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# ADAPTIVE ACCURACY CONTROL OF NONLINEAR NEWTON-KRYLOV METHODS FOR MULTISCALE INTEGRATED HYDROLOGIC MODELS

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**Summary.** In the popular Newton-Krylov methods for solving large-scale systems of nonlinear equations, inner linear systems resulting from outer Newton linearization are solved by Krylov iterative linear solvers. The accuracy control of Krylov solvers are based on the progress of the Newton iteration to achieve good local convergence while avoiding over-solving. In practice, the efficiency and robustness of Krylov solvers rely on the use of preconditioning. Unfortunately, the existing accuracy control schemes of Krylov solvers cannot be applied efficiently when a left preconditioner is utilized. This is a challenge for applications where it is necessary to employ a left preconditioner. An example of an application exhibiting this problem is Integrated Water Flow Model (IWFM), a water resources management and planning model developed by California Department of Water Resources. In IWFM, hydrologic quantities with different numerical scales, namely groundwater head, stream flow and lake elevation are simultaneously simulated. Consequently, its linear systems are badly scaled and require row equilibration and left preconditioning. In this paper, we formulate a new accuracy control scheme that can be used directly with left preconditioned systems to take advantages of the "cheap" residual norm available from Krylov solvers. The new scheme not only provides flexibility in using preconditioning but also is efficient in solving a series of nonlinear systems. In addition, we also present a scheme to formulate adaptive damping when backtracking is not feasible. Numerical results show that the combination of new schemes reduces the number of Newton iterations by up to 50% and reduces simulation time by up to 30% in IWFM.

## 1 Introduction

In regions with limited fresh water supplies, accurate simulation of the conjunctive use of surface water and groundwater to meet human and environmental demands is an important component of water resources planning efforts. The planning and management of water resource systems is greatly facilitated by integrated hydrologic applications that simulate water movement through linked groundwater, surface water, land surface and root zone processes such as Modflow-Surfact,[11] GSFLOW,[9] HydroGeoSphere[16] and IWFM.[6] Applications that can simulate fully coupled surface-water and groundwater flow also provide opportunities for interdisciplinary investigations.

These types of application incorporate multiple hydrologic processes and produce systems of nonlinear equations of the form

$$F(x) = 0, \tag{1}$$

where $F : \mathbb{R}^n \to \mathbb{R}^n$ is a nonlinear function and is assumed to be continuously differentiable everywhere. Newton-type or gradient-based methods are generally regarded as being very efficient for solving this type of system.[10] Starting with an initial guess $x_0$, the Newton method iteratively builds a sequence of approximate solutions $\{x_k\}$:

$$x_{k+1} = x_k + s_k, \tag{2}$$

where the update direction $s_k$ is the solution of the system of linear equations

$$J(x_k)s_k = -F(x_k), \tag{3}$$

and $J(x_k)$ is the Jacobian of $F$ at $x_k$. Krylov iterative linear solvers such as Generalized Minimum Residual (GMRES) algorithm[15] are commonly employed to solve (3). The combined scheme is called the Newton-Krylov method or Newton-GMRES method.[3] In practice, solving (3) to a high accuracy in every Newton iteration might be computationally expensive and unnecessary, especially in the early iterations. Instead, equation (3) is solved inexactly up to an accuracy controlled by the so-called forcing term $\eta_k$, i.e., finding $s_k$ such that:[4]

$$\|r_k\| = \|F(x_k) + J(x_k)s_k\| \leq \tau_k \equiv \eta_k\|F(x_k)\|. \tag{4}$$

It is proven[4] that such an inexact Newton method converges locally and superlinearly if $0 < \eta_k \leq \eta_{\max} < 1$ and $\eta_k \to 0$ as $k \to 0$. Note that at each GMRES iteration, the residual norm $\|r_k\|$ is readily available and criterion (4) can be verified immediately.

A number of challenges emerge when the Newton-GMRES method is used to solve the nonlinear systems that arise in multiscale integrated hydrologic models. One of them comes from multiscale simulations. Modeling water movement through a catchment implies the integration of multiple processes, such as infiltration, surface runoff, groundwater flow and surface water flow that have very different spatial and temporal scales.[1] In the simulation of the Central Valley of California (see section 3), the stream flow ranges from zero to $10^{12}$ (cubic feet/month) while the groundwater head and lake elevation range from $10^{-3}$ to $10^{3}$ (feet). Consequently, the linear system (3) can have solution components which spread over a very wide range of magnitudes. This makes it difficult to ensure that each solution component is solved to its corresponding data accuracy. It has been shown that row equilibration is a good remedy for the scaling issue.[5] As row equilibration is a simple type of left preconditioning, subsequently, it is natural to use left preconditioning. Furthermore, left preconditioning avoids the possible inaccuracy caused by the post-processing, especially when the condition number of the preconditioner is expected to be large. When a left preconditioner $M_k$ is utilized, GMRES is applied to the preconditioned system:

$$M_k J(x_k) s_k = -M_k F(x_k). \tag{5}$$

Since left preconditioning changes the residual norm, the termination criterion (4) is not immediately applicable. In this paper, we propose to formulate a tolerance $\tau_k^P$ to control the accuracy of the preconditioned residual norm directly:

$$\|r_k^P\| = \|M_k \left[F(x_k) + J(x_k)s_k\right]\| \leq \tau_k^P. \tag{6}$$

A proper choice of the tolerance $\tau_k^P$ can also significantly reduce the number of outer Newton iterations.

To improve the likelihood as well as the convergence rate of the Newton-GMRES method, a backtracking strategy is often used.[7,12] Backtracking determines the step size for the Newton update direction $s_k$ through repeated tests to ensure a sufficient reduction in $\|F(\cdot)\|$. This becomes impractical and may not be feasible for integrated hydrologic models, such as IWFM where significant additional hydrologic computational procedures are embedded in the formulation of $\|F(\cdot)\|$. It is also reported that backtracking in the Newton-GMRES method tends to fail when a strict criterion is used for the GMRES solver.[17] The second contribution of this paper is to introduce simple adaptive damping factors in place of backtracking loop to determine the step sizes. These damping factors are based on the reduction of $\|F(\cdot)\|$ up to the current Newton iterations to improve the convergence of the inexact Newton method when backtracking is not feasible.

## 2 Newton-GMRES method

A high-level description of the inner-outer Newton-GMRES iterative method with step size selection proceeds as follows:

1: **for** $k = 0, 1, 2, \ldots$ **do**
2:     Solve (5) iteratively by GMRES with stopping criterion $\tau_k$
3:     Compute damping factor $\theta_k$
4:     Update $x_{k+1} = x_k + \theta_k s_k$
5: **end for**

Two critical parameters for the success of the method are the termination criterion $\tau_k$ for the inner iteration (line 2) and the damping factor $\theta_k$ (line 3) for the outer iteration.

One choice of the termination criterion $\tau_k$, is to apply the stopping criterion (4) using the following widely used forcing term

$$\eta_k = \gamma \left( \frac{\|F(x_k)\|}{\|F(x_{k-1})\|} \right)^{\alpha}, \tag{7}$$

where $\gamma \in (0, 1]$ and $\alpha \in (1, 2]$ are adjustment parameters.[8] However, when left preconditioning is utilized, the residual norm $\|r_k\|$ is not directly available. To apply the termination criterion (4), one needs to formulate the approximate solution $s_k$ explicitly at every GMRES iteration to compute $\|r_k\|$. This is computationally expensive. Furthermore, we observe that the termination criterion (4) is not appropriate for multiscale simulations. It is imposed on the original system which has variables spanning a wide range of magnitudes. It is more sensitive to changes in the variables of large scale, which can cause premature termination before the variables of small scales are solved up to the desired accuracy.

In this paper, we propose a termination criterion that applies directly on the preconditioned residual norm $\|r_k^P\|$ defined in (6), which is readily available at each GMRES iteration, namely the "cheap" residual norm. Our proposed termination criterion for the GMRES solver is

$$\|r_k^P\| \le \tau_k^P = \frac{\gamma_M}{(1+k)^{\rho}} \, \frac{\|F(x_k)\|}{\max\{\|F(x_0)\|, \|F(x_{k-1})\|\}} \tag{8}$$

where $\rho > 0$ is a parameter to control the influence of the quantity $1/(1+k)^{\rho}$ and $\gamma_M > 0$ is a constant such that

$$\|M_k^{-1}\|\gamma_M < \frac{1}{2}\|F(x_0)\| \quad \text{for all } k \ge 0. \tag{9}$$

Using the relation $r_k = M_k^{-1} r_k^P$, it can be shown that the criterion (8) implies

$$\|r_k\| \le \eta_k^M \|F(x_k)\|, \tag{10}$$

where the forcing term is

$$\eta_k^M = \frac{\|M_k^{-1}\| \, \tau_k^P}{\|F(x_k)\|}.$$

We can show that $\eta_k^M \le \eta_{\max} = 1/2 < 1$ and $\eta_k^M \to 0$ as $k \to 0$. This guarantees that the Newton-GMRES with termination criterion (8) still converges locally and superlinearly (see Section 1).

On the choice of $\gamma_M$ to satisfy the condition (9), we note that if $M_k$ is an incomplete LU (ILU) preconditioner,[14] then an estimate of $\|M_k^{-1}\|$ can be obtained at a fixed $k$. Furthermore, as $k$ varies, the condition numbers of the ILU preconditioners $M_k$ can be controlled by adaptively adjusting the process of dropping small entries.[2] In practice, a rough estimate of $\|M_k^{-1}\|$ is often sufficient.

Now let us explain why $\tau_k^P$ is also an adequate stopping tolerance for the inner GMRES iteration. First, we observe that when the constant $\gamma_M$ satisfies the condition (9), $\tau_k^P$ is on the same numerical scale of $\|r_k^P\|$. Second, the asymptotic behavior of $\tau_k^P$ is dominated by $\|F(x_k)\|/\|F(x_0)\|$. When $\|F(x_k)\|/\|F(x_0)\|$ decreases rapidly, $x_k$ is close to the exact solution and a strict criterion (small tolerance $\tau_k^P$) should be imposed for solving the inner linear system (5). Third, when no or little progress is made towards the solution in the early Newton iterations, the quantity $1/(1+k)^\rho$ ensures that there are still a sufficient number of inner iterations. This is particularly desirable for applications with expensive outer Newton iterations.

Next let us discuss the formulation of the damping factor $\theta_k$. Backtracking requires that there is a sufficient reduction in $\|F(\cdot)\|$ in each Newton iteration. $\|F(x_k + \theta_k s_k)\|$ needs to be computed repeatedly at different step sizes $\theta_k$ (a.k.a. damping factors) before a suitable one is found.[7,12] To avoid backtracking, we propose to use the following adaptive damping factor

$$\theta_k = \left(1 + \mu \frac{\|F(x_k)\|}{\max\{\|F(x_0)\|, \|F(x_{k-1})\|\}}\right)^{-1} \quad \text{for } k > 0 \tag{11}$$

with an initial value $\theta_0 \in (0,1)$, where $\mu > 0$ is a parameter. It is easy to see that $\theta_k \in (0,1)$ for all $k$. If the Newton process converges, i.e. $\|F(x_k)\| \to 0$ as $k \to \infty$, then $\theta_k \to 1$ as $k \to \infty$. The convergence rate of $\theta_k$ is controlled by $\mu$. The smaller $\mu$ is, the faster $\theta_k$ approaches 1. Typically, $\theta_0$ is chosen in $(10^{-3}, 10^{-1})$ and $\mu$ is in $[10^{-3}, 1)$. The defaults are $\theta_0 = 10^{-1}$ and $\mu = 10^{-1}$.

## 3 Numerical experiments

In this section, we illustrate the effectiveness of the Newton-GMRES method with the proposed termination criterion (8) and adaptive damping factor (11) in solving nonlinear systems of equations arising from IWFM simulations. IWFM is an integrated hydrologic model that simulates groundwater flow, surface water flow and groundwater-surface water interactions as well as other components of the hydrologic system. The discretized groundwater flow equations, stream flow equations and lake storage equations are implicitly coupled to form systems of nonlinear equations corresponding to different time steps. Solving these nonlinear systems is the most time-consuming component and accounts for about 80% of the total time in a typical IWFM simulation. Moreover, IWFM simulations not only incorporate systems with the multiscale phenomena but also have significant hydrologic computations, namely the calculation of water demand, groundwater pumping and stream diversion adjustments, embedded in the outer Newton iteration. Therefore, backtracking is impractical.

The Newton-GMRES methods with termination criterion (4) and (8) are implemented in IWFM (version 3.02). In addition, the damping factor (11) is also included. The implementation of GMRES with ILU preconditioner is based on SPARSKIT (version 2).[13]

| Simulation | FMP | | RefinedC2V | | | |
|---|---|---|---|---|---|---|
| Time step | 1 | 100 | 1 | 2 | 150 | 300 |
| Newton iters. | 8 (13) | 5 (9) | 9 (43) | 10 (26) | 9 (19) | 8 (30) |
| GMRES iters. | 121 (45) | 84 (74) | 148 (120) | 141 (113) | 124 (85) | 128 (79) |

Table 1: The numbers of inner and outer iterations of the Newton-GMRES method using the new stopping criterion (8) with adaptive damping factor (11) versus the standard stopping criterion (4) (in parentheses).

All of our numerical experiments were carried out on a dual-core Intel 2.40GHz processor with 2GB RAM and Intel compilers Fortran (ifort) and $C^{++}$ (icc) (version 11.1).

The following two simulations are used for numerical experiments:

FMP: this is hypothetical simulation using 104 time steps. FMP is modeled as a four-layer aquifer system, and has a total of 46460 nodes, which includes 46000 ground-water nodes and 460 stream nodes.

RefinedC2V: this is a simulation for the Central Valley of California with the spatial domain of approximately 20,000 square mile. We consider a three-layer aquifer system for the period from 1972 to 2003 using 372 monthly time steps. RefinedC2V has a total of 95068 nodes, which includes 90537 ground-water nodes (in three layers), 4529 stream nodes and 2 lake nodes.

In both simulations, the outer Newton iteration stops when $\|F(x_k)\|/\|F(x_0)\| \leq 10^{-7}$ and $\|x_k - x_{k-1}\| \leq 10^{-3}$. In addition, the parameters $\rho = 1.5$, $\tau_{\min} = 10^{-6}$ and $\theta_0 = \mu = 10^{-1}$ $\gamma_M$=10 were used.

Let us first examine the performance of the Newton-GMRES method at selected time steps. Table 1 details the numbers of Newton and GMRES iterations in the selected time steps. As we can see, the proposed stopping criterion (8) significantly reduces the number of outer Newton iterations while uses more inner GMRES iterations. This indicates that the termination criterion (8) is more strict than the criterion (4). Strict criterion demands more PGMES iterations but produces more accurate update directions and thus reduces the number of Newton iterations. The corresponding convergence history in terms of the relative nonlinear residual norm $\|F(x_k)\|/\|F(x_0)\|$ is shown in Figure 1 for the selected time steps of RefinedC2V simulation. Both approaches suffer temporary increases at the beginning. However, when there is no or little progress towards the solution, damping reduces the step size for the update direction $s_k$ and makes the temporary increases less severe in the proposed approach. In addition, more accurate update directions also help to achieve more steady convergence.

Next we show the the effectiveness of the proposed approach in terms of overall performance in the simulations. Table 2 records the total numbers of Newton and GMRES iterations as well as the elapsed time for the two simulations. It shows that the proposed

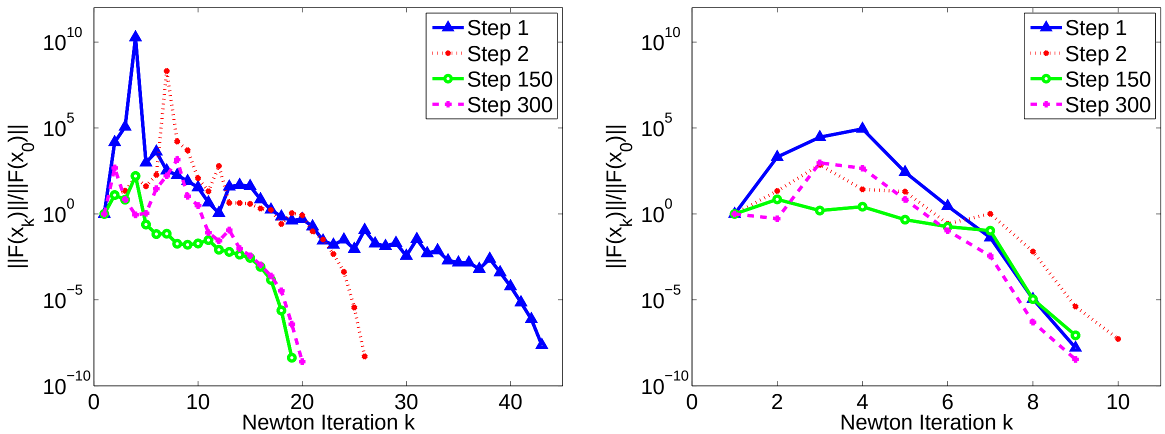


Figure 1: Convergence history of Newton-GMRES method with the standard stopping criterion (4) (left) and the new stopping criterion (8) with adaptive damping factor (11) (right) for selected steps of RefinedC2V simulation.

| Simulation | FMP | | RefinedC2V | |
|---|---|---|---|---|
| Method | NP | MNP | NP | MNP |
| Newton iters. | 3755 | 2269 | 6251 | 3203 |
| GMRES iters. | 33329 | 34652 | 31099 | 50811 |
| Time(sec.) | 524 | 408 | 2659 | 1753 |

Table 2: Overall performance of the Newton-GMRES method using the standard stopping criterion (4) (in the NP column) and using the new stopping criterion (8) with adaptive damping factor (11) (in the MNP column)

approach decreases the number of Newton iterations by about 40-50% and the simulation time by about 20-30%.

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