AN EVALUATION OF LINEARLY IMPLICIT TIME DISCRETIZATION METHODS FOR APPROXIMATING RICHARDS' EQUATION

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Abstract

The solution of Richards' equation continues to be a challenge for many problems of interest. Typically, fully implicit time discretizations are preferred due to the severe, potentially degenerate nonlinearities that result from standard constitutive relationships. Recently however, there has been renewed interest in linearly implicit methods, since they avoid the solution of full nonlinear problems, while retaining desirable stability properties over explicit discretizations. In this work, we consider implicit and linearly implicit temporal approximations for Richards' equation. We evaluate performance in terms of robustness and efficiency for different levels of accuracy under conditions that reflect common difficulties associated with simulating flow in the vadose zone.

1. INTRODUCTION

Implicit time discretizations are generally preferred in the numerical solution of variably saturated groundwater flow problems due to the substantial nonlinearity of standard constitutive relations and the additional stiffness that results from highly heterogeneous media [*Kees and Miller*, 2002]. Implicit methods invariably lead to the solution of discrete nonlinear problems. In many cases, these systems are large and difficult to solve.

Linearly implicit, or noniterative, time discretization methods are a related class of methods that attempt to circumvent nonlinear algebraic systems arising from fully implicit methods by replacing them with the solution of a fixed number of linear problems [*Hairer and Wanner*, 1996; *Lubich and Ostermann*, 1995]. While far less common than implicit discretizations, linearly implicit methods for modeling subsurface flow phenomena are not new. For instance, *Douglas and Jones* [1963] introduced a second-order linearly implicit method using a predictor-corrector formulation, and a number of low-order, non-adaptive linearly implicit discretizations for Richards' equation were evaluated in the work of *Paniconi et al.* [1991]. On the other hand, the performance of a second-order linearly implicit Thomas-Gladwell scheme in *Kavetski et al.* [2002a] suggests that such approaches may be competitive with fully implicit, adaptive methods.

In this work, we focus on a class of linearly implicit Runge-Kutta discretizations known as Rosenbrock methods that have proven competitive for solving ordinary differential equation (ODE) and differential algebraic equation (DAE) systems at low to moderate levels of accuracy [*Hairer and Wanner*, 1996]. This class includes low-order methods with few stages as well as higher order approximations and readily incorporates modern error control strategies [*Söderlind*, 2002]. Here, we evaluate the accuracy and efficiency of three Rosenbrock methods along with a linearly implicit Thomas-Gladwell scheme [*Kavetski et al.*, 2002a] for the solution of Richards' equation within a method of lines context. Our primary aim is to determine the range of conditions over which these approaches are competitive with, or superior to, state-of-the-art adaptive, high-order methods.

2. FORMULATION

Richards' equation is a common model for variably saturated groundwater flow in which flow of the gas phase is not explicitly resolved. Although several alternative versions are available, we restrict our attention to the pressure-head form of Richards' equation, which has the advantage of being applicable for saturated and unsaturated conditions but can also lead to poor mass conservation for low accuracy solutions [*Kees and Miller*, 2002]. Further, we consider only one spatial dimension for convenience and write

$$\begin{aligned} A(\psi)\frac{\partial \psi}{\partial t} &= \frac{\partial}{\partial x}\left[\rho k_r K_s\left(\frac{\partial \psi}{\partial x} - \rho g_u\right)\right], \quad \text{for } (x,t) \in \Omega \times [0,T] \\ A(\psi) &= \frac{d\rho}{d\psi}\theta + \rho\frac{d\theta}{d\psi} \end{aligned} \tag{1}$$

Here $\Omega = [0, X]$ is the spatial domain, $[0, T]$ is the temporal domain, ψ is the aqueous phase pressure head, θ is the aqueous phase volume fraction, ρ is the aqueous phase density divided by a reference density, k_r is relative permeability, and K_s is the saturated hydraulic conductivity. g_u is assumed constant and accounts for the coordinate system alignment with gravity [*Kees and Miller*, 2002]. The initial condition for eqn (1) is

$$\psi(x,0) = \psi^0(x) \tag{2}$$

Dirichlet boundary conditions are assumed for simplicity

$$\psi(0,t) = \psi^L(t),\ \psi(X,t) = \psi^R(t) \tag{3}$$

The difficulty of solving eqn (1) depends largely on the nonlinearities that appear in the assumed constitutive relationships. Here, we adopt the well-known van Genuchten [*van Genuchten*, 1980] and Mualem [*Mualem*, 1976] p-S-k relations

$$S_e = \frac{(\theta - \theta_r)}{(\theta_s - \theta_r)} = \left[1 + (\alpha_v|\psi|)^{n_v}\right]^{-m_v}, \qquad k_r = \sqrt{S_e}\left[1 - (1 - S_e^{1/m_v})^{m_v}\right]^2 \tag{4}$$

and account for compressibility of the aqueous phase via

$$\rho = \varrho/\varrho_0 = e^{\beta_w(\psi - \psi_0)} \tag{5}$$

where ϱ_0 is a reference density, S_e is the effective saturation, θ_r is the residual volumetric water content, θ_s is the saturated volumetric water content, α_v is a parameter related to the mean pore size, n_v is a parameter related to the uniformity of the soil pore-size

distribution, and $m_v = 1 - 1/n_v$. For $\psi \geq 0$, the porous medium is fully saturated, and eqn (4) reverts to $S_e = 1$ and $k_r = 1$, respectively.

3. DISCRETIZATION

As mentioned in §1, we use a method of lines strategy for solving eqn (1) subject to the auxiliary conditions given in eqns (2) and (3) and the constitutive relations in eqns (4) and (5).

3.1. **Spatial discretization.** The domain Ω is discretized uniformly with a set of n_x nodes and spacing $\Delta x = L/(n_x - 1)$. In the interior, a control volume discretization for eqn (1) can be written

$$A(\psi_i)\frac{\partial \psi_i}{\partial t} = \left(f_{i-1/2} - f_{i+1/2}\right)/\Delta x \tag{6}$$

$$f_{i+1/2} = -\rho_{i+1/2} k_{r,i+1/2} K_{s,i+1/2}\left[\left(\frac{\psi_{i+1} - \psi_i}{\Delta x}\right) - \rho_{i+1/2} g_u\right] \tag{7}$$

for $i = 2, \ldots, n_x - 1$. The proper approximation for interface terms in eqn (7) has been the subject of some investigation [*Miller et al.*, 1998]. Based on previous experience with finite difference approximations, we use

$$\begin{aligned} \rho_{i+1/2} &= (\rho_i + \rho_{i+1})/2, \qquad k_{r,i+1/2} = (k_{r,i} + k_{r,i+1})/2, \\ K_{s,i+1/2} &= 2K_{s,i}K_{s,i+1}/(K_{s,i} + K_{s,i+1}) \end{aligned} \tag{8}$$

Dirichlet boundary conditions are enforced via

$$\psi_1 = \psi^L(t), \qquad \psi_{n_x} = \psi^R(t) \tag{9}$$

3.2. **Temporal discretization.** In order to solve eqns (6)–(9), we consider time integration methods for the first order DAE system

$$\mathbf{M}(t, \mathbf{y})\frac{\partial \mathbf{y}}{\partial t} = \mathbf{F}(t, \mathbf{y}) \tag{10}$$

In the following, we review Rosenbrock methods for eqn (10) and then summarize a linearly implicit Thomas-Gladwell scheme [*Kavetski et al.*, 2002a].

3.2.1. *Rosenbrock Methods.* Rosenbrock schemes are one of many Runge-Kutta methods that have been pursued for the integration of ODE and DAE systems. Our interest here is primarily in the semi-discrete system, eqn (10). For clarity and completeness, however, we begin with a Rosenbrock formulation for a system of explicit ODE's

$$\frac{\partial \mathbf{y}}{\partial t} = \mathbf{F}(t, \mathbf{y}) \tag{11}$$

A generic s-stage Rosenbrock approximation for the solution of eqn (11) is [*Hairer and Wanner*, 1996; *Lang and Verwer*, 2001]

$$\mathbf{y}^{n+1} = \mathbf{y}^n + \sum_{i=1}^{s} m_i \mathbf{Y}_{ni} \tag{12}$$

$$\hat{\mathbf{y}}^{n+1} = \mathbf{y}^n + \sum_{i=1}^{s} \hat{m}_i \mathbf{Y}_{ni} \tag{13}$$

where $\mathbf{y}^{n+1}$ is an approximation of $\mathbf{y}(t^{n+1})$ that is of order p, and $\hat{\mathbf{y}}^{n+1}$ is a lower $(p-1)$ order, embedded approximation used for the error estimate $\mathbf{e}^{n+1} = \mathbf{y}^{n+1} - \hat{\mathbf{y}}^{n+1}$. The s stage values are given by

$$\left[\frac{1}{\gamma\Delta t}\mathbf{I} - \mathbf{F}_y(t^n, \mathbf{y}^n)\right]\mathbf{Y}_{ni} = \mathbf{F}(t_i, \mathbf{Y}_i) - \sum_{j=1}^{i-1}\frac{c_{ij}}{\Delta t}\mathbf{Y}_{nj} + \gamma_i \Delta t \mathbf{F}_t(t^n, \mathbf{y}^n) \tag{14}$$

Here, $\Delta t = t^{n+1} - t^n$, $\mathbf{I}$ is the identity matrix, $\mathbf{F}_y = \partial\mathbf{F}/\partial\mathbf{y}$, and $\mathbf{F}_t = \partial\mathbf{F}/\partial t$. Superscripts represent time levels, and subscripts are used to denote internal stage level quantities. The values of t_i and $\mathbf{Y}_i$ are given by

$$t_i = t^n + \alpha_i \Delta t, \qquad \mathbf{Y}_i = \mathbf{y}^n + \sum_{j=1}^{i-1} a_{ij}\mathbf{Y}_{nj} \tag{15}$$

A given Rosenbrock method can be defined by specifying the coefficients $\{m_i\}$, $\{\hat{m}_i\}$, $\{\alpha_{ij}\}$, and $\{\gamma_{ij}\}$, where $i, j = 1, \ldots, s$ and

$$\alpha_{ij} = 0,\ j \geq i \quad \gamma_{ij} = 0,\ j > i, \quad \gamma_{ii} = \gamma,\ \forall i,$$

Of course, these coefficient values are not wholly free, but are constrained by appropriate order and stability conditions [*Hairer and Wanner*, 1996]. In addition, we have the following definitions for eqns (14) and (15)

$$\begin{aligned} \alpha_i = \sum_{j=1}^{i-1}\alpha_{ij}, \qquad & \gamma_i = \textstyle\sum_{j=1}^{i}\gamma_{ij}, \qquad & \mathbf{\Gamma} = (\gamma_{ij})_{i,j=1}^{s}, \\ (c_{ij})_{i,j=1}^{s} = \mathbf{\Gamma}^{-1}, \quad & \text{and } (a_{ij})_{i,j=1}^{s} = (\alpha_{ij})_{i,j=1}^{s}\mathbf{\Gamma}^{-1} \end{aligned} \tag{16}$$

Rosenbrock methods can also be readily applied to more complicated DAE systems, although the formulation can be slightly more involved. To obtain a discretization for eqn (10), we follow a common approach [*Hairer and Wanner*, 1996] and introduce an auxiliary variable, $\mathbf{z}$, to write the extended system

$$\begin{aligned} \frac{\partial \mathbf{y}}{\partial t} &= \mathbf{z} \\ 0 &= \mathbf{F}(t, \mathbf{y}) - \mathbf{M}(t, \mathbf{y})\mathbf{z} \end{aligned} \tag{17}$$

While eqn (17) is a system in $2n_x$ unknowns, the Rosenbrock approximation for eqn (17) can be reduced, so that only linear systems of size n_x need be solved. To be more concrete, we follow *Lang* [2001] and write the basic Rosenbrock method for eqn (10) as eqns (12) and (13) along with

$$\mathbf{z}^{n+1} = \mathbf{z}^n + \sum_{i=1}^{s} m_i \left\{ \frac{1}{\Delta t}\sum_{j=1}^{i}(c_{ij} - s_{ij})\mathbf{Y}_{nj} + (\sigma_i - 1)\mathbf{z}^n \right\} \tag{18}$$

$$\hat{\mathbf{z}}^{n+1} = \mathbf{z}^n + \sum_{i=1}^{s} \hat{m}_i \left\{ \frac{1}{\Delta t}\sum_{j=1}^{i}(c_{ij} - s_{ij})\mathbf{Y}_{nj} + (\sigma_i - 1)\mathbf{z}^n \right\} \tag{19}$$

The stage value for $\mathbf{Y}_{ni}$ is given by

$$\left[\frac{1}{\gamma\Delta t}\mathbf{M}(t^n,\mathbf{y}^n)-\mathbf{J}^n\right]\mathbf{Y}_{ni} = \mathbf{F}(t_i,\mathbf{Y}_i)-\mathbf{M}(t^n,\mathbf{y}^n)\sum_{j=1}^{i-1}\frac{c_{ij}}{\Delta t}\mathbf{Y}_{nj}+ \gamma_i\Delta t\mathbf{J}_t^n+\left[\mathbf{M}(t^n,\mathbf{y}^n)-\mathbf{M}(t_i,\mathbf{Y}_i)\right]\mathbf{Z}_i \tag{20}$$

The internal stage values are again given by eqn (15) and

$$\mathbf{Z}_i=(1-\sigma_i)\mathbf{z}^n+\sum_{j=1}^{i-1}\frac{s_{ij}}{\Delta t}\mathbf{Y}_{nj} \tag{21}$$

The matrix $\mathbf{J}^n$ and vector $\mathbf{J}_t$ are just the derivative of the right hand side $\mathbf{F}-\mathbf{M}\mathbf{z}$ with respect to $\mathbf{y}$ and t respectively,

$$\mathbf{J}^n=\frac{\partial}{\partial\mathbf{y}}\left[\mathbf{F}-\mathbf{M}\mathbf{z}\right]^n,\qquad \mathbf{J}_t^n=\frac{\partial}{\partial t}\left[\mathbf{F}-\mathbf{M}\mathbf{z}\right]^n \tag{22}$$

evaluated at t^n, $\mathbf{y}^n$, and $\mathbf{z}^n$. In addition to eqn (16), the necessary coefficient definitions are

$$\begin{aligned}(\sigma_{ij})_{i,j=1}^s=(\alpha_{ij})_{i,j=1}^s\mathbf{B}^{-1},\qquad \sigma_i=\sum_{j=1}^{i-1}\sigma_{ij},\\ (s_{ij})_{i,j=1}^s=(\sigma_{ij})_{i,j=1}^s\mathbf{\Gamma}^{-1}\qquad \mathbf{B}=(\alpha_{ij}+\gamma_{ij})_{i,j=1}^s\end{aligned} \tag{23}$$

3.3. **Linearly implicit Thomas-Gladwell scheme.** The original Thomas-Gladwell scheme was formulated for second-order ODE systems [*Thomas and Gladwell*, 1988]. Here, we follow *Kavetski et al.* [2002a] and consider a first-order system of the type given in eqn (10). The linearly implicit scheme presented in *Kavetski et al.* [2002a, 2004] can be viewed as a modification of the original fully implicit version, in which only one iteration of the requisite nonlinear solve is performed. While a Picard-based scheme was presented in [*Kavetski et al.*, 2002a], we consider a Newton-based approach here, since Picard iteration can be recovered from a Newton step with the use of the appropriate Jacobian approximation [*Paniconi et al.*, 1991].

To summarize the linearly implicit Thomas-Gladwell scheme (TG2), we first introduce the discrete residual corresponding to a backward Euler discretization of eqn (10)

$$\mathbf{R}^{n+1}(\mathbf{y}) = \mathbf{M}(t^{n+1},\mathbf{y})\left(\frac{\mathbf{y}-\mathbf{y}^n}{\Delta t}\right)-\mathbf{F}(t^{n+1},\mathbf{y}) \tag{24}$$

The second-order TG2 solution, $\mathbf{y}^{n+1}$, is then given by

$$\begin{aligned}\tilde{\mathbf{J}}\Delta\mathbf{y}=-\mathbf{R}^{n+1}(\mathbf{y}^{n+1,p}),\qquad \tilde{\mathbf{J}}=\frac{\partial\mathbf{R}}{\partial\mathbf{y}}^{n+1}(\mathbf{y}^{n+1,p}),\\ \Delta\mathbf{y}=\hat{\mathbf{y}}^{n+1}-\mathbf{y}^{n+1,p},\qquad \mathbf{y}^{n+1,p}=\mathbf{y}^n+\Delta t\mathbf{z}^n,\\ \mathbf{z}^{n+1}=\frac{\hat{\mathbf{y}}^{n+1}-\mathbf{y}^n}{\Delta t},\qquad \mathbf{y}^{n+1}=\mathbf{y}^n+\frac{\Delta t}{2}\left(\mathbf{z}^n+\mathbf{z}^{n+1}\right)\end{aligned} \tag{25}$$

$\hat{\mathbf{y}}^{n+1}$ is again a lower (first) order solution that provides a local truncation error estimate, $\mathbf{e}^{n+1}=\mathbf{y}^{n+1}-\hat{\mathbf{y}}^{n+1}$.

4. RESULTS

To illustrate the time integration methods' performance, numerical experiments were performed for a common vertical infiltration problem that offers a stringent test, since it includes a sharp solution front along with the development of fully saturated conditions in a subset of the physical domain [*Kees and Miller*, 2002; *Miller et al.*, 1998]. The physical parameters for the test problem are summarized in Table 1. The initial condition was hydrostatic equilibrium and the direction of gravity was from right to left ($g_u = -1$). The boundary conditions were $\psi^L = 0$, and $\psi^R = 0.1$ [m].

TABLE 1. Physical parameters for test problem

L [m]	T [d]	α_v [1/m]	n_v	θ_s	θ_r	K_s [m/d]	ϱ_0 [kg/m^3]	β_w [m d^2/kg]
10	0.25	5.47	4.24	0.301	0.093	5.04	998.2	6.564×10^{-20}

A series of numerical experiments for $n_x = 201$ and a range of integration tolerances were performed with the TG2 scheme outlined in §3.3 and three Rosenbrock methods. The Rosenbrock methods included a two-stage second order method (ROS2) [*Verwer et al.*, 1999], a three-stage third order scheme (ROS3P) [*Lang and Verwer*, 2001], and the six-stage, fourth-order scheme, RODAS [*Hairer and Wanner*, 1996]. The integration tolerances were set using a fixed scaling test criterion. The absolute tolerances were set to $\varepsilon_a = \varepsilon_r \times 10^{-2}$ [m], and the relative error tolerances were $\varepsilon_r = 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}$.

A predictive error controller [*Gustafsson*, 1994] was used with the Rosenbrock methods, while the default, classical error control strategy from *Kavetski et al.* [2002a] was used with the TG2 scheme. A weighted root mean square norm [*Kees and Miller*, 1999] was used in both error control strategies. For comparison, results from a DAE solver based on a fixed leading coefficient backward difference formula (FLCBDF) discretization were also obtained [*Kees and Miller*, 1999]. The FLCBDF integrator used a full Newton iteration with relative residual convergence test and nonlinear solver tolerance of 10^{-8}. $\mathbf{F}_t$ was evaluated numerically for the Rosenbrock methods. Analytical Jacobians were used otherwise. All linear systems were solved using a banded LU solver from LAPACK. The p-S-k relations were evaluated using cubic splines with 2001 nodes.

Figures 1 and 2 show discrete L^1 error versus elapsed CPU time for the five schemes. The temporal error, e_t, was measured using a consistent grid solution obtained by the FLCBDF solver on the same spatial grid but with temporal integration tolerances set to 10^{-8}. The total error, e_g, was measured using a dense grid solution with $n_x = 36451$.

5. DISCUSSION

The experiments indicate that Rosenbrock methods are capable of obtaining accurate results for infiltration problems that present common challenges for numerical solution of Richards' equation, including sharp solution fronts and the formation of fully saturated regions. The TG2 scheme is simple to implement and performed well for low-to-moderate accuracy simulations, where the temporal error was non-negligible in comparison with the spatial error. For better resolved discretizations, such as those in the adaptive approach from *Miller et al.* [2005], the balance between temporal and spatial error may change

FIGURE 1. Temporal error

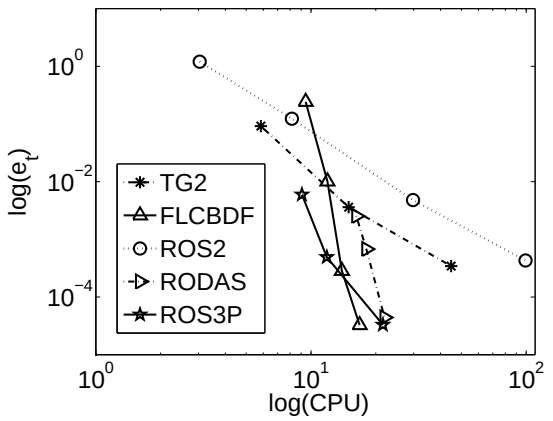
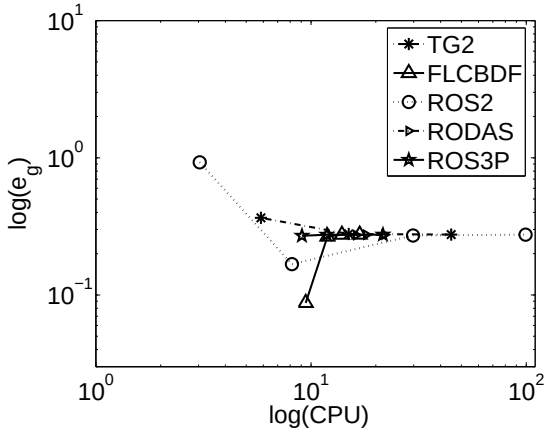


FIGURE 2. Total error



to favor higher order approximations. The most robust approach was the fully implicit FLCBDF solver.

These preliminary experiments raise several questions. For instance, ROS2 is the only Rosenbrock scheme considered that maintains its formal accuracy with approximate Jacobians (a "W method") [*Verwer et al.*, 1999]. Order reduction can also be a significant issue for problems with time dependent boundary conditions. However, ROS3P was designed specifically to avoid order reduction [*Lang and Verwer*, 2001]. The relative performance of the methods may also be affected by the use of iterative linear solvers, which are typically found in multidimensional problems.

More broadly, linearly implicit schemes represent an attempt to control nonlinearity through temporal truncation error alone, and so highlight the importance of an effective control strategy for a good time integrator. The performance of more sophisticated error control, like the PC controller strategy, is of interest both for linearly implicit discretizations and fully implicit methods [*Söderlind and Wang*, 2006].

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