Transformation Approaches for Simulating Flow in Variably Saturated Porous Media

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Abstract.   Sharp fronts with rapid changes in fluid saturations over short distance and time scales often exist in multiphase flow in subsurface systems. Such highly nonlinear problems are notoriously difficult to solve, and standard solution approaches are often inefficient and unreliable. We summarize four existing and one new transformation method (IT2) for solving Richards' equation within a common framework and compare performance for a wide range of media properties. We show that: transformation methods can significantly improve solution efficiency and robustness compared to standard solution approaches; transformation parameters depend upon auxiliary conditions, media properties, and spatial and temporal discretization; and IT2 compares favorably with existing transforms.

1. Introduction

Modeling flow of multiple fluids in subsurface systems is an important water resources problem for which many unresolved questions remain [*Miller et al.*, 1997]. Resolving sharp fronts of a dependent variable as a function of space and time is a particularly challenging aspect of this class of problems. These fronts can develop when a more viscous wetting phase displaces a less viscous non-wetting phase, as when water infiltrates a porous media that is initially relatively dry, resulting in sharp fronts in volumetric fractions of the fluid phases for certain media properties and auxiliary conditions.

While such sharp fronts result from many possible combinations of conservation laws and constitutive relations of interest in multiphase flow problems, Richards' equation (RE) with common constitutive relations is a simple case of substantial practical importance where this difficult class of problems can arise [*Miller and Kelley*, 1994; *Tocci et al.*, 1997]. Because of this, RE is a good test problem, although it is understood that significant theoretical questions remain unresolved about its adequacy for describing unsaturated flow [*Gray and Hassanizadeh*, 1991a; *Gray and Hassanizadeh*, 1991b; *Miller et al.*, 1997].

Sharp volumetric fluid-phase fraction fronts result in part from nonlinearities in constitutive relations that describe the interdependence of fluid pressures, saturations, and conductivities. These nonlinearities are present in discretized forms of the governing equations that are solved. Accurate resolution of these sharp fronts can require fine discretizations in space and time, and can lead to systems of nonlinear algebraic equations that are difficult to solve. Choosing discretization or nonlinear solution methods inappropriately can lead to inefficient or unreliable approximate solution approaches.

Several approaches to these problems can be grouped together under the rubric of transformation methods. Transformation methods seek to reduce the sharpness of a

front in a problem through the identification and application of an appropriate change
of variable applied to the dependent variable. The original problem's solution may then
be retrieved by applying an inverse transformation.

While several transformation methods have been applied to RE with some success,
we lack detailed investigations, comparisons, and guidance for the applying these
approaches generally. Further, some of the transformation methods applied to date
include a parameter(s) that must be specified, and the effect of the parameter's value
on solution efficiency and robustness is often unknown. These difficulties provide a
barrier to the routine application of transformation methods for solving RE and other
multiphase flow problems.

The goal of this work is to advance the current understanding of transformation
approaches for solving Richards' equation. The specific objectives of this work are (1)
to develop a framework to summarize transformation methods for solving RE; (2) to
identify key components of a solution approach for RE that may affect the efficiency
and robustness of the resulting approximation; (3) to compare existing transformation
methods for a range of media and auxiliary conditions; (4) to investigate the importance
of parameter selection on the efficiency of parameterized transformation methods; (5) to
identify and evaluate a new transform for a wide range of test problems; and (6) to give
guidance for the application of transformation methods to solve RE.

2. Background

Transformation methods for solving RE have existed for several decades [*Rubin,*
1968; *Raats and Gardner,* 1974; *Haverkamp et al.,* 1977; *Baca et al.,* 1978; *Vauclin et
al.,* 1979]. The general objective of transformation methods is to overcome inefficiencies
in the numerical solution process—inefficiencies caused by the strong nonlinearity of the
media hydraulic properties as functions of pressure, particularly in the case of infiltration
into a media that is initially relatively dry. These types of infiltration problems give rise

to very high water pressure gradients near the wetting front and lead to computationally inefficient numerical solutions when using standard techniques. Prohibitively small time step sizes or a large number of nonlinear iterations are often required for such problems. Combining transform methods with iterative, implicit, mass-conserving numerical methods results in more efficient solutions. Current transformations include integral [*Haverkamp et al.*, 1977], hyperbolic function [*Ross*, 1990], variable switching [*Kirkland et al.*, 1992; *Forsyth et al.*, 1995], and rational function transformations [*Pan and Wierenga*, 1995].

Early attempts at transformation methods used an integral transform commonly referred to as the Kirchoff integral transformation (IT1) [*Rubin*, 1968; *Raats and Gardner*, 1974; *Vauclin et al.*, 1979; *Haverkamp et al.*, 1977; *Redinger et al.*, 1984; *Campbell*, 1985]. This transformation directly reduces the nonlinearity of the conductivity terms in RE and, as a result, is effective in reducing the number of nonlinear iterations required for a solution, under certain conditions. However, IT1 depends on media hydraulic properties and will therefore vary spatially if the hydraulic properties do so. Thus, simple application of IT1 is restricted to homogeneous media. Corrections can be made to adapt IT1 to layered and gradational media by adding a flux balancing correction [*Ross and Bristow*, 1990]. IT1 is also more complex to implement, since an analytic function of the inverse is generally not available.

Solving the water-content-based form of RE can result in significantly improved performance compared to the traditional pressure-based methods [*Hills et al.*, 1989]. This is due to the fact that the media hydraulic functions are less nonlinear when expressed in terms of water content than when expressed in terms of pressure, particularly when modeling infiltration into a relatively dry media. Thus numerical solutions using the water-content-based RE generally require fewer nonlinear iterations. The limitation of this approach is that the water-content-based RE cannot be used to solve infiltration problems involving saturated regions. A θ-based transform (THT) is

an attempt to retain the advantages of water-content-based methods while remaining applicable to media containing saturated or near-saturated regions. THT's include the affine transformation of θ approach [*Kirkland et al.*, 1992] as well as the primary variable switching technique [*Forsyth et al.*, 1995]. The THT has the characteristics of water content when the media is unsaturated and of pressure when the media is at or near saturation. This approach has shown roughly the same reduction in nonlinear iterations as in the water-content-based solution. Since the THT is defined in terms of volumetric water fraction, it will vary spatially if the media type does so. As is the case with IT1, simple application of THT is restricted to homogeneous media.

Because direct application of IT1 and THT is restricted to homogeneous media, an alternate class of transforms was developed that would be directly applicable to heterogeneous media. These transforms are defined strictly in terms of ψ and arbitrary parameter(s). Since ψ is continuous across the boundaries between different media types, these transform functions will be continuous variables in heterogeneous media, provided that the parameters remain constant across media types. The first such transform dates back to a simple log transform [*Baca et al.*, 1978]. This was effective, but a more general and efficient transform, defined in terms of the hyperbolic sine function (HST), was subsequently introduced [*Ross*, 1990]. HST reduces computational expense, but it introduces two arbitrary parameters. It is recommended [*Ross*, 1990] that one of the parameters be fixed at a constant percentage of the other to reduce HST to one arbitrary parameter [*Ross*, 1990]. However, to optimize the HST completely for a given problem, the two parameters must remain arbitrary. Since the introduction of HST, another of this class of transforms has been proposed. This transform is defined in terms of a rational function (RFT) of ψ [*Pan and Wierenga*, 1995]. The RFT provides performance improvements similar to HST, but introduces only one arbitrary parameter.

Because all of the transforms except IT1 involve arbitrary parameters, selecting parameter values is important to determine the efficiency of a particular transformation.

The literature to date lacks rigorous optimization of transform parameters over a wide range of test problems. The literature suggests that selection of HST [*Ross, 1990*] and RFT parameters [*Pan and Wierenga, 1995*] for optimal or near-optimal performance is independent of media properties, but this claim must be verified through formal optimization and sensitivity analysis. Such analysis is critical in determining the efficiency and robustness of a given transformation but has not been reported in the literature to date. If the data suggest a relationship between effective transform parameters and media properties for the HST and RFT type transformations, then the advantage that these transforms are applicable in their current form to heterogeneous media conditions becomes less certain.

3. Formulation

3.1. 1D Richards' Equation

We consider one-dimensional (1D) infiltration in this work, beginning with a general, p version of the 1D RE. For the case in which fluid compressibility is included for a vertical system, the p version of the common mixed form equation is given by

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

where S_s is the specific storage coefficient, which accounts for fluid compressibility; S_a is saturation of the aqueous phase; $p = p(\psi)$ is a general transformation function; ψ is the pressure head; t is time; θ is the volumetric water 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

$$p (z, t = 0) = p_0 (z) = p (\psi_0 (z)) \tag{2}$$

$$p (z = 0, t > 0) = p_1 = p (\psi_1) \tag{3}$$

$$p (z = Z, t > 0) = p_2 = p (\psi_2) \tag{4}$$

where Z is the length of the domain, ψ_0 may be a function of space, and ψ_1 and ψ_2 are constants. The auxiliary conditions p_0, p_1, and p_2 are found by the appropriate change of variables of the initial and boundary conditions given in terms of ψ.

3.2. Constitutive Relations

Solution of RE requires constitutive relations to describe the interdependence among pressure, saturation, and hydraulic conductivity. For the purpose of this work, we use the well-known van Genuchten (VG) pressure-saturation relationship [*van Genuchten,* 1980], given by

$$S_e\left(\psi\right) = \frac{\theta_a\left(\psi\right) - \theta_r}{\theta_s - \theta_r} = \begin{cases} \left(1 + |\alpha_v \psi|^{n_v}\right)^{-m_v}, & \psi < 0 \\ 1, & \psi \geq 0 \end{cases} \tag{5}$$

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; and α_v and n_v are experimentally determined coefficients in the VG p-S model, which are related to the mean pore size and the uniformity of the pore size distribution, respectively.

The saturation-permeability relation for the aqueous, or wetting phase, is described using Mualem's model [*Mualem,* 1976]

$$K\left(S_e\right) = K_s S_e^{1/2} \left[1 - \left(1 - S_e^{1/m_v}\right)^{m_v}\right]^2 \tag{6}$$

where K_s is the water-saturated hydraulic conductivity, and $S_e = S_e(\psi)$ from (5).

3.3. Transform Definitions

Starting from the general p version of the 1D RE (1), the more commonly used mixed, ψ-based, and θ-based (water-content-based) forms of RE can be retrieved. The basic idea behind the transformation approach is to define a function $p(\psi)$ that will result in a more efficient and robust solution to the governing equation, (1). Several transformations have been developed to date, and the definitions of $p(\psi)$ for each are listed in Table 1. Arbitrary parameters are represented by β and β_1.

Table 1

THT and IT1 linearize either the temporal or spatial derivative term in RE, respectively. While it is not possible to linearize both the temporal and spatial terms in RE completely, the efficiency and accuracy of the numerical solution can be significantly enhanced by choosing a transform that achieves the proper balance between linearization of temporal and spatial terms. RFT and HST can partially linearize both temporal and spatial terms; they are defined explicitly in terms of ψ instead of K or θ. This allows for a straightforward application for heterogeneous media, but such applications will be effective only if the arbitrary parameter is not dependent upon and sensitive to the given media parameters.

As an alternative to extant transforms, we tested several alternative transforms in an attempt to find one that would effectively balance the linearization of temporal and spatial terms and would not be as sensitive to changes in media parameters. We evaluated higher-order rational functions, exponential-based functions, and integral functions. We looked at transforms defined explicitly in terms of ψ as well as those that included media hydraulic functions K and θ in their definitions. Based upon our evaluation, we have found an integral transform that is effective in terms of efficiency and robustness. This transform, IT2, is defined in terms of θ and the integral of K.

Note that all of the transform functions are C^1 continuous functions of ψ and have non-zero derivatives for all values of ψ; i.e., $\partial p / \partial \psi \neq 0$. These conditions are necessary for accurate and efficient solution of (1). Note also that for the case of $\beta = 0$, IT2 reduces to IT1. Thus, IT1 is a subset of IT2.

4. APPROACHES

4.1. Spatial and Temporal Approximation

The numerical solution of (1) begins with a discrete formulation, for which we use a spatially-centered, fully-implicit finite difference approximation. For the spatial domain

[0,Z], a uniform grid is defined with $n_n - 1$ 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 $1 \leq i \leq n_n$. (1) is then approximated for $1 < i < n_n$ as

$$\frac{1}{\Delta t}\left[\theta_i^{l+1} - \theta_i^l + \left(S_s S_a \frac{\partial \psi}{\partial p}\right)_i^{l+1}\left(p_i^{l+1} - p_i^l\right)\right] =$$
$$\frac{1}{\Delta z^2}\left[\left(K\frac{\partial \psi}{\partial p}\right)_{i+1/2}^{l+1}\left(p_{i+1}^{l+1} - p_i^{l+1}\right) - \left(K\frac{\partial \psi}{\partial p}\right)_{i-1/2}^{l+1}\left(p_i^{l+1} - p_{i-1}^{l+1}\right)\right] +$$
$$\frac{1}{\Delta z}\left[K_{i+1/2}^{l+1} - K_{i-1/2}^{l+1}\right] \tag{7}$$

where n_n is the number of spatial nodes in the solution, p_i is the approximation to the solution $p(z_i)$, l indicates time level, and $K_{i\pm1/2}^{l+1}$ are interblock conductivities estimated from known values of $K(p_{i-1}^{l+1})$, $K(p_i^{l+1})$, and $K(p_{i+1}^{l+1})$.

Of the several ways to estimate interblock conductivities [*Haverkamp and Vauclin,* 1979; *Zaidel and Russo,* 1992; *Warrick,* 1991], we investigated four approaches. The first approach we used was the arithmetic mean technique (KAM):

$$K_{i\pm1/2} = (K_i + K_{i\pm1})/2 \tag{8}$$

KAM has been used routinely [*Haverkamp and Vauclin,* 1979; *Warrick,* 1991; *Zaidel and Russo,* 1992] and is simple and inexpensive to compute.

Due to the nonlinearity of ψ, the interblock conductivity estimation technique defined by $K[(\psi_i + \psi_{i\pm1})/2]$ is ineffective. Nonlinear solvers will often fail at small simulation times when using this approach. But since the transformed variable p will be somewhat smoother in terms of the spatial dimension, the second approach we used was the transformed analog of this approach, i.e., conductivity evaluation at the arithmetic mean of the transformed variable p (KAMP). KAMP is defined as

$$K_{i\pm1/2} = K\left[(p_i + p_{i\pm1})/2\right] \tag{9}$$

Because K varies in space as a function of ψ, an integral representation of mean interblock values can be computed [*Warrick,* 1991; *Zaidel and Russo,* 1992]. The third

approach we used is an integral representation in transformed space (KINT):

$$K_{i\pm1/2} = \begin{cases} \dfrac{\int_{min\{p_i,p_{i\pm1}\}}^{max\{p_i,p_{i\pm1}\}} \left(K\frac{d\psi}{dp}\right)dp}{\int_{min\{p_i,p_{i\pm1}\}}^{max\{p_i,p_{i\pm1}\}} \left(\frac{d\psi}{dp}\right)dp}, & \text{if } p_i \neq p_{i\pm1} \\ K_i, & \text{if } p_i = p_{i\pm1} \end{cases} \tag{10}$$

This approach has not been widely used for the solution of RE because of the apparent expense involved in computing the integrals. This approach has not been used in a transform solution to RE to our knowledge.

The fourth approach we used for estimating interblock conductivities is termed the arithmetic mean saturation (KAMS) [*Zaidel and Russo,* 1992] and is computed by

$$K_{i\pm1/2} = K\left[\left(S_{e_i} + S_{e_{i\pm1}}\right)/2\right] \tag{11}$$

This technique is easy to implement but if spline approximations are used, this approach is most efficiently implemented by splining in terms of S_e, which itself is splined in terms of p. This results in some added expense. Spline issues are discussed in more detail below.

4.2. Nonlinear Solution Methods

To find an approximating solution $\{p_i; 1 \leq i \leq n_n\}$ to (7) requires solving a system of nonlinear equations. For the purpose of this work, we use either modified Picard iteration (MPI) [*Celia et al.,* 1990] or full Newton iteration (NI). The MPI technique produces a simple computational algorithm that is mass conserving for numerical approximations that preserve spatial symmetry.

The NI system is formed from (7) by defining

$$\begin{aligned} f_i &= \frac{1}{\Delta t}\left[\theta_i^{l+1} - \theta_i^l + \left(S_s S_a \frac{\partial\psi}{\partial p}\right)_i^{l+1} \left(p_i^{l+1} - p_i^l\right)\right] \\ &\quad - \frac{1}{\Delta z^2}\left[\left(K\frac{\partial\psi}{\partial p}\right)_{i+1/2}^{l+1} \left(p_{i+1}^{l+1} - p_i^{l+1}\right) - \left(K\frac{\partial\psi}{\partial p}\right)_{i-1/2}^{l+1} \left(p_i^{l+1} - p_{i-1}^{l+1}\right)\right] \\ &\quad - \frac{1}{\Delta z}\left[K_{i+1/2}^{l+1} - K_{i-1/2}^{l+1}\right] \end{aligned} \tag{12}$$

and then solving for $f(p) = 0$ by Newton iteration

$$[J]\{\Delta p\} = -\{f\} \tag{13}$$

where $[J]$ is the Jacobian. NI applied to a solution algorithm that uses fixed time steps is not an effective strategy, since reliable convergence often requires very small time steps. We overcome this problem by using a quadratic/cubic line search technique [*Dennis and Schnabel*, 1996] in concert with NI, which we term a NI-line search (NILS) approach. NILS is much more robust than NI.

We terminated the nonlinear solvers based on an absolute error measure of p. Thus, if the ranges of the various transforms are not equal, those with smaller ranges will tend to converge sooner, though often with increased error. To avoid this potential problem, the transforms were normalized so that the ranges of each are equivalent; i.e., each of the transform functions maps the domain $[\psi_{min}, \psi_m]$ onto the range $[0, p_m]$, where $\psi_m = min[0, \psi_{max}]$, and $p_m = \psi_m - \psi_{min}$.

4.3. Efficiency Considerations and Evaluation

We define efficiency as the computational effort required to achieve a specified accuracy. The evaluation of constitutive relations requires a significant amount of computational effort using the standard approach for solving RE. Therefore these relations are often evaluated, the values stored in tables, and intermediate values determined by linear, cubic, or Hermite spline interpolation. This procedure results in a significant savings in computational effort compared to direct function evaluations without a significant change in the accuracy of the solution. Based upon our previous work and some additional screening for transformed solutions, we used Hermite splines in this work, which are described in detail elsewhere [*Miller et al.,*].

Table interpolation reduces computational effort even more for transformation approaches than for standard approaches for solving RE. This is especially so for the

more complex transforms such as IT2, which would require the determination of roots within a numerical integration procedure. Table interpolation greatly reduces the computational effort per iteration, although this effort is still greater than the effort required for a table interpolation approach to an untransformed solution. The difference in effort between a transformed and an untransformed approach depends upon the nonlinear solution scheme used, although this difference is usually less than 50% per iteration. Clearly then, transformation methods must require fewer iterations than untransformed solutions in order to be more efficient.

Error vs. work plots are used to compare the various transforms in terms of efficiency, robustness, and parameter sensitivity. These plots not only show the overall effectiveness of a given transform in terms of speed and accuracy over a wide range of media conditions, they also serve to illustrate optimal parameter range and parameter sensitivity. To compare the transformation approaches to the traditional untransformed approach, the cost per iteration used to calculate work as a function of nonlinear iterations is adjusted to account for the additional effort required in the transformed solution approach.

For methods based upon the MPI approach, the work primarily concerns forming the coefficient matrix and right hand side vector, and solving the linear systems of equations. This observation allows for a simple, straightforward measure of work that requires relative weights for the two procedures and integer counts for each of the procedures, such as

$$W_p = w_c n_c + w_l n_l \tag{14}$$

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, and n_l is the number of linear solutions performed. As reported in previous work [*Tocci et al.*, 1997], estimates of

the weighting coefficients based on detailed profiling results for the untransformed RE using MPI solver, KINT permeability approximations, and Hermite spline interpolation are $(w_c)_{ut} = 0.530$ and $(w_l)_{ut} = 0.181$. We performed similar profiling tests using the transformation approach and, based on these results, our estimates for the solution of the transformed RE using MPI, KINT, and Hermite splines are $(w_c)_{tr} = 0.743$ and $(w_l)_{tr} = 0.181$. Thus for this case, the transformation approach requires about 30% more effort per iteration than the untransformed solution.

Error was evaluated by comparison to a dense-grid solution. This error, referred to as dense-grid error, is defined by

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

where k is the norm measure and $\hat{y}_i$ is an accurate approximation of the true solution based on a dense spatial grid. $k = 1$, $k = 2$, and $k = \infty$ were considered in this work and termed L_1, L_2, and L_∞ error norms, respectively. The dense grid solutions were generated using the MPI solver with temporal and spatial grid sizes equal to $1/32$ of the standard sizes listed in Tables 2 and 3.

4.4. Parameter Optimization

The parameters for any of the transformations can be optimized for some performance-based objective function such as amount of work required or dense-grid error. In this work, we use the objective function

$$\min_{\beta_{min} \leq \beta \leq \beta_{max}} \left\{ W_p \left(\beta \right) \times \| \epsilon_D \left(\beta \right) \|_1 \right\} \tag{16}$$

where β is the arbitrary transform parameter, W_p is the required work as defined by Equation (14), and $\| \epsilon_D \|_1$ is the dense-grid error as defined by Equation (15).

For the parameter optimization of the work, we used the nonlinear optimization package IFFCO [*Gilmore and Kelley, 1993*]. IFFCO is a projected quasi-Newton

algorithm that uses a decreasing sequence of finite difference steps (scales) to approximate the gradient. It uses an approximation to the Hessian and a line search algorithm that gives the code global convergence capabilities.

4.5. Test Problems

We compared the transformation approaches for solving RE to traditional solution methods using eight sets of test conditions, which are summarized in Tables 2 and 3. Four of these conditions (Problems A–D) have been used previously in the literature as test problems [*Miller and Kelley,* 1994] [*Celia et al.,* 1990; *Rathfelder and Abriola,* 1994] [*Forsyth et al.,* 1995]. Problems E–H represent various soil textural groups sand, loamy sand, loam, and clay loam, respectively, according to the USDA classification [*Soil Conservation Service,* 1975] as estimated by Carsel and Parrish [*Carsel and Parrish,* 1988] from analyses of a large number of soils.

With the exception of Problems C and D, each set of simulation conditions yields a difficult sharp-front problem with relatively dry initial conditions. Problems C and D were considered because they offer an excellent benchmark for comparing our results to recent research performed using state-of-the-art methods. However, Problems C and D are substantially easier than the remaining problems because the domain is much smaller, the initial conditions are less severe, and (for Problem C) fully saturated conditions do not develop.

To illustrate the effect of the transformation approach on resulting solution profiles, sample results are plotted for Problem A. Figure 1 shows the solution in terms of the untransformed pressure head ψ at various simulation times. Figure 2 shows the solution in terms of the transformed variable p at various simulation times, using the optimized IT2 transform. Clearly, the infiltration profile is smoother when plotted in terms of the transformed variable p.

Tables 2 and

Figure 1

Figure 2

5. Results and Discussion

The number of transforms (four), interblock conductivity methods (four), nonlinear solution methods (two), test problems (eight), and other variables of concern, such as spatial and temporal discretization combine to yield a large number of possible combinations. While several thousand simulations were performed in this work, a complete analysis of each of these variables was beyond the scope of this effort. In the sections that follow we report on results of: (1) baseline comparisons for interblock conductivity and nonlinear solution methods; (2) performance comparisons for all transforms and test problems using a single nonlinear solver and interblock conductivity method; and (3) the sensitivity of the transform parameter, β, to spatial and temporal discretization levels.

5.1. Baseline Comparisons

For each of the eight test problems, baseline comparisons were made for simulations incorporating all possible combinations of transformation, interblock conductivity estimation, and nonlinear solver. All of the simulations were made using fixed time steps and one arbitrary transformation parameter. For the case of the HST this was accomplished by setting $\beta_1 = 0.1\beta$ [*Ross, 1990*]. Parameter optimization was performed for all transforms on each test problem using IFFCO. These results were used to identify the most promising combinations of interblock conductivity approach, nonlinear solver, and transform.

While these results are not reported in detail, we draw the following general conclusions from our baseline runs: (1) the integral conductivity estimation method consistently demonstrated a greater reduction in dense-grid error than the other three interblock conductivity approaches with only slightly greater computational cost; (2) MPI typically required more iterations but less work than the NILS, due to the higher per iteration work required for the NILS solver; and (3) the IT2 transform compared

favorably with all other transforms in terms of efficiency and robustness. Based upon these results, we limited our additional phases of this work to the KINT and MPI approaches, although all transforms were considered.

5.2. Performance Comparisons

Using the general observations made from the baseline comparisons, a set of simulations was performed using the KINT interblock conductivity estimate and the MPI nonlinear solver. For this set of simulations, work and error were observed as a function of β for all four transforms and all eight test problems. Table 4 shows the allowable transform parameter ranges over which convergence was achieved, the optimal parameter values, and resulting optimal work and error values. IT1 is not listed as a separate transform since it is represented by the $\beta = 0$ point of the IT2 transform. Though several of the optimal β values for IT2 are zero or close to zero, particularly for problems involving $n_v < 2$, significant differences in performance are seen for IT1 and IT2 over the entire range of problems considered.

$\boxed{\text{Table 4}}$

The error vs. work results are illustrated for two of the test problems — A and C —in Figures 3 and 4, respectively. The lines on the work-error plots represent the work and error for each transform as the transform parameter is varied. Results are plotted for parameter values at equally spaced intervals over the range of allowable values. For THT, HST, and RFT, data points are plotted at equally spaced intervals in β, and for IT2, data points are plotted at equally spaced intervals in log β.

$\boxed{\text{Figures 3 an}}$

Based upon this set of simulations, the following observations are made:

1. transforms generally lead to more efficient solutions, sometimes as much as an order of magnitude more efficient as measured in terms of the objective function minimized in this work;

2. transforms tended to be increasingly efficient compared to untransformed solutions

as the sharpness of the front increased, such as for cases in which a saturated zone developed and n_v was relatively large;

3. all transforms were generally sensitive to β for a given problem.

4. the optimal value of β varied among problems for all transforms;

5. while variations in efficiencies existed among transforms for each problem, IT2 was in general the most efficient transform; and

6. IT2 was typically the least sensitive to changes in β.

These data show that for sharp-front problems, transformation methods can significantly reduce computational effort and increase robustness of the solution scheme given an appropriate value for β. However, guidance does not yet exist to choose an appropriate value of β for any transform a priori. Further, the sensitivity of transforms to media properties suggest that the relative efficiency and robustness of transform methods will likely decrease as the degree of media heterogeneity increases.

5.3. Parameter Sensitivity to Discretization

We performed a discretization study to investigate the effects of spatial and temporal discretization on the behavior of all transformation methods for Problems A, B, C, and H and report these results in Table 5. For each problem, a coarse spatial grid $\boxed{\text{Table 5}}$ and two coarse time-step sizes were tested. Results from these numerical experiments showed that IT2 and RFT were able to converge and give accurate solutions on all of the coarse spatial and temporal grids. For the untransformed RE, the nonlinear solver failed to converge for all of the problems except C. The number of spatial nodes in the coarse-grid simulations was roughly 10 times less than in the previous simulations, which resulted in significant computational savings. Work measure were scaled linearly as a function of the number of spatial nodes. Therefore, the IT2 and RFT transformations

are able to provide accurate solutions at much larger discretization scales, resulting in very efficient simulations that would not be possible using the untransformed RE or other transformations.

Figure 5 shows the solution profiles in untransformed space for Problem A, comparing dense grid and coarse grid solutions at various simulation times. The dense grid solutions, shown as solid lines, are achieved using 25601 spatial nodes at a fixed time-step size of 1.56e-6 days. The coarse grid solutions, shown as dashed lines, are achieved using 41 spatial nodes at a fixed time-step size of 2.0e-4. While the coarse grid solution is not highly accurate, it is impressive that a solution was attained at all and this quality of result may be adequate for some uses.

Based upon these results, we find that the optimal β is sensitive to spatial and temporal discretization, and that the optimal β for a given discretization may lie outside the range for which convergence can be achieved at another discretization, especially for the RFT approach. The general trend noted was that the range of β for which convergent results were achieved tended to become narrower as the discretization became coarser. We also found that the objective function (16) in the parameter optimization exhibits a more clearly defined minimum as the discretization is coarsened, yet the the range of β values yielding efficient solutions also becomes narrower.

To illustrate the sensitivity of optimal β to spatial and temporal discretization, RFT and IT2 β values were optimized over a range of spatial and temporal discretizations for Problem A. These results are shown as contour plots in Figures 6 and 7. Optimal β values as a function of Δz and Δt are clearly smoother for IT2 than for RFT. We also noted that for RFT, β's closer to the optimal β are required for good performance. For IT2, performance is not as sensitive to small deviations from the optimal β.

Figure 5

Figures 6 an

5.4. Parameter Estimation

Given the relative insensitivity of the IT2 parameter to changes in media conditions, it is desirable to define an estimator for this parameter in terms of known system properties. Such an estimator would be beneficial in providing an effective transform without the need for expensive nonlinear parameter optimization. Using finer discretization scales, trends were detected in optimal IT2 parameter values as a function of media parameters n_v and α_v. However, as discretization parameters are coarsened, the optimal work and error values become more sensitive to changes in the IT2 parameter. Thus, it is difficult to define an estimator for the IT2 parameter that will yield optimal or near-optimal work and error results over a wide range of media and discretization parameters based upon the set of results generated to date.

Preliminary work shows that it may be much easier to define an estimator for the IT2 parameter that will yield optimal results when using a variable time-step solution method than for the fixed-time-step cases considered in this work. The further development of this notion, or alternative approaches to estimating a near-optimal β as a function of media properties, auxiliary conditions, and spatial and temporal discretization levels is the subject of future work.

6. Conclusions

Several conclusions can be drawn from our comparison of transformation approaches and traditional approaches to solving RE for a range of media properties and auxiliary conditions.

- Transformation approaches have the potential to lead to more efficient and robust solutions of Richards' equation.

- The potential advantage of transformation approaches increases as the difficulty of the problem increases, as measured by the average number of nonlinear iterations

per time step that are required for the untransformed case.

- Capitalizing on the potential advantages of transform methods requires specification of an appropriate transformation and knowledge of a reasonable value for any free parameters that exist in the transform.

- A set of one new (IT2) and four existing transforms are described within a common framework, and the optimal transform parameter is shown to depend upon auxiliary conditions, media properties, and spatial and temporal discretization.

- IT2 showed good efficiency and robustness compared to all other transforms for a wide range of media properties and discretization levels.

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Figure 1. Solution profile in ψ for Problem A.

Figure 2. Solution profile in p for Problem A.

Figure 3. Error vs. work for Problem A using MPI solver and KINT conductivity estimation.

Figure 4. Error vs. work for Problem C using MPI solver and KINT conductivity estimation.

Figure 5. Comparison of solution profiles for dense and coarse grid solutions to Problem A.

Figure 6. Contour plot of optimal RFT parameter β vs. Δz and Δt for Problem A.

Figure 7. Contour plot of optimal IT2 parameter β vs. Δz and Δt for Problem A.

Table 1. Transformation Definitions

Transformation	p Definition	
IT1	$\int_{-\infty}^{\psi} K(\psi')d\psi',$	$-\infty < \psi < \infty$
THT	$\frac{1}{c(\beta)}\left[\theta(\psi) - \theta(\beta)\right] + \beta,$	$\psi < \beta$
	$\psi,$	$\psi \geq \beta$
HST	$\sinh\left[-\frac{\psi-\beta}{\beta_1}\right],$	$\psi < \beta$
	$-\frac{\psi-\beta}{\beta_1},$	$\psi \geq \beta$
RFT	$\frac{\psi}{1+\beta\psi},$	$\psi < 0$
	$\psi,$	$\psi \geq 0$
IT2	$\int_{-\infty}^{\psi} K(\psi')\ d\psi'\ +\ \beta\ \left[\theta(\psi) - \theta_r\right],$	$\psi \leq 0$
	$\left.\frac{\partial p}{\partial \psi}\right|_{\psi=0} * \psi\ +\ p(0),$	$\psi > 0$

Table 2. Test Problem A–D Parameters

Variable	Problem A	Problem B	Problem C	Problem D
θ_r (—)	0.093	0.279	0.102	0.000
θ_s (—)	0.301	0.416	0.368	0.330
α_v (m^{-1})	5.47	6.12	3.35	1.43
n_v (—)	4.264	1.914	2.000	1.506
K_s (m/day)	5.040	2.298	7.970	0.067
S_s (m^{-1})	1.0×10^{-6}	1.0×10^{-6}	0.00	0.00
z (m)	[0,10.0]	[0,10.0]	[0,0.3]	[0,6.0]
t (days)	[0,0.18]	[0,0.265]	[0,0.092]	[0,7.16]
ψ_0 (m)	-z	$-z$	-0.10	-0.3069
ψ_1 (m)	0.00	0.00	-0.10	-0.3069
ψ_2 (m)	0.10	0.10	-0.75	-0.07
Δz (m)	0.0125	0.0125	0.0025	0.0125
Δt (days)	5.0×10^{-5}	1.0×10^{-4}	5.0×10^{-4}	7.16×10^{-2}

Table 3. Test Problem E–H Parameters

Variable	Problem E	Problem F	Problem G	Problem H
θ_r (—)	0.045	0.057	0.078	0.095
θ_s (—)	0.430	0.410	0.430	0.410
α_v (m^{-1})	14.5	12.4	3.60	1.90
n_v (—)	2.680	2.280	1.560	1.310
K_s (m/day)	7.128	3.502	0.250	0.062
S_s (m^{-1})	1.0×10^{-6}	1.0×10^{-6}	0.00	0.00
z (m)	[0,10.0]	[0,10.0]	[0,5.0]	[0,2.0]
t (days)	[0,0.24]	[0,0.45]	[0,2.25]	[0,1.0]
ψ_0 (m)	-z	$-z$	-z	-z
ψ_1 (m)	0.0	0.0	0.0	0.0
ψ_2 (m)	0.10	0.10	0.10	0.10
Δz (m)	0.0125	0.0125	0.0125	0.00625
Δt (days)	1.0×10^{-4}	1.5×10^{-4}	3.0×10^{-3}	2.0×10^{-3}

Table 4. Simulation Results

| Problem | Transform | β_{min} | β_{max} | β_{opt} | Optimal Performance Values | |
					L_1 Error ($\times 10^{-3}$)	Work $\times$ L_1 Error
A	UNT	$\cdots$	$\cdots$	$\cdots$	5.30	129.85
	THT	ψ_{min}	-0.05	-0.05	3.93	134.80
	HST	ψ_{min}	-0.15	-0.15	3.08	97.02
	RFT	-3.50	0.00	-3.50	4.36	140.39
	IT2	0.00	100.00	0.58	0.74	19.24
B	UNT	$\cdots$	$\cdots$	$\cdots$	0.69	17.46
	THT	ψ_{min}	-0.015	-1.20	0.46	15.90
	HST	ψ_{min}	-0.04	-1.50	0.46	15.89
	RFT	-36.00	0.00	0.00	0.69	22.63
	IT2	0.00	20.00	0.001	0.50	15.99

Table 4. (continued)

| Problem | Transform | β_{min} | β_{max} | β_{opt} | Optimal Performance Values | |
					L_1 Error $(\times 10^{-3})$	Work $\times$ L_1 Error
C	UNT	$\cdots$	$\cdots$	$\cdots$	12.14	21.25
	THT	ψ_{min}	0.00	0.00	5.78	8.84
	HST	ψ_{min}	-0.001	-1.60	6.51	9.83
	RFT	-10.00	0.00	-10.00	5.76	8.87
	IT2	0.00	100.00	0.005	6.27	6.27
D	UNT	$\cdots$	$\cdots$	$\cdots$	0.08	0.07
	THT	ψ_{min}	0.00	-0.13	0.08	0.08
	HST	ψ_{min}	-0.001	-0.06	0.08	0.07
	RFT	-45.00	0.00	-45.00	0.08	0.08
	IT2	0.00	100.00	0.04	0.08	0.08

Table 4. (continued)

Problem	Transform	β_{min}	β_{max}	β_{opt}	Optimal Performance Values L_1 Error ($\times 10^{-3}$)	Work $\times$ L_1 Error
E	UNT	$\cdots$	$\cdots$	$\cdots$	5.22	110.66
	THT	ψ_{min}	-0.03	-0.03	0.60	21.78
	HST	ψ_{min}	-0.05	-0.05	0.33	9.87
	RFT	-71.00	0.00	-71.00	0.33	8.51
	IT2	0.00	5.00	0.05	0.27	7.69
F	UNT	$\cdots$	$\cdots$	$\cdots$	4.86	125.87
	THT	ψ_{min}	-0.04	-0.04	0.34	13.77
	HST	ψ_{min}	-0.02	-0.02	0.70	26.46
	RFT	-63.00	0.00	-63.00	0.69	21.25
	IT2	0.00	1.30	0.01	0.31	11.07

Table 4. (continued)

| Problem | Transform | β_{min} | β_{max} | β_{opt} | Optimal Performance Values | |
					L_1 Error ($\times 10^{-3}$)	Work $\times$ L_1 Error
G	UNT	$\cdots$	$\cdots$	$\cdots$	1.61	19.96
	THT	ψ_{min}	-0.01	-0.90	1.42	23.86
	HST	ψ_{min}	-0.12	ψ_{min}	1.60	25.76
	RFT	-68.09	0.00	-47.50	1.36	10.74
	IT2	0.00	1.27	0.002	1.46	14.89
H	UNT	$\cdots$	$\cdots$	$\cdots$	0.51	4.04
	THT	ψ_{min}	-0.007	-0.01	0.46	5.11
	HST	ψ_{min}	-0.22	ψ_{min}	0.51	5.30
	RFT	-201.00	0.00	-17.50	0.45	4.20
	IT2	0.00	0.73	0.00	0.51	2.47

Table 5. Coarse Grid Simulation Results

| Media | Δz | Δt | Transform | β_{min} | β_{max} | β_{opt} | Optimal Performance Values | |
							L_1 Error $(\times 10^{-3})$	Work $\times$ L_1 Error
A	0.1	1e-4	UNT	DNC	$\cdots$	$\cdots$	$\cdots$	$\cdots$
			THT	-2.90	-0.50	-0.50	2.68	4.50
			HST	DNC	$\cdots$	$\cdots$	$\cdots$	$\cdots$
			RFT	-5.49	-2.10	-5.49	43.98	68.70
			IT2	0.00	1.40	0.003	2.22	2.95
		2e-4	UNT	DNC	$\cdots$	$\cdots$	$\cdots$	$\cdots$
			THT	-0.85	-0.31	-0.31	2.41	2.73
			HST	-1.04	-0.92	-0.92	7.93	7.88
			RFT	-4.00	-0.53	-0.53	6.08	5.96
			IT2	0.00	1.80	0.01	2.38	1.97

Table 5. (continued)

Media	Δz	Δt	Transform	β_{min}	β_{max}	β_{opt}	Optimal Performance Values L_1 Error $(\times 10^{-3})$	Work $\times$ L_1 Error
B	0.1	2e-4	UNT	DNC	$\cdots$	$\cdots$	$\cdots$	$\cdots$
			THT	DNC	$\cdots$	$\cdots$	$\cdots$	$\cdots$
			HST	DNC	$\cdots$	$\cdots$	$\cdots$	$\cdots$
			RFT	-71.00	-6.80	-50.90	3.95	5.17
			IT2	0.00	1.40	0.00	15.30	30.97
		5e-4	UNT	DNC	$\cdots$	$\cdots$	$\cdots$	$\cdots$
			THT	DNC	$\cdots$	$\cdots$	$\cdots$	$\cdots$
			HST	DNC	$\cdots$	$\cdots$	$\cdots$	$\cdots$
			RFT	-45.80	-6.70	-43.80	3.97	2.29
			IT2	0.00	1.40	0.00	12.68	10.61

Table 5. (continued)

Media	Δz	Δt	Transform	β_{min}	β_{max}	β_{opt}	L_1 Error ($\times 10^{-3}$)	Work $\times$ L_1 Error
						Optimal Performance Values		
C	0.03	1e-3	UNT	$\cdots$	$\cdots$	$\cdots$	267.79	9.59
			THT	ψ_{min}	0.00	-2.16	9.89	0.46
			HST	ψ_{min}	-0.001	-2.51	10.48	0.49
			RFT	-200.00	0.00	-0.28	17.19	0.79
			IT2	0.00	93.00	0.006	12.81	0.45
		2e-3	UNT	$\cdots$	$\cdots$	$\cdots$	277.55	6.55
			THT	ψ_{min}	0.00	-1.97	10.71	0.32
			HST	ψ_{min}	-0.001	-2.26	12.33	0.37
			RFT	-200.00	0.00	-0.35	18.49	0.54
			IT2	0.00	93.00	0.008	13.61	0.29

Table 5. (continued)

Media	Δz	Δt	Transform	β_{min}	β_{max}	β_{opt}	Optimal Performance Values L_1 Error ($\times 10^{-3}$)	Work $\times$ L_1 Error
H	0.05	4e-3	UNT	DNC	$\cdots$	$\cdots$	$\cdots$	$\cdots$
			THT	DNC	$\cdots$	$\cdots$	$\cdots$	$\cdots$
			HST	DNC	$\cdots$	$\cdots$	$\cdots$	$\cdots$
			RFT	-33.40	-7.03	-17.20	3.39	1.35
			IT2	0.00	0.16	0.00	9.70	2.50
		8e-3	UNT	DNC	$\cdots$	$\cdots$	$\cdots$	$\cdots$
			THT	DNC	$\cdots$	$\cdots$	$\cdots$	$\cdots$
			HST	DNC	$\cdots$	$\cdots$	$\cdots$	$\cdots$
			RFT	-26.80	-6.46	-17.70	3.57	0.70
			IT2	0.00	0.17	0.00	9.48	1.22