration procedure.

The shape of the underrelaxation function depends on parameter assignments. The parameter $\gamma_{\min}$ can be assigned values within the range $0 < \gamma_{\min} < 1$. Yet, as $\gamma_{\min}$ approaches unity, the adaptive scheme transforms into simple Picard iterations. The parameter α can be assigned values within the range $\alpha > 0$. But as the value assigned to α gets higher, the adaptive scheme transforms to invariant underrelaxation with a value of $\gamma_{\min}$. For many ground water problems, optimal convergence is achieved with $\gamma_{\min}$ equal to about 0.1 or less, α between 0.5 and 5, and ρ equal to about 0.7.

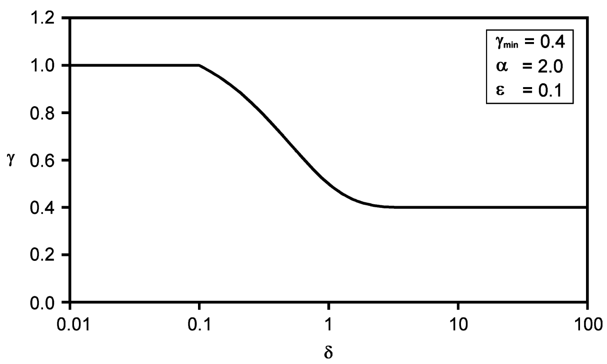

Figure 1. Underrelaxation function.

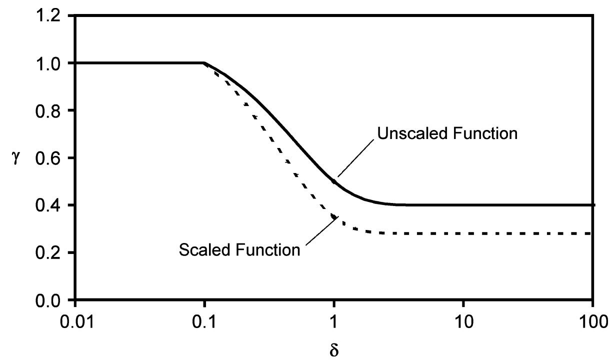

Figure 2. Scaling of the underrelaxation function.

Comparison with Other Picard Schemes

The performance of the proposed scheme was tested using two different models. The first model (model A) is a steady-state model of an unconfined regional ground water system with a finite-element mesh containing about 68,000 nodes. This model contains nonlinear head-dependent fluxes that represent the principal discharges from the ground water system. The head-dependent fluxes include both ground water discharges to phreatophytes and stream-aquifer interactions. The second model (model B) is a steady-state model of an unconfined aquifer with a finite-element mesh containing about 30,000 nodes. This model contains no nonlinear head-dependent fluxes, but the assigned hydraulic conductivity values have a large range. For each model, respective simulations were made with (1) no underrelaxation; (2) nonadaptive underrelaxation; (3) adaptive underrelaxation based on the proposed approach; and (4) adaptive underrelaxation based on the approach developed by Huyakorn et al. (1986). The Huyakorn approach is a modification of the earlier work by Cooley (1983). For models A and B, the iteration parameters for the respective simulations are listed in Table 1.

The ground water models were constructed using the program FEMFLOW3D, Version 2.0 (Southern Nevada Water Authority 2006), which is a finite-element program for the solution of 3D ground water flow problems. While FEMFLOW3D, Version 1.0 (Durbin and Bond 1998) uses simple Picard iterations for addressing the nonlinear head-dependent fluxes associated with drainage nodes, ground water use by phreatophytes, and stream-aquifer interactions, FEMFLOW3D, Version 2.0 (Southern Nevada Water Authority 2006) has been updated to implement Picard iterations with adaptive underrelaxation. Additionally, the Huyakorn method (Huyakorn et al. 1986) was implemented in a special version of FEMFLOW3D for comparing the proposed approach with the Huyakorn approach.

Table 1
Parameter Values for Example Cases

Model	Case Number	Case Description	Parameters	Iterations
A	1	No underrelaxation	$\gamma = 1$ for all δ; $\varepsilon = 0.10$	99
	2	Constant underrelaxation	$\gamma = 0.60$ for all δ; $\varepsilon = 0.10$	46
	3	Adaptive underrelaxation	$\gamma_{\min} = 0.60$; $\alpha = 0.90$, $\rho = 0.90$, $\varepsilon = 0.10$	26
	4	Huyakorn approach	None	60
B	1	No underrelaxation	$\gamma = 1$ for all δ; $\varepsilon = 0.10$	No convergence
	2	Constant underrelaxation	$\gamma = 0.80$ for all δ; $\varepsilon = 0.10$	15
	3	Adaptive underrelaxation	$\gamma_{\min} = 0.80$; $\alpha = 0.90$, $\rho = 0.90$, $\varepsilon = 0.10$	17
	4	Huyakorn approach	None	18

The results for model A are shown on Figure 3 and are listed in Table 1. For the simulation without underrelaxation, convergence occurs after 99 iterations. For the simulation using a constant underrelaxation factor, optimal convergence occurred after 46 iterations. For the simulation using the proposed adaptive approach, convergence occurred after 26 iterations. For the simulation using the Huyakorn approach, convergence occurred after 60 iterations. These results based on model A indicate that for particular cases, the proposed approach reduces the number of Picard iterations.

The results for model B are shown on Figure 4 and also are listed in Table 1. For the simulation without underrelaxation, convergence did not occur, probably because the model contains thin layers of low hydraulic conductivity that are overlain and underlain by layers of much higher conductivity where the thin layers cross the water table. For the simulation using a constant underrelaxation factor, optimal convergence occurred after 15 iterations. For the simulation using the proposed adaptive approach, convergence occurred after 17 iterations. For the simulation using the Huyakorn approach, convergence occurred after 18 iterations. These results based on model B indicate first that ground water simulations that otherwise do not converge can be solved using an underrelaxation approach. They indicate second that for particular cases, a variety of underrelaxation approaches can be used effectively.

For the two test models, the proposed underrelaxation approach performs as well as or better than the nonadaptive underrelaxation or the Huyakorn approach. Additionally, the proposed approach has been applied to numerous other nonlinear ground water modeling problems. Those applications have included both large-scale regional models and local-scale models. The experience has been that convergence always has been achieved. However, for some applications, a trial-and-error effort was required to find the underrelaxation parameter values that optimized convergence. For other applications, a variety of parameter value sets produced effective convergence.

Conclusions

Picard iterations with adaptive underrelaxation can accelerate the convergence for nonlinear ground water flow problems. What is the most efficient approach for adaptive underrelaxation (or even the need for adaptive underrelaxation) appears to be very problem dependent, which is a conclusion reached also by Mehl (2006). However, for the ground water models used for testing the proposed approach, the approach performed as well as or better than the alternative approaches.

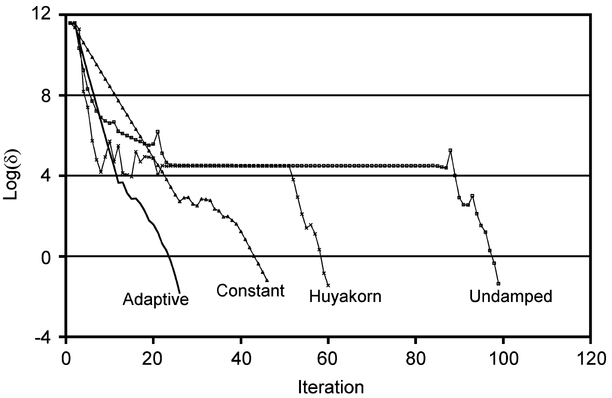

Figure 3. Comparison for model A of Picard iterations among alternative underrelaxation approaches.

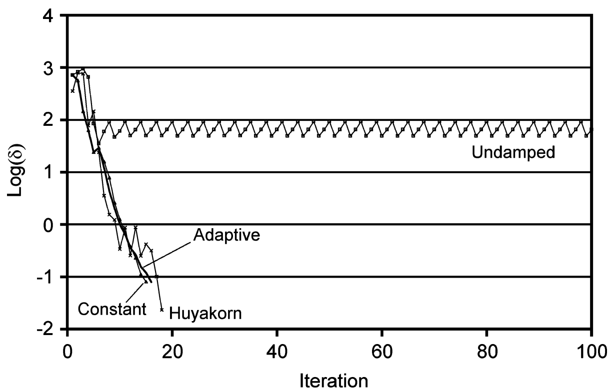

Figure 4. Comparison for model B of Picard iterations among alternative underrelaxation approaches.

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