Nonsmooth Nonlinearities and Temporal Integration of Richards' Equation

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Richards' equation is a model for flow in the unsaturated zone. Adaptive implicit methods for temporal integration of Richards' equation have been used with considerable success. The nonlinearities in the van Geneuchten and Mualem formulae that are often used to close the system can be nonsmooth and even non-Lipschitz. This lack of smoothness means that the traditional analysis of adaptive temporal integration may not apply. In this paper we describe the mathematical issue and report on computational experiments that show how a basic one-step adaptive temporal integration method seems to behave properly. The motivation for this work is the **AD**aptive **H**ydrology model, a production code being developed by the US Army Engineer and Research Development Center. ADH simulates three dimensional groundwater and surface water flow using unstructured, adaptive finite elements in space and implicit temporal integration.

1. INTRODUCTION

Richards' equation (RE) is a simple model of flow in the unsaturated zone [1]. In three space dimensions, letting z be the vertical direction and ∇ the spatial gradient operator, the pressure head form of RE is

$$S_s S_a(\psi) + \eta \frac{\partial S_a(\psi)}{\partial t} = \nabla \cdot [K(\psi) \nabla (z + \psi)] \tag{1}$$

In (1), ψ is pressure head, S_s is the specific storage, $S_a(\psi)$ is the aqueous phase saturation, η is the porosity, and $K(\psi)$ is the hydraulic conductivity. We will assume that appropriate initial and boundary conditions have been imposed.

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In this paper we model saturation with the van Geneuchten formula, [2],

$$S_a(\psi) = \begin{cases} S_r + \frac{(1-S_r)}{[1+(\alpha|\psi|)^n]^m}, & \psi < 0 \\ 1, & \psi \geq 0 \end{cases}. \tag{2}$$

In (2), S_r is the residual saturation, n is an experimentally determined measure of pore size uniformity, $m = 1 - 1/n$, and α is an experimentally determined coefficient that is related to the mean pore size. We then define the conductivity with the Mualem model, [3],

$$K(\psi) = \begin{cases} K_s \frac{[1-(\alpha|\psi|)^{n-1}[1+(\alpha|\psi|)^n]^{-m}]^2}{[1+(\alpha|\psi|)^n]^{m/2}}, & \psi < 0 \\ 1, & \psi \geq 0 \end{cases} \tag{3}$$

where K_s is the water-saturated hydraulic conductivity. One can see from (2) and (3) that the nonlinearity is not Lipschitz continuous, much less differentiable, at $\psi = 0$, if $1 < n < 2$. Values of n in this range are physically realistic and solvers must be prepared to deal with nonsmooth nonlinearities. RE codes are much more efficient if the nonlinearities are approximated by splines [4]. This approximation also improves the robustness of the nonlinear solver within a temporal integration. We use such an approximation in this paper, but the high density of the knots in the spline, which are needed for accuracy, will lead to a very large Lipschitz constant for the nonlinerity.

Advanced methods [5,6] for temporal integration of differentiable algebraic equations (DAEs) have been applied to RE with considerable success [7,4,8–11]. The merits in using a DAE, rather than an ordinary differential equation (ODE) approach for temporal integration has been explained in, for example, [12]. The results in these papers were obtained with backward difference formulae (BDF) methods, which are based on a Taylor series analysis of local truncation errors. In the case of RE, Taylor expansions, while possibly available for discrete approximations of RE, may well not exist for the continuous problem. The effect of this could be that the estimates for local truncation error in time will depend on the spatial mesh. This would lead to erratic behavior in the temporal integration, something not observed in previous work.

The purpose of this paper is to investigate the dependence of temporal error estimates of the type seen in BDF codes on the spatial mesh with a computational study of one and three dimensional RE solvers. We observe independence of an estimate of temporal truncation error on the spatial mesh.

We restrict ourselves to one-step, first-order methods for two reasons. Firstly, this simple case allows us to focus on a single term in the error, rather than the many that a full variable-order method would require. Secondly, the ADH code refines the spatial mesh at each iteration, making a one-step method the most attractive for implementation.

Both finite difference and finite element discretizations have been used with adaptive temporal integration methods. The computations in this paper use piecewise linear finite elements in space. The temporal integration can either be viewed as a space-time finite element approximation where the elements are piecewise linear in space and piecewise constant in time, or as a method of lines (MOL) approach, in which the time-dependent system is discretized in space and a temporal integration code is applied to the resulting ODE or DAE.

1.1. ADH

Our three-dimensional numerical examples use the **Ad**aptive **H**ydrology Model, or ADH [13], a production ground and surface water simulator being developed at the US Army Engineer Research and Development Center (ERDC). ADH uses adaptive, unstructured, tetrahedral finite elements in space and implicit integration in time. This code regrids after each time step, hence one step integrators must be used. The resulting discretized nonlinear equations are solved with a Newton-Krylov-Schwarz method, which uses a Krylov method with a domain decomposition preconditioner to compute the Newton step in an inexact Newton solver.

1.2. DISCRETIZATION OF RE IN ADH

We denote the residual form of Richards' equation as

$$RE(\psi) = S_s S_a(\psi)\frac{\partial \psi}{\partial t} + \eta\frac{\partial S_a}{\partial t} - \nabla \cdot [K(\psi)\nabla(z+\psi)] = 0 \tag{4}$$

The weak form of Richards' equation is found by multiplying (4) by an appropriate weight function and integrating over time and space. ADH uses a Galerkin method [14] with piecewise linear polynomials in space and piecewise constant polynomials in time. Let Ω_n be the current spatial mesh with boundary Γ_n over the time interval $[t^{n-1}, t^n]$. We assume Dirichlet boundary conditions, $\psi = \bar{\psi}$ on Γ_n. Our finite element interpolation spaces are

$$V_h = \{v_h | v_h \in H^{1,h}(\Omega_n), v_h = 0 \text{ on } \Gamma_n\},$$

$$\hat{V}_h = \{\hat{v}_h | \hat{v}_h \in H^{1,h}(\Omega_n), \hat{v}_h = \bar{\psi} \text{ on } \Gamma_n\}.$$

We pose our we formulation as: given $\hat{\psi}^{n-1}$ find $\hat{\psi}^n$, an approximation to $\psi(t^n)$ such that

$$\int_{t^{n-1}}^{t^n} \int_{\Omega_n} RE(\hat{\psi}^n) v_h dt d\Omega_n = 0$$

$\forall \hat{\psi}^n \in \hat{V}_h$, $\forall v_h \in V_h$. The weak formulation can be simplified using integration by parts to get

$$\int_{\Omega_n} S_s S_a(\hat{\psi}^n)[\hat{\psi}^n - \hat{\psi}^{n-1}] v_h dz \quad + \int_{\Omega_m} \eta[S_a(\hat{\psi}^n) - S_a(\hat{\psi}^{n-1})] v_h dz$$

$$+\Delta t \int_{\Omega_n} [K_s k_r(\hat{\psi}^n)\nabla(\hat{\psi}^n + z)]\nabla v_h dz = 0.$$

1.3. TIME STEP CONTROL

Adaptive temporal integration and error control are needed in ADH for several reasons. The solution of Richards' equation often results in the formation of sharp fronts. A particularly small time step is needed when the front is forming, hence a fixed time step method is not the most computationally efficient approach. The error control that accompanies a variable time-step method improves both accuracy and robustness.

We consider a basic first-order one-step method, which we derive under the assumption that the nonlinearity is smooth, to show how the standard theory would work.

The essential ideas of our approach come from [5,15]. ADH advances in time using backward Euler. We seek to use a simple explicit approximation to estimate the local truncation error and compute the next time step in order to bound the predicted error below a user specified tolerance. We describe the theory by demonstrating on an ODE. Here $y \in R^N$. In the case of RE, N would be the size of the spatial mesh after discretization.

Consider

$$y' = f(t,y), t^0 < t < t^f, y(t^0) = y_0.$$

Let $h_n = t^n - t^{n-1}$ and y^{n-1} approximate $y(t^{n-1})$, such that we seek y^n, an approximation to $y(t^n)$. The backward Euler approximation is $y^n_{BE} = y^{n-1} + h_n y'(t^n)$, with local truncation error

$$E_n = \|y^n_{BE} - y(t^n)\| = \frac{h_n^2}{2}\|y''(\xi_n)\| + O(h_n^3). \tag{5}$$

where $\xi_n \in [t^{n-1}, t^n]$. Our first goal is to approximate $C_n \approx \|y''(\xi_n)\|$ using a simple, explicit predictor. Using C_n and (5), the local truncation error can be bound by a user specified tolerance, TOL, if the next time step h_{n+1} satisfies

$$\frac{h_{n+1}^2}{2} C_n < TOL.$$

This inequality is satisfied if

$$h_{n+1} = \sqrt{\frac{2TOL \cdot frac}{C_n}}, \tag{6}$$

where $frac < 1$ is a user specified safety parameter to try to ensure that the next step is not a failure. To obtain C_n, we define the predictor by $y^n_{PRE} = y^{n-1} + h_n y'^{n-1}_{PRE}$, where $y'^{n-1}_{PRE} = (y^{n-1} - y^{n-2})/h_{n-1}$ approximates $y'(t^{n-1})$. One can show using a Taylor series that

$$\|y^n_{PRE} - y^n_{BE}\| = |h_n^2 - \frac{h_n h_{n-1}}{2}| \|y''(\xi_n)\|.$$

Hence,

$$C_n = 2\frac{\|y^n_{PRE} - y^n_{BE}\|}{|h_n(2h_n - h_{n-1})|} \approx \|y''(\xi_n)\|. \tag{7}$$

To advance from t^n to $t^{n+1} = t^n + h_{n+1}$, we compute y^n_{PRE} to find C_n and then estimate the local truncation error, E_n, with (5). If $E_n < TOL$, we determine the next time step, h_{n+1}, using (6). If $E_n > TOL$, we reject the previous approximation and reduce the size such that $h_n/4 \leftarrow h_n$. Decreasing the time step by a factor of four ensures that there will be no division by zero in (7). Following standard practice [16,5,17], we limit the growth of the time to avoid necessary oscillations in the error indicator and decrease the time step if the nonlinear solver performs poorly. For this paper, if $h_{n+1}/h_n > 10$, then $h_{n+1} = 3h_n$. If the nonlinear solver does not converge in 4 iterations, $h_n/4 \leftarrow h_n$.

2. RESULTS

2.1. GRID REFINEMENT STUDY

We report on observations of the independence of C_n on the spatial grid using two infiltration problems in one spatial dimension. We consider two media, clay and silt, which have a value of $1 < n < 2$, making the nonlinearities in (2) and (3) non-Lipschitz. Both problems are solved over a 10 m. long domain that begins fully unsaturated. We prescribe the pressure head at the top of the domain so that infiltration begins at the start of the simulation. The physical data for these problems is given in Table 1. In these simulations saturated conditions develop in part of the domain, causing a sharp front that is difficult to model accurately and efficiently with a fixed step method.

The 1-D simulator used was a finite elements code structured similarly to ADH. The linear equation for the Newton step was solved with Gaussian elimination. Since the saturation and conductivity relations are expansive to evaluate, both ADH and the one dimensional simulator use piecewise linear splines to approximate (2) and (3). For these infiltration problems, we sampled 5000 points for the spline on the interval $-15 \leq \psi \leq 0$. In ADH the spline uses 800 nodes on the interval $-20 \leq \psi \leq 0$. Both splines are extended to be constants outside of their ranges. In the 1D simulation we considered meshes of size $\Delta z = 1/100, 1/200, 1/400$, and $1/800$. The 1D simulations were run on a Sun Ultra 10 workstation with a 440MHz processor using cc: WorkShop Compilers 5.0 98/12/15 C 5.0.

Table 1
Media Parameters

Parameter	clay	silt
n	1.09	1.37
α	0.244	0.478
S_r	0.179	0.074
η	0.33	0.40
K_s	1.10808e-5	1.1801e-03
T_{final}	600 days	90 days
$max\Delta t$	10 days	1 day

For the results in this section we used $TOL = 10^{-3}$, $frac = 0.5$, and an initial time step of 10^{-9}. Figures 1 and 2 show the independence of C_n of Δz for both clay and silt.

2.2. RESULTS WITH ADH

In this simulation, done for three unstructured grids, we simulate flow through a heterogeneous column in three dimensions. The simulator uses a Newton-BiCGSTAB nonlinear solver [18,19] and a two-level additive Schwarz preconditioner [20]. As in § 2.1 we see independence of C_n on the mesh.

The material domain is 10 meter long heterogeneous column consisting of sand, silt,

Figure 1. C_n for Clay

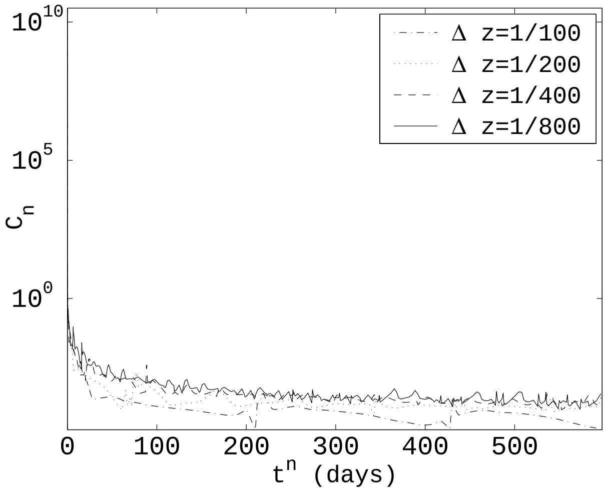
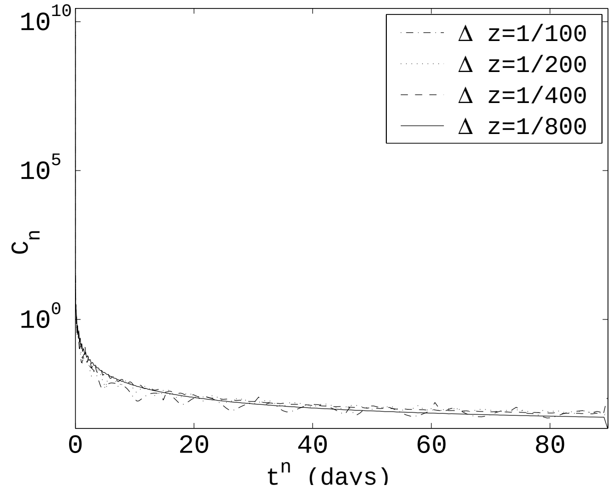


Figure 2. C_n for Silt



and clay. The column begins fully saturated and is then slowly drained from the bottom. The three grids are described in Table 2.

We used an initial time step of $10^{-5}$and allowed the simulation to run for 30 days with $max\Delta t = 0.5$ days. We used $TOL = 0.01$ and $frac = 0.5$ The runs were done at the North Carolina Supercomputing Center on a single processor of an IBM RS/6000 SP, equipped with 180 four-way 375 MHz Power3-II processors per node, running C for AIX Compiler, Version 5. Figure 3 illustrates the mesh-independence of C_n in this case.

Figure 3. C_n in ADH, three grids

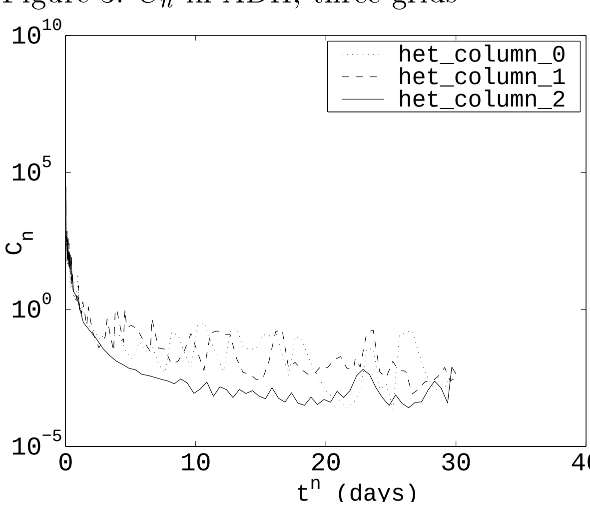


Table 2
Three Unstructured Grids

Problem	No. nodes	No. elements
het_column_0	845	3840
het_column_1	5881	30720
het_column_2	43889	245760

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