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Numerical Solution of Richards' Equation: A Review of Advances and Challenges

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The flow of water in partially saturated porous media is of importance in fields such as hydrology, agriculture, environment and waste management. It is also one of the most complex flows in nature. The Richards' equation describes the flow of water in an unsaturated porous medium due to the actions of gravity and capillarity neglecting the flow of the non-wetting phase, usually air. Analytical solutions of Richards' equation exist only for simplified cases, so most practical situations require a numerical solution in one- two- or three-dimensions, depending on the problem and complexity of the flow situation. Despite the fact that the first reasonably complete conservative numerical solution method was published in the early 1990s, the numerical solution of the Richards' equation remains computationally expensive and in certain circumstances, unreliable. A universally robust and accurate solution methodology has not yet been identified that is applicable across the range of soils, initial and boundary conditions found in practice. Existing solution codes have been modified over years to attempt to increase robustness. Despite theoretical results on the existence of solutions given sufficiently regular data and constitutive relations, our numerical methods often fail to demonstrate reliable convergence behavior in practice, especially for higher-order methods. Because of robustness, the lack of higher-order accuracy and computational expense, alternative solution approaches or methods are needed. There is also a need for better documentation of improved solution methodologies and benchmark test problems to facilitate consistent advances and avoid re-inventing of the wheel.

Core Ideas

- **The numerical solution of Richards' equation remains challenging.**
- **Space/time discretization affects both computational effort and accuracy.**
- **Adaption of space and time discretizations produces benefits.**
- **Dissemination of codes and improved documentation are needed.**
- **Recent reformulation of one-dimensional Richards' equation shows promise.**

This review paper is intended to serve as a touchstone on the state of the science of calculating the flow of water through unsaturated porous media. As active researchers we believe it is good to occasionally take stock in what has been accomplished up to date, where things may be headed, and what important issues remain. This review concentrates on computational modeling of flow through the unsaturated zone via Richards' equation.

This effort can help provide some focus to the research community and serve to help propel new research forward, particularly by those just joining the field. There are many practical problems that require calculation of one-, two-, and three-dimensional fluxes in the unsaturated zone. For a much broader review of modeling soil processes, we recommend the recent paper from Vereecken et al. (2016). A detailed review of mathematical models of infiltration can be found (Assouline, 2013), while Paniconi and Putti (2015) provide historical perspective and an overview of modeling Richards' equation in the context of catchment hydrology.

The equation attributed to Richards (1931) that describes the flow of water through unsaturated porous media under the action of capillarity and gravity was first published by the English mathematician and physicist Lewis Fry Richardson in 1922 (Richardson, 1922). Therefore, the equation would rightly be called "Richardsons' equation", although in this paper we continue to call it by its common name, Richards' equation.

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Richards' equation can be seen as a simplification of the standard two-phase flow formulation for a gas and water phase in a porous medium where the pressure gradient required to drive flow of the gas phase is ignored due to the large mobility contrast between the water and gas phases. One of the most interesting aspects of the Richards' equation is that despite its ease of derivation, it is arguably one of the most difficult equations to reliably and accurately solve in all of hydrosciences.

Richards' equation can be written in a number of forms, namely the water content, mixed water content and capillary head form, and the head form. In one-dimension, the so-called "mixed water content form", because it mixes the water content θ with the capillary head ψ(θ), is:

$$\frac{\partial \theta}{\partial t}=\frac{\partial}{\partial z}\left[K(\theta)\left(\frac{\partial \psi(\theta)}{\partial z}-1\right)\right] \qquad [1]$$

where z is vertical coordinate (positive downward)[L]; t is time [T]; θ equals $\theta(z,t)$ equals volumetric soil moisture content [-]; ψ(θ) is empirical soil hydraulic capillary head function [L]; $K(\theta)$ = empirical unsaturated hydraulic conductivity function [L T^{-1}].

Equation [1] is often written solely as a function of the water content by introducing the chain rule:

$$\frac{\partial \theta}{\partial t}=\frac{\partial}{\partial z}\left(D(\theta)\frac{\partial \theta}{\partial z}-K(\theta)\right) \qquad [2]$$

where $D(\theta) = K(\theta)(\partial\psi(\theta)/\partial\theta)$ is referred to as the soil-water diffusivity [L^2 T^{-1}]. As in Eq. [1], the first term in parentheses captures the effects of capillarity, while second term in parentheses represents the effect of gravity-driven flux.

In uniform soils the water content or mixed water content forms of Richards' equation are valuable because water content is a continuous variable. However, in nature soils are seldom uniform over significant length scales, and layered soils are ubiquitous. In layered soils the water content is discontinuous across layer interfaces because of unique unsaturated capillary head relations in the different soil layers (Assouline, 2013). Rather, the capillary head (ψ) is continuous, and it is better to write the Richards' equation with capillary head as the dependent variable and evaluate the moisture content in terms of ψ, θ = θ(ψ). This can be done in either a mixed form:

$$\frac{\partial \theta(\psi)}{\partial t}-\frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial \psi}{\partial z}-1\right)\right]=0 \qquad [3]$$

or via the chain rule as the fully head-based form:

$$c(\psi)\frac{\partial \psi}{\partial t}-\frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial \psi}{\partial z}-1\right)\right]=0 \qquad [4]$$

where $c(\psi)$ equals $\partial\theta/\partial\psi$ equals the specific moisture capacity [L^{-1}]; $K(\psi)$ equals the hydraulic conductivity function written as a function of ψ[L T^{-1}].

Equations [3] and [4] can both be used to solve unsaturated and saturated flow problems. One may also encounter Eq. [4] in a form that includes fluid compressibility effects

$$\left[S_s S_a(\psi)+c(\psi)\right]\frac{\partial \psi}{\partial t}-\frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial \psi}{\partial z}-1\right)\right]=0 \qquad [5]$$

where S_s [L^{-1}] is the specific storage and S_a [-] is the saturation of the aqueous phase (Miller et al., 1998). While $\partial\theta/\partial t = c(\psi)\partial\psi/\partial t$ holds at the continuous level through the chain rule, the nonlinearity of $c(\psi)$ makes it impossible to maintain this equality uniformly at the discrete level, and the pure head-based form in Eq. [4] or [5] is not generally mass conservative. There are techniques like a chord-slope approximation (Rathfelder and Abriola, 1994) that can be used in specific cases or flux updating that can promote, but not ensure, mass conservation (Kirkland et al., 1992). In general though, high accuracy in the time integration of Eq. [4] is essential to avoid mass balance errors (Tocci et al., 1997), and Eq. [3] together with expansion of the nonlinearity θ(ψ) in the storage change term, $\partial\theta/\partial t$, (Allen and Murphy, 1985; Celia et al., 1990) is preferred when low-order time integration is used.

Richards' equation is a nonlinear, degenerate elliptic-parabolic partial differential equation (List and Radu, 2016). The head-based forms of the equation, Eq. [3–5], transition from parabolic to elliptic as the solution domain nears saturation unless storage effects are included ($S_s > 0$), in which case Eq. [5] remains parabolic. The nonlinearity and transition of type in different portions of the problem domain make it very difficult to solve using traditional analytical techniques, and it is impossible to solve in closed form except for a small number of special cases (Miller et al., 1998). This difficulty is only exacerbated by the range of initial and boundary conditions encountered in practice as well as by the nature of common soil water constitutive relations that can lead to solutions with low regularity (Alt and Luckhaus, 1983). Specifically, the solution depends on two empirical, highly nonlinear soil water constitutive relations: the unsaturated hydraulic conductivity function $K(\theta)$ that can be constant or very near zero for non-positive values of the capillary head, and the capillary head function ψ(θ) that can take on arbitrary small values for relative saturations near 100%. These extremes lead to degeneracy in the solution of Richards' equation. The soil constitutive relations may not be smoothly differentiable at these extremes and can further have very high slopes and hysteresis, and be discontinuous at low relative saturations. Furthermore, infiltration into dry soils often leads to sharp wetting fronts that result in extremely large spatial gradients of soil hydraulic properties (Zha et al., 2017). These nonlinearities and the degeneracy make the design and analysis of numerical schemes for the Richards' equation very difficult (Miller et al., 2013).

Exact one-dimensional solutions of Richards' equation have been derived for a few specialized forms of the constitutive relations describing the soil water retention and the unsaturated hydraulic conductivity functions (Rogers et al., 1983; Broadbridge and White, 1988; Sander et al., 1988; Barry and Sander, 1991; Barry et al., 1993; Ross and Parlange, 1994). However, these solutions are not generally applicable because either the functional forms are dissimilar from widely used constitutive relations that represent real soils, and/or the solutions impose strict requirements on

the initial and boundary conditions. These exact solutions are valuable for verifying numerical solutions.

Given the lack of a general closed-form solution of the Richards' equation, numerical solvers are required when accurate unsaturated flow simulation capability is desired. Of course, many approximate, empirical, or completely arbitrary methods have been developed over the years to simulate the flow of water through unsaturated soils because of the real or perceived difficulties posed by the numerical solution of Richards' equation. Here we ignore those, and we solely consider problems where fully dynamical simulations in unsaturated porous media are required. Note that in the following we focus on head-based forms of Richards' equation that are valid for unsaturated or fully saturated (i.e., variably saturated) conditions. When necessary, we will use the term "strictly unsaturated" to refer to conditions or techniques that are restricted to relative saturation values less than 100%.

The complexities of solving the Richards' equation were discussed by Gray and Hassanizadeh (1991), who referred to the formulation as "paradoxical and overly simplistic". Since then, many authors have presented critiques of Richards' equation and existing solution techniques. A far-from-exhaustive sample includes (Forsyth et al., 1995; Tocci et al., 1997; van Dam and Feddes, 2000; Vogel et al., 2001; Kavetski et al., 2001a; Farthing et al., 2003b; Bause and Knabner, 2004; Manzini and Ferraris, 2004; D'Haese et al., 2007; Kees et al., 2008; Vogel and Ippisch, 2008; Juncu et al., 2011; Berninger et al., 2014; Lipnikov et al., 2016). Our intention here is not to repeat what those authors have written, rather it is to assess the state of the art, limitations, needs, and alternatives.

CALCULATION OF VADOSE ZONE FLUXES

In the Richards' equation, the physical properties of the medium are represented as nonlinear coefficients. The nonlinearities introduce a number of challenges as alluded to in the introduction. For example, with the widely used van Genuchten and Mualem constitutive relations, the capillary head function, $\psi(\theta)$, and the specific moisture capacity, $\partial\theta/\partial\psi$, approach zero as the moisture content in the porous medium nears saturation, while the soil-water diffusivity, $D(\theta)$, can grow arbitrarily large (van Genuchten, 1980). Loosely, this behavior leads to a condition known as degeneracy, when the solution of Richards' equation is hampered by coefficients that take values near zero or infinity. Classical analytical results on the existence, uniqueness, and regularity of weak solutions can be found in (Van Duyn and Peletier, 1982; Alt and Luckhaus, 1983), while Gilding (1991) provides analysis of infiltration in strictly unsaturated domains, including the positivity and boundedness of soil moisture and conditions for finite speed of propagation of wetting fronts. In practice, the difficulties driven by these nonlinearities often manifest as rapid changes in capillary head and soil moisture around infiltration fronts as well as complex material coefficients that are potentially non-continuously differentiable near full saturation (Miller et al., 1998).

Infiltration is often assumed to be a one-dimensional process in the vertical direction. Or et al. (2015) demonstrated that higher dimensional approaches are generally necessary only at scales less than approximately 10 m. The one-dimensional solution methodology developed by Celia et al. (1990), which uses modified Picard iterations to improve mass conservation, has become the standard numerical approach. It remains essentially the method that is used in many production codes including the USDA Hydrus-1D Richards' equation solver (Simunek et al., 2005).

As a result of the one-dimensional vertical assumption, large-scale models are able to replace a fully coupled, three-dimensional solution with many, independent one-dimensional calculations. Because of reliability issues however, current large-scale models of land/atmosphere interaction often use approximate or conceptual methods to model vadose zone fluxes. Those approximations usually require assumption of runoff generation mechanism, and are used in land-surface schemes such as: VIC (Liang et al., 1994), JULES (Cox et al., 1999), NOAH (Ek et al., 2003), CLM (Niu et al., 2007), NOAH-MP (Yang et al., 2011). The reality is that the numerical solution of Richards' equation is avoided in these schemes because of concerns regarding computational expense and solution reliability, as well as questions regarding the appropriateness of applying the equation to represent the behavior of large model elements or grids.

The penalty in using a Richards' solver in hydrological simulation with thousands or millions of one-dimensional solutions comes from the fact that while many of these may converge with rapidity and ease, there are conditions where some of them will not (Niswonger and Prudic, 2009) for a variety of reasons. In those cases, where convergence is slow or not possible, the code must be able to identify this condition and move to the next time step with some approximate solution. This problem affects the reliability of hydrological simulators that use Richards' equation. The lack of solution reliability imposes a large penalty on the use of Richards' equation solvers when convergence is unattainable. This penalty takes the form of computational expense, slowdown of parallel algorithms waiting for detection and approximations in the case of non-convergent solutions, and solutions with large errors, including significant mass-balance errors.

The convergence abilities and computational efficiency (or lack thereof) for a particular Richards' equation solver depend on many factors. The quality of the software engineering and implementation of the numerics are obviously critical. The essential numerical components include the spatial and temporal approximations used to transition from an initial boundary value problem posed at the continuous level to a discrete system, as well as the nonlinear and linear algebra techniques that are used to solve the resulting discrete systems and produce an approximate solution (Trangenstein, 2013). Here, we focus on the numerical discretization techniques themselves and not the very important software engineering issues surrounding the development of high-quality scientific codes (McConnell, 2004; Bartlett, 2009; Heroux and Willenbring, 2009). We summarize briefly the current state of

the art and identify outstanding issues for the primary numerical components of a Richards' equation solver below.

SPATIAL DISCRETIZATION

The overwhelming majority of Richards' equation solvers employ either a finite difference, finite volume, or finite element approximation in space. Hybrid combinations are also possible (Helmig, 2011). Table 1 provides a representative list of research and production codes along with their spatial approximations. The details of these approaches vary. They all build on a discrete partition or tessellation of the spatial domain of interest. The tessellation may be a structured grid or more generally an unstructured mesh. Figure 1 illustrates a simple unstructured mesh of a polygonal spatial domain, Ω, consisting of a union of non-empty, non-overlapping triangles, $M_h = \{\Omega_e\}$.

Each scheme must then approximate the spatial variation of material properties and solution variables on this mesh and enforce the conservation statement and solution dynamics expressed by Richards' equation in some way. For example, conservation might be enforced point-wise in a traditional finite difference scheme. Or, it might be enforced in an integral sense using test functions that are constant over a control volume, V, in a finite volume method

$$\int_V \frac{\partial \theta}{\partial t} \mathrm{d}x - \int_V \nabla \cdot \left[K(\psi)(\nabla \psi - \mathbf{1}_z) \right] \mathrm{d}x = 0 \qquad [6]$$

Here, $\mathbf{1}_z$ is a vector denoting the vertical axis. V could correspond to a mesh element, Ω_e, in "cell-centered" scheme or a dual control volume, $\tilde{\Omega}_I$, in a "vertex-centered" scheme (Fig. 1) (Huber and Helmig, 2000; Manzini and Ferraris, 2004). Finite element methods are also weighted residual methods that enforce Richards' equation weakly,

$$\int_\Omega \frac{\partial \theta}{\partial t} w \mathrm{d}x - \int_\Omega \nabla \cdot \left[K(\psi)(\nabla \psi - \mathbf{1}_z) \right] w \mathrm{d}x = 0, \ \forall w \in W(\Omega) \qquad [7]$$

Finite element methods impose a richer structure on the space of weighting functions, $W(\Omega)$ (Ern and Guermond, 2004). As an example, Fig. 2 illustrates a typical piecewise linear Lagrange polynomial, w_I, that is the building block for most finite element models for Richards' equation. It takes a value of 1 at vertex, I, and is zero at the other vertices of the triangulation, M_h. Of course, Eq. [6] and [7] are only intended to provide some context for the following discussion, and we have neglected any details of the solution approximation or evaluation of the integrals in Eq. [6] and [7] (Kees et al., 2008).

Table 1. Alphabetical list of representative research and production Richards' equation codes.

Code	Spatial approximation	Reference
ADH	CG FEM†	Howington et al. 1999
CATHY	CG FEM	Camporese et al., 2010
FEHM	CV FEM	Zyvoloski, 2007
FEFLOW	CG FEM	Trefry and Muffels, 2007
HydroGeoSphere	CV FEM	Brunner and Simmons, 2012
HYDRUS	CG FEM	Simunek et al., 2008
ParFlow	CCD	Kollet and Maxwell, 2006
RichardsFOAM	FV	Orgogozo et al., 2014
TOUGH	IFD	Finsterle et al., 2008
VS2D	CCD	Healy, 2008
WASH123D	CG FEM	Yeh et al., 2011

† CG FEM, Continuous Galerkin Finite Element Method; CV FEM, Control Volume Finite Element Method; CCD, Cell-Centered Differences; FV, Finite Volume; IFD, Integrated Finite Differences.

The spatial accuracy of all of these approximation methods depends on several factors. In particular, it is generally a function of the local mesh geometry, which can be expressed through a characteristic length scale and a measure of the aspect ratio or distortion (Trangenstein, 2013). Loosely, the formal accuracy of a convergent scheme can be related to the characteristic length scale of the mesh raised to some power, which we will refer to as the scheme's order. There is a traditional rule of thumb that large angles (hence aspect ratios) negatively impact approximation accuracy (Shewchuk, 2002). On the other hand, it is also possible through mesh optimization techniques to exploit solution behavior and gain higher accuracy through the appropriate use of element anisotropy (Pain et al., 2001; Mostaghimi et al., 2015).

The spatial discretization size is relevant beyond just the formal accuracy. Convergence of a method relates to how well the scheme approximates a solution to Richards' equation. It does not address whether or not Richards' equation is a valid approximation for unsaturated flow at the length scales used in the mesh, however. For example, it is unlikely that a three-dimensional solution of Richards' equation on a large, multiple-kilometer-scale voxel can accurately represent nature or be physically meaningful because it will violate the representative elementary volume assumption (Or et al., 2015).

For reference, Fig. 3 shows three commonly used one-dimensional discretizations. From left to right these spatial discretizations represent increasing degrees of complexity, and increasing degrees of accuracy. The uniform discretization is simplest, but the nature of the solution requires fine resolution everywhere. The variable discretization provides high resolution near the land surface, where accurately simulating the change in water content with time is most important for accurate partitioning of rainfall or energy (Downer and Ogden, 2004). The variable spatial discretization also allows coarsening away from the land surface, which can reduce computational

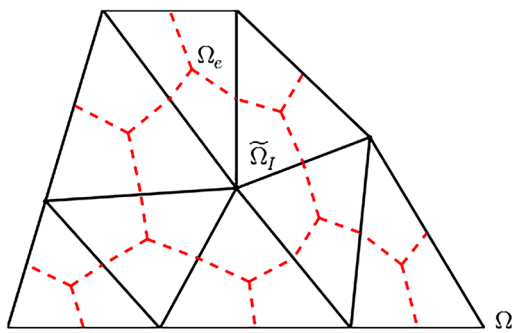

Fig. 1. Example triangulation with dual mesh.

burden without significantly affecting the solution accuracy. The adaptive spatial discretization is a much more complicated situation wherein the solver places computational points that allow the most accurate simulation of the time evolution of the wetting front.

The past three decades have seen the introduction and maturation of a number of spatial approximation methods for elliptic problems that are robust for high contrasts in material properties and heterogeneity while providing locally conservative velocities for transport. These schemes include cell and vertex-centered finite volume schemes, mimetic finite differences, multi-point flux approximation (MPFA) techniques, mixed finite elements, and discontinuous Galerkin methods (Chavent and Roberts, 1991; Arbogast et al., 1995; Aavatsmark et al., 1998; Campbell et al., 2002; Dawson et al., 2004; Klausen and Russell, 2004; Trangenstein, 2013).

These techniques have been largely successful for multiphase flow problems when applied to the global flow (or pressure) equation in fractional flow formulations (Chavent et al., 1984; Gerritsen and Durlofsky, 2005; Hoteit and Firoozabadi, 2005; Chen et al., 2006). They have also been applied to Richards' equation by a number of researchers (Bergamaschi et al., 1999; Li et al., 2007a; Arrarás et al., 2009; Klausen et al., 2008; Kumar et al., 2009). However, their direct translation to variably saturated flow has proven challenging.

To achieve comparable robustness, non-trivial modifications like low-order quadrature and mass lumping (Forsyth and Kropinski, 1997; Arbogast et al., 1998; Woodward and Dawson, 2000; Farthing et al., 2003b; Pop et al., 2004; Belfort et al., 2009; Younes et al., 2013) have often been required along with significant work on methods for solving the resulting nonlinear discrete problems (Paniconi et al., 1991; Bergamaschi et al., 1999; Bause and Knabner, 2004; List and Radu, 2016). As a result, cell-centered finite differences and low-order finite volumes/integrated finite differences, and piecewise linear, continuous Galerkin finite element schemes remain the dominant schemes used in practice (Selker and John, 2004; Kollet and Maxwell, 2006; Yeh et al., 2011; Diersch, 2013). We note that post-processing is increasingly being used in conjunction with continuous Galerkin methods to provide velocity fields that are locally conservative over elemental control volumes (Larson and Niklasson, 2004; Sun and Wheeler, 2006; Kees et al., 2008; Scudeler et al., 2016).

Local features like steep infiltration fronts make Richards' equation a natural candidate for adaptive spatial discretizations like the one sketched on Fig. 3C. Many researchers have shown that adaptive resolution can greatly improve accuracy and robustness (Bause and Knabner, 2004; Li et al., 2007b). Indeed even one-dimensional approximations have shown that they can pose a significant computational burden and benefit from adaptive resolution, depending on the combination of soil properties, initial conditions, and boundary forcing (Miller et al., 2006). However, despite the introduction of sophisticated adaption techniques that have have matured in other computational mechanics fields (Schwab, 1998; Rannacher, 2001; Fidkowski and Darmofal, 2011), including so-called h adaption which modifies the local mesh spacing (Pettway et al., 2010) as well as methods that vary the local mesh spacing and approximation order (i.e., h-p adaption) (Solin and Kuraz, 2011), spatial adaption for Richards' equation is still not widely used in practice.

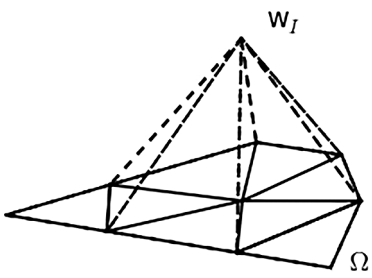

Fig. 2. Example piecewise linear weighting function.

TEMPORAL DISCRETIZATION

As with spatial approximations, solution of time-varying problems requires partition of the temporal domain of interest. Generating a discrete partition for an interval, $[0,T]$ $0 = t^0 < t^1 < \ldots < t^m = T$, is much simpler than a complex three-dimensional domain. Nevertheless, accuracy remains a function of the time step size. Schemes can be characterized in terms of their local discretization error, which is the error that would originate over one time step, $\Delta t^{(n+1)} = t^{(n+1)} - t^n$, starting from the true solution at t^n. The error that accumulates over the entire interval $[0,T]$ is known as the global error (Hairer et al., 1996). We will, somewhat loosely, refer to a method as order p if its local error is order $p+1$

$$\in^{n+1} \leq C(\Delta t^{n+1})^{p+1} \quad [8]$$

Here C is a constant that is independent of the time step (Hairer et al., 1996).

The norm for the numerical solutions of Richards' equation is low-order time discretizations, which are globally first-order. Notable exceptions include the approaches in (Tocci et al., 1997; Farthing et al., 2003b) based on higher order Backward Difference Formulas (BDFs) and the second-order Taylor-Gladwell scheme introduced in (Kavetski et al., 2001a, 2004). The vast majority of temporal approximations are also implicit in head-based models that allow fully saturated conditions to develop in the domain (Celia et al., 1990). Fully implicit

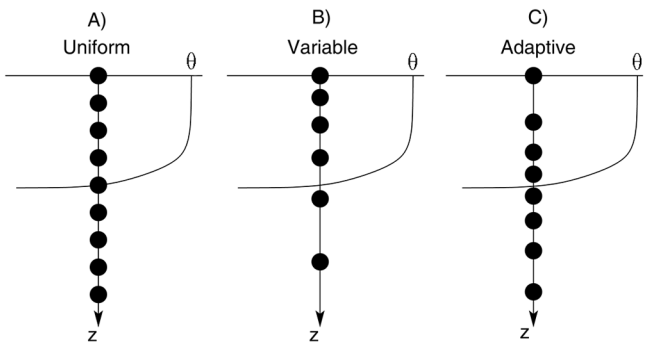

Fig. 3. Three widely used spatial discretizations shown for example in 1-dimension.

discretizations incorporate the current solution at a time level into their approximations and so require solution of at least one nonlinear problem at each time step.

To make the following discussion more precise, we assume a method of lines (MOL) approach to eliminate partial derivative terms after applying one of the spatial discretizations from Section 3. The subsequent discussion would be analogous if we followed a Rothe paradigm and introduced a temporal discretization before the spatial discretization (Lang, 2013). Applying the MOL leads to following semi-discrete problem when stepping forward from one time level, t^n, to the next, t^{n+1}

$$\mathbf{F}(t,\mathbf{y},\mathbf{y}')=0,\ \text{for}\ t\in(t^n,t^{n+1}) \qquad [9]$$

Here, $\mathbf{y}'\in R^n$ is an n-dimensional vector of discrete unknowns or degrees of freedom resulting from the spatial approximation, $\mathbf{y}'$ is the time derivative for $\mathbf{y}$, and the time step is $\Delta t^{(n+1)}$. Initial conditions for Eq. [9] are taken from time level n, and we assume that they are consistent

$$\mathbf{F}(t^n,\mathbf{y}^n,\mathbf{y}'^{,n})=0 \qquad [10]$$

Equation [9] is known as a system of Differential Algebraic Equations (DAEs) and can be thought of as a generalization of an Ordinary Differential Equation (ODE) system (Brenan et al., 1996). As an example, BDFs are multistep methods that can be thought of as introducing an approximation for $\mathbf{y}'$,

$$\mathbf{y}'^{,n+1}\approx\alpha^{n+1}\mathbf{y}^{n+1}+\beta^n \qquad [11]$$

and so lead to a discrete nonlinear problem

$$\mathbf{F}\left(t^{n+1},\mathbf{y}^{n+1},\mathbf{y}'^{,n+1}\right)=\mathbf{G}^{n+1}\left(\mathbf{y}^{n+1}\right)=0 \qquad [12]$$

that must be solved to obtain $\mathbf{y}^{(n+1)}$. Note that Backward Euler is just the first order BDF

$$\mathbf{y}'^{,n+1}\approx\frac{1}{\Delta t^{n+1}}\mathbf{y}^{n+1}-\frac{1}{\Delta t^{n+1}}\mathbf{y}^n \qquad [13]$$

Similarly, an implicit k stage Runge-Kutta approximation for Eq. [9] requires solution of the nonlinear problems (Brenan et al., 1996; Hairer et al., 1996)

$$\mathbf{F}\left(t_i^{n+1},\mathbf{y}^n+\Delta t^{n+1}\sum_{j=1}^k a_{ij}\mathbf{Y}'_j,\mathbf{Y}'_i\right)=0,\ \text{for}\ i=1,\ldots,k \qquad [14]$$

for the intermediate stage derivatives $\mathbf{Y}'_i$ to obtain

$$\mathbf{y}^{n+1}=\mathbf{y}^n+\sum_{i=1}^k b_j\mathbf{Y}'_j \qquad [15]$$

Here the implicitness results from one or more coefficient $a_{ij}>0, j\geq i$.

The nonlinear system of equations in Eq. [12] or [14] must, in general, be solved iteratively until some error tolerance is met. On the other hand, there has been interest over the years in linearly implicit or non-iterative temporal approximations, which require solving a fixed number of linear systems per time step (Paniconi et al., 1991; Kavetski et al., 2002). Linearly implicit approximations can be found in either multistep or multistage (e.g., Rosenbrock schemes) contexts (Farthing et al., 2006). However they are still much less common than fully implicit techniques.

Adaptive time discretizations for Richards' equation are much more common than adaptive spatial discretizations. A classical approach is to increase or decrease the time step by a fixed fraction based on the number of iterations taken by the nonlinear solver (Paniconi and Putti, 1994). The methods introduced in (Kavetski et al., 2001a, 2001b) and (Tocci et al., 1997) adapt the time step size and/or order based on estimates of temporal error. These approaches combine low and high-order approximations to establish estimates of the local error associated with a solution using a given time step and approximation order. They accept or reject a solution based on user-selected tolerances and pick a new order and/or time step size using heuristics often motivated by simple control theory (Söderlind, 2006). These approaches can be orders of magnitude more efficient than fixed time step or heuristic alternatives, depending on the level of temporal accuracy requested (Brenan et al., 1996; Kees and Miller, 2002; Farthing et al., 2003b). On the other hand, heuristic time stepping based on nonlinear solver performance may outperform adaptation driven by local truncation error estimates for lower accuracy regimes (D'Haese et al., 2007).

It is common to adjust time steps based on nonlinear solver convergence as well as temporal truncation error estimates in mature ODE and DAE solvers (Brenan et al., 1996; Hairer et al., 1996). However, traditional approaches are not always well-suited to highly nonlinear problems, especially when low temporal accuracy is acceptable (Farthing et al., 2003b; Söderlind and Wang, 2006). Efforts to combine nonlinear solver performance and formal truncation error include Gustafsson and Söderlind (1997), however, such approaches have not been evaluated thoroughly for Richards' equation and are not common practice.

LINEAR AND NONLINEAR SOLVERS

The desire to adjust a time step based on the performance of the nonlinear solver arises from the fundamentally local nature of Newton's method and its variants that serve as the linearization techniques for the vast majority of Richards' equation solvers. That is, returning to the notation for the discrete MOL system at time level t^{n+1}

$$\mathbf{G}^{n+1}\left(\mathbf{y}^{n+1}\right)=0 \qquad [16]$$

Newton's method attempts to solve Eq. [16] through a series of linear problems

$$\mathbf{J}_i^{n+1}\Delta\mathbf{y}_i^{n+1}=-\mathbf{G}^{n+1}\left(\mathbf{y}_i^{n+1}\right),\ \mathbf{y}_{i+1}^{n+1}=\mathbf{y}_i^{n+1}+\Delta\mathbf{y}_i^{n+1},\ i=1,\ldots \qquad [17]$$

until some convergence tolerance is met. Here $\mathbf{J}_i^{n+1}=\frac{\partial\mathbf{G}}{\partial\mathbf{y}}\left(\mathbf{y}_i^{n+1}\right)$ is the Jacobian evaluated at $\mathbf{y}_i^{n+1}$ Common convergence criteria include specifying tolerances on the norm of the residual,

$\mathbf{G}^{n+1}(\mathbf{y}^{n+1})$, or solution increment, $\Delta\mathbf{y}^{n+1}$. Classical convergence results show that Newton's method for Eq. [16] will converge quadratically assuming that $\mathbf{G}^{n+1}$ is sufficiently smooth and the initial guess, $\mathbf{y}_i^{n+1}$ is sufficiently close to the true solution (Kelley, 1995). As a result, a smaller time step, Δt^{n+1}, often translates into a better initial guess for $\mathbf{G}^{n+1}$ and improved convergence. An added benefit of smaller time steps is that the diagonal terms of $\mathbf{J}$ are frequently proportional to $1/\Delta t^{n+1}$, and the linear system in Eq. [17] becomes easier to solve as these diagonal terms become more dominant (Söderlind, 2006).

Picard iteration and modified Picard iteration can be recast as Newton's method with an approximate Jacobian (Paniconi and Putti, 1994) and so inherit this local nature. Like other modified and inexact Newton's methods (Kelley, 1995), they trade reduced convergence rates in hope of gains in simplicity, efficiency, and possibly robustness since the need for derivatives of nonlinear soil constitutive relations is either eliminated (classical Picard) or reduced (modified Picard) (Lehmann and Ackerer, 1998). Another approach to reduce the impact of highly nonlinear constitutive relations on Newton convergence is to switch the primary variable between water content in drier regions and capillary head elsewhere (Forsyth et al., 1995).

An interesting alternative to Newton or Picard methods is the relaxation scheme used in Pop et al. (2004) as an approach for linearizing mixed finite element approximations for Richards' equation. It introduces a global, regularizing term into the linearized problem for $\mathbf{G}^{n+1}$ and exploits the monotonicity of soil-moisture constitutive relationships to secure robust convergence behavior with potentially less restrictive time step constraints and better conditioned linear systems than Newton or modified Picard approaches (Slodicka, 2002; List and Radu, 2016).

The issues associated with the local nature of Newton's method and its variants are not unique to Richards' equation and the need for additional modifications (so-called globalization techniques) like line-search and trust-region methods (Kelley, 1995; Jones and Woodward, 2001; Knoll and Keyes, 2004; Wang and Tchelepi, 2013) has been recognized in the broader community. There has also been renewed interest in acceleration techniques like Anderson acceleration (Walker and Ni, 2011), which can be seen as an approach to improve the quality of Picard (fixed-point) iterates by exploiting the nonlinear residual history using Krylov subspace techniques (Lott et al., 2012). Finally, a globalization approach that has been considered by several researchers is to marry Newton's method with a slower converging technique like Picard iteration (Lehmann and Ackerer, 1998; Bergamaschi et al., 1999) or the scheme from Pop et al. (2004) to improve robustness for poor initial guesses while recapturing quadratic convergence as intermediate iterates approach the true solution (List and Radu, 2016).

As discussed above, the choice of time step naturally impacts nonlinear solver performance (Gustafsson and Söderlind, 1997), and Richards' equation solvers that use an implicit time discretization must negotiate a balance between the size of time step that can be taken and the difficulty of the resulting nonlinear system. For large problems, the linear systems that must be solved at each nonlinear iteration must be solved iteratively as well. The most frequently used iterative linear solvers are Krylov based. Briefly, Krylov subspace methods for the linear system $\mathbf{Ax} = \mathbf{b}$ search for a solution at iteration j in the Krylov space,

$$\mathrm{K}_j = \mathrm{span}\left(\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \mathbf{A}^2\mathbf{r}_0, \ \ldots, \ \mathbf{A}^{j-1}\mathbf{r}_0\right) \qquad [18]$$

where $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$. Conjugate Gradients are the canonical Krylov method and can be related to a minimization problem over K_j for a symmetric, positive definite $\mathbf{A}$. For non-symmetric matrices, which is typically the case with $\mathbf{J}$ unless Picard iteration is used, methods like Generalized Minimal RESidual (GMRES) or Bi-Conjugate Gradient STABilized (BiCGSTAB) are required (Saad and van der Vorst, 2000). The time spent in solution of this system is usually the dominant expense in the linearization process for large problems (Tocci et al., 1998; Jones and Woodward, 2001)

A similar need to manage the interplay between the temporal approximation, initial guess, and nonlinear problem, $\mathbf{G}^{(n+1)} = 0$, plays out in the resulting linearized problem through the conditioning of $\mathbf{J}$. That is, direct (e.g., LU-based) solvers are essentially global and seldom fail unless the linear problem is extremely ill-conditioned. Sparse direct solvers saw much improvement during the previous decade (Hénon et al., 2002; Li, 2005) and are practical for many two-dimensional problems and moderate three-dimensional problems (Farthing et al., 2003a). However, they are still unable to handle large, coupled three-dimensional problems where iterative, Krylov-based techniques are required (Knoll and Keyes, 2004). The performance of Krylov methods in turn depends largely on effective preconditioning techniques. There have been efforts to develop or apply robust, scalable preconditioners for Richards' equation (Jenkins et al., 2001; Jones and Woodward, 2001), and high-quality software packages like PETSc provide access to a number of modern preconditioners as well as linear and nonlinear solvers (Balay et al., 1997). However, uniformly robust preconditioning techniques and nonlinear solver performance for Richards' equation for remains an open research topic (Juncu et al., 2011; Lipnikov et al., 2016).

For example, rather than attempt to extend or modify existing preconditioners like geometric and algebraic multigrid to the linearized systems arising from standard discretizations of Richards' equation, the work of Berninger et al. (2011) takes an alternate view and modifies the underlying discretization to realize the performance of multigrid for classical linear self-adjoint problems. That is, introducing a Kirchoff (or matric flux potential) transform for homogeneous media (Williams et al., 2000)

$$u(\psi) = \int_{-\infty}^{\psi} K(p)\,dp \qquad [19]$$

has the effect of linearizing the gradient term in Darcy's law through the chain rule $\nabla u = K(\psi)\nabla\psi$. Together with temporally explicit treatment of gravitational terms, this produces a system that is equivalent to a convex minimization problem and for which a class of nonlinear multigrid techniques are well-behaved

(Kornhuber, 2002). While this suffices for homogeneous domains, additional conditions based on conserving mass (via flux matching) and maintaining continuity of pressure at material interfaces are required for heterogeneous domains. The nonlinearity of these transmission conditions also requires a more complex, nonlinear substructuring domain-decomposition approach (Berninger et al., 2014).

Finally, for large problems with iterative solvers there is the need to manage not just the impact of the time step on the difficulty of the nonlinear system, but also its impact on the resulting linear problems, which are often better conditioned for smaller time steps. Moreover, clear efficiency gains are possible by coordinating the linear and nonlinear solver tolerances dynamically to avoid over-solving intermediate linear systems (Tocci et al., 1998; Eisenstat and Walker, 1996).

DISCUSSION AND ALTERNATIVES

Computational inefficiency and lack of robustness in Richards' equation solvers used in practice most often manifest as poor linear and nonlinear solver convergence and/or poor performance of the time integrator. Our view is that a significant portion of this poor convergence and instability arises from under resolution in space of sharp fronts or other phenomena where highly nonlinear soil properties change drastically over neighboring elements or cells. However, the spatial component of this behavior is not as readily apparent because estimates or indicators of spatial accuracy are more difficult to obtain than the convergence estimates and temporal error indicators that are available for classical iterative linear and nonlinear techniques and many time discretizations. Indeed, as discussed above, the vast majority of spatial discretizations used in practice are based on classical low-order finite element discretizations and cell-centered finite differences and are combined with evaluation techniques for soil constitutive relations like mass-lumping and upwinding that are designed to favor robustness over accuracy.

One way to increase computational efficiency at the expense of solution validity is to use resolutions considerably coarser than the REV scale dictates. This requires the use of so-called "effective" parameter values that diverge from physical reality as the computational scale increases, and results in large errors in the simulation's representation of the physical system even though it has converged. We hope instead that there will be continued development and adoption of new spatial and temporal discretization schemes. Following trends of maturing computational fields, we expect to see improved, adaptive algorithms driven by solution dynamics and a posteriori error estimates (Mostaghimi et al., 2015; Baron et al., 2017). Moreover, approaches are needed that consider entire solution error and dynamics–for example, joint space-time discretization and error control (Solin and Kuraz, 2011) rather than just a MOL approach with temporal adaptivity but static spatial approximation (Farthing et al., 2003b). While the implementation of full spatially and temporally adaptive techniques is a clear hurdle, the proper location of high-resolution space should also improve robustness and accuracy in many cases.

Similarly, many of the issues with robustness of Richards' equation solvers may be addressed with better understanding of the dynamic interplay between temporal approximation and linearization techniques. As discussed above, researchers have tried to manage these dynamics through the time step (Tocci et al., 1997; Kavetski et al., 2002; D'Haese et al., 2007) and/or linearization technique (Paniconi and Putti, 1994; Lehmann and Ackerer, 1998; Lipnikov et al., 2016). Alternative linearization approaches (e.g., List and Radu, 2016) and better algorithms for managing the complex dynamics of adaptive solvers taken, for example, from control-theory (Bhaya and Kaszkurewicz, 2006) could directly improve existing production codes and also lower the barrier to adoption of more accurate spatial approximations.

We believe the notions of computational stability and proportionality are useful concepts to guide the development of modern Richards' equation solvers. Simulators for Richards' equation should have clearly defined input parameters for controlling their accuracy, and changes in these parameters should reliably increase (or decrease) accuracy and computational expense at a predictable rate. In other words, tightening an error tolerance slightly should lead to a commensurate decrease in error without excessive increases in run time (Söderlind and Wang, 2006).

The idea of computational stability follows the line of introducing mathematical concepts like continuous data dependence and well-posedness to computational software. The need for more rigorous computational science with standards like reproducibility and repeatability of numerical experiments has been recognized across a number of fields (Collberg and Proebsting, 2016). It can be seen, for example, in efforts to develop clear understanding of benchmarking, verification, and validation for computational codes in fields like nuclear engineering and aerospace engineering (Babuska and Oden, 2004; Oberkampf and Trucano, 2007). A key component of such efforts is a suite of test problems identified and accepted by the community that allows fair evaluation and comparison of numerical techniques and simulation codes. While several test problems recur throughout the literature and isolated comparisons can be found, the community has lacked a central repository of benchmark problems or recurring efforts to compare results across research groups as can be found in other fields (e.g., American Institute of Aeronautics and Astronautics, 1998; Larson et al., 2014; American Society of Mechanical Engineers, 2017; International Association for the Engineering Modelling, Analysis and Simulation Community, http://www.nafems.org [verified 14 Sept. 2017]). The recent integrated hydrologic model comparison project (Maxwell et al., 2014; Kollet et al., 2017) and the International Soil Modeling Consortium (http://soil-modeling.org; verified 10 Feb. 2017) represent welcome steps in this direction. This is also an area where government agencies (e.g., NOAA, the US National Weather Service, Office of Water Prediction) could make a major contribution.

Even as we work to improve the numerics, there continues to be reason to evaluate Richards' equation as a formulation for unsaturated flow. Problems where gas-phase dynamics are important usually demand a full two-phase formulation (Helmig, 2011; Smits et al., 2013), while more recent work on thermodynamically constrained averaging theory has focused on developing a consistent upscaling framework for deriving extensions to Richards' equation (Bronson, 2014; Gray and Miller, 2014). These approaches are primarily aimed at extending the operational range of validity for the mathematical system as a representation for unsaturated flow (Or et al., 2015). In some cases, new formulations or closure schemes may introduce additional challenges for numerical schemes due to new terms with additional, nonlinear coupling and complexity. On the other hand, it is also possible that some numerical difficulties are unintended side effects of inadequate formulations rather than being inherent to the unsaturated flow problem.

In a different direction, recent work to derive alternative formulations that trade some of the generality of the traditional Richards' equation solution for gains in speed and reliability has shown success. It is possible, for example, to convert Richards' equation into a formulation for the evolution of soil moisture front location with θ as the independent variable under suitable assumptions (Philip, 1957; Swartzendruber, 1969). Ogden et al. (2017) converted the one-dimensional Richards' equation into a form that they call the Soil Moisture Velocity Equation (SMVE) that describes the speed of propagation of particular moisture contents within a homogeneous soil layer:

$$\left(\frac{dz}{dt}\right)_{\theta} = \frac{-\partial K(\theta)}{\partial \theta}\left(\frac{\partial \psi(\theta)}{\partial z} - 1\right) - D(\theta)\frac{\partial^2 \psi / \partial z^2}{\partial \psi / \partial z} \qquad [20]$$

Equation [20] is equivalent to the one-dimensional Richards equation. This equation separates the flux due to gravity and the integrated wetting front capillary drive from the flux caused by the shape of the wetting front. The first term on the right-hand side Eq. [20], which is called the "advection-like" term, was derived by Ogden et al. (2015a). The second term on the right-hand side of Eq. [20], called the "diffusion-like" term, is equal to a diffusive flux due to the second spatial derivative of capillary head divided by the slope of the capillary head along the wetting front. This diffusion-like term will be zero when the gradient of the capillarity is a constant along lines of constant θ, or in the case of a sharp wetting front when $\partial\psi/\partial z = \infty$. Both of these cases represent situations that can cause convergence difficulties in Richards' equation solvers.

Fluxes calculated using the SMVE advection-like term agree very closely with the numerical solution of Richards' equation (Ogden et al., 2015a), data from column experiments (Ogden et al., 2015b) and exact analytical solutions (Ogden et al., 2017). Results in all cases show that the diffusion-like term in Eq. [20] is negligible unless one is interested in the exact shape of the wetting front. Most importantly, the advection-like term of the SMVE can be converted into an ODE using the MOL and solved using a finite moisture-content discretization that divides the vadose zone into N regions of thickness $\Delta\theta$ called "bins" (Talbot and Ogden, 2008).

That resulting ODE for infiltrating water is (Ogden et al., 2015a):

$$\left(\frac{dz}{dt}\right)_j = \frac{K(\theta_d) - K(\theta_i)}{\theta_d - \theta_i}\left(\frac{|\psi(\theta_d)| + h_p}{z_j} + 1\right) \qquad [21]$$

where j is the bin index, θ_d is the moisture content of the bin containing the highest moisture content, θ_i is the initial moisture content, h_p is the ponded depth if existent, and z_j is the depth to the wetting front in the jth finite moisture content bin. Note that the ODE solution of Eq. [21] requires evaluation of no spatial derivatives, eliminating what is a source of difficulty in the traditional solution of Richards' equation. Equation [21] can be solved using an explicit forward Euler scheme or other traditional ODE solutions such as Runge-Kutta. This ODE is guaranteed to converge and to conserve mass using a finite volume solution. While the SMVE solution method is at present limited to one-dimensional infiltration in homogeneous soil layers, the reliable, accurate and efficient ODE solution are major advantages. Furthermore, Eq. [21] will solve sharp wetting fronts with no difficulty and is not degenerate, making the method well suited for use in Earth System and large-scale models of land-atmosphere interaction.

CONCLUSIONS

We provided a high-level overview of numerical methods for the solution of Richards' equation with an eye toward summarizing previous work and identifying major trends. A recurring theme is the need to balance speed, robustness, and accuracy. Historically, the dominant approaches have been low order in space and time and used fixed spatial grids or meshes. This has set up an unfortunate tension in many cases between accuracy and robustness– or at least ease of convergence. Loosening tolerances and coarsening resolution are expedient, but unreliable, ways to improve speed or achieve convergence that have a negative effect on solution accuracy and realism. The pursuit of improved numerical methods has largely been about reducing this tension and increasing computational efficiency rigorously.

We hope to see continued development and research into the numerical solution of Richards' equation. Indeed, we believe it is essential if application of Richards' equation to large-scale problems at valid discretizations is to become commonplace. Successful Richards' equation solvers in the future will likely be adaptive in space and time, while efficiently managing the interplay between discretizations on the one hand and linear and/or nonlinear algebra solvers on the other. The recent identification of the Soil Moisture Velocity Equation (Eq. [20]) indicates that, at least in the case of one-dimensional solutions of Richards' equation, there may be novel approaches yet to be discovered. The most likely way for this development to continue is to encourage the exchange of ideas and techniques with the applied mathematics, computational mechanics, computer science and Earth Science communities. Improved software

engineering and creation of archival verification and validation data sets for use by the community are also essential if we are to proceed rationally and make the most of our efforts.

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