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A Data-driven Modeling Approach for Water Flow Dynamics in Soil

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Abstract

Modeling and predicting soil moisture is essential for precision agriculture, smart irrigation, drought prevention, etc. Estimating root zone soil moisture from surface or near-surface soil moisture data is typically achieved by solving a hydrological model that describes water movement through soils. Advanced agro-hydrological models today use the Richards equation, a highly nonlinear, degenerate elliptic-parabolic partial differential equation that captures irrigation, precipitation, evapotranspiration, runoff, and drainage. State-of-the-art Richards equation solvers employ either a finite difference, finite element, or finite volume discretization framework in space. In this paper, we introduce a novel computational framework to solve generic n-dimensional Richards equation by introducing global random walk and deep neural network to a modified finite volume method (FVM). Furthermore, for n-dimensional Richards equation, we introduce multi-point flux approximation to the FVM framework. Through these innovations, our novel computational framework effectively utilizes the underlying physics behind the Richards equation, which enhances the speed and accuracy of the solution process. Through an illustrative case study, we demonstrate the efficiency and effectiveness of our computational framework and show that it correctly characterizes the physical relationships among soil moisture content, pressure head, and flux.

Keywords: Soil moisture, Richards equation, finite volume method, neural network, random walk

1. Introduction

Soil moisture is a key hydrological parameter that has significant importance to human society and environment. Accurate modeling and monitoring of soil moisture in crop fields, especially in the root zone (top 100 cm of soil), is essential for improving agricultural production and crop yield with the help of precision irrigation and farming tools. Recent studies also show that monitoring root zone soil moisture at suitable locations and adjusting irrigation schedules accordingly can reduce water use by 40-60% (Sadler et al., 2005). Improved irrigation infrastructures based on soil moisture knowledge could also prevent more than $30 billion/year in drought related agricultural losses in the US (Khand et al., 2018). This is especially important to US states like Oklahoma, where 41% of total water use goes directly to agricultural irrigation and almost 90% of the land area suffers from drought throughout the year (Droughts.gov, 2022). Estimating root zone soil moisture is typically achieved by solving a hydrological model that describes water movement through soils. Most of the advanced agro-hydrological models today incorporate the Richards equation (Richards, 1931), which captures irrigation, precipitation, evapotranspiration, runoff, and drainage dynamics of water in saturated and unsaturated porous medium such as soil:

Summary of Comments on Paper2-commented.pdf

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Number: 1 Author: Nicolae Suciu Subject: Notiz Date: 6/3/2024 9:02:00 PM +02'00'

This is the second article posted on the web site
https://checlams.github.io/publications/

The authors of the article use ideas, numerical schemes, and codes from a previously published study (https://doi.org/10.1016/j.advwatres.2021.103935 and https://zenodo.org/records/4709693)
-without giving the appropriate credit,
-falsifying the interpretation of the method they used as reference,
-fabricating false solutions to the problem,
-falsifying comparisons with the reference method, and
-finally concluding that the reference method, used to develop their own approach, is wrong while claiming at the same time that the comparison validates their approach.

The elements of scientific misconduct, such as Plagiarism, Falsification, and Fabrication that I identified in this article are presented in the red-color comments below.

I also note that the icon illustrating the article on the web page https://checlams.github.io/publications/ is Fig. 18 downloaded from the page https://doi.org/10.1016/j.advwatres.2021.103935 without indicating the source. The same figure illustrates one of the authors' projects posted on the page https://checlams.github.io/projects/.

$$\frac{\partial\theta(\varphi)}{\partial t} = \nabla \cdot [K(\theta)\nabla(\varphi + z)] - S \tag{1}$$

where φ stands for pressure head, θ denotes the soil moisture content, K is unsaturated hydraulic water conductivity, $t \in [0, T]$ denotes the time, z denotes the vertical depth, and S is the sink term associated with root water extraction, which we ignore without loss of generality. The flux is given by the Darcy's law: $q = -K(\theta)\nabla(\varphi + z)$. For unsaturated flow, both K and θ are highly nonlinear functions of φ. For instance, the widely used van Genuchten-Mualem correlations (van Genuchten, 1980) for $\theta(\varphi)$and $K(\theta)$ are:

$$\theta(\varphi) = \begin{cases} \dfrac{\theta_s - \theta_r}{[1 + (\alpha|\varphi|)^n]^{\frac{n-1}{n}}} + \theta_r, & \varphi < 0 \\ \theta_s, & \varphi \geq 0 \end{cases}$$

$$K(\theta) = K_s \sqrt{\frac{\theta - \theta_r}{\theta_s - \theta_r}} \left\{ 1 - \left[1 - \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{\frac{n}{n-1}} \right]^{\frac{n-1}{n}} \right\}^2 \tag{2}$$

where α and n are van Genuchten parameters characterizing different soils, and θ_s, K_s and θ_r denote saturation soil moisture, residual water content, and saturated hydraulic conductivity, respectively. As a result, exact analytical solutions to Equation (1) often do not exist, and numerical solutions rely on discretization of spatial and temporal domains. In particular, the finite volume method (FVM) adopts an integral form of the Richards equation, which captures some valuable physical insights about water flow dynamics (Rathfelder and Abriola, 1994). In addition, FVM is a flexible framework that can be coupled with various other techniques such as the predictor-corrector method (Lai and Ogden, 2015), linearization scheme (Radu et al., 2015), and 1lobal random walk approach (Vamos, 2013). Recently, we developed a computationally efficient FVM-based framework for solving the Richards equation by integrating it with adaptive linearization scheme, global random walk method, and multi-layer neural networks (Song and Jiang, 2023). In an illustrative example, we showed that our novel data-driven framework not only generated fast and accurate solutions to the 1-D Richards equation, but also implicitly captured the underlying physical relationships among soil moisture content, pressure head, and flux. In this work, we generalize this computational framework to successfully 4blving 3-D Richards equation for the first time in the literature.

2. FVM Discretization

To apply FVM to Richards equation, we first integrate both sides of Equation (1) to obtain an integral form of the Richards equation over a higher-dimensional control V:

$$\int_V \frac{\partial\theta(\varphi)}{\partial t} dV = \int_V \nabla \cdot [K(\theta)\nabla(\varphi + z)] dV \tag{3}$$

Next, we can apply the divergence theorem to convert the volume integral on the RHS of Equation (3) into a surface integral over S_V by introducing the outward pointing unit normal vector denoted as **n**:

$$\int_V \frac{\partial\theta(\varphi)}{\partial t} dV = \int_{S_V} [K(\theta)\nabla(\varphi + z)] \cdot \mathbf{n}\, dS_V \tag{4}$$

By doing so, FVM is able to incorporate conservation laws, whereas other discretization methods cannot. Specifically, to obtain the discretized version of Equation (4) using FVM,

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Number: 1 Author: Nicolae Suciu Subject: Hervorheben Date: 2/13/2024 12:18:51 PM

Number: 2 Author: Nicolae Suciu Subject: Notiz Date: 2/16/2024 8:10:40 PM

(Vamos, 2013) does not exist in the reference list. Actually, C. Vamos did not published an article as single author in 2013!

Instead, the authors systematically use in the following the ideas, the methods and the algorithms from the article [Suciu et al., 2021] (https://doi.org/10.1016/j.advwatres.2021.103935).

Number: 3 Author: Nicolae Suciu Subject: Notiz Date: 2/16/2024 6:51:15 PM

FALSE:

A search on Google (on February 14, 2024) for "three dimensional Richards' equation" returns about 6,600 results. On the top of the list is a recent 3-dim numerical solution:

OpenCAL system extension and application to the three-dimensional Richards equation for unsaturated flow (https://doi.org/10.1016/j.camwa.2020.05.017).

Number: 4 Author: Nicolae Suciu Subject: Hervorheben Date: 11/1/2023 2:28:40 PM

we discretize the volume integral on the LHS of Equation (4) into a total of N_V small cells V_i with $i = 1, \cdots N_\omega$ whose volume is denoted as ϑ_i. Each V_i is associated with surfaces $\omega_{i,j}$ for $j = 1, \cdots N_{\omega_i}$ on the RHS of Equation (4) whose area is denoted as $\mathcal{A}(\omega_{i,j})$, and we use $[\cdot]_{\omega_i}$ and $\mathbf{n}_{\omega_i}$ respectively to denote the operator and outward pointing unit normal vector associated with $\omega_{i,j}$ upon discretization. Next, to discretize the time domain, we approximate the time derivative $\partial\theta(\varphi)$ as $\frac{\theta_i^{m+1,s+1}-\theta_i^m}{\Delta t}$, where $\theta_i^{m+1,s+1}$ represents the discretized θ in the ith small cell at the next time step $m+1$ and iteration step $s+1$, whereas θ_i^m is the converged θ value in the ith small cell at the current time step m. With this, the discretized version of Equation (4) using FVM becomes:

$$\frac{\theta_i^{m+1,s+1} - \theta_i^m}{\Delta t}\vartheta_i = \sum_{j=1}^{N_{\omega_i}} [K(\theta)\nabla(\varphi + z)]_{\omega_{i,j}} \cdot \mathbf{n}_{\omega_{i,j}} \mathcal{A}(\omega_{i,j}) \tag{5}$$

3. Data-Driven Global Random Walk Algorithm

In this section, we introduce a data-driven global random walk (DGRW) approach that seeks to implicitly encapsulate the physical knowledge describing particle movement and conservation within a control volume. Global random walk allows particles to move to neighboring cells simultaneously on any direction or stay in their current cells with a given probability. Thus, in 3-D case, there are a total of seven options for every particle. Let $\mathfrak{n}_{i,j,k}^{m,s}$ be the number of particles in the cell (i,j,k) at fixed-point iteration step s and time step m. Correspondingly, $\delta\mathfrak{n}_{i',j',k'}^{m,s}$, where $i' = i-1, i, i+1$, $j' = j-1, j, j+1$, and $k' = k-1, k, k+1$, denotes the number of particles moving from cell (i',j',k') to cell (i,j,k). Explicitly, we can write:

$$\mathfrak{n}_{i,j,k}^{m,s+1} = \delta\mathfrak{n}_{i+1,j,k}^{m,s} + \delta\mathfrak{n}_{i-1,j,k}^{m,s} + \delta\mathfrak{n}_{i,j+1,k}^{m,s} + \delta\mathfrak{n}_{i,j-1,k}^{m,s} + \delta\mathfrak{n}_{i,j,k+1}^{m,s} + \delta\mathfrak{n}_{i,j,k-1}^{m,s} + \delta\mathfrak{n}_{i,j,k}^{m,s} \tag{6}$$

As we may expect, having such physical knowledge is important for solving Richards equation, which governs the movement of water molecules in unsaturated and saturated soil systems. In fact, Suciu et al. (2021) adopted global random walk concepts and proposed a numerical framework for solving 1- and 2-D Richards equation. In their numerical framework, the authors assumed that the pressure head φ is proportional to the number of particles $\mathfrak{n}$ in a cell or control volume. With this assumption, soil moisture content in the cell of interest is simply proportional to the arithmetic mean of the number of particles. While this assumption is valid for diffusion equations (Vamoş et al., 2001), Richards equation is a highly nonlinear convection-diffusion equation, and the exact relationship between φ and $\mathfrak{n}$ remains unclear. In fact, we have shown that the numerical framework proposed by Suciu et al. (2021) failed to obtain an accurate solution for 1-D Richards equation (Song and Jiang, 2023).

Since the relationship between φ and $\mathfrak{n}$ may not be describable by any basic function, we decide to model the relationship using two multi-layer neural networks (MNNs). Although deep neural network with more layers and neurons could also be used, it is not required as MNN with less number of layers (e.g., 3) is sufficient for learning the relationship between φ and $\mathfrak{n}$ given enough neurons in the neural network (Hornik, 1991). In one of the MNNs, we approximate φ as a function of $\mathfrak{n}$, $\varphi_{i,j,k} = f(\mathfrak{n}_{i,j,k})$, at each fixed time step and iteration step. In the other MNN, we learn the inverse mapping

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This is Eq. (19) in [Suciu et al., 2021] formally generalized to 3 spatial dimensions.

The way the authors introduce DGRW leaves the impression that they created the GRW algorithm and "Suciu et al. (2021) adopted ..."

Nevertheless, this relation is not used and the DGRW described in the following is simply a finite difference scheme.

The idea of global random walk model of flow in porous media and the relation (6) are taken from [Suciu et al., 2021] without giving the appropriate credit. However, since this paper is cited on the next page, the authors were aware of both the idea and the relation defining the global random walk algorithm for flow in porous media. We have thus the proof of two elements of scientific misconduct: MISAPPROPRIATION of IDEAS and PLAGIARISM.

Number: 2 Author: Nicolae Suciu Subject: Notiz Date: 6/3/2024 7:00:12 PM +02'00'

FALSE:

Eq. (18) in [Suciu et al., 2021] is essentially a finite difference approximation of the pressure head, denoted by n^{s}_{i,j,k}. This scheme can be developed into randomized GRW scheme if n^{s}_{i,j,k} is a realization of a binomially distributed random variable defined by Eqs. (19-20) in [Suciu et al., 2021].

The difference between the finite difference scheme and the GRW scheme is that the latter contains more or less noise, depending on the number of particles. But the ensemble average of the GRW solution is strictly identical to the finite difference solution (see [Suciu et al., 2021, Eq(20)]). This is the "exact relationship" between the pressure head \varphy and the random variable n: the latter is a noisy representation of the former.

As stated in the paragraph above Remark 3 in [Suciu et al., 2021], by removing the randomness one obtains a deterministic GRW, which is precisely the finite difference scheme (18). It is only this deterministic GRW (finite difference) scheme which is used in [Suciu et al., 2021]. The same in this article of Song and Jiang, which is based on the finite difference scheme (6) given on the next page. Note that there is no connection between the two relations with the same label (6). Hence, \varphy and n represent the same quantity.

Number: 3 Author: Nicolae Suciu Subject: Hervorheben Date: 11/1/2023 2:29:14 PM

Number: 4 Author: Nicolae Suciu Subject: Notiz Date: 6/3/2024 7:00:17 PM +02'00'

The statement is false and illogical:

1. One-dimensional GRW solutions are used as reference for the method proposed in [Song and Jiang, 2023] (https://checlams.github.io/assets/pdf/paper/drw_focapo.pdf);
it is found that the latter produces results that deviate from the GRW solution; conclusion: GRW solutions are wrong!

2. There is a benchmark problem with mixed finite elements; GRW was successfully tested on this benchmark; the method proposed by the authors deviates from the GRW and the mixed finite element solutions; conclusion: the latter two methods are wrong and the proposed method is correct!

3. The GRW scheme successfully passed a code verification test (https://arxiv.org/abs/2011.12889); the authors' method has not been verified in the most simple and common way, i.e., by comparisons with exact manufactured solutions.

Number: 5 Author: Nicolae Suciu Subject: Hervorheben Date: 11/1/2023 2:29:37 PM

Number: 6 Author: Nicolae Suciu Subject: Notiz Date: 6/3/2024 7:00:20 PM +02'00'

FALSE:

In [Suciu et al., 2021] as well as in this article, see the next relation (6),
\varphi = n (see comment above).

Since the motivation of finding the relation between \vrphi and n fails, one may wonder why develop a data-driven scheme which is much slower (it uses many reference solutions and optimization procedures) and, as seen in the comment above it is not accurate?

Number: 7 Author: Nicolae Suciu Subject: Hervorheben Date: 11/1/2023 2:30:42 PM

f^{-1} from pressure head information to the number of particles, $\mathfrak{n}_{i,j,k} = f^{-1}(\varphi_{i,j,k})$. During offline training, we first obtain reference solutions from the global random walk solvers developed by Sucui et al. (2021) (code available at GitHub repository: https://github.com/PMFlow/FlowBenchmark). We then add Gaussian noise to these reference solutions to 1) account for the possibly nonlinear relationship between φ and ɳ, and 2) enhance its generalization performance and the quality of solution obtained (Song and Jiang, 2023). Once offline training is complete, we substitute f to Equation (5) and derive the following data-driven random walk formulation for the discretized Richards equation:

$$\begin{aligned}\mathfrak{n}_{i,j,k}^{m,s+1} = \Bigg[1 - \Bigg(& r_{i+\frac{1}{2},j,k}^{m,s} + r_{i-\frac{1}{2},j,k}^{m,s} + r_{i,j+\frac{1}{2},k}^{m,s} + r_{i,j-\frac{1}{2},k}^{m,s} + r_{i,j,k+\frac{1}{2}}^{m,s} + r_{i,j,k-\frac{1}{2}}^{m,s}\Bigg)\Bigg]\mathfrak{n}_{i,j,k}^{m,s} \\ &+ r_{i+\frac{1}{2},j,k}^{m,s}\mathfrak{n}_{i+1,j,k}^{m,s} + r_{i-\frac{1}{2},j,k}^{m,s}\mathfrak{n}_{i-1,j,k}^{m,s} + r_{i,j+\frac{1}{2},k}^{m,s}\mathfrak{n}_{i,j+1,k}^{m,s} + r_{i,j-\frac{1}{2},k}^{m,s}\mathfrak{n}_{i,j-1,k}^{m,s} \\ &+ r_{i,j,k+\frac{1}{2}}^{m,s}\mathfrak{n}_{i,j,k+1}^{m,s} + r_{i,j,k-\frac{1}{2}}^{m,s}\mathfrak{n}_{i,j,k-1}^{m,s} \\ &+ f^{-1}\left(\left(r_{i,j,k+\frac{1}{2}}^{m,s} - r_{i,j,k-\frac{1}{2}}^{m,s}\right)\Delta z - \frac{\theta^{m,s}\left(\mathfrak{n}_{i,j,k}^{m,s}\right) - \theta^{m-1}\left(\mathfrak{n}_{i,j,k}^{m-1,s}\right)}{L_{i,j,k}^{m,s}}\right)\end{aligned} \tag{6}$$

where $r_{i\pm\frac{1}{2},j,k}^{m,s} = \frac{K\left(\theta\left(\varphi_{i\pm\frac{1}{2},j,k}^{m,s}\right)\right)\Delta t}{(\Delta x)^2 L_{i\pm\frac{1}{2},j,k}^{m,s}}$, $r_{i,j\pm\frac{1}{2},k}^{m,s} = \frac{K\left(\theta\left(\varphi_{i,j\pm\frac{1}{2},k}^{m,s}\right)\right)\Delta t}{(\Delta y)^2 L_{i,j\pm\frac{1}{2},k}^{m,s}}$, and $r_{i,j,k\pm\frac{1}{2}}^{m,s} = \frac{K\left(\theta\left(\varphi_{i,j,k\pm\frac{1}{2}}^{m,s}\right)\right)\Delta t}{(\Delta z)^2 L_{i,j,k\pm\frac{1}{2}}^{m,s}}$. Here, we adopt an adaptive linearization scheme inspired by Mitra and Pop (2019) by adding the term $L_{i,j,k}^{m,s}\left(\varphi_{i,j,k}^{m,s+1} - \varphi_{i,j,k}^{m,s}\right)$ on the LHS of Equation (5).

In DGRW algorithm, Equation (6) passes through the inverse mapping f^{-1} learned from MNN to generate Richards equation solutions in terms of the particle distribution in each cell, $\mathfrak{n}_{i,j,k}$. To convert these solutions to physically meaningful solutions such as the pressure head, flux, and soil moisture content, we apply the trained mapping f^{-1} and Equation (2). We have proven that the DGRW algorithm is convergent, and the total error can be estimated using $\varepsilon = \max_i \left\{\frac{\left\|f\left(\mathfrak{n}_{i,j,k}^{m,s+1}\right) - f\left(\mathfrak{n}_{i,j,k}^{m,s}\right)\right\|_F}{\left\|f\left(\mathfrak{n}_{i,j,k}^{m,s+1}\right)\right\|_F}\right\} = \max_i \left\{\frac{\left\|\psi_{i,j,k}^{m,s+1} - \psi_{i,j,k}^{m,s}\right\|_F}{\left\|\psi_{i,j,k}^{m,s+1}\right\|_F}\right\}$, where $\|\cdot\|_F$ is the Frobenius norm.

4. An Illustrative Case Study

We modify the 2-D benchmark problem of Havercamp (1977) that describes groundwater reservoir recharge from a drainage trench by extending it to 3-D. The boundary conditions of the problem are set up as $\Omega = [0\text{m}, 2\text{m}]^3$, and $\Gamma_D = \Gamma_{D_1} \cup \Gamma_{D_2} \cup \Gamma_{D_3} \cup \Gamma_{D_4}$, in which:

$$\begin{aligned}\Gamma_{D_1} &= \{(x,y,z) \in \partial\Omega | x \in [0\text{m}, 1\text{m}] \wedge y \in \Omega \wedge z = 2\text{m}\}, \\ \Gamma_{D_2} &= \{(x,y,z) \in \partial\Omega | x \in \Omega \wedge y \in [0\text{m}, 1\text{m}] \wedge z = 2\text{m}\}, \\ \Gamma_{D_3} &= \{(x,y,z) \in \partial\Omega | x = 2\text{m} \wedge y \in \Omega \wedge z = [0\text{m}, 1\text{m}]\}, \\ \Gamma_{D_4} &= \{(x,y,z) \in \partial\Omega | x \in \Omega \wedge y = 2\text{m} \wedge z = [0\text{m}, 1\text{m}]\}.\end{aligned}$$

The Dirichlet boundary condition on Γ_D results in the drainage process, whereas the Neumann boundary condition is applied on $\Gamma_N = \partial\Omega \setminus \Gamma_D$. The z-direction is point

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False reference; the authors used the codes from
https://github.com/PMFlow/RichardsEquation
published here
https://zenodo.org/records/4709693

There are no three-dimensional schemes in this repository.

The authors used a two dimensional "deterministic GRW" which is identical to a finite difference scheme. This is also obvious if we look at the structure of the code main_Richiards_2D_Flow_benchmark.m in this repository.

Number: 2 Author: Nicolae Suciu Subject: Hervorheben Date: 11/1/2023 2:31:05 PM

Number: 3 Author: Nicolae Suciu Subject: Notiz Date: 6/3/2024 7:01:34 PM +02'00'

FALSIFICATION:

This is Eq. (18) in [Suciu et al., 2021] formally generalized to 3 spatial dimensions:

-Eq. (6) is a finite difference scheme, with i,j,k representing the nodes of a staggered grid, not cells. This equation cannot be derived from Eq. (5) which is based on the forward discretization of the time derivative of \theta, while the last term in (6) is a backward discretization of the derivative of \theta.

-the inverse mapping f^{-1} is not necessary. In [Suciu et al., 2021] it is demonstrated numerically that the 2-dimensional version of this iterative scheme converges if f^{-1}=identity mapping.

Note that the scheme (6) is not yet completely defined because the restrictions for the parameters r are missing; these are the CFL conditions of the finite difference scheme from [Suciu et al., 2021].

Number: 4 Author: Nicolae Suciu Subject: Hervorheben Date: 11/1/2023 2:31:30 PM

Number: 5 Author: Nicolae Suciu Subject: Notiz Date: 6/4/2024 4:50:58 PM +02'00'

PLAGISARISM:

The scheme (6) is not obtained by adding the stabilization term to (5), see my previous comment. Usually, finite volume discretization leads to implicit linearization schemes , see [Radu et al., 2015, http://dx.doi.org/10.1016/j.cam.2015.02.051].

Eq. (6) is an explicit L-scheme obtained by adding the stabilization term to a staggered finite difference scheme with backward Euler discretization [Suciu et al., 2021, Sects. 2 and 4.1] , where the authors formally added terms for the third spatial dimension.

This is not yet and adaptive scheme. To construct an adaptive L-scheme, a function L(x) should be defined at every iteration and time step. At the time being there are no adaptive schemes for this explicit L-scheme!

Number: 6 Author: Nicolae Suciu Subject: Notiz Date: 6/3/2024 7:02:20 PM +02'00'

I designed the explicit L-schemes for Richards equation (https://zenodo.org/records/4709693) and as far as I know there are no (published) convergence proofs.

The proof is not trivial and it surely cannot be done for the incomplete scheme presented by the authors of this article.

Number: 7 Author: Nicolae Suciu Subject: Hervorheben Date: 11/1/2023 2:32:10 PM

Number: 8 Author: Nicolae Suciu Subject: Notiz Date: 6/3/2024 7:02:35 PM +02'00'

non-sense:

-what is for instance y\in\Omega ? a thre-dimensional vector?

Number: 9 Author: Nicolae Suciu Subject: Hervorheben Date: 11/1/2023 2:32:53 PM

downward into the ground. The initial conditions describing hydrostatic equilibrium are modified as follows:

$$\varphi(x,y,z,t) = \begin{cases} -2 + 2.2\dfrac{t}{\Delta t_D} \text{ on } \Gamma_{D_1} \text{ and } \Gamma_{D_2}, T \le \Delta t_D, \\ 0.2 \text{ on } \Gamma_{D_1} \text{ and } \Gamma_{D_2}, T > \Delta t_D, \\ 1 - z \text{ on } \Gamma_{D_3} \text{ and } \Gamma_{D_4}, \end{cases}$$

$$q(x,y,z,t) = 0 \text{ on } \Gamma_N,$$

$$\varphi(x,y,z,0) = \begin{cases} 1 - z \text{ on } \Omega \backslash \Gamma_D \\ -2 \text{ on } \Gamma_D \end{cases}.$$

We use the parameters listed in ist (2016) to represent water flow dynamics in silt loam soil, in which $\theta_s = 0.396$, $\theta_r = 0.131$, $\alpha = 0.423$, $n = 2.06$, and $K_s = 0.0496$ in Equation (2). We choose $\Delta t_D = \frac{1}{16}d$, $\Delta t = \frac{1}{48}d$, and $T = \frac{3}{16}d$. A rectangular 3-D mesh with 9261 nodes is used, where $\Delta x = \Delta y = \Delta z = 0.1$. The convergence tolerance ε_0 is set to be 10^{-5}. Each MNN contains 3 layers and 10 neurons. Overall, 261 noise-added eference solutions from global random walk solvers developed by Suciu et al. (2021) were obtained, with 70%, 15%, and 15% of them being used for training, validation, and testing, respectively. Bayesian regularization is used to train both MNNs.

(a) (b)

Figure 1. Pressure head obtained from (a) GRW algorithm, and (b) DGRW approach.

(a) (b)

Figure 2. Pressure head obtained from (a) DGRW algorithm, and (b) GRW approach.

Figures 1 and 2 illustrate the pressure head and soil moisture results obtained using the RW algorithm of Suciu et al. (2021) and our DGRW framework at $y = 1.7$m and $t = T = \frac{3}{16}d$. In general, our DGRW results show excellent agreement with the GRW results. Nevertheless, we observe that e GRW solutions did not produce jumps in pressure head and soil moisture content in the z-direction as x approaches 1m (Γ_{D_1}), whereas our

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Not true: z is positive upward in Eqs. (1) and (6).

Number: 2 Author: Nicolae Suciu Subject: Hervorheben Date: 11/1/2023 2:33:22 PM

Number: 3 Author: Nicolae Suciu Subject: Notiz Date: 2/16/2024 8:25:28 PM

Here "T" should be replaced by "t"; this was a typo in [Suciu et al., 2021] that the authors imported in their article !!!

Number: 4 Author: Nicolae Suciu Subject: Notiz Date: 2/16/2024 6:35:31 PM

If the initial condition \varphi=-2 is imposed on the whole boundary \Gamma_D one obtains unsaturated regions near \Gamma_3 and \Gamma_4 and results like those presented in Figs. 1 and 2 cannot be obtained. As for \Gamma_D1 and \Gamma_D2, the initial condition is already specified by the boundary condition.

Number: 5 Author: Nicolae Suciu Subject: Notiz Date: 2/15/2024 3:17:21 PM

List (2016) is not included in the list of references. These parameters and the structure of the boundary conditions are taken from [Suciu et al., 2021], as indicated by the picking up the typo "T instead of t".

Number: 6 Author: Nicolae Suciu Subject: Hervorheben Date: 11/1/2023 2:33:46 PM

Number: 7 Author: Nicolae Suciu Subject: Notiz Date: 2/16/2024 8:27:14 PM

In [Suciu et al., 2021] there are no 3-dim GRW solutions !

The two-dimensional solver is a "deterministic GRW " which produces non-random solutions. Hence, the 9261 reference solutions are identical !

Number: 8 Author: Nicolae Suciu Subject: Hervorheben Date: 11/5/2023 6:39:20 PM

Number: 9 Author: Nicolae Suciu Subject: Hervorheben Date: 11/1/2023 2:34:11 PM

Number: 10 Author: Nicolae Suciu Subject: Notiz Date: 2/16/2024 6:39:48 PM

Fig. 2 shows the saturation, not the pressure; I guess that the authors wanted to say that Fig. 2a is the saturation for the GRW algorithm and in Fig. 2b is the saturation for the DGRW approach.

Number: 11 Author: Nicolae Suciu Subject: Notiz Date: 6/3/2024 7:04:46 PM +02'00'

With the codes used in [Suciu et al., 2021) one obtains only 2-dim GRW solutions!

Comparisons could be done on vertical, x-z slices, far from y=1, where the top BC for the 2-dim GRW changes.

Even so, 2-dim slices of the 3-dim problem could be only somewhat similar to the 2-dim solutions.

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Number: 13 Author: Nicolae Subject: Notiz Date: 2/8/2025 10:13:01 PM

FABRICATION and FALSIFICATION:

Figure 1 and Figure 2 are obtained with the three-dimensional codes 'GRW_Ref_27.m' and 'DRW_Ref_27.m' posted by the authors in the GitHub repository
https://github.com/taekwonzysong/AI4Soil/tree/main/Ref.%20%5B27%5D

These figures present solutions at the final time having a similar appearance to the initial state. The reason is that the water content is not updated at the end of each time step, resulting in a wrong iterative scheme which fails to converge.

The results given by the two codes are identical. However, while Figs. 1a and 2a correspond to a cross-section at y=1.7, Figs 1b and 2b are FABRICATED by taking a cross section at y=0.7 in 'DRW_Ref_27.m'.

Thus, the comparison of the GRW and DRW approaches is FALSIFIED.

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DGRW did predict these jumps. As the total simulated time is greater than Δt_D, the initial condition for pressure head should be 0.2m for $x = [0m, 1m]$ and -2m for $x = [1m, 2m]$ (Figure 1b). Similarly, jumps in soil moisture and flux in the z-direction are expected at $x = 1m$ as well. Therefore, by effectively characterizing the complex relationship between pressure head and the number of particles, our DGRW approach is capable of capturing the water flow dynamics embedded in the Richards equation.

5. Conclusion

In this work, we propose a novel data-driven DGRW framework to accurately solve 3-D Richards equation for the first time. DGRW synergistically integrates data-driven global random walk theory and FVM to encapsulate physical knowledge and insights describing water flow dynamics in soil systems. We compare the solutions of our DGRW framework and state-of-the-art GRW approach on a 3-D benchmark problem and successfully validate the accuracy and usefulness of our approach in capturing the underlying physics of water flow dynamics.

References

Drought.gov, 2022, Current U.S. Drought Monitor Conditions for Oklahoma, https://www.drought.gov/states/oklahoma, accessed March 2022.

R. Haverkamp, M. Vauclin, J. Touma, P.J. Wierenga, G. Vachaud, 1977, A comparison of numerical simulation models for one-dimensional infiltration, Soil Science Society of America, 41, 2, 285-294.

K. Hornik, 1991, Approximation capabilities of multilayer feedforward networks, Neural networks, 4, 2, 251-257.

K. Khand, S. Taghvaeian, A. Ajaz, 2018, Drought and Its Impact on Agricultural Water Resources in Oklahoma, https://extension.okstate.edu/fact-sheets/drought-and-its-impact-on-agricultural-water-resources-in-oklahoma.html, accessed March 2022.

W. Lai, F.L. Ogden, 2015, A mass-conservative finite volume predictor–corrector solution of the 1D Richards' equation, Journal of Hydrology, 523, 119-127.

F.A. Radu, J.M. Nordbotten, I.S. Pop, K. Kumar, 2015, A robust linearization scheme for finite volume based discretizations for simulation of two-phase flow in porous media, Journal of Computational and Applied Mathematics, 289, 134-141.

K. Rathfelder, L. M. Abriola, 1994, Mass conservative numerical solutions of the head-based richards equation, Water Resources Research, 30, 9, 2579-2586.

L.A. Richards, 1931, Capillary conduction of liquids through porous mediums, Physics, 1, 5, 318-333.

E. Sadler, R. Evans, K. Stone, and C. Camp, 2005, Opportunities for conservation with precision irrigation, Journal of Soil and Water Conservation, 60, 6, 371-378.

Z. Song, Z. Jiang, 2023, A data-driven random walk approach for solving water flow dynamics in soil systems, In: Proceedings Foundations of Computer-Aided Process Operations and Chemical Process Control Conference. San Antonio, TX.

N. Suciu, D. Illiano, A. Prechtel, F.A. Radu, 2021, Global random walk solvers for fully coupled flow and transport in saturated/unsaturated porous media, Advances in Water Resources, 152, 103935.

C. Vamos, N. Suciu, H. Vereecken, O. Nitzsche, H. Hardelauf, 2001, Global random walk simulations of diffusion, In Scientific Computing, Validated Numerics, Interval Methods, pp. 343-354.

M.T. van Genuchten, 1980, A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, Soil Science Society of America Journal, 44, 5, 892-898.

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As shown in my second comment on page 2 (820), this is not true!

Number: 2 Author: Nicolae Suciu Subject: Hervorheben Date: 11/1/2023 2:26:42 PM

Number: 3 Author: Nicolae Suciu Subject: Notiz Date: 2/16/2024 8:36:39 PM

The numerical scheme presented in this article has nothing to do with either the FVM or the (random) GRW approaches; it is just a finite difference scheme !

Number: 4 Author: Nicolae Suciu Subject: Hervorheben Date: 11/1/2023 2:27:06 PM

Number: 5 Author: Nicolae Suciu Subject: Notiz Date: 2/16/2024 8:36:47 PM

As seen in the last comment (red) on the previous page, the proposed method is not validated at all !

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Number: 7 Author: Nicolae Suciu Subject: Hervorheben Date: 11/1/2023 2:27:53 PM