Higher order, locally conservative temporal integration methods for modeling multiphase flow in porous media

C.T. Miller[a*], M.W. Farthing[a†], C.E. Kees[a‡], and C.T. Kelley[b§]

[a]Center for the Advanced Study of the Environment
Department of Environmental Sciences and Engineering, Box 7400
University of North Carolina
Chapel Hill, NC 27566-7400, USA

[b]Center for Research in Scientific Computation
Department of Mathematics, Box 8205
North Carolina State University
Raleigh, NC 27695-8205, USA

Traditional approaches for solving single- and multiphase fluid flow in porous medium systems rely on low-order methods in both space and time. Temporal approximations often use either fixed time-step methods or empirically based adaptive strategies that adjust the time step based on the number of iterations required for the nonlinear solver to converge. Over the last several years, several single- and multiphase flow problems have been solved using higher order temporal integration methods based on formal error estimation and control. This approach has led to robust and efficient solvers. In this work, we summarize the recent advances in applying higher order temporal integration methods to a range of multiphase flow problems. We also extend this work to derive an approximate solution to Richards' equation using mixed finite element methods in space and to formulate a solution approach for three-phase flow.

1. INTRODUCTION

Over the last several years, advancements in modeling multiphase flow and transport in porous medium systems have led to increased efficiency and robustness in simulating such systems; improved spatial and temporal discretization schemes and advances in iterative algebraic solver approaches [1,2] have been largely responsible.

We have seen steady progress in temporal integration schemes. Using low-order fixed-time-step solution approaches for difficult multiphase flow problems is known to be inefficient [3]. Moreover, while heuristic time-adaption schemes are more efficient than fixed-time-step methods, they have given way to more sophisticated schemes: temporal

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‡Under the auspices of UCAR, Visiting Scientist Program, P.O. Box 3000, Boulder, CO 80307-3000, USA
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integration methods estimate and control the temporal error through adapting both the temporal step size and the order of the temporal approximation. They are an especially appealing class of methods [4], and considerable work has been done on using them, along with standard finite difference approaches, to approximate Richards' equation (RE) [3–8] and, more recently, two-phase flow [9].

Since many subsurface systems are irregularly shaped, the ideal spatial discretization approach would capture such features efficiently. Because of this trait, finite element approaches have received considerable attention in the literature, but standard Bubnov-Galerkin methods do not conserve mass locally. Mixed finite element methods (MFEMs) do not suffer from this restriction, but only recently have these methods been combined with adaptive higher order temporal integration schemes for saturated flow [10]. To the best of our knowledge, the literature does not yet include treatments of multiphase flow problems approximated using higher order adaptive step-size temporal integration combined with MFEM approaches in space. We believe such approaches are promising. Further, we know of no published report of a higher order temporal integration approximation for three-phase flow in porous media, although this too seems like a potentially useful advance.

The overall goal of this brief work is to advance higher order temporal integration methods to solve multiphase flow problems. Specifically, our objectives are (1) to summarize an effective and efficient approach for adaptive, higher order temporal integration; (2) to formulate a higher order MFEM model for RE; (3) to illustrate the adaption of temporal approximation order and step size for a field-scale application; and (4) to formulate an adaptive higher order temporal approximation for three-phase flow in porous media.

2. TEMPORAL INTEGRATION

Low-order temporal integration approaches have been the standard for solving the partial differential equations (PDE's) that arise from water resources problems. As an alternative, the method of lines (MOL) approach applies an approximate method to the spatial derivatives present in the original PDE and then approximates the resultant set of ordinary differential equations (ODE's) using the methods available for solving such systems. These two methods are equivalent when the same low-order methods in space and time are used to solve the original PDE. However, decoupling the solution approach using the MOL allows for the straightforward use of sophisticated time integration strategies that have some attractive properties: excellent stability and accuracy, a range of orders of approximation, adjustable step size, and built-in error estimation and control and to meet user-specified criteria. MOL approaches clearly provide a robust and efficient way to solve many water resources problems, although many unanswered questions remain.

Choosing an integration strategy is one such question. We have investigated a range of temporal integration approaches and advocate using a differential algebraic equation (DAE) approach based on higher order, fixed-leading-coefficient backward difference formulas (FLCBDF's)[4,11]. We consider DAE's of the form

$$\mathbf{f}[t, \mathbf{y}(t), \mathbf{y}'(t)] = 0 \tag{1}$$

where $\mathbf{f}$ is a vector of equations that depend on time, t, and some combination of the vector of dependent variables, $\mathbf{y}$, and the vector of first derivatives of the dependent variables with respect to time, $\mathbf{y}'$. Applying a FLCBDF approximation to Equation (1) yields a system of potentially nonlinear algebraic equations of the general form

$$\bar{\mathbf{f}}(t, \mathbf{y}, \alpha\mathbf{y} + \beta) = 0 \tag{2}$$

where α is a constant that depends on the step size and order of the approximation, and β is a constant related to the predicted solution at the unknown time step, y^p_{l+1}, where a predictor-corrector approach is used [4]. Equation (2) is typically solved using an inexact Newton method of the form

$$\mathbf{J}^m \boldsymbol{\delta}^m = -\bar{\mathbf{f}} \tag{3}$$

where $\mathbf{J}$ is the Jacobian of the nonlinear equations described by Equation (2), m is an iteration index, and $\boldsymbol{\delta}$ is a Newton correction. The linear system solves needed to compute $\boldsymbol{\delta}$ can be performed using direct methods for simple one-dimensional problems or preconditioned Krylov-subspace methods for multidimensional applications [9].

The order of the approximation and the step size can be chosen to meet user-specified absolute and relative error tolerances. Using a weighted norm approximation of the difference between the corrector and predictor solution of the general form

$$\tau_l = K_l \|\boldsymbol{\delta}_l\|_W < 1 \tag{4}$$

where τ is the error estimate, K_l is a coefficient dependent on the FLCBDF approximation, and the subscript W denotes a weighted norm that depends on the user-specified error tolerances. Complete details of this approach are available in the literature [9,12].

We have found DAE approaches more efficient than the more traditional MOL approaches. The latter require the system of ODE's to be written in explicit form [3]. Moreover, DAE approaches benefit from object-oriented solution methods [9], and MOL/DAE methods can be used to derive mass conservative approximations of multiphase flow by specifying explicit algebraic constraints [9].

3. RICHARDS' EQUATION

We have shown that an MOL/DAE approach can yield a robust and efficient approximation of RE [3]. We have also shown how this time integration approach can be extended to derive a locally conservative mixed hybrid finite element (MHFEM) approximation to single-phase flow in three spatial dimensions; such efforts also result in an efficient solution [10]. Here, we extend our previous work by deriving an adaptive temporal integration approach for RE, which may be applied to irregular domains while maintaining a locally conservative solution.

Although using a MHFEM discretization with a MOL/DAE approach showed several benefits over standard approaches for flow in a confined, heterogeneous aquifer, a number of issues should be considered before translating its advantages for single-phase flow over to RE. As might be expected, these issues arise from the need to account for the nonlinearity inherent in multiphase flow. Specifically, the nonlinear nature of the constitutive relations commonly used to describe the relationship among fluid pressures, saturations, and relative permeabilities (p-S-k relations) for RE places added demands on temporal and spatial discretizations used as well as the techniques required to solve the resulting nonlinear and linear systems.

In addition to the standard MFEM [13], both the MHFEM [14] and the enhanced cell-centered difference method (ECDM) [15,16] have been applied to RE. The ECDM can also be seen as a nonstandard finite difference technique obtained from a standard MFEM approach by using certain numerical quadrature rules [17]. Like other more common spatial approximations, the MFEM discretizations have varied in their choice of formulation for RE, p-S-k relations, linear and nonlinear solution strategies, and time discretization. The temporal approximations, however, have all been low order [13,14,16] with either fixed time step or empirical adaption. The low-order time discretization is of particular concern for applying the MHFEM to the pressure head form of RE (PRE), which causes significant mass balance errors for certain problems [18].

The PRE can be given by

$$\left(\theta \frac{\partial \hat{\rho}}{\partial \psi} + \hat{\rho} \frac{\partial \theta}{\partial \psi}\right) \frac{\partial \psi}{\partial t} \quad + \quad \nabla \cdot (\hat{\rho} \mathbf{q}) = 0 \qquad \text{in } \Omega \times [0,T] \tag{5}$$

where Ω and $[0,T]$ are the physical and temporal domains, ψ is the pressure head, $\hat{\rho}$ is a normalized density, and θ is the volume fraction for the aqueous phase. We use the common extension of Darcy's law to variably saturated flow [19]

$$\mathbf{q} = -k_r(\psi) K_s (\nabla \psi - \hat{\rho} \mathbf{d}) \tag{6}$$

Here K_s is the saturated hydraulic conductivity, k_r is the relative permeability, and $\mathbf{d}$ is a vector accounting for the acceleration of gravity. To describe the interdependence of fluid pressure, saturation, and the relative permeability we use the p-S-k relations of van Genuchten [20] and Mualem [21], while we assume slight compressibility for the aqueous phase density [22].

The boundary and initial conditions are given by

$$\begin{aligned} \psi &= \psi^b && \text{on } \Gamma_D, t \in [0,T] \\ \mathbf{u} \cdot \mathbf{n} &= u^b && \text{on } \Gamma_N, t \in [0,T] \\ \psi &= \psi^0 && \text{in } \Omega, t = 0 \end{aligned} \tag{7}$$

where $\mathbf{u}$ is the mass flux.

The ECDM discretization is suitable for use with logically rectangular meshes. Details can be found in [17,15,23]. Briefly, it formulates an expanded system for Equations (5)–(7) which includes an adjusted gradient

$$\begin{aligned} \tilde{\mathbf{u}} &= -(\nabla \psi - \hat{\rho} \mathbf{d}) \qquad \text{with} \\ \mathbf{u} &= \hat{\rho} k_r K_s \tilde{\mathbf{u}} \end{aligned} \tag{8}$$

It proceeds by identifying subdomains of Ω over which the problem coefficients vary smoothly. It forms local approximations of Equations (5)–(8) over these subdomains using the lowest order Raviart-Thomas space and certain numerical quadrature rules [17]. These local approximations are then coupled by defining Lagrange multipliers along subdomain boundaries where continuity of the normal component of mass flux is enforced explicitly.

We extended previous work by developing an a temporally adaptive ECDM solution for a PRE. We used an available ECDM spatial discretization method [17], an object-oriented FLCBDF DAE temporal integration approach [4], and solved the resultant system of equations using a preconditioned generalized minimal residual (GMRES) iterative solver from the PETSc library [24]. Simulations were performed on an IBM RS/6000 SP supercomputer with 720 processors at the North Carolina Supercomputing Center (www.ncsc.org).

As an example, we consider a typical unsatured flow problem for a hillslope domain. The idealized hillslope geometry is defined in terms of a mapping $\mathbf{F}$ from a reference domain $\hat{\Omega} = [0, 24] \times [0, 1]$ (meters) given by $x_1 = \hat{x}_1$ and

$$x_2 = \begin{cases} \hat{x}_2 + 0.1\hat{x}_1 \sin(\pi\hat{x}_1/25) & \text{for } \hat{x}_1 \leq 16 \\ \hat{x}_2 + 1.477 & \text{otherwise} \end{cases} \tag{9}$$

Given this mapping, it is natural to identify two subdomains of $\hat{\Omega}$ for $\hat{x}_1 < 16$ and $\hat{x}_1 > 16$. The saturated conductivity and parameter values for the van Genuchten-Mualem p-S-k relations were then taken from the literature for a sand medium [25].

The initial value of ψ was set to be at hydrostatic equilibrium with the water table, located at $x_2 = 1/3$. No flow conditions were defined for the right and bottom boundaries. Homogeneous Neumann conditions were also used on the left boundary except for the region given by $x_2 \leq 1/3$ where Dirichlet conditions were set to hydrostatic equilibrium with the water table. The top boundary flux into the domain was given by

$$u^b = \begin{cases} 2\sin(\pi t) & \text{for } 5.33 \leq x_2 \leq 13.33 \text{ and } t \leq 1/24 \\ 0 & \text{otherwise} \end{cases} \tag{10}$$

A contour plot of θ at $t = 0.1$ on a 90×60 mesh is shown in Figure 1. Figure 1 also traces the the choice of time step and temporal approximation order over the course of the simulation for the DAE integrator with both full adaption and the integration order restricted to one (BE-A). The data points shown are values averaged over every 10 time steps. The fully adaptive simulation required 336 seconds of total CPU time on 32 processors while the BE-A run required 1085.0 seconds. The BE-A run would be more efficient than typical low-order heuristically based integration schemes and much more efficient than fixed-time-step low-order integration schemes. These results are consistent with previous findings documenting the advantages of the MOL/DAE approach used in this work [3,10].

4. THREE-PHASE FLOW

Given a mass-conservative spatial discretization, we can obtain a mass conservative temporal discretization for RE and two-phase flow models by employing a semi-explicit index-one formulation, as we demonstrated in [22]. Here we briefly outline this approach for three-phase flow models.

The semi-discrete system of three-phase flow equations can be written as

$$\frac{\partial}{\partial t}\left(\theta_{i,j}\rho_{i,j}\right) = O_{di,j} \text{ for } i = w, n, a \text{ and } j = 1, \ldots, N \tag{11}$$

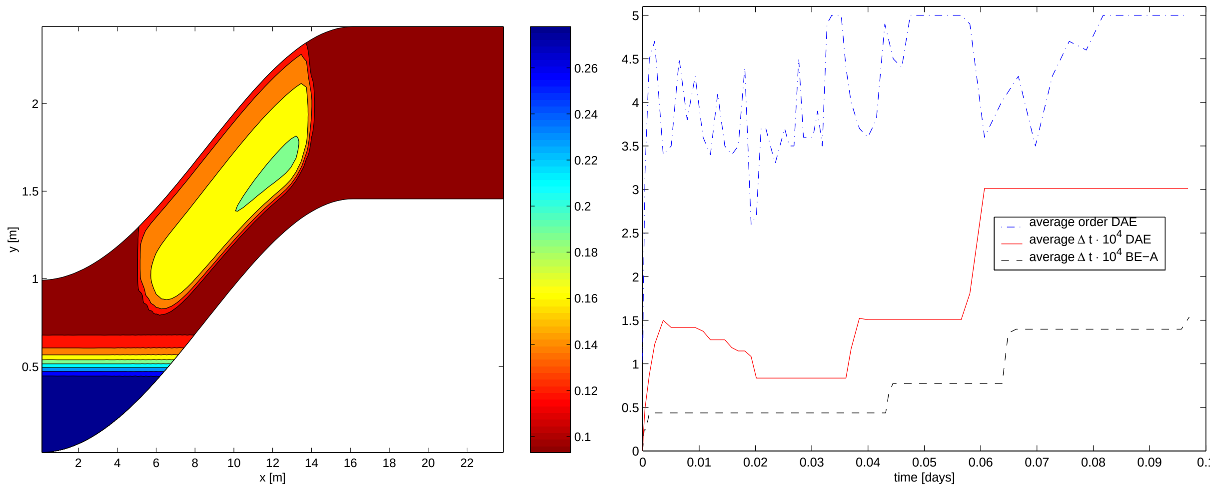

Figure 1. left: Spatial distribution of water phase volume fraction for hill-slope simulation. right: Temporal integration order and step size as a function of simulation time for hill-slope simulation.

where N is the number of discrete spatial nodes, O_d is the approximate divergence of fluid phase mass flux at each node, and the subscripts w, n, and a are phase qualifiers corresponding to a wetting and a non-wetting fluid phase and air, respectively. To simplify the presentation we have assumed that the form of the equations are the same on the interior and boundary of the domain. We have also assumed that relations sufficient to obtain formal closure are available; that is, at each spatial node there is a three component vector of unknowns, $\mathbf{y}_j$. For example, we could choose $\mathbf{y}_j = (\theta_{w,j}, \psi_{w,j}, \psi_{g,j})$ for common closure relations. Following the approach given in [22], we derive a semi-explicit index-one DAE from eqn 11 given by

$$\begin{array}{rcl} \frac{\partial M_{i,j}}{\partial t} - O_{di,j} & = & 0 \\ M_{i,j} - \rho_{i,j}(\mathbf{y}_i)\theta_{i,j}(\mathbf{y}_i) & = & 0 \end{array} \quad \text{for } i = w, n, a \text{ and } j = 1, \ldots, N \tag{12}$$

where M represents the fluid phase bulk density in the porous medium. Applying the BDF time discretization above yields the nonlinear system

$$\begin{array}{rcl} \alpha M_{j,i} + \beta_i - O_{dj,i} & = & 0 \\ M_{j,i} - \rho_j(\mathbf{y}_i)\theta_j(\mathbf{y}_i) & = & 0 \end{array} \quad \text{for } i = w, n, a \text{ and } j = 1, \ldots, N \tag{13}$$

This system can be solved efficiently using a combination of straightforward algebraic manipulations and Newton's method as shown in [22]. As long as eqn 13 is solved accurately, the numerical model is mass conservative in the sense that the discrete change in fluid bulk density is exactly equal to the discrete divergence of fluid mass flux, regardless of the size of the time step.

5. CONCLUSIONS

The method of lines is a straightforward approach for applying sophisticated adaptive temporal integration methods to PDE models of flow and transport in porous media. We have demonstrated, in particular, that transient nonlinear models of multiphase flow can be solved efficiently using variable order, variable step size BDF methods in the context of the MOL. Further, these methods can be applied in conjunction with sophisticated spatial discretization techniques, such as MFEMs, to yield accurate, mass conserving, solutions to complex multiphase problems on irregular domains.

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