Efficient and robust numerical modeling of variably saturated flow in layered porous media

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Abstract

We extend our recent work on higher-order time integration of Richards' equation to layered heterogeneous porous media, using a differential-algebraic-equation-based method of lines (DAE/MOL) approach. We show that the DAE/MOL approach is robust and efficient compared to standard low-order time integration methods for heterogeneous media. We also show the advantage of using an integral representation of permeability compared to a standard arithmetic mean for the test problems considered herein.

1 Introduction

Richards' equation (RE) is commonly used to describe flow in partially saturated porous media [], although questions about the validity of this approach remain []. RE is commonly solved using low-order spatial approximations [] and low-order temporal-integration methods []; several codes are available that implement these methods [].

In our recent work, we have shown: (1) DAE/MOL approaches for solving RE are robust and more efficient than traditional low-order approaches [**?**]; (2) modification to a standard DAE integrator can further improve efficiency [**?**]; (4) use of vectorizable interpolation methods for evaluating constitutive relations can drammatically affect simulator performance [**?**]; (3) monitoring of the condition number of the Jacobian is an effective strategy to aid in the selection

of nonlinear termination criteria [**?**]; (5) lack of smoothness in van Genuchten-Mualem relations for common media conditions can lead to problems with convergence of nonlinear solvers—a situation that can be remedied using an integral conductivity representation and cubic spline interpolation []; (6) DAE/MOL approaches generalize to two dimension, as does condition-number-based termination of the nonlinear solver []; and (7) transformation approaches can significantly improve the efficiency of RE solution methods for both standard low-order methods and DAE/MOL approaches [].

While these advances have contributed to the robustness and efficiency of solutions for RE, the focus of this work has been on homogeneous media, except our recent investigation of a slightly heterogeneous two-dimensional system in which the focus was on linear and nonlinear solver issues []. Neither our previous work, nor the work of others that we are aware of have investigated the efficiency and robustness of the DAE/MOL approach for solving RE for heterogeneous media, although such conditions are typical of natural systems. This seems especially important to consider for media that lacks smoothness in certain situations.

The objective of this work is to compare standard, low-order methods for solving RE to a DAE/MOL approach for heterogeneous media conditions. This comparison has two important components: robustness, or the reliability of the solution method; and efficiency, the error in the solution achieved for a given investment in computational resources.

2 Methods

2.1 Formulation

We consider two common forms of RE in one spatial dimension, the pressure-head-based form

$$[c(\psi) + S_s S_a(\psi)] \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z} \left[K(\psi) \left(\frac{\partial \psi}{\partial z} + 1 \right) \right] \tag{1}$$

and the mixed form

$$\frac{\partial \theta_a}{\partial t} + S_s S_a(\psi) \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z} \left[K(\psi) \left(\frac{\partial \psi}{\partial z} + 1 \right) \right] \tag{2}$$

where $c = d\theta_a/d\psi$ is the specific moisture capacity, S_s is the specific storage coefficient, which accounts for fluid compressibility; S_a is saturation of the aqueous phase; ψ is the pressure head; t is time; θ_a is the volumetric fraction of the aqueous phase; z is the vertical spatial dimension; and K is the hydraulic conductivity.

We consider problems with auxiliary conditions of the form

$$\psi(z, t = 0) = \psi_0(z) \tag{3}$$
$$\psi(z = 0, t > 0) = \psi_1 \tag{4}$$
$$\psi(z = Z, t > 0) = \psi_2 \tag{5}$$

where Z is the length of the domain, ψ_0 may be a function of space, and ψ_1 and ψ_2 are constants. These conditions lead to the development of a sharp infiltration front and saturated conditions over a portion of the domain, which is a difficult class of test problem.

For closure, we use the standard van Genuchten (VG) pressure-saturation relationship [van Genuchten(1980),], which is given by

$$S_e(\psi) = \frac{\theta_a(\psi) - \theta_r}{\theta_s - \theta_r} = \begin{cases} (1 + |\alpha_v \psi|^{n_v})^{-m_v}, & \psi < 0 \\ 1, & \psi \geq 0 \end{cases} \tag{6}$$

and the Mualem saturation-conductivity relation [Mualem(1976),]

$$K(S_e) = K_s S_e^{1/2} \left[1 - \left(1 - S_e^{1/m_v}\right)^{m_v}\right]^2 \tag{7}$$

where $m_v = 1 - 1/n_v$, 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 pore-size distribution, and K_s is the water-saturated hydraulic conductivity.

2.2 Spatial Discretization

We use a standard finite-difference approximation to discretize RE with respect to the spatial dimension [Celia et al.(1990)Celia, Bouloutas, and Zarba,], z, where $z \in [0, Z]$. We consider a uniform spatial discretization comprised of $n_n - 1$ intervals $\{[z_i, z_{i+1}]\}_{i=1}^{n_n-1}$, of length Δz, with $\Delta z = Z/(n_n - 1)$, and $z_i = (i-1)\Delta z$ for $1 \leq i \leq n_n$. The spatial operator

$$O_{sd}(\psi) = \frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial \psi}{\partial z} + 1\right)\right] \tag{8}$$

is approximated at $z = z_i$ for $1 < i < n_n$ by

$$O_{sd_i}(\psi) = \Delta z^{-2}\left[K_{i+1/2}(\psi_{i+1} - \psi_i) - K_{i-1/2}(\psi_i - \psi_{i-1})\right] + \Delta z^{-1}\left(K_{i+1/2} - K_{i-1/2}\right) \quad (9)$$

where n_n is the number of spatial nodes in the solution, and ψ_i is the approximation to $\psi(z_i)$.

Interblock conductivities, $K_{1\pm1/2}$ are evaluated using an arithmetic mean (KAM)

$$K_{i\pm1/2} = \left(K_i + K_{i\pm1}\right)/2 \quad (10)$$

and an integral (KINT) approximation

$$K_{i\pm1/2} = \begin{cases} \frac{1}{|\psi_i - \psi_{i\pm1}|}\int_{\min\{\psi_i,\psi_{i\pm1}\}}^{\max\{\psi_i,\psi_{i\pm1}\}} K\, d\psi, & \text{if } \psi_i \neq \psi_{i\pm1}; \\ K(\psi_i), & \text{if } \psi_i = \psi_{i\pm1}. \end{cases} \quad (11)$$

2.3 Temporal Integration

We considered two temporal integration methods, the first method is a standard implicit finite difference approximation applied to the mixed-form equation and solved using modified Picard iteration (MPI), which is considered the standard approach []. Time step size was selected using a common empirical adaptive time-step control algorithm [Rathfelder and Abriola(1994),]

- if $m < m_l$ then $\Delta t_{n+1} = \min(f_t \Delta t_n, \Delta t_{max})$
- else if $m > m_u$ then $\Delta t_{n+1} = \max(\Delta t_n / f_t, \Delta t_{min})$

where m is the number of iterations required by the nonlinear solver to converge for time step n, m_l is a lower iteration limit, m_u is an upper iteration limit, f_t is a time-step acceleration factor, Δt_{max} is the maximum allowable time-step size, and Δt_{min} is the minimum allowable time-step size.

The second time integration method investigated was a DAE/ MOL approach for the pressure-head form of RE (1), which was applied to the semi-discrete form of RE given by

$$A(\psi)_i \frac{d\psi_i}{dt} = O_{sdi}(\psi) \quad (12)$$

where A includes accumulation and compressibility terms. A modified version of DASPK [Brown et al.(1994)Brown, Hindmarsh, and Petzold, Tocci et al.(1997)Tocci, Kelley, and Miller,] was used as our DAE solver. DASPK is a DAE solver based upon the fixed leading coefficient, first- through fifth-order backward difference formulas and containing error estimation and control through adjustment of method order and step size [Brenan et al.(1996)Brenan, Campbell, and Petzold,].

2.4 Efficiency

We define efficiency as the computational effort required to achieve a specified accuracy, which requires evaluation of both work and error—the former being challenging and the latter trivial. We evaluate work for the MPI method by

$$W_p = w_c n_c + w_l n_l \tag{13}$$

and for the DAE/MOL method by

$$W_n = w_j n_j + w_f n_f + w_l n_l \tag{14}$$

where W_p is a work measure for MPI methods, w_c is a weighting factor for formation of the coefficient matrix and right hand side vector, which are typically done at the same time, w_l is a weighting factor for solution of the linear system of equations, n_c is the number of coefficient matrix formation calls, n_l is the number of linear solutions performed, W_n is a work measure for Newton iteration DAE methods, w_j is a weighting factor for formation of the Jacobian matrix, w_f is a weighting factor for evaluation of the function, n_j is the number of Jacobian evaluations, and n_f is the number of function evaluations. We estimated these weights based upon CPU time on a Hewlett-Packard ... running version ... of ... operating system, and using version — of ... complier as $w_c = 0.484$, $w_j = 0.552$, $w_f = 0.271$, and $w_l = 0.181$. **Glenn these need to be updated.**

Error was evaluated by comparison to dense-grid solutions using

$$\| \epsilon_D \|_k = \left[\frac{1}{n_n} \sum_{i=1}^{n_n} \left(|\hat{\psi}_i - \psi_i| \right)^k \right]^{1/k} \tag{15}$$

where k is the norm measure, with $k = 1$ results are reported in this work; and $\hat{\psi}_i$ is an approximation of the true solution based on a

Table 1: Media Properties

Variable	Sand	Loam	Clay
θ_r (—)	0.093	0.078	0.102
θ_s (—)	0.301	0.430	0.368
α_v (m^{-1})	5.470	3.600	3.350
n_v (—)	4.264	1.560	2.000
K_s (m/day)	5.040	0.250	7.970
S_s (m^{-1})	1.0×10^{-6}	1.0×10^{-6}	0.000

dense spatial grid. The dense-grid solutions were generated using the DAE/MOL approach with a spatial grid size equal to 1/32 of the size used in the test simulations. **Glenn check this too.**

3 Results

Two layered, heterogeneous test problems were investigated using the MPI and DAE/MOL approach described above. For both test problems, the spatial domain was $z \in [0, 4]$ m. The temporal domains were $t \in [0, 0.25]$ days for Problem 1 and $t \in [0, 0.08]$ days for Problem 2. The media for Problem 1 consisted of four, 1-m thick alternating layers of loam and sand. The media for Problem 2 consisted of four 1-m thick alternating layers of clay and sand. The properties of these materials are listed in Table 1, which were taken from the literature []. Problem 1 exhibits a larger degree of heterogeneity than Problem 2 due to the wider difference in K_s and n_v between adjoining layers, making Problem 1 a more difficult test problem. The dense grid solution profile for both test problems is shown on Figure 1, which illustrates the effects of media heterogeneity and the sharp-front nature of the solution profiles.

Quantitative results in the form of work and error measures for each of the test problems are shown in Figures 2 and 3. The comparisons of the MPI and DAE/MOL approaches showed:

1. the DAE/MOL approach was more robust than the MPI approach, the MPI method failing to produce convergent solutions for Problem 1;

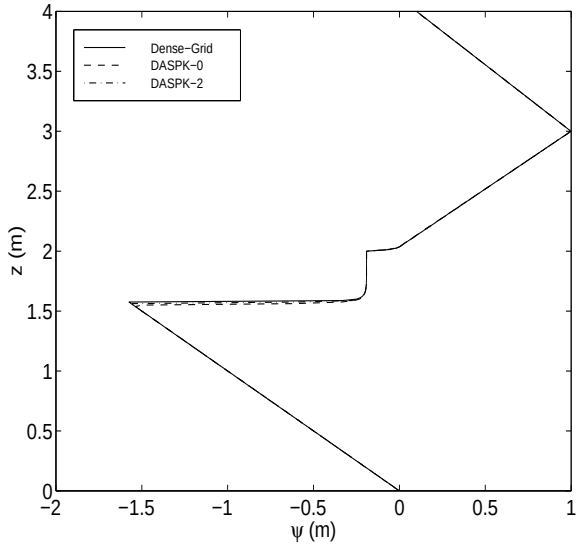

Figure 1: Solution Profiles for Test Problems 1 and 2.

2. the DAE/MOL approach was more efficient than the MPI approach when both methods converged, producing equivalent accuracy results with as little as 30% of the computational effort in one case; and **Glenn check this.**

3. the KINT produced more accurate and more efficient results than the KAM approach. **Glenn again check this.**

Acknowledgments

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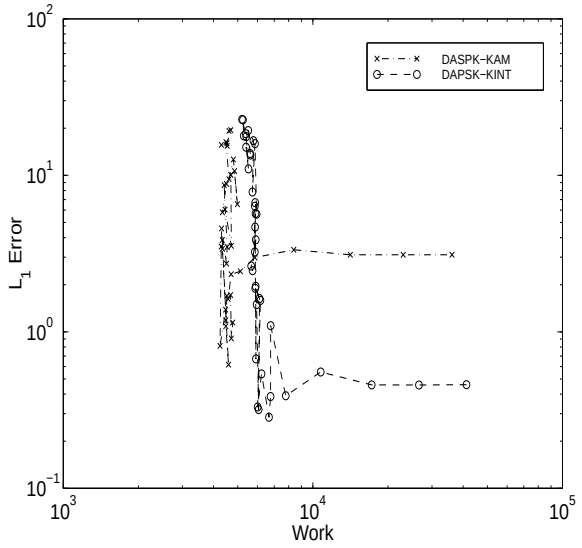

Figure 2: Solution Profile for Test Problem 1.

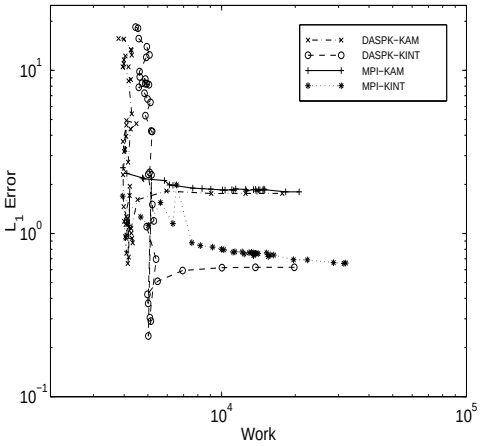

Figure 3: Solution Profile for Test Problem 2.

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