A COLLOCATION MODEL OF TWO-DIMENSIONAL UNSATURATED FLOW

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ABSTRACT

This paper introduces a numerical scheme for solving the equation governing two-dimensional flow in a variably saturated porous medium. The scheme uses a mass-conserving time-stepping method together with a computationally efficient collocation formulation of the spatial derivatives. A Newton-like iteration gives a temporally stable implicit scheme. The paper examines a sample problem involving subsurface irrigation in the unsaturated zone.

INTRODUCTION

This paper presents a new numerical scheme for simulating variably saturated flows in two space dimensions. The scheme, based on finiteelement collocation, is an extension of a one-dimensional formulation presented earlier (Allen and Murphy, 1985). In that paper we discussed some of the computational advantages of collocation and examined the issue of mass conservation that arises in many numerical approaches to variably saturated flows.

The equation we solve is

$$\nabla \cdot [K(\nabla h - \mathbf{e}_s)] - \frac{\partial \theta}{\partial t} = 0 \tag{1}$$

where, in two dimensions, $\nabla \equiv (\partial/\partial x, \partial/\partial z)$ with z measuring distance above some datum, and \mathbf{e}_x is the unit vector in the z-direction. In this equation, h(x, z, t) is the pressure head (m), K stands for the soil's hydraulic conductivity (m/s), and θ signifies the moisture content of the soil (dimensionless). Typically, the physics of variably saturated flows dictate that K and θ vary with h, and the relationships K(h) and $\theta(h)$ make Equation (1) nonlinear. Murphy (1985) gives a derivation of this equation.

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In the following section we discuss a finite-element formulation of Equation (1) incorporating iterative time-stepping to accommodate the nonlinearity. Then we describe a collocation scheme for obtaining algebraic analogs to the differential equation and review an application to a sample problem.

FINITE-ELEMENT FORMULATION

Our first task in numerically solving two-dimensional unsaturated flows is to discretize the governing equation (1). To do this, we first expand the spatial derivatives using the product rule and use a backward Euler difference scheme to approximate the time derivative on a uniform temporal grid $0 < \Delta t < 2\Delta t < \cdots < n\Delta t < \cdots$:

$$\frac{\partial K^{n+1}}{\partial x} \frac{\partial h^{n+1}}{\partial x} + \frac{\partial K^{n+1}}{\partial z} \frac{\partial h^{n+1}}{\partial z} + K^{n+1} \left(\frac{\partial^2 h^{n+1}}{\partial x^2} + \frac{\partial^2 h^{n+1}}{\partial z^2} \right) \\ - \frac{\partial K^{n+1}}{\partial z} - \frac{\theta^{n+1} - \theta^n}{\Delta t} = 0$$
(2)

This equation furnishes an implicit time-stepping scheme for the approximate pressure head $h^n(x,z) \approx h(x,z,n\Delta t)$, which we regard as the principal unknown.

To solve Equation (2) we must accommodate the dependence of the nonlinear functions $K^{n+1} = K(h^{n+1})$, $\theta^{n+1} = \theta(h^{n+1})$ on unknown values h^{n+1} of the pressure head. To do this, we use an iterative method to advance between time levels, solving for iterative increments $\delta h =$ $h^{n+1,m+1} - h^{n+1,m}$ to progress from the known iteration m to the next unknown iteration m + 1. This scheme allows us to lag the nonlinear coefficients by an iteration in solving for δh :

$$-\frac{1}{\Delta t}\frac{d\theta^{n+1,m}}{dh} + K^{n+1,m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{\partial K^{n+1,m}}{\partial x}\frac{\partial}{\partial x} + \frac{\partial K^{n+1,m}}{\partial z}\frac{\partial}{\partial z}\bigg]\delta h = -R^{n+1,m}$$
(3)

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where the expression

$$R^{n+1,m} = -\frac{1}{\Delta t} (\theta^{n+1,m} - \theta^n) + K^{n+1,m} \left(\frac{\partial^2 h^{n+1,m}}{\partial x^2} + \frac{\partial^2 h^{n+1,m}}{\partial z^2} \right) \\ + \frac{\partial K^{n+1,m}}{\partial x} \frac{\partial h^{n+1,m}}{\partial x} + \frac{\partial K^{n+1,m}}{\partial z} \left(\frac{\partial h^{n+1,m}}{\partial z} - 1 \right)$$

plays a role analogous to that of the residual in standard Newton-Raphson schemes. In executing the iterative method, we begin each time step by setting $h^{n+1,0} = h^n$ and stop the iteration, setting

 $h^{n+1,m+1} = h^{n+1}$, when $||R^{n+1,m}||_{\infty} < \epsilon$ for some prescribed tolerance $\epsilon > 0$.

The formulation leading to Equation (3) differs from standard head-based formulations, which typically use the chain rule to expand the accumulation term as $\partial\theta/\partial t = (d\theta/dh)\partial h/\partial t$. Such an expansion calls for the evaluation of the specific moisture capacity $d\theta/dh$ at some time level in the interval $[n\Delta t, (n + 1)\Delta t]$ in the temporally discrete approximation. There seems to be no simple (noniterative) way of choosing this time level to guarantee global mass conservation in the sense

$$\oint_{\partial\Omega} (K^{n+1} \nabla h^{n+1} - K^{n+1} \mathbf{e}_s) \cdot \mathbf{n} \, d\mathbf{x} = \frac{1}{\Delta t} \int_{\Omega} (\theta^{n+1} - \theta^n) \, d\mathbf{x}$$

where Ω represents the spatial domain of the problem and n is the unit outward normal vector to the boundary $\partial \Omega$. As discussed in (Allen and Murphy, 1985), discretizing the flow equation as in Equation (3) avoids this difficulty, enforcing global mass conservation to within the iterative convergence criterion at each time step.

To discretize Equation (3) in space, we project the spatially varying quantities $h^{n,m}(x,z)$, $\theta^{n,m}(x,z)$, $K^{n,m}(x,z)$ and $d\theta^{n,m}/dh$ onto finiteelement subspaces. In particular, we select for the principal unknown $h^{n,m}(x,z)$ trial spaces spanned by tensor products of piecewise cubic Hermite interpolating functions in the x- and z-directions. Thus, for a rectangular region Ω , we adopt a two-dimensional grid $\{x_0 < x_1 < \cdots < x_M\} \times \{z_0 < z_1 < \cdots < z_N\}$ with nodes (denoted x_i) at the points (x_j, z_k) and, for $x \in \Omega$, set

$$\delta h(\mathbf{x}) \approx \delta \hat{h}(\mathbf{x}) = \sum_{i=1}^{N} \left[\delta_i \varphi_{00i}(\mathbf{x}) + \delta_i^{(x)} \varphi_{10i}(\mathbf{x}) + \delta_i^{(x)} \varphi_{01i}(\mathbf{x}) + \delta_i^{(x)} \varphi_{11i}(\mathbf{x}) \right]$$
(4)

Here δ_i , $\delta_i^{(z)}$, $\delta_i^{(x)}$, and $\delta_i^{(zx)}$ represent approximate values of δh , $\partial(\delta h)/\partial x$, $\partial(\delta h)/\partial z$, $\partial^2(\delta h)/\partial x \partial z$, respectively, at the node \mathbf{x}_i . The basis functions φ_{00i} , φ_{10i} , φ_{01i} , and φ_{11i} are tensor products of the one-dimensional Hermite basis functions (Prenter, 1976, Chapter 3): $\varphi_{pqi}(\mathbf{x}) = H_{pi}(x) H_{qi}(z)$, where H_{0i} is the one-dimensional basis function associated with the nodal value of the interpolate, and H_{1i} is associated with its nodal slope.

The projection (4) furnishes a continuously differentiable interpolation scheme for the iterative increment $\delta \hat{h}$ in which the nodal parameters are unknown except where given by boundary data. The head h inherits this interpolation scheme according to the updating rule

$$h^{n+1,m+1}(\mathbf{x}) \approx \hat{h}^{n+1,m+1}(\mathbf{x})$$

= $\sum_{i=1}^{N} \left\{ \left[(h_i)^{n+1,m} + \delta_i \right] \varphi_{00i}(\mathbf{x}) + \left[(h_i^{(x)})^{n+1,m} + \delta_i^{(x)} \right] \varphi_{10i}(\mathbf{x}) + \left[(h_i^{(x)})^{n+1,m} + \delta_i^{(x)} \right] \varphi_{01i}(\mathbf{x}) + \left[(h_i^{(xx)})^{n+1,m} + \delta_i^{(xx)} \right] \varphi_{11i}(\mathbf{x}) \right\}$

Therefore, given initial and boundary data for \hat{h} , one can use Equation (3) to solve for $\delta \hat{h}$ at each iteration, updating \hat{h} to step forward in time.

We also let the moisture content θ have a Hermite cubic expansion, using the chain rule to express spatial derivatives of θ in terms of the nodal unknowns $h_i^{(x)}$, $h_i^{(x)}$, and $h_i^{(xx)}$:

$$\hat{\theta}(\mathbf{x}) = \sum_{i=1}^{N} \left\{ \theta(h_i) \varphi_{00i}(\mathbf{x}) + \frac{d\theta}{dh} (h_i) h_i^{(x)} \varphi_{10i}(\mathbf{x}) \right. \\ \left. + \frac{d\theta}{dh} (h_i) h_i^{(x)} \varphi_{01i}(\mathbf{x}) + \left[\frac{d^2\theta}{dh^2} (h_i) h_i^{(x)} h_i^{(x)} + \frac{d\theta}{dh} (h_i) h_i^{(xx)} \right] \varphi_{11i}(\mathbf{x}) \right\}$$

This C^1 projection of θ parallels the successful one-dimensional calculations reported in (Allen and Murphy, 1985).

Finally, for the coefficients K and $d\theta/dh$ in Equation (3) we adopt piecewise bilinear approximations:

$$\hat{K}(\mathbf{x}) = \sum_{i=1}^{N} K(h_i) L_i(\mathbf{x}) L_i(\mathbf{z})$$
$$\left(\frac{d\theta}{dh}\right)(\mathbf{x}) = \sum_{i=1}^{N} \frac{d\theta}{dh} (h_i) L_i(\mathbf{x}) L_i(\mathbf{z})$$

where L_i is just the one-dimensional piecewise linear Lagrange (chapeau) basis function associated with node *i*.

Substituting all of these finite-element projections into Equation (3) yields a temporally discrete scheme with a finite number of unknown nodal degrees of freedom h_i at each time step.

COLLOCATION SOLUTION SCHEME

To determine the nodal values of $\delta \hat{h}$ and therefore advance the head \hat{h} in time, we need a set of algebraic equations at each iterative step. Some of these equations come from boundary conditions; the rest we will

construct using finite-element collocation. Let us begin by reviewing the boundary conditions.

By using the tensor-product basis defined above we have tacitly oriented the computational boundaries parallel to the coordinate axes. For nonrectangular domains, we would isoparametrically transform the (x, y)-plane to a plane endowed with a deformed coordinate system as described in Pinder et al. (1978). In the untransformed system, the unit normal vector \mathbf{n} and unit tangent vector \mathbf{r} to the boundary will be $\pm e_x$ or $\pm e_x$, depending on the position along the boundary. Suppose x_i is a Dirichlet node. Then $\hat{h}^{n+1}(\mathbf{x}_i) = h_i^{n+1}$ is a fixed, known quantity and therefore $\delta_i = 0$. Moreover, we can differentiate the boundary data tangentially along the Dirichlet boundary $\partial \Omega_D$ to deduce fixed values for $\nabla \hat{h}^{n+1} \cdot r$, thus forcing $\delta_i^{(x)} = 0$ if $r = \pm e_x$ and $\delta_i^{(x)} = 0$ if $r = \pm e_x$. Similarly, if x, is a Neumann node, then $\nabla \hat{h}^{n+1}(\mathbf{x}_i)$ is a fixed, known quantity, forcing $\delta_i^{(x)} = 0$ if $n = \pm e_x$ and $\delta_i^{(x)} = 0$ if $n = \pm e_x$. Differentiating the boundary data tangentially in this case will give fixed values for $\nabla(\nabla \hat{h}^{n+1} \cdot \mathbf{n}) \cdot \mathbf{r}$ along the Neumann boundary $\partial \Omega_N$, forcing $\delta^{(xz)}_{\cdot} = 0$. Therefore at any boundary node within a boundary line segment the boundary data determine two nodal parameters. At corner nodes the boundary data along the intersecting boundary segments will combine to determine three nodal parameters.

To determine the remaining boundary and interior nodal parameters, we collocate the finite-element approximation to Equation (3) at a set of collocation points $\overline{x}_k \in \Omega$. This yields a system of linear equations each having the form

$$\begin{bmatrix} -\frac{1}{\Delta t} \frac{d\hat{\theta}^{n+1,m}}{dh} (\bar{\mathbf{x}}_k) + \hat{K}^{n+1,m} (\bar{\mathbf{x}}_k) \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} \right) + \frac{\partial \hat{K}^{n+1,m}}{\partial x} (\bar{\mathbf{x}}_k) \frac{\partial}{\partial x} \\ + \frac{\partial \hat{K}^{n+1,m}}{\partial z} (\bar{\mathbf{x}}_k) \frac{\partial}{\partial z} \end{bmatrix} \delta \hat{h} (\bar{\mathbf{x}}_k) = -\hat{R}^{n+1,m} (\bar{\mathbf{x}}_k)$$

where \hat{R} represents the expression obtained by substituting the appropriate interpolatory projections for the spatially varying quantities in the residual R.

We choose for the collocation points \overline{x}_k the Gauss points associated with four-point quadrature on each rectangular element $[x_p, x_{p+1}] \times [z_q, z_{q+1}]$ (Pinder et al., 1978). This choice of collocation points furnishes exactly the right number of additional equations for the remaining unknown nodal parameters and gives the best possible accuracy estimates for the linearized problem at each time step (Prenter and Russell, 1976).

SAMPLE PROBLEM

To show the effectiveness of our collocation scheme, we solve a sample problem similar to one solved by van Genuchten (1983) using a Galerkin procedure on Hermite bicubics. This problem describes water infiltrating from a source located 0.15m below the soil surface. The governing differential equation is

$$\nabla \cdot [K(\nabla h - \mathbf{e}_{\pi})] - \frac{\partial \theta}{\partial t} + Q = 0$$

where Q is the water source, measured in s^{-1} . The spatial domain of the problem is $\Omega = (0, 0.61 \text{m}) \times (-3.5 \text{m}, 0)$. We assume that the left side $\{0\} \times (-3.5 \text{m}, 0)$ and right side $\{0.61 \text{m}\} \times (-3.5 \text{m}, 0)$ are lines of symmetry with no normal flux, that the bottom $(0, 0.61 \text{m}) \times \{-3.5 \text{m}\}$ is a free-draining boundary, and that the soil surface $(0, 0.61 \text{m}) \times \{0\}$ remains at atmospheric pressure. These assumptions lead to the boundary conditions

$$\frac{\partial h}{\partial x}(0, z, t) = \frac{\partial h}{\partial x}(0.61 \text{m}, z, t) = 0, \qquad -3.5 \text{m} < z < 0, \ t > 0$$
$$\frac{\partial h}{\partial z}(x, -3.5 \text{m}, t) = 0, \qquad 0 < x < 0.61 \text{m}, \ t > 0$$
$$h(x, 0, t) = -0.14495 \text{m}, \qquad 0 < x < 0.61 \text{m}, \ t > 0$$

We impose the initial condition $h(\mathbf{x}, 0) = -0.387$ m, $\mathbf{x} \in \Omega$. For the material properties K and θ we assume the same functional forms as van Genuchten, which in SI units are

$$K(h) = (1.157 \times 10^{-7})[96.768 \exp(12.58h)]m/s, \quad h \le 0$$

$$\theta(h) = 0.10 + 0.40/[1 + 0.0025(100h)^2]^{1/2}, \quad h \le 0$$

We assume a point source of the form $Q(\mathbf{x}) = Q_0 \delta(x-0) \delta(z+0.15\text{m})$ with a source strength $Q_0 = 5 \times 10^{-5} \text{s}^{-1}$. In finite-element collocation we must approximate Q by a square-integrable function. We choose a piecewise bilinear approximation of the form $\hat{Q}(\mathbf{x}) = \sum_{i=1}^{N} Q_i L_i(x) L_i(z)$, where the point $\mathbf{x}_i^{\text{source}} = (0, -0.15\text{m})$ is a node, $Q_i = 0$ if $\mathbf{x}_i \neq \mathbf{x}_i^{\text{source}}$, and $\int_{\Omega} \hat{Q} d\mathbf{x} = \int_{\Omega} Q d\mathbf{x}$.

We solve the resulting collocation equations on the five-element-byeleven-element grid given in (van Genuchten, 1983) using a time step $\Delta t = 3600$ s (one hour). Figure 1 shows the structure of the matrix that has to be inverted at each iteration in the nonlinear time-stepping procedure. The bandwidth for this matrix is 31. We use a direct solver executing LU factorization with partial pivoting on banded asymmetric matrices.



Figure 1. Matrix structure for the sample problem.

Figures 2 through 7 show the spatial variation of $\hat{h}(\mathbf{x}, t)$ at two-hour intervals. At two hours (Figure 2), the source already has a noticeable effect on the pressure head. In the horizontal direction \hat{h} peaks at the source, drops off, and then levels out. In the vertical direction the pressure head gradually increases further down into the column as time progresses. Finally, at t = 12 hours (Figure 7) \hat{h} reaches a very close approximation to the steady-state solution in the sense that this solution is virtually identical to solutions at later times.

CONCLUSION

The finite-element collocation method produces good approximations to pressure head distributions in unsaturated flows through porous media. As we have shown, the mass-conserving iterative formulation, demonstrated earlier for one-dimensional flows, extends in a natural way to two space dimensions. One area deserving further investigation is the linear algebra involved at each iterative stage. Since the matrices for the multidimensional problems have an asymmetric block structure without diagonal dominance, better methods for solving the linear iterative systems would be a boon to further applications.

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