Application and Validation of an Upscaling Method for Unsaturated Water Flow Processes in Heterogeneous Soils

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Upscaling of soil water flow processes and soil hydraulic properties is one of the most important issues in vadose zone research. The difficulties in such upscaling come from the heterogeneity and nonlinearity of the soil properties. Sharing some common element with the multiscale methods, an upscaling method was previously proposed for a class of nonlinear parabolic equations including the Richards equation, which is often used for modeling flow processes in soils. To verify its applicability in more realistic and varied flow scenarios, in this study we applied the method to one- and two-dimensional simulations of unsaturated water flow through heterogeneous soil profiles under different boundary conditions including infiltration, evaporation, and drainage. The Gardner–Basha model and the Mualem–van Genuchten model were used as the constitutive relations to close the Richards equation. Results show that the upscaling method can effectively capture the large-scale structure of fine-scale behavior in these realistic and varied scenarios. Note that in this study we pre-calculated the effective hydraulic functions by solving the local problems outside the coarse-scale simulation to avoid the expensive computation of upscaling these functions, which need to be updated at each time step on each coarse block. In our examples, we observed that, compared with the upscaling method that calculates the effective hydraulic functions by solving the fine-scale problems during the coarse-scale simulation, the upscaling method with pre-calculation saved more than 83 and 90% of the central processing unit time in the one- and two-dimensional simulations, respectively, without compromising accuracy.

Abbreviations: CPU, central processing unit; UM, upscaling method; UM-p, upscaling method with pre-calculation.

Needed by many large-scale hydrologic applications and management decisions, upscaling of soil water flow processes as well as soil hydraulic properties is one of the most important issues in vadose zone research. The Richards equation, which combines continuity equations and simplified flux equations such as the Darcy–Buckingham law, is a clear, physically based, fully parameterized spatial-time model and can be used for fundamental research to represent unsaturated flow and transport processes (van Dam and Feddes, 2000). The scale at which the flow and transport are described in terms of the Richards equation is called the representative elementary volume (REV) scale, which is also referred to as the Darcy, core, or local scale (Bierkens and van der Gaast, 1998). This is just the scale at which some system and system-state variables and vadose zone properties are usually measured directly in drilled soil cores or in situ with tools. In recent years, an in-depth understanding of modeling soil water flow processes at a larger scale as well as effective unsaturated hydraulic properties is required more and more because the severity has been increasingly realized of such vadose zone environmental problems as limited water resources in arid and semiarid regions, soil salinization and alkalization, and groundwater pollution containment. This scale, however, is usually very different from (i.e., larger than) the local scale at which the flow and transport behaviors are best described. To predict and understand flow processes at larger...
scales, upscaling methods are frequently used to upscale the local-scale measurements and flow processes to scales that are orders of magnitude larger than the local scale. Major questions involved in upscaling are what the effective mathematical description is for the unsaturated flow process of the vadose zone and how to obtain the effective hydraulic properties at the larger scale.

On the other hand, the need for upscaling stems from the disparity between the scale at which measurement is made and the scale at which domains are discretized for the numerical solution of flow and transport (e.g., Wen and Gómez-Hernández, 1996). In theory, high-resolution models are ideal to reduce the uncertainty in hydrologic modeling due to the inherent high spatial variability of soil properties, the nonlinearities of the soil physical properties, the rapid changing boundary fluxes across the soil–plant–atmosphere interfaces, non-uniform root water uptake, and the complexity of the dynamic systems. However, computer resources are challenged when high-resolution models are applied on a large number of grid blocks. This is the case in many semiarid or arid areas where the vadose zone is considerably deeper (down to a few tens of meters) (e.g., Onsoy et al., 2005; Mayers et al., 2005; Baran et al., 2007; Botros et al., 2009) when the disposal of hazardous wastes, recharge to the groundwater system, and the estimation of the resulting risk of groundwater pollution are concerned. This is also the case in catchment hydrologic modeling, which often requires a tremendous amount of computer memory and central processing unit (CPU) time. Thus, in practice, limited by computer resources, the modeling scale (working scale) always has to be larger than the observation scale of typical laboratory and field measurements to reduce the computational cost. Such a problem refers to upscaling high-resolution models into coarser models with certain accuracy, which is one of the most challenging problems in mathematics and geophysics.

Many types of upscaling methods have been performed for porous media flow processes involving a wide range of scales. A common approach is to "scale up" the locally variable permeability into some effective or equivalent permeability. Local small-scale information is incorporated into the effective parameter at the coarse scale to characterize the macroscopic flow behaviors of the medium (e.g., Durlofsky, 1992; Wen and Gómez-Hernández, 1996; Renard and de Marsily, 1997; Bierkens and van der Gaast, 1998; Wu et al., 2002; Farmer, 2002; King and Neuweiler, 2002). The main purpose of such upscaling methods is to obtain the homogeneous equivalent or upscaled flow parameters, which are often expected to represent the intrinsic properties of the homogenized domain. There are also many methods proposed to derive the upscaled nonlinear hydraulic properties of soils to simulate the large-scale ensemble flux (e.g., Zhu and Mohanty, 2002; Ward et al., 2006; Zhu et al., 2007). Toward upscaling soil water processes in the vadose zone, various methodologies for deriving the macroscopic description of the flow process have been developed based on different physical and mathematical considerations such as the stochastic perturbation method, volume averaging methods, and homogenization methods. The homogenization methods have recently been applied to the Richards equation at the laboratory scale within the strictly capillary-dominated flow regime in soils composed of several distinct materials (Lewandowska and Laurent, 2001; Lewandowska et al., 2004; Szymkiewicz and Lewandowska, 2006; Sviercoski et al., 2009) and have also been combined with ensemble averaging techniques in a statistical framework to model the water flow problem for continuously changing stochastic fields (Neuweiler and Cirpka, 2005; Neuweiler and Eichel, 2006). A more extensive overview of upscaling hydraulic properties and soil water flow processes has been provided by Vereecken et al. (2007).

Another type of method—multiscale numerical methods, such as the multiscale finite element method (Hou and Wu, 1997; Efendiev and Wu, 2002; Efendiev et al., 2004), the multiscale finite volume method (Jenny et al., 2003), the heterogeneous multiscale method (Yue and E, 2005; E et al., 2005), and the numerical homogenization method (Efendiev and Pankov, 2004)—has recently been proposed for nonlinear flow problems. Some attempts have been made to develop and apply multiscale numerical methods to saturated or unsaturated soil water flow (e.g., Efendiev et al., 2004; Efendiev and Pankov, 2004; He and Ren, 2006; Chen and Ren, 2008; Cao and Yue, 2014). In multiscale numerical methods, fine-scale information may be carried throughout the simulation, and coarse-scale equations are generally not expressed analytically but rather formed and solved numerically (Efendiev et al., 2004).

Chen et al. (2005) developed a complete coarse-grid algorithm for a class of nonlinear parabolic equations based on an upscaling procedure that shares some common element with the other multiscale numerical methods. The core step of this upscaling method is that the nonlinear constitutive relations such as the relationship between the hydraulic conductivity and the pressure, \( K(x, h) \), are upscaled before solving the nonlinear problems. The real significance of the method lies in its ability to solve the problems on coarse meshes. Concerning the nonlinear convection term, they proposed a new way in which the local problem does not involve the convection term, which is different from the multiscale finite element method introduced by Efendiev et al. (2004) and Efendiev and Pankov (2004). It seems to be the first attempt to address such a problem of computing the approximation of the convection term. They provided a detailed convergence analysis of the method under the periodicity assumption and demonstrated the efficiency and the accuracy of the method for the Richards equation of the exponential model by carrying out numerical experiments with periodic and random permeability fields.

To verify its applicability in more realistic and varied flow scenarios, in this study we applied this method to one- and two-dimensional simulations of unsaturated water flow through
heterogeneous soil profiles under different boundary conditions including infiltration, evaporation, and drainage. The one-dimensional simulations focused on illustrating and evaluating the performance of the method under a varied range of boundary conditions. We also investigated the effects of different degrees of heterogeneity of the hydraulic conductivity field and the coarsening ratio on the simulation results. The two-dimensional simulations further focused on evaluating the applicability of the method when the soil medium has isotropy and anisotropy heterogeneity. Moreover, two types of constitutive relations were considered in all the simulations. To close the Richards equation, constitutive relations are needed that consist of a reliable descriptive model of the soil water retention curve \( \theta(b) \) as well as an accurate model of the unsaturated hydraulic function \( K(x,h) \).

In this study, the Gardner–Basha model, which has been widely used in the stochastic analysis of unsaturated flow in heterogeneous soils (e.g., Yeh and Zhang, 1996; Harter and Yeh, 1998), and the Mualem–van Genuchten model, which is one of the most frequently used models because it is more realistic for natural soils, were considered as the constitutive relations in the simulations. Results show that the upsampling method can capture the large-scale structure of fine-scale behavior effectively in the flow scenarios considered in this study.

Note that in this study we pre-calculated the upscaled effective hydraulic functions on each coarse block by solving the local problems separately from the coarse-scale simulations to avoid the expensive computation of upsampling these functions. In the upsampling method proposed by Chen et al. (2005), the upscaled nonlinear coefficients corresponding to the diffusion and convection terms can be computed analytically under the periodicity assumption. For real natural porous media, these coefficients are computed numerically from the fine-scale solutions of the local boundary value problems. This computation, in theory, needs to be done at each time step on each coarse block during the coarse-scale simulation because an unsaturated hydraulic parameter such as \( K(h) \) is a function of the pressure head depending on the location and time. This makes the computation extremely expensive and often out of reach due to the limitations of computer resources. However, in practice, such expensive computation can be avoided by pre-calculating the effective hydraulic functions. This was accomplished in this study by solving the local flow problems on each coarse block for several fixed values of the water pressure head within the expected range and then using them in the coarse-scale simulations. Once the upscaled effective hydraulic functions are given in such a discrete form, an interpolation of parameter values between the pre-calculated points would be easy. Because the upscaled effective hydraulic functions can be reused, the resulting method is relatively efficient. In our study, we also determined how much computational cost can be saved when the pre-calculation procedure is applied. There is a remarkable CPU saving in the computational cost without compromising accuracy when using the pre-calculation procedures.

Materials and Methods

The Richards Equation

The Richards equation is the commonly accepted basis for detailed studies of soil water movement in unsaturated soils. This equation can be expressed in terms of both the pressure head \( b \) and the volumetric water content \( \theta \), resulting in an \( b \)-based form, a \( \theta \)-based form, or a mixed form of the Richards equation. In this study, we considered the mixed form of the Richards equation for the unsaturated flow:

\[
\frac{\partial \theta(b)}{\partial t} = - \nabla \cdot \left[ K(x,h) \nabla (b-z) \right] = f
\]

where \( \theta \) is the volumetric water content, \( b \) is the pressure head, \( K(x,h) \) is the unsaturated hydraulic conductivity, \( x = (x, y, z) \) is the spatial coordinate, \( z \) denotes the vertical coordinate that is positively oriented downward, \( t \) is time, and \( f \) stands for possible sources or sinks.

Soil Hydraulic Property Models

Unsaturated flow in the vadose zone is often simulated based on the continuum approach with constitutive relations. Such relations consist of the soil water retention curve \( \theta(b) \), which describes the relationship between the soil water content and the soil water pressure head, and the unsaturated hydraulic conductivity function \( K(x,b) \), which relates the hydraulic conductivity to the water content or the soil water pressure head. The source of the nonlinearity of the Richards equation comes from \( \theta(b) \) and \( K(x,b) \). In this study, we considered two sets of constitutive relations. One set is the Gardner–Basha model [the Gardner model (Gardner, 1958) coupled with the \( \theta(b) \) relation suggested by Basha (1999)], which has been widely used in stochastic analysis of unsaturated flow in heterogeneous soils, and the other is the Mualem–van Genuchten model (Mualem, 1976; van Genuchten, 1980), which is the most frequently used model because it is more realistic for natural soils.

The Gardner–Basha model: The constitutive relations used by Gardner (1958) and Basha (1999) are

\[
\theta(b) = \theta_r + (\theta_s - \theta_r) \exp(-\beta|b|)
\]

(2)

\[
K(x,b) = K_s(x) K_r(b) = K_s(x) \exp(-\alpha_C|b|)
\]

(3)

where \( \theta_r \) is the residual water content, \( \theta_s \) is the saturated water content, \( \beta \) and \( \alpha_C \) are parameter characteristics of the soil pore size distribution, \( K_s \) is the relative hydraulic conductivity, and \( K_r \) is the saturated hydraulic conductivity.

The Mualem–van Genuchten model: Van Genuchten (1980) combined his S-shaped soil water content–pressure head curve with the statistical pore-size distribution model of Mualem (1976) to obtain the following constitutive relations:
\[ \theta(b) = \theta_1 + (\theta_2 - \theta_1) \left[ 1 + \left( \alpha_\nu \| b \| \right)^{m'} \right] \left[ 1 + \left( \alpha_\nu \| b \| \right)^{m'} \right]^{-m'} \]  \hspace{1cm} [4]

\[ K(x,b) = K_s(x) K_i(b) \]
\[ = K_s(x) \left[ 1 - (\alpha_\nu \| b \|)^{n'-1} \frac{1}{\left( 1 + (\alpha_\nu \| b \|)^{n'} \right)^{m/2}} \right] \]  \hspace{1cm} [5]

\[ m' = 1 - \frac{1}{n'} \]  \hspace{1cm} [6]

where \( n' \) and \( m' \) are empirical parameters determining the shape of the soil water retention curve and \( \alpha_\nu \) is a parameter relating to the mean pore size.

As is well known, the multiscale nature of the porous media flow problem often comes from the spatial heterogeneity of the saturated hydraulic conductivity \( K_s \) and the pore size distribution parameter \( \alpha_\nu \) in the Gardner–Basha model. Much experimental evidence indicates that the \( K_s \) and \( \alpha_\nu \) of many soils follow a lognormal distribution (Byers and Stephens, 1983; Sudicky, 1986; Hopmans et al., 1988; Unlu et al., 1990; Russo and Bouton, 1992; White and Sully, 1992), and such lognormal distributions have been widely used in the literature. In all examples below, we assume that \( K_s \) and \( \alpha_\nu \) follow lognormal distributions and use the turning bands method (Mantoglou and Wilson, 1982; Tompson et al., 1989) with the exponential covariance model to generate realizations of \( K_s \) and \( \alpha_\nu \) fields of the study domain.

**Upscaling Formulation**

Here we introduce the upscaling formulation for a generic nonlinear convection–diffusion equation in a more general context. Considering a study domain \( \Omega \) in \( d \)-dimensional space with an underlying fine grid (Fig. 1 schematically shows an example of a fine-scale definition and a coarse-scale partition in two-dimensional space), we set \( Q_T = \Omega \times (0,T) \) and \( S_T = \partial \Omega \times (0,T) \) for \( 0 < T < \infty \). Consider the following parabolic equation:

\[ \frac{\partial b^e}{\partial t} - \nabla \left[ K^e(x,b^e) \nabla b^e + A^e(x,b^e) \right] = f(x,t) \quad \text{in} \quad Q_T \]

\[ b^e(x,t) = 0 \quad \text{on} \quad S_T \]

\[ b^e(x,0) = b_0(x) \quad \text{in} \quad \Omega \]

where \( x = (x_1, x_2, ..., x_d) \), \( K^e(x,b^e) = K_{ij}^e(x,b^e) \) is a symmetric, positive definite, bounded tensor for some positive constant \( l_1 \) and \( l_2 \), and \( A^e(x,b^e) = A^e_i(x,b^e) \) is a bounded vector. We note that for the Richards equation, \( K^e(x,b^e) \) is related to the unsaturated hydraulic conductivity tensor associated with the diffusion term in the equation and \( A^e_i(x,b^e) = -K^e(x,b^e) \partial_i \) is related to the convection term of the equation; \( \varepsilon \) is the characteristic length representing the small-scale variability of the medium. We also assume that \( \partial K^e_{ij}(x,s)/\partial s, \partial A^e_i(x,s)/\partial s \), where \( s \) is an arbitrary real number, are uniformly bounded and \( \theta(s) \) satisfies

\[ 0 < \theta_1 < \theta(s) \leq \theta_2 < \infty, \quad \theta''(s) < C, \quad \forall s \in \mathbb{R} \]

Define the space

\[ W = b: b \in L^2(0,T; H^1_0(\Omega)), b \in H^1(0,T; H^{-1}(\Omega)) \]

The variational problem of Eq. [7] is to seek \( b^e \in W \) for almost every \( t \in (0,T) \), \( b^e(x,t) \in H^1_0(\Omega) \) such that \( b^e(x,0) = b_0(x) \) in \( \Omega \), and

\[ h^e_i = 1 \quad \text{on} \quad S \]

\[ h^e_i = 0 \quad \text{on} \quad T \]

Fig. 1. Schematic illustration of fine- and coarse-scale meshes and of the upscaling procedures for the unsaturated flow problem; \( h^e_i \) is the pressure head, \( K^e(x,s) \) is the unsaturated hydraulic conductivity tensor, where \( \varepsilon \) is the characteristic length representing the small-scale variability of the media, \( x = (x_1,x_2) \) is the spatial coordinate, and \( i \) is an arbitrary real number.
where the homogenized coefficients \( \mathbf{\bar{K}}(x,b) \) and \( \mathbf{\bar{A}}(x,b) \) can be computed analytically from \( \mathbf{K}(x,b) \) and \( \mathbf{A}(x,b) \), respectively, under the assumption that the oscillating coefficients of porous media are periodic. Such an assumption allows us to use homogenization theory to obtain the asymptotic solutions. Chen et al. (2005) gave a detailed convergence analysis and a sharp capability of the results only to media with spatial periodicity. For heterogeneous natural media in which such analytical formulae do not exist, the nonlinear relations \( \mathbf{\bar{K}}(x,\cdot) \) and \( \mathbf{\bar{A}}(x,\cdot) \) can be computed numerically.

Let \( M_u \) be a regular triangulation of \( \Omega \) with mesh size \( h = T/N \) be the time step length, \( t^n = nT, n = 0, 1, \ldots, N \). Further, let \( W_u \) be the standard conforming linear finite element space over \( M_u \) and \( W_0 = W_u \cap H_0^1(\Omega) \). Set \( v = 0(h) \). For \( n = 1, 2, \ldots, N \), the discrete problem is to seek \( v_n \in W_u \), the approximate solution of \( v \) at time \( t = t^n \), so that

\[
\begin{align*}
\frac{v_n - v_{n-1}}{\tau} + & \mathbf{\bar{K}}(x,b^n) \nabla b^n + \mathbf{\bar{A}}(x,b^n) \cdot \nabla \omega_n = 0, \\
& \forall \omega_n \in W_u^0
\end{align*}
\]

where \( b^n = 0^{-1}(v_n) \), \( v_0 = 0(b_0) \) and

\[
\mathcal{F}^n = \tau^{-1} \int_{t^n \to t^{n+1}} f(x,t) dt
\]

To solve the water flow problems at the coarse scale, we need to calculate \( \mathbf{\bar{K}}(x,s) \) and \( \mathbf{\bar{A}}(x,s) \) for each coarse block, \( V_i \), in \( \Omega \). The numerical solutions of such upscaled hydraulic properties are obtained by solving the local elliptic problems with appropriate boundary conditions. For any \( s \in \mathbb{R} \), the nonlinear functions of \( \mathbf{\bar{K}}(x,s) \) and \( \mathbf{\bar{A}}(x,s) \) are piecewise constants over \( M_u \), defined as follows.

For any \( V \in M_u \) and \( s \in \mathbb{R} \), we solve the local problems to obtain the solutions of \( p_i \) on \( V_i = 1, 2, \ldots, d \):

\[
- \nabla \cdot [\mathbf{\bar{K}}(x,s) \nabla p_i] = 0 \quad \text{in } V \]

\[
p_i = x_i \quad \text{on } \partial V \]

Then, on \( V, \mathbf{\bar{K}} \) is a constant tensor determined by the following system:

\[
\mathbf{\bar{K}} \left( \nabla p_i \right)_V = \left( \mathbf{K}(x,s) \nabla p_i \right)_V \quad i = 1, 2, \ldots, d
\]

where \( p_i \) is the solution of Eq. [16] in \( V \) with the appointed boundary condition (Eq. [17]), and \( \cdot = (1/V) \int_V \cdot dx \) is the volume-average \( V \). To determine \( \mathbf{\bar{K}} \) from Eq. [18], we need \( d \) sets of fine-scale solutions of Eq. [16]. In three dimensions, three pressure solutions are sufficient to determine \( \mathbf{\bar{K}} \) from Eq. [18], provided that the volume averages of the pressure gradients are linearly independent. Similar to the linear case stated by Efendiev et al. (2004), the main idea of the calculation of the coarse-scale hydraulic properties is that it delivers the same average response as that of the underlying fine-scale problem locally. Take the two-dimensional simulation, for example—such calculation based on the local problems is schematically depicted in Fig. 1. For each coarse block \( V \), we solve the local problems with some appropriate boundary conditions. Various boundary conditions including periodic, Dirichlet, and so forth can be used to calculate the local solutions and thus the effective parameters. One of such boundary conditions is the widely used pressure-drop no-flow condition, for example, setting \( p_i = 1 \) and \( p_i = 0 \) on opposite sides along one direction and no-flow boundary conditions on the other side. The effects of various boundary conditions of the local microscale problem have been investigated by Wu et al. (2002) and Yue and E (2007).

We can then use Green’s theorem:

\[
\left( \nabla p_i \right)_V = e_i + \frac{1}{V} \int_{\partial V} (p_i - x_i) n d \sigma = e_i
\]

where \( e_i \) is the unit vector in the \( i \)th direction. Thus, Eq. [18] can be simplified as

\[
\mathbf{e}_i \cdot \mathbf{\bar{K}}(x,s) \nabla p_i = \left( \nabla p_i \right)_V
\]

Similar to the linear case (see Wu et al., 2002), \( \mathbf{\bar{K}} \) is symmetric and positive definite, and

\[
e_i \cdot \mathbf{\bar{K}}(x,s) \nabla p_i = \left( \nabla p_i \right)_V
\]
Further, for the convection term, \( \mathbf{A}(x, s) \) is a constant vector in \( V \) determined by

\[
\mathbf{A}(x, s) = \left\{ \mathbf{A}^e(x, s) \cdot \nabla p \right\}_V \tag{22}
\]

The ultimate goal of upscaling is to compute solutions on coarse-scale meshes. The approach considered in this study was to replace the local coefficients \( K(x, b) \) and \( \mathbf{A}(x, b) \) with the homogenized coefficients \( K^*(x, b) \) and \( \mathbf{A}^*(x, b) \), respectively. The homogenized coefficients are discrete functions relying on the discretization of the medium and depending on the soil type and the moisture condition of the grid block on which the coefficients are computed. An essential requirement for the computed homogenized coefficients is that they can lead to the pressure head and the flow velocity at a certain accuracy at the coarse scale. Furthermore, it is ideal that these hydraulic functions depend only on the detailed nature of the heterogeneity and the discretization of the medium, so that these hydraulic functions can be used in different flow scenarios once they are computed.

**Implementation of the Upscaling Method**

Our problem of interest is to upscale the soil water flow processes and model the corresponding coarse-scale problems. Before the coarse-scale simulation, the effective constitutive relations on each coarse grid are calculated by solving the local problems separately. The computational cost of this calculation is reduced by performing a pretreatment procedure that builds up the database of the effective constitutive relations in discrete form. To be specific, we do the following three steps:

1. For some fixed coarse-scale pressure head values, we solve the local problem (Eq. [16]) in each coarse grid under the appropriate boundary conditions (depicted in Fig. 1) to obtain the pressure gradients.

2. Using the solutions obtained from Step 1, we compute the homogenized nonlinear relations \( \mathbf{K}(x, s) \) (Eq. [21]) and \( \mathbf{A}(x, s) \) (Eq. [22]) that correspond to the diffusion term and the convection term, respectively, in the Richards equation.

3. During the coarse-scale simulation, we approximate the effective or homogenized coefficients by using an interpolation scheme and then use them in the coarse-scale solutions.

**Results and Discussion**

We now apply the upscaling method to the one- and two-dimensional Richards equations, which describe water flow through heterogeneous soils. To facilitate the comparison among different schemes, we denote the upscaling method with pre-calculation of the effective constitutive relations outside the coarse-scale simulation as UM-p. Accordingly, we denote the upscaling method with calculation of the effective constitutive relations during the coarse-scale simulation as UM. As a side note, we solve Eq. [1] on fine-scale grids by implementing some iteration method and use this fine-scale solution as a reference solution, which is denoted as “fine scale.” The coarse-scale solutions are then compared with this fine-scale solution. To evaluate the performance of the method, the frequently used relative Euclidean norm \( L^2 \) and the relative maximum norm \( L^\infty \) are used:

\[
L^2 = \left[ \frac{\sum_{i=1}^{M} (H_i - b_i)^2}{\sum_{i=1}^{M} (b_i)^2} \right]^{1/2} \tag{23}
\]

\[
L^\infty = \max_{i=1,\ldots,M} \frac{H_i - b_i}{\max_{i=1,\ldots,M} |b_i|} \tag{24}
\]

where \( M \) is the total number of nodes on the coarse grid, \( H_i \) is the coarse solution of the pressure head at the \( i \)th node, and \( b_i \) is the fine solution of the pressure head at the corresponding node.

**Set 1: One-Dimensional Simulations in Vertical Soil Profiles**

Soil Water Flow Problems with Infiltration Boundaries

We show two examples for the one-dimensional ponded infiltration problem, using the Gardner–Basha model and the Mualem–van Genuchten model, respectively. In all the one-dimensional test examples below, the numerical calculations are performed for a soil column of 10 m. The computation unit for the fine-scale equation is divided into 512 grid cells, whereas the size of the coarse-scale grid cells is 32.

For the case of the Gardner–Basha model, we solve the one-dimensional unsaturated soil water flow problem with a ponded depth of 1 cm on the top of the soil profile, i.e., \( b = 0.01 \) m on \( \Gamma_{\text{top}} \), while the bottom boundary condition is a free drainage boundary, \( \partial h/\partial z = 0 \) on \( \Gamma_{\text{bottom}} \), where \( \Gamma_{\text{top}} \) and \( \Gamma_{\text{bottom}} \) denote the top side and the bottom side, respectively, of the study domain \( \Omega \). The initial condition is given by a pressure head of \(-10 \) m in the entire soil profile, i.e., \( h(z, 0) = -10 \) m. Realization of the saturated hydraulic conductivity field \( K_s^e \) and the parameter characteristic of the soil pore size distribution field \( \alpha_G^e \) at the fine scale is generated using the turning bands method. The geometric mean of \( K_s^e \) \( ( K_s^e ) \) is 0.01 m min\(^{-1} \). The standard deviation of the logarithm of the saturated hydraulic conductivity \( \sigma_{\ln K_s^e} \) is 1.5 and the correlation length \( \lambda \) is 0.5 m, which is equivalent to the coefficient of variation of the hydraulic conductivity \( CV_{K_s^e} = 170.7\% \), which represents a moderate heterogeneity in hydraulic conductivity. This conductivity varies by two orders of magnitude, ranging from a minimum of \( 2.7830 \times 10^{-4} \) m min\(^{-1} \) to a maximum of \( 1.932 \times 10^{-1} \) m min\(^{-1} \). For \( \alpha_G \), we set \( \bar{\alpha}_G = 0.1 \) m\(^{-1} \) and \( \sigma_{\ln \alpha_G} = 0.4 \) for the variation. The total simulation time is set to 5 h and is divided into equal time steps with size \( \tau = 1 \) min. For the Gardner–Basha model parameters, we chose \( \beta = 0.15, \theta_c = 0.4120, \) and \( \theta_s = 0.0210 \).
Next, we use the upscaling method to simulate the coarse-scale water flow. The obtained coarse-scale solutions of the water pressure head \( \tilde{h} \) corresponding to the fine-scale solutions \( h^s \) at \( t = 0.1, 1, \) and \( 5 \) h by the UM-p method are depicted in Fig. 2 [denoted as coarse-scale (UM-p)]. Also shown in Fig. 2 are the coarse-scale solutions derived from the theoretical upscaling method through solving the local problems at each time step during the coarse-scale simulation [denoted as coarse-scale (UM)] and the fine-scale solutions (denoted as fine-scale). Results show that the two upsampling methods are in good agreement with each other and that both can effectively match the fine-scale solutions on the coarse grid. This resemblance is quantified by the \( L_2 \) norm and the \( L_∞ \) norm, respectively. Table 1 presents the relative errors of the coarse-scale models compared with the fine-scale model at \( t = 0.1, 1, \) and \( 5 \) h.

Both coarse-scale methods give good accuracy in the \( L_2 \) and \( L_∞ \) norms. We can see from this test example that the CPU time for the UM-p method was 15% of that for the UM method. This illustrates that the pre-calculation of the effective hydraulic functions offers a big saving in computing time for the construction of a database of the effective hydraulic functions. Here, we again mention that with the UM method, all the effective hydraulic functions are recomputed at each time step by solving the local problems, while with the UM-p method, the effective hydraulic functions are computed in advance in the expected range and then used in the coarse-scale simulations.

For the case of the Mualem–van Genuchten model, we solve the one-dimensional unsaturated soil water flow problem with the same initial conditions as the first example. We impose the following boundary conditions for this infiltration problem: \( h = -1 \) m on \( \Gamma_{\text{top}} \) and a free-drainage boundary on \( \Gamma_{\text{bottom}} \). The related parameters for the Mualem–van Genuchten model are as follows: \( \theta_s = 0.3658, \theta_r = 0.0386, n' = 2, m' = 0.5, \sigma_{\text{in}}K_{\epsilon}' = 1.5, \) and \( \sigma_{\text{ln}}\alpha' = 0.4 \). We assume that the geometric means of \( K_{\epsilon}' \) and \( \alpha' \) are \( 0.002 \) m \( \text{min}^{-1} \) and \( 0.15 \) m\(^{-1} \), respectively. The correlation lengths of both \( K_{\epsilon}' \) and \( \alpha' \) are \( 0.5 \) m.

The coarse-scale water pressure heads derived by the UM-p method, the UM method, and the fine solutions are plotted at \( t = 1, 4, \) and \( 8 \) h in Fig. 3. We can see that both coarse-scale models compare well with the fine solutions on a coarse grid. Table 2 presents the relative errors of the coarse-scale models compared with the fine-scale model at \( t = 1, 4, \) and \( 8 \) h. As in the previous example, both coarse models give equally good results in the \( L_2 \) and \( L_∞ \) norms. For this test example, the CPU time for the UM-p method was 16% of that of the UM method. This again indicates that the UM-p method noticeably reduces the computing time compared with the UM method while ensuring accuracy.

### Soil Water Flow Problems with an Upward Evaporation Boundary

We assume that an evaporation experiment is performed after the soils reach the water content of field capacity. Thus, for this problem, the initial condition is assigned according to the following boundary conditions for this infiltration problem: \( h = -1 \) m on \( \Gamma_{\text{top}} \) and a free-drainage boundary on \( \Gamma_{\text{bottom}} \). The related parameters for the Mualem–van Genuchten model are as follows: \( \theta_s = 0.3658, \theta_r = 0.0386, n' = 2, m' = 0.5, \sigma_{\text{in}}K_{\epsilon}' = 1.5, \) and \( \sigma_{\text{ln}}\alpha' = 0.4 \). We assume that the geometric means of \( K_{\epsilon}' \) and \( \alpha' \) are \( 0.002 \) m \( \text{min}^{-1} \) and \( 0.15 \) m\(^{-1} \), respectively. The correlation lengths of both \( K_{\epsilon}' \) and \( \alpha' \) are \( 0.5 \) m.

The coarse-scale water pressure heads derived by the UM-p method, the UM method, and the fine solutions are plotted at \( t = 1, 4, \) and \( 8 \) h in Fig. 3. We can see that both coarse-scale models compare well with the fine solutions on a coarse grid. Table 2 presents the relative errors of the coarse-scale models compared with the fine-scale model at \( t = 1, 4, \) and \( 8 \) h. As in the previous example, both coarse models give equally good results in the \( L_2 \) and \( L_∞ \) norms. For this test example, the CPU time for the UM-p method was 16% of that of the UM method. This again indicates that the UM-p method noticeably reduces the computing time compared with the UM method while ensuring accuracy.

### Soil Water Flow Problems with an Upward Evaporation Boundary

We assume that an evaporation experiment is performed after the soils reach the water content of field capacity. Thus, for this problem, the initial condition is assigned according to the

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**Table 1. The errors in the relative Euclidean \( (L_2) \) and maximum \( (L_∞) \) norms for the coarse solutions from the upscaling method (UM) and the upscaling method with pre-calculation (UM-p) compared with the fine solutions for the one-dimensional ponded infiltration problem at \( t = 0.1, 1, \) and \( 5 \) h using the Gardner–Basha model.**

<table>
<thead>
<tr>
<th>Time</th>
<th>Coarse scale (UM)</th>
<th>Coarse scale (UM-p)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( L_2 )</td>
<td>( L_∞ )</td>
</tr>
<tr>
<td>0.1</td>
<td>3.465 ( \times ) 10^{-2}</td>
<td>9.980 ( \times ) 10^{-2}</td>
</tr>
<tr>
<td>1</td>
<td>2.482 ( \times ) 10^{-2}</td>
<td>3.801 ( \times ) 10^{-2}</td>
</tr>
<tr>
<td>5</td>
<td>3.790 ( \times ) 10^{-2}</td>
<td>4.939 ( \times ) 10^{-2}</td>
</tr>
</tbody>
</table>

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**Fig. 2. Comparison of the water pressure head \( h \) between the coarse-scale models using the upscaling method (UM) and the upscaling method with pre-calculation (UM-p) for the one-dimensional ponded infiltration problem at time \( t = 0.1, 1, \) and \( 5 \) h using the Gardner–Basha model.**

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**Fig. 3. Comparison of the water pressure head \( h \) between the coarse-scale models using the upscaling method (UM) and the upscaling method with pre-calculation (UM-p) for the one-dimensional ponded infiltration problem at time \( t = 1, 4, \) and \( 8 \) h using the Mualem–van Genuchten model.**
physical definition of the field capacity for many soils (Jury et al., 1991; Saxton and Rawls, 2006): the soil matric potential is −33 kPa, i.e., $h = -3.412$ m. The boundary conditions are imposed as follows: $\Gamma_{\text{top}}$ is an upward flux boundary with water flux $q = 0.0003 \text{ m min}^{-1}$ and $\Gamma_{\text{bottom}}$ is a Dirichlet boundary with $b = 0$ m.

For this unsaturated water flow problem with the evaporation boundary condition, we consider two cases, using the Gardner–Basha model and the Mualem–van Genuchten model, respectively. For both cases, we use the same model parameters as for the soil water flow problems with infiltration boundaries. The pressure heads in the soil profile at $t = 0.1, 1, \text{ and } 5$ h and $t = 1, 4, \text{ and } 8$ h obtained from the coarse-scale models and the fine-scale model are shown in Fig. 4 and 5 for the Gardner–Basha model and the Mualem–van Genuchten model, respectively. As can be seen from these figures, the two coarse-scale models can effectively capture the large-scale structure of the fine-scale solutions. The relative errors for the two coarse-scale simulations at $t = 0.1, 1, \text{ and } 5$ h and $t = 1, 4, \text{ and } 8$ h are presented in Tables 3 and 4, respectively, indicating that both models give good results in the $L^2$ and $L^\infty$ norms. We note that the total CPU time for the UM-p method was 15 and 16% of that for the UM method for the two cases with the Gardner–Basha model and the Mualem–van Genuchten model, respectively.

Effects of Upscaling Ratios and Heterogeneity of the Hydraulic Conductivity

We next turned our attention to exploring some important aspects that have effects on the accuracy of the upsampling method, including the upsampling ratio (the ratio of the coarse grid size to the fine grid size) and the degree of spatial variability of the hydraulic conductivity.

Table 2. The errors in the relative Euclidean ($L^2$) and maximum ($L^\infty$) norms for the coarse solutions from the upscaling method (UM) and the upsampling method with pre-calculation (UM-p) compared with the fine solutions for the one-dimensional ponded infiltration problem at $t = 1, 4, \text{ and } 8$ h using the Mualem–van Genuchten model.

<table>
<thead>
<tr>
<th>Time</th>
<th>$L^2$ (UM)</th>
<th>$L^\infty$ (UM)</th>
<th>$L^2$ (UM-p)</th>
<th>$L^\infty$ (UM-p)</th>
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<tr>
<td>1 h</td>
<td>$3.468 \times 10^{-2}$</td>
<td>$1.051 \times 10^{-1}$</td>
<td>$3.469 \times 10^{-2}$</td>
<td>$1.051 \times 10^{-1}$</td>
</tr>
<tr>
<td>4 h</td>
<td>$2.015 \times 10^{-2}$</td>
<td>$3.801 \times 10^{-2}$</td>
<td>$2.015 \times 10^{-2}$</td>
<td>$3.801 \times 10^{-2}$</td>
</tr>
<tr>
<td>8 h</td>
<td>$2.544 \times 10^{-2}$</td>
<td>$3.357 \times 10^{-2}$</td>
<td>$2.544 \times 10^{-2}$</td>
<td>$3.357 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

Fig. 4. Comparison of the water pressure head ($h$) between the coarse-scale models using the upscaling method (UM) and the upsampling method with pre-calculation (UM-p) and the fine-scale model for the one-dimensional upward evaporation problem at time $t = 0.1, 1, \text{ and } 5$ h using the Gardner–Basha model.

Fig. 5. Comparison of the water pressure head ($h$) between the coarse-scale models using the upscaling method (UM) and the upsampling method with pre-calculation (UM-p) and the fine-scale model for the one-dimensional upward evaporation problem at time $t = 1, 4, \text{ and } 8$ h using the Mualem–van Genuchten model.

Table 3. The errors in the relative Euclidean ($L^2$) and maximum ($L^\infty$) norms for the coarse solutions from the upscaling method (UM) and the upsampling method with pre-calculation (UM-p) compared with the fine solutions for the one-dimensional upward evaporation problem at $t = 0.1, 1, \text{ and } 5$ h using the Gardner–Basha model.

<table>
<thead>
<tr>
<th>Time</th>
<th>$L^2$ (UM)</th>
<th>$L^\infty$ (UM)</th>
<th>$L^2$ (UM-p)</th>
<th>$L^\infty$ (UM-p)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1 h</td>
<td>$4.644 \times 10^{-2}$</td>
<td>$9.282 \times 10^{-2}$</td>
<td>$4.668 \times 10^{-2}$</td>
<td>$9.257 \times 10^{-2}$</td>
</tr>
<tr>
<td>1 h</td>
<td>$6.166 \times 10^{-2}$</td>
<td>$6.855 \times 10^{-2}$</td>
<td>$6.071 \times 10^{-2}$</td>
<td>$6.759 \times 10^{-2}$</td>
</tr>
<tr>
<td>5 h</td>
<td>$2.414 \times 10^{-2}$</td>
<td>$2.052 \times 10^{-2}$</td>
<td>$2.269 \times 10^{-2}$</td>
<td>$1.914 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

Table 4. The errors in the relative Euclidean ($L^2$) and maximum ($L^\infty$) norms for the coarse solutions from the upscaling method (UM) and the upsampling method with pre-calculation (UM-p) compared with the fine solutions for the one-dimensional upward evaporation problem at $t = 1, 4, \text{ and } 8$ h using the Mualem–van Genuchten model.

<table>
<thead>
<tr>
<th>Time</th>
<th>$L^2$ (UM)</th>
<th>$L^\infty$ (UM)</th>
<th>$L^2$ (UM-p)</th>
<th>$L^\infty$ (UM-p)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 h</td>
<td>$4.006 \times 10^{-2}$</td>
<td>$6.791 \times 10^{-2}$</td>
<td>$4.006 \times 10^{-2}$</td>
<td>$6.790 \times 10^{-2}$</td>
</tr>
<tr>
<td>4 h</td>
<td>$3.680 \times 10^{-2}$</td>
<td>$5.766 \times 10^{-2}$</td>
<td>$3.680 \times 10^{-2}$</td>
<td>$5.766 \times 10^{-2}$</td>
</tr>
<tr>
<td>8 h</td>
<td>$3.660 \times 10^{-2}$</td>
<td>$4.528 \times 10^{-2}$</td>
<td>$3.660 \times 10^{-2}$</td>
<td>$4.528 \times 10^{-2}$</td>
</tr>
</tbody>
</table>
To accomplish this objective, we conducted a series of numerical examples in one-dimensional soil profiles under different levels of coarsening and spatial variability of the hydraulic conductivity.

First, the effect of upscaling ratios was investigated. Two sets of test cases were conducted, using the Gardner–Basha model and the Mualem–van Genuchten model, respectively. Each set of tests included six levels of coarsening. The fine-scale model used 512 grid cells, whereas the coarse-scale models used 256, 128, 64, 32, 16, and 8 grids, i.e., $1/2, 1/4, 1/8, 1/16, 1/32,$ and $1/64$ of the fine grid size. The related model parameters in these two sets were the same as those in the first and second examples, respectively, in the soil water flow problems with infiltration boundaries. These two sets of examples had boundary conditions for the unsaturated water flow problem as follows:

$$h = -1 \text{ m on } \Gamma_{\text{top}} \text{ and } h = -10 \text{ m on } \Gamma_{\text{bottom}}.$$  

The initial condition was given by a pressure head of $-10$ m in the entire soil profile, i.e., $h(z,0) = -10$ m. For comparison, Fig. 6 shows the average $L^2$ and $L^\infty$ norms during 5 h when the Gardner–Basha model (left) and the Mualem–van Genuchten model (right) were used. As expected, the discrepancy is larger in the case of a higher degree of coarsening. We also note that in these tests, the coarse-scale solutions give relatively better agreement with the fine-scale solutions when the ratio of the fine grid size to the coarse grid size is $\leq 16$.

Second, the effect of the degree of spatial variability of the saturated hydraulic conductivity on the simulation results was investigated. In this study, the spatial variability of the hydraulic conductivity is described by its standard deviation. Also, using the Gardner–Basha model and the Mualem–van Genuchten model, we performed six cases for each model with different standard deviations of the logarithm of the hydraulic conductivity, i.e., $\sigma_{\ln K_s} = 0.5, 1.0, 1.5, 2.0, 2.5, 3.0$. The fine-scale model used 512 grid cells, whereas the coarse-scale models used 32 grid cells. These two sets of test examples had the same boundary and initial conditions for the unsaturated water flow problem as the previous examples with different upscaling ratios. Apparently, for larger spatial variability, the discrepancies between fine-scale and coarse-scale solutions become more pronounced (not shown here for brevity). Figure 7 shows the average $L^2$ and $L^\infty$ norms during 5 h using the Gardner–Basha model (left) and the Mualem–van Genuchten model (right). These two error norms slightly increase as the standard deviation of the logarithm of the hydraulic conductivity becomes increasingly larger. We can also see that the upsampling method gives reasonable results even with a high degree of heterogeneity when $K_s$ varies by five orders of magnitude ($\sigma_{\ln K_s} = 3.0$).

**Set 2: Two-Dimensional Simulations in Vertical Soil Profiles**

Simulations of two-dimensional unsaturated water flow in heterogeneous soil profiles were conducted. Consider a study domain $\Omega$ in two-dimensional $x,z$ space, in which $z$ denotes the vertical coordinate that is positive downward. The solution domain $\Omega$ in the numerical examples is a rectangle of size $40 \times 40$ m. In all the test experiments below, we use a 128 by 128 fine grid and a 16 by 16 coarse grid, that is, the fine grid size is $1/64$ of the coarse grid size. For the two-dimensional simulations, besides applications of the upsampling methods to the statistically isotropic soils, applications to anisotropic soils were also conducted to make the experiments more realistic because natural soils are often observed to exhibit bedding or stratification (e.g., Yeh et al., 1985; Bear et al., 1987). In anisotropic cases, the hydraulic properties including $K_s$ and $\alpha_G$ (or $\alpha_v$) fields of the study domain should be considered to be statistically anisotropic, i.e., the correlation scale of these random fields depends on the direction.

**Unsaturated Soil Water Flow with Downward Infiltration Boundaries**

The problem we consider here is the typical water infiltration into an initially dry soil. The first two examples considered for this problem are conducted in both isotropic and anisotropic soils with
the Gardner–Basha model. We impose the following boundary conditions for the unsaturated flow problem: \( h = -1 \) m on \( \Gamma_{\text{top}} \); \( h = -10 \) m on \( \Gamma_{\text{bottom}} \); \( \Gamma_{\text{left}} \) and \( \Gamma_{\text{right}} \) are impermeable. The initial condition is assigned: \( h = -10 \) m. The related parameters that we assume for the Gardner–Basha model are as follows: \( b = 0.15 \), \( q_s = 0.412 \), and \( q_r = 0.021 \). The saturated hydraulic conductivity \( K_s^e(x) \) and the model parameter \( \alpha_G^e(x) \) are generated using the turning bands method. The geometric means of \( K_s^e \) and \( \alpha_G^e \) are \( 0.0055 \) m min\(^{-1}\) and \( 0.1 \) m\(^{-1}\), respectively. The heterogeneity of the soil porous medium mainly comes from these two random fields, exhibited by the standard deviations of \( \ln K_s^e \) and \( \ln \alpha_G^e \): \( \sigma_{\ln K_s^e} = 1.5 \) and \( \sigma_{\ln \alpha_G^e} = 0.3 \). The correlation structures of the random fields for the two examples are isotropic with \( \lambda_x = \lambda_z = 4 \) m and anisotropic with \( \lambda_x = 16 \) m and \( \lambda_z = 4 \) m, where \( \lambda_x \) and \( \lambda_z \) are the correlation lengths in each direction. The realization of the lognormal saturated conductivity field with isotropic heterogeneity is depicted on the left of Fig. 8. The conductivity field varies by four orders of magnitude, from a minimum \( 3.220 \times 10^{-5} \) m min\(^{-1}\) to a maximum \( 1.128 \) m min\(^{-1}\). The ratio of maximum to minimum for \( \alpha_G^e(x) \) is 8.107. Similarly, the realization of the lognormal saturated conductivity \( K_s^e(x) \) field with anisotropic heterogeneity is shown on the right of Fig. 8. The conductivity field varies from a minimum \( 5.080 \times 10^{-5} \) m min\(^{-1}\) to a maximum \( 0.471 \) m min\(^{-1}\).

We next discuss the simulation results of the two cases with the Gardner–Basha model. The contour plots of the water content at \( t = 1, 2, \) and \( 5 \) h obtained from the coarse-scale solutions by the UM-p method and the fine-scale solutions are shown in Fig. 9.
Fig. 9. Comparison of the water content derived from the fine-scale model (left) and the coarse-scale model using the upscaling method with pre-calculation (UM-p) (right) at time $t = 1, 2,$ and $5$ h for the two-dimensional downward infiltration problem with the Gardner–Basha model and correlation lengths $\lambda_x = \lambda_z = 4$ m.
Fig. 10. Comparison of the water content derived from the fine-scale model (left) and the coarse-scale model using the upscaling method with pre-calculation (UM-p) (right) at time $t = 1$, 2, and 5 h for the two-dimensional downward infiltration problem with the Gardner–Basha model and correlation lengths $\lambda_x = 16$ m and $\lambda_z = 4$ m.
and 10 for the isotropic case and the anisotropic case, respectively. Good agreement can be observed between the coarse-scale result and the fine-scale result. We also compare the plots of the average water pressure heads obtained from the two coarse-scale models (the UM method and the UM-p method) and the fine-scale model at \( t = 0.1, 1, \) and 5 h in Fig. \( 11 \) and 12 for the isotropic case and anisotropic case, respectively. These results were obtained by averaging horizontal water content values at each depth. As can be seen from these figures, both coarse-scale solutions provide good agreement with the fine-scale reference solutions in most locations. Furthermore, Tables 5 and 6 list the errors of the coarse-scale models compared with the fine-scale model for these two cases at \( t = 0.1, 1, \) and 5 h. Such errors indicate that both coarse models give equally good results in the \( 2 \) and \( 5 \) h for the two-dimensional downward infiltration problem with the Gardner–Basha model and correlation lengths \( l_x = l_z = 4 \) m.

Next, we consider an unsaturated infiltration flow simulation with the Mualem–van Genuchten model. We impose the following boundary conditions for the unsaturated flow problem: \( h = -3 \) m on \( \Gamma_{\text{top}}; h = -10 \) m on \( \Gamma_{\text{bottom}}; \Gamma_{\text{left}} \) and \( \Gamma_{\text{right}} \) are impermeable. The initial condition is assigned: \( h = -10 \) m. The related model parameters are as follows: \( \theta_s = 0.3658, \theta_r = 0.0386, n' = 2, \) and \( m' = 0.5. \) The geometric means of \( K^e \) and \( \alpha^e \) are 0.01 m min\(^{-1}\) and 0.15 m\(^{-1}\), respectively. Here we also consider two cases: the correlation structures of the random fields are isotropic with \( \lambda_x = \lambda_z = 4 \) m, or they are anisotropic with \( \lambda_x = 16 \) m and \( \lambda_z = 2 \) m. The random fields \( K^e \) in these two cases are generated with the standard deviations \( \sigma_{\ln K^e} = 2.0 \) and \( \sigma_{\ln K^e} = 1.5 \) for the isotropic case and the anisotropic case, respectively. The parameter fields \( \alpha^e \) for both cases are assigned as \( \sigma_{\ln \alpha^e} = 0.4. \) The conductivity fields vary by six and three orders of magnitude for these two cases, respectively. The ratios of maximum to minimum \( \alpha^e(x) \) are 16.645 and 11.223, respectively. We present the realization of the lognormal saturated conductivity fields for these two cases on the left and right, respectively, of Fig. 13. Figures 14 and 15 present the contour plots of the water content distributions at \( t = 1, 2, \) and 5 h obtained from the coarse-scale solutions by the UM-p method and the fine-scale solutions for the isotropic and anisotropic cases, respectively. These figures illustrate that

**Table 5.** The errors in the relative Euclidean \( (L^2) \) and maximum \( (L^\infty) \) norms for the coarse solutions from the upscaling method (UM) and the upscaling method with pre-calculation (UM-p) compared with the fine solutions for the two-dimensional downward infiltration problem with the Gardner–Basha model and correlation lengths \( \lambda_x = \lambda_z = 4 \) m.

<table>
<thead>
<tr>
<th>Time</th>
<th>Coarse scale (UM)</th>
<th>Coarse scale (UM-p)</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>( L^2 )</td>
<td>( L^\infty )</td>
</tr>
<tr>
<td>h</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td></td>
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<tr>
<td>1</td>
<td></td>
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<tr>
<td>5</td>
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</table>

**Table 6.** The errors in the relative Euclidean \( (L^2) \) and maximum \( (L^\infty) \) norms for the coarse solutions from the upscaling method (UM) and the upscaling method with pre-calculation (UM-p) compared with the fine solutions for the two-dimensional downward infiltration problem at \( 0.1, 1, \) and 5 h using the Gardner–Basha model and correlation lengths \( \lambda_x = 16 \) m and \( \lambda_z = 4 \) m.

<table>
<thead>
<tr>
<th>Time</th>
<th>Coarse scale (UM)</th>
<th>Coarse scale (UM-p)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( L^2 )</td>
<td>( L^\infty )</td>
</tr>
<tr>
<td>h</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td></td>
<td></td>
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<tr>
<td>1</td>
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</table>
the upscaled solutions of the water pressure head effectively capture the large-scale behavior of the fine-scale results. We also compare the average solutions in the horizontal direction of the water pressure heads at $t = 0.1$, 1, and 5 h obtained from the two coarse-scale models with those from the fine-scale model in Fig. 16 and 17 for the isotropic case and the anisotropic case, respectively. As in the previous examples, the results of the UM-p method are very close to those of the UM method in both cases. Comparison of these two figures indicates that the coarse-scale solutions of the anisotropic case do not match the fine-scale solutions as well as those of the isotropic case. This is more obvious as the simulation time increases. Tables 7 and 8 list the relative errors of the coarse-scale models compared with the fine-scale model for these two cases at $t = 0.1$, 1, and 5 h. In both cases, we note that the total CPU time for the UM-p method was about 9% of that for the UM method.

Unsaturated Soil Water Flow with an Upward Evaporation Boundary

Numerical experiments were also conducted for the unsaturated water flow problem with an upward evaporation boundary. For brevity, we present only the simulation results for the anisotropic case with the Gardner–Basha model and the Mualem–van Genuchten model. We used the same model parameters for these two models as those discussed above with downward infiltration boundaries. The boundary conditions that we imposed for the problem are as follows: $\Gamma_{\text{top}}$ is an evaporation boundary with $q = 0.00001 \text{ min}^{-1}$, and $\Gamma_{\text{bottom}}$ is a Dirichlet boundary with $h = 0 \text{ m}$; $\Gamma_{\text{left}}$ and $\Gamma_{\text{right}}$ are impermeable. The initial condition is assigned as the field capacity, i.e., $h = -3.412 \text{ m}$. We present the simulation results of the anisotropic case ($\lambda_x = 16 \text{ m}$ and $\lambda_z = 2 \text{ m}$) with the Gardner–Basha model and of the anisotropic case ($\lambda_x = 16 \text{ m}$ and $\lambda_z = 2 \text{ m}$) with the Mualem–van Genuchten model. Water content distributions in the whole soil profiles at $t = 1$, 2, and 5 h obtained from the coarse-scale model by the UM-p method and the fine-scale model are presented in Fig. 18 and 19 for these two examples, respectively. We can observe that the coarse-scale model captures the large-scale structure of the fine-scale results. The comparison of the average solutions in the horizontal direction of the two coarse-scale results by the UM-p and the UM methods with the fine-scale results at $t = 0.1$, 1, and 5 h are listed in Tables 9 and 10, indicating a reasonable agreement between the coarse-scale and fine-scale results. Compared with the tests (not shown here for brevity) under the same upward evaporation boundary with isotropic heterogeneity, the discrepancy is larger in these anisotropic cases. We note that the total CPU time for the UM-p method was about 8% of that for the UM method for these two examples.

Unsaturated Soil Water Flow with Mixed Boundaries

We also considered one more test example of the unsaturated infiltration with mixed boundary conditions: a prescribed pressure at a part of the top surface and a prescribed flux boundary condition at the other part of the top surface. This simulation is useful for some aspects of agricultural engineering such as furrow and ridge tillage with film mulching between furrows used in many semiarid and arid regions. The more
Fig. 14. Comparison of the water content derived from the fine-scale model (left) and the coarse-scale model using the upscaling method with pre-calculation (UM-p) (right) at time $t = 1, 2, \text{ and } 5 \text{ h}$ for the two-dimensional downward infiltration problem with the Mualem–van Genuchten model and correlation lengths $\lambda_x = \lambda_z = 4 \text{ m}$.
Fig. 15. Comparison of the water content derived from the fine-scale model (left) and the coarse-scale model using the upscaling method with pre-calculation (UM-p) (right) at time $t = 1, 2,$ and $5 \text{ h}$ for the two-dimensional downward infiltration problem with the Mualem–van Genuchten model and correlation lengths $\lambda_x = 16 \text{ m}$ and $\lambda_z = 2 \text{ m}$.
realistic constitutive relation—the Mualem–van Genuchten model—was used. We used the same model parameters for this case as for those discussed above with downward infiltration boundaries. Only the anisotropic case with $l_x = 16$ m and $l_z = 2$ m is presented here. A Dirichlet boundary condition with $h = -1$ m is defined on the left half of the top surface and a no-flow boundary is defined on the right half. The bottom boundary condition is a free-drainage boundary; $\Gamma_{\text{left}}$ and $\Gamma_{\text{right}}$ are impermeable. The initial conditions were assigned with $h = -5$ m on the left part of the simulation domain and $h = -10$ m on the right part.

The total simulation time was set as 50 h. The water content distributions in the whole soil profiles at $t = 1$, 10, and 50 h obtained from the coarse-scale model by the UM-p method and the fine-scale model are presented in Fig. 22, which shows both horizontal flow (which may not have been significant in the previous test cases) and vertical flow. The comparison of the average solutions in the horizontal direction of the two coarse-scale results by the UM-p method and the UM method with the fine-scale results at $t = 1$, 10, and 50 h is shown in Fig. 23. Moreover, the relative errors of the two coarse-scale models compared with those of the fine-scale model at $t = 1$, 10, and 50 h are listed in Table 11, indicating a reasonable agreement between the coarse-scale and fine-scale results. We note that the total CPU time for the UM-p method was about 8% of that for the UM method.

**Conclusions**

In this study, we applied an upscaling method to a series of unsaturated water flow scenarios to illustrate the method and verify its applicability by simulating one- and two-dimensional test cases of water flow through heterogeneous soil profiles under different boundary conditions including infiltration, evaporation, and drainage as well as mixed...
Fig. 18. Comparison of the water content derived from the fine-scale model (left) and the coarse-scale model using the upscaling method with pre-calculation (UM-p) (right) at time $t = 1, 2,$ and $5$ h for the two-dimensional upward evaporation problem with the Gårdner–Basha model and correlation lengths $\lambda_x = 16$ m and $\lambda_z = 4$ m.
Fig. 19. Comparison of the water content derived from the fine-scale model (left) and the coarse-scale model using the upscaling method with precalculation (UM-p) (right) at time $t = 1, 2,$ and $5$ h for the two-dimensional upward evaporation problem with the Mualem–van Genuchten model and correlation lengths $\lambda_x = 16$ m and $\lambda_z = 2$ m.
boundary conditions. The commonly used Gardner–Basha and Mualem–van Genuchten models were used as the constitutive relations in all the simulations. In the upscaling procedures, the effective hydraulic functions are computed based on the solutions of the local problems and need to be updated at each time step on each coarse-scale block due to the nonlinearity of the hydraulic functions. In our test example, we pre-calculated these effective coefficients on each coarse block to avoid the extremely expensive computations and then used them in the coarse-scale simulations.

From a series of test examples, we have demonstrated that the upscaling method with pre-calculation of the effective hydraulic functions (the UM-p method) provides an efficient framework and can be effectively applied to model unsaturated water flow with the various boundary conditions considered in this study. The coarse-scale solutions from the upscaling method can effectively capture the large-scale structure of the fine-scale behavior. Moreover, the results show that the upscaling method with pre-calculation of the effective hydraulic functions (the UM-p method) is very close in accuracy to the method with calculation of these functions by solving the local problems at each time step (the UM method), whereas the UM-p method reduces the computational cost remarkably. This indicates that updating effective hydraulic properties for some fixed values of pressure heads from the expected range is adequate for the whole accuracy of the approximation of the hydraulic properties and thus adequate for the accuracy of the simulation at the coarse scale. To summarize, compared with the UM method, the UM-p method saved >83% of the CPU time in the one-dimensional simulations with 512 fine grid cells and >90% of the CPU time in the two-dimensional simulations with 128 by 128 fine grid cells in this study.

We also investigated the effects of both different degrees of coarsening ratios and the spatial variability of the hydraulic conductivity field on the accuracy of the upscaling method using two sets of one-dimensional numerical tests. It is evident

<table>
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<th>Time (h)</th>
<th>Coarse scale (UM)</th>
<th>Coarse scale (UM-p)</th>
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<tr>
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<td>$L^\infty$</td>
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<tr>
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<td>$6.624 \times 10^{-1}$</td>
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<td>$4.290 \times 10^{-1}$</td>
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<tr>
<td>5</td>
<td>$2.570 \times 10^{-1}$</td>
<td>$6.066 \times 10^{-1}$</td>
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</table>
Fig. 22. Comparison of the water content derived from the fine-scale model (left) and the coarse-scale model using the upscaling method with pre-calculation (UM-p) (right) at time $t = 1, 10, \text{and } 50 \text{ h}$ for the two-dimensional infiltration problem with mixed boundary conditions with the Mualem–van Genuchten model and correlation lengths $\lambda_x = 16 \text{ m}$ and $\lambda_z = 2 \text{ m}$.
that a higher degree of coarsening and heterogeneity produces lower accuracy of the simulations. Moreover, the two-dimensional test examples show that the upsampling method performs better in the isotropic case than in the anisotropic case under the same boundary and initial conditions. Further development of the upsampling strategy is needed to improve the accuracy of the coarse-scale model with higher degrees of coarsening, heterogeneity, and anisotropy.

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