Deep-learning-based upscaling method for geologic models via theory-guided convolutional neural network

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Abstract

Large-scale or high-resolution geologic models usually comprise a huge number of grid blocks, which can be computationally demanding and time-consuming to solve with numerical simulators. Therefore, it is advantageous to upscale geologic models (e.g., hydraulic conductivity) from fine-scale (high-resolution grids) to coarse-scale systems. Numerical upscaling methods have been proven to be effective and robust for coarsening geologic models, but their efficiency remains to be improved. In this work, a deep-learning-based method is proposed to upscale the fine-scale geologic models, which can assist to improve upscaling efficiency significantly. In the deep learning method, a deep convolutional neural network (CNN) is trained to approximate the relationship between the coarse block of fine-scale hydraulic conductivity fields and the corresponding hydraulic heads, which can then be utilized to replace the numerical solvers while solving the flow equations for each coarse block. In addition, physical laws (e.g., governing equations and periodic boundary conditions) can also be incorporated into the training process of the deep CNN model, which is termed the theory-guided convolutional neural network (TgCNN). With the physical information considered, dependence on the data volume of training the deep learning models can be reduced greatly. Several cases of subsurface flow, with varying two-dimensional and three-dimensional structures and isotropic and anisotropic conditions, are used to evaluate the performance of the proposed deep-learning-based upscaling method. The results show that the deep learning method can provide equivalent upscaling accuracy to the numerical method, and efficiency can be improved significantly compared to numerical upscaling.

Keywords

Upscaling · Deep learning · Theory-guided convolutional neural network · Subsurface flow

1 Introduction

Numerical simulation has become an important tool for investigating subsurface flow problems, such as groundwater flow, carbon capture and storage, oil and gas production, etc. The characterization of large-scale or high-resolution geologic models usually requires a large number of grid blocks in numerical simulation, and it would be computationally expensive and time-consuming to run the fine-scale models directly with numerical simulators. For tasks that necessitate simulating multiple realizations of geologic models or running the simulation iteratively, e.g., uncertainty quantification and data assimilation, the computational burden would be further increased. Upscaling the geologic models from fine-scale to coarse-scale can assist to reduce the requisite computational effort for running the models, which has constituted an essential and necessary task for subsurface flow simulation [3–5, 16, 18, 27].

Upscaling of fine-scale hydraulic conductivity requires calculation of equivalent conductivity over the coarse block consisting of high-resolution grid blocks, and the simulated hydraulic heads and velocity with the upscaled conductivity should match the reference fine-scale solutions as closely as possible. There are many upscaling techniques in the existing literature, and systematic reviews of upscaling methods can be found in previous studies [4, 7, 21, 27]. Two categories of classic upscaling methods are firstly introduced here,
including analytical methods and numerical methods [18, 21]. Analytical methods are both straightforward and efficient, such as arithmetic average, geometric average, harmonic average, arithmetic-harmonic average, and harmonic-arithmetic average [6, 27]. Cardwell and Parsons [1] proved that the block equivalent conductivity is bounded by the harmonic-arithmetic average and the arithmetic-harmonic average of fine-scale grids in the block, which is termed Cardwell and Parsons bounds, and Guerillot et al. [11] proposed to calculate the geometric average between the two bounds. Journel et al. [13] reported a power average to calculate equivalent conductivity for coarse blocks. With the exponent value varying from -1 to 1, the calculated equivalent conductivity can vary between the harmonic and the arithmetic averages. Moreover, the determination of the exponent value is case-specific, and depends on the type of heterogeneity, the block shape and size, and flow conditions [27]. Although the analytical methods are simple and fast, accuracy and robustness are limited by assumptions associated with the analytical methods. For instance, the above-mentioned methods assume that the conductivity of the grids in the coarse block should be scalars, and the calculated equivalent conductivity for the block is also assumed to be a scalar. Liao et al. [18] developed an analytical upscaling method based on perturbation expansion techniques and Fourier analysis, which can provide accurate estimations for equivalent conductivity in heterogeneous and anisotropic 2D cases. The analytical method was also further extended to 3D scenarios [17].

Numerical upscaling methods are relatively more accurate and robust for heterogeneous and anisotropic subsurface flow problems. In numerical methods, the flow equations need to be solved for each coarse block, and the finite difference (FD) method is usually utilized. While solving the flow equations for the coarse blocks, the boundary conditions imposed on the blocks would also affect the upscaled equivalent conductivity. The commonly used boundary conditions include fixed head-no flow boundary conditions, fixed head boundary conditions on all sides, and periodic boundary conditions [5, 18, 28, 31]. White and Horne [29] reported a numerical upscaling algorithm, in which a set of different boundary conditions are imposed, and the simulation results are averaged to calculate the coarse equivalent conductivity. Durlofsky [5] utilized periodic boundary conditions for numerical calculation of equivalent conductivity tensors, which can provide symmetric equivalent conductivity tensors. Therefore, upscaled equivalent conductivity with periodic boundary conditions seems to possess more desirable features. Even though numerical methods can provide more robust and accurate estimation of equivalent coarse-scale conductivity, computational burden remains a major challenge, especially for large-scale cases with millions of grid blocks, because the flow equations need to be solved numerically and repeatedly for each coarse block.

Machine learning methods have also been utilized for upscaling tasks to improve the efficiency. The machine learning models can be trained to predict the solutions of the local problems. Chan and Elsheikh [2] utilized a fully-connected neural network as a predictor of the coarse scale basis functions, which was trained to approximate the relationships between the patches of permeability/conductivity fields and the multiscale basis functions. The predicted basis functions can be further used to calculate the approximated fine-scale solutions. Compared to solving the local problems, using the network to get the basis functions requires lower computational costs. Govinda Anantha and Nicholas [10] further proposed to use the dense convolutional encoder-decoder network (Dense-ED) to learn the mapping between the permeability patches and the basis functions. Compared to the fully-connected network, the convolutional encoder-decoder network can extract the correlated spatial information more effectively. However, both the fully-connected network and the convolutional encoder-decoder network in these works are data-driven models, and none of physical laws are considered in the training process of the neural networks.

Introducing the physical constraints into the training process of deep learning/data driven models has attracted great attention in recent years. One of the most popular frameworks is the physics-informed neural network (PINN) [20, 23], which incorporate the residuals of governing equations into the loss function of neural network. In their work, the derivatives in the equations were calculated with the automatic differentiation of fully-connected neural network. Wang et al. [26] proposed a theory-guided auto-encoder (TgAE) framework, in which the governing equations were discretized with finite difference method, and the discretized equation residuals were incorporated into the loss function of the network to impose the physical constraints. The similar idea was also studied by Karnakov et al. [14], who termed this framework as Optimizing a Discrete Loss (ODIL). While these works aim to construct a global model for a specific problem, there are few attempts to construct a local deep learning model with physical constraints for upscaling purposes.

In this work, we attempt to utilize theory-guided or physics-constrained deep learning models to achieve efficient upscaling of geologic models. The convolutional neural network (CNN) can be trained as a local small-scale model to predict the solutions of flow equations for local coarse-scale blocks. In the training process, the flow equations and boundary conditions can be discretized and incorporated as prior physical knowledge to regulate the CNN models, which is termed the theory-guided convolutional neural network (TgCNN) [25]. With the theory-guidance, the dependence on the data volume of training the CNN models can be reduced, and the predictions from the TgCNN can be forced to follow physical laws. When the training is finished, the numerical solving process of the local flow problems can be replaced with the trained models. The
In this work, incompressible single-phase steady-state subsurface flow problems are studied, which are governed by the following equation:

\[-\nabla \cdot (K(x)\nabla H(x)) = 0, \quad x \in \Omega\]  

(1)

and subjected to the following boundary conditions:

\[
\begin{cases} 
H(x) = f(x) , & x \in \Omega_D \\
K(x)\nabla H(x) \cdot n(x) = g(x) , & x \in \Omega_N 
\end{cases}
\]  

(2)

where \( K \) denotes the hydraulic conductivity tensor [LT\(^{-1}\)]; \( H \) denotes the hydraulic head [L]; \( \Omega \subset \mathbb{R}^n \) denotes the studied domain with Dirichlet boundary \( \Omega_D \) and Neumann boundary \( \Omega_N \).

The remainder of this paper is organized as follows. In Sect. 2, the governing equations of single-phase subsurface flow and numerical upscaling method are introduced, and the proposed deep-learning-based method is also illustrated. In Sect. 3, several cases of subsurface flow with varying complexities are designed to evaluate the performance of the proposed upscaling method. In Sect. 4, discussions and conclusions are provided.

\section{Methodology}

\subsection{Governing equations}

In this work, incompressible single-phase steady-state subsurface flow problems are studied, which are governed by the following equation:

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where \( K \) denotes the hydraulic conductivity tensor [LT\(^{-1}\)]; \( H \) denotes the hydraulic head [L]; \( \Omega \subset \mathbb{R}^n \) denotes the studied domain with Dirichlet boundary \( \Omega_D \) and Neumann boundary \( \Omega_N \); \( f(x) \) denotes the prescribed head on Dirichlet boundary segments [L]; and \( g(x) \) denotes the prescribed flux across Neumann boundary segments [LT\(^{-1}\)].

By taking the average flow rate over the domain, the equivalent hydraulic conductivity for the domain can be defined with the following equation [21, 22]:

\[
\frac{1}{V} \int_{\Omega} v(x) dx = K_{eq} \left( \frac{1}{V} \int_{\Omega} \nabla H(x) dx \right)
\]  

(3)

where \( V \) denotes the volume of the domain; \( v \) denotes the Darcy filtration velocity [LT\(^{-1}\)], which can be calculated with \( v = -K \nabla H \) (Darcy’s law); and \( K_{eq} \) denotes the equivalent hydraulic conductivity of the domain \( \Omega \) [LT\(^{-1}\)]. The hydraulic conductivity of the domain to be upscaled is assumed to be diagonal, as represented below:

\[
K = \begin{pmatrix} K_x & 0 \\ 0 & K_y \end{pmatrix} \quad \text{(2D)} \quad \text{and} \quad K = \begin{pmatrix} K_x & 0 & 0 \\ 0 & K_y & 0 \\ 0 & 0 & K_z \end{pmatrix} \quad \text{(3D)}
\]  

(4)

and the upscaled equivalent conductivity can be represented with a tensor:

\[
K_{eq} = \begin{pmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yx} \\ K_{zx} & K_{zy} & K_{zz} \end{pmatrix} \quad \text{(2D)} \quad \text{and} \quad K_{eq} = \begin{pmatrix} K_{xx} & K_{xy} & K_{xz} & K_{yx} & K_{yy} & K_{yx} & K_{zx} & K_{zy} & K_{zz} \end{pmatrix} \quad \text{(3D)}
\]  

(5)

\subsection{Heterogeneity}

In subsurface flow problems, geologic models are usually heterogeneous. In this work, the Karhunen–Loeve expansion (KLE) is utilized to characterize and generate the heterogeneous and spatially correlated hydraulic conductivity fields [8, 30]. The log-transformed hydraulic conductivity \( \ln K(x, \omega) \) can be seen as a stochastic field (represented as \( Y(x, \omega) = \ln K(x, \omega) \) for simplicity), which can be expressed in the following form using the KLE [8]:

\[
Y(x, \omega) = \langle Y(x, \omega) \rangle + \sum_{i=1}^{\infty} \sqrt{\lambda_i} f_i(x) \xi_i(\omega),
\]  

(6)

where \( \langle Y(x, \omega) \rangle \) denotes the mean of the stochastic field; \( \lambda_i \) and \( f_i(x) \) are the eigenvalue and eigenfunction of the covariance, respectively; and \( \xi_i(\omega) \) denotes the independent standard Gaussian random variables when \( Y(x, \omega) \) is a Gaussian random field. Considering that there are infinite terms in Eq. (6), the expansion can be truncated into finite terms \( n \) according to the decay rate of \( \xi_i(\omega) \). The truncated number \( n \) can be determined by calculating the preserved percentage of energy (preserved information of the stochastic field)

\[
\sum_{i=1}^{n} \lambda_i / \sum_{i=1}^{\infty} \lambda_i.
\]
weight, the expansion can then be truncated, and the stochastic field \( Y(\mathbf{x}, \omega) = \ln K(\mathbf{x}, \omega) \) can be parameterized with the \( n \) dimensional random vector:

\[
\xi = \{ \xi_1(\omega), \xi_2(\omega), \ldots, \xi_n(\omega) \}
\]

Therefore, the stochastic field can be represented as:

\[
Y(\mathbf{x}, \omega) = \langle Y(\mathbf{x}, \omega) \rangle + \sum_{i=1}^{n} \sqrt{\lambda_i(\mathbf{x})} \xi_i(\omega),
\]

and the realizations of hydraulic conductivity can be generated by sampling the independent random variables \( \xi_i(\omega) \). Each group of random variables corresponds to a realization of conductivity field.

### 2.3 Numerical methods

Numerical methods have been widely used for upscaling of fine-scale geologic models [5]. In numerical methods, the fluid flow equation Eq. (1) can be solved for each coarse grid block. Moreover, periodic boundary conditions can be exerted on the coarse grid blocks while solving the flow equations [5], as presented below (2D scenarios):

\[
H(x, y)|_{y=0} = H(x, y)|_{y=L_y} - \Delta H_1, \quad v_x(x, y)|_{y=0} = v_x(x, y)|_{y=L_y},
\]

\[
H(x, y)|_{y=0} = H(x, y)|_{y=L_y} - \Delta H_2, \quad v_y(x, y)|_{y=0} = v_y(x, y)|_{y=L_y},
\]

where \( L_x \) and \( L_y \) denote the length of the coarse blocks in the x- and y-direction, respectively; \( \Delta H_1 \) and \( \Delta H_2 \) denote the constant hydraulic head differences between the boundaries; and \( v_x \) and \( v_y \) denote the Darcy velocity in the x- and y-direction, respectively \([LT^{-1}]\).

To solve flow equations for different coarse grid blocks, the finite difference (FD) method can be adopted, in which the governing equation can be discretized as follows (2D scenarios):

\[
K_{x,i+1/2,j}(H_{i+1,j} - H_{i,j}) - K_{x,i-1/2,j}(H_{i,j} - H_{i-1,j}) = \frac{(\Delta x)^2}{\Delta y^2} K_{y,i,j+1/2}(H_{i,j+1} - H_{i,j}) - K_{y,i,j-1/2}(H_{i,j} - H_{i,j-1})
\]

where \( i \) and \( j \) denote the index of grid blocks in the x- and y-direction, respectively; \( K_x \) and \( K_y \) denote the hydraulic conductivity component in the x- and y-direction, respectively; and \( K_{x,i+1/2,j} \) denotes the conductivity at the interface of grid block \((i, j)\) and \((i + 1, j)\), which can be calculated with the harmonic average of two conductivities at two adjacent grid blocks as follows:

\[
K_{x,i+1/2,j} = \frac{2}{1/K_{x,i,j} + 1/K_{x,i+1,j}}
\]

By introducing transmissibility, Eq. (10) can be further rewritten as:

\[
\frac{\Delta x}{\Delta y} T_{x,i+1/2,j}(H_{i+1,j} - H_{i,j}) - \frac{\Delta x}{\Delta y} T_{x,i-1/2,j}(H_{i,j} - H_{i-1,j})
\]

\[
+ \frac{\Delta x}{\Delta y} T_{y,i,j+1/2}(H_{i,j+1} - H_{i,j}) - \frac{\Delta x}{\Delta y} T_{y,i,j-1/2}(H_{i,j} - H_{i,j-1}) = 0
\]

where \( T_x \) and \( T_y \) denote the transmissibility between the two adjacent grid blocks, which can be defined as:

\[
T_{x,i+1/2,j} = \frac{2\Delta y}{1/K_{x,i,j} + 1/K_{x,i+1,j}},
\]

\[
T_{y,i,j+1/2} = \frac{2\Delta x}{1/K_{y,i,j} + 1/K_{y,i+1,j}}
\]

The linear system of equations can then be constructed based on Eq. (12) for the coarse grid blocks, and the sparse coefficient matrix can also be assembled for solving the linear equations. With the solutions of hydraulic heads, the equivalent hydraulic conductivity of the coarse grid blocks can be calculated by Eq. (3). The workflow of the numerical upscaling method is presented in Fig. 1.

It is worth noting that for each coarse grid block, the periodic boundary conditions should be exerted twice (or three times for 3D scenarios) with different directions, and the flow equations should also be solved twice accordingly to obtain the equivalent conductivity with different principal directions, as presented in Fig. 2.

### 2.4 Deep-learning-based methods

The most time-consuming part of numerical upscaling methods is solving the flow equations for each coarse block. Therefore, in order to improve the efficiency of the upscaling process, numerical solving for each coarse block can be replaced by deep learning models, as shown in Fig. 3. The deep learning model can approximate the mapping from the coarse patch of the fine-scale hydraulic conductivity field to the local hydraulic head solution for the patch, which can assist to avoid cumbersome numerical solving and provide a more efficient forward calculation. The deep learning model can be represented as follows:

\[
\hat{H} = g(K; \theta),
\]

where \( \hat{H} \) denotes the predicted hydraulic head; and \( g(\theta) \) denotes the deep learning model with model parameters \( \theta \) (weights and bias).

Considering that the patch of the fine-scale hydraulic conductivity field and the distribution of hydraulic heads can both
be seen as images, the convolutional neural network (CNN) structure can be adopted to approximate the relationship, which has constituted a powerful tool for image processing [9, 12, 15]. A convolutional encoder-decoder architecture can be constructed easily with several convolution layers and deconvolution layers. The most straightforward approach to train the CNN model is using the data pairs obtained from numerical solutions. The loss function can be written as follows:

\[ L_{\text{Data}}(\theta) = \frac{1}{N_{\text{grid}}} \frac{1}{N} \sum_{i=1}^{N} \| \hat{H}_i - H_i \|_2^2 = \frac{1}{N_{\text{grid}}} \frac{1}{N} \sum_{i=1}^{N} \| g(K_i; \theta) - H_i \|_2^2, \]

where \( N \) denotes the total number of data pairs (image-to-image pairs between the hydraulic conductivity and heads); \( N_{\text{grid}} \) denotes the number of grids in each realization; \( \hat{H}_i \) denotes the images of predicted hydraulic heads for

Fig. 1 Illustration of the numerical upscaling method

Fig. 2 Illustration of periodic boundary conditions in different directions
hydraulic conductivity $K_i$; and $H_i$ denotes the ground truth of hydraulic heads for the $i$th data pair.

When the available data pairs are abundant, minimizing the loss function Eq. (16) would be the most direct and convenient way to train the deep CNNs. It would be challenging, however, to train an accurate CNN model in scenarios with limited labeled data pairs. Under this circumstance, already known physical laws could provide some additional and valuable information for the training stage to construct the theory-guided convolutional neural network (TgCNN). By incorporating physical laws or equations as prior knowledge to guide the training process, the problem of training data shortage can be effectively alleviated. In order to achieve theory-guided training, consider the discretized governing equation Eq. (12), which can be utilized to regulate CNNs in the training process. The predictions of hydraulic heads shall honor Eq. (12), from which the ground truth comes, and thus when the predicted values of hydraulic heads are substituted into Eq. (12), the residuals of the equation should approach zero, as presented in Eq. (17):

$$R(K; \theta) = \frac{T_{x,i+1/2,j}(\hat{H}_{i+1,j} - \hat{H}_{i,j})}{\Delta x} - \frac{T_{x,i-1/2,j}(\hat{H}_{i,j} - \hat{H}_{i-1,j})}{\Delta x} + \frac{T_{y,j+1/2,i}(\hat{H}_{i,j+1} - \hat{H}_{i,j})}{\Delta y} - \frac{T_{y,j-1/2,i}(\hat{H}_{i,j} - \hat{H}_{i,j-1})}{\Delta y} \rightarrow 0.$$  (17)

Therefore, the residuals can be minimized in the training process to force the CNN model to produce predictions that adhere to governing equation Eq. (12). The residual term in the loss function can be expressed as follows:

$$L_{GE}(\theta) = \frac{1}{N_{grid}} \frac{1}{N_r} \sum_{i=1}^{N_r} \| R(K_i; \theta) \|_2^2,$$  (18)

where $N_r$ denotes the total number of hydraulic conductivity patches used to calculate the equation residuals and boundary condition residuals, which is different from the number of paired training data $N$. It is worth mentioning that the labeled data are not required while calculating the residuals, and only the conductivity patches are utilized.

Since the periodic boundary conditions need to be exerted while solving the flow equations for each coarse grid block, the periodic boundary conditions can also be incorporated as prior knowledge into the training stage. The loss terms for the boundary conditions can be written as:

$$L_{BC-H}(\theta) = \frac{1}{N_{grid-b}} \frac{1}{N_r} \sum_{i=1}^{N_r} \left( \| \hat{H}_i \|_0 - \| H_i \|_0 \right)^2 - \Delta H_1^2 + \frac{1}{N_{grid-b}} \frac{1}{N_r} \sum_{i=1}^{N_r} \left( \| \hat{H}_i \|_1 - \| H_i \|_1 \right)^2 - \Delta H_2^2.$$  (19)
The TgCNN model can be trained by minimizing the loss function Eq. (23), which can then be used to predict the hydraulic head solutions for different conductivity patches. The equivalent hydraulic conductivity at the coarse scale can be further calculated with the predicted hydraulic head, as shown in Fig. 3. With the numerical solution process being replaced by the deep learning models, the efficiency of upscaling geologic models can be improved significantly.

### 3 Case studies

In this subsection, several synthetic cases are introduced to test the performance of the proposed deep-learning-based upscaling method, including 2D cases and 3D cases.

#### 3.1 2D case

##### 3.1.1 2D base case

A 2D case is firstly studied in this subsection. The physical domain is a square area, with each side of length 100 [L] \((L_x = L_y = 100 [L])\). The correlation length of the x- and y-direction are both set to be 20 [L] \((\eta_x = \eta_y = 20 [L])\). The mean of the stochastic log-transformed hydraulic conductivity field is 0, and the variance is 1 \((\ln K = 0 \text{ and } \sigma_{\ln K}^2 = 1.0)\). In addition, the covariance of the stochastic field is an exponential form function:

\[
L_{BC-v}(\theta) = \frac{1}{N_{grid-b}} \frac{1}{N_r} \sum_{i=1}^{N_r} \| \hat{v}_x \|_{y=0} - \| \hat{v}_x \|_{y=L_y} \right\|_2^2
+ \frac{1}{N_{grid-b}} \frac{1}{N_r} \sum_{i=1}^{N_r} \| \hat{v}_y \|_{x=0} - \| \hat{v}_y \|_{x=L_x} \right\|_2^2,
\]

where \(N_{grid-b}\) denotes the number of grids at boundaries; and \(\hat{v}_x\) and \(\hat{v}_y\) can be calculated, respectively, using Darcy’s law as follows:

\[
\hat{v}_x = -K_x \cdot \nabla \hat{H},
\]

\[
\hat{v}_y = -K_y \cdot \nabla \hat{H}.
\]

Consequently, the loss function of TgCNN after incorporating the theory-guidance can be given as:

\[
L(\theta) = \lambda_{Data} L_{Data}(\theta) + \lambda_{GE} L_{GE}(\theta)
+ \lambda_{BC-H} L_{BC-H}(\theta) + \lambda_{BC-v} L_{BC-v}(\theta)
\]

where \(\lambda_{Data}\), \(\lambda_{GE}\), \(\lambda_{BC-H}\), and \(\lambda_{BC-v}\) denote the weights of different loss terms in the total loss function. These hyperparameters can be set as 1 by default, and could also be further adjusted by balancing the magnitudes of each loss term.

The TgCNN model can be trained by minimizing the loss function Eq. (23), which can then be used to predict the hydraulic head solutions for different conductivity patches.
The realizations of hydraulic conductivity fields can then be generated with KLE by using these statistical information. In order to characterize the fields more elaborately, 90% of the information of the stochastic fields is preserved while generating the hydraulic conductivity realizations for the fine-scale grid blocks. In this case, the hydraulic conductivity is assumed to be isotropic, i.e., $K_x = K_y$.

The fine-scale geologic models are $100 \times 100$ grid blocks, which need to be upscaled into $10 \times 10$ coarse grid blocks, with each coarse block consisting of $10 \times 10$ fine-scale grids. In the numerical upscaling method, the flow equations need to be solved for each coarse grid block with the periodic boundary conditions. In this case, the constant hydraulic head difference of the two directions are set to be $\Delta H_1 = 1$ and $\Delta H_2 = 0$, respectively. In the deep-learning-based upscaling method, the TgCNN model is constructed to predict the solutions of flow equations and improve the efficiency of the upscaling process. Considering that each coarse block consists of $10 \times 10$ high-resolution grids, the image size of inputs to the TgCNN model is also $10 \times 10$. Moreover, the size of outputted hydraulic head images is $12 \times 12$ because the heads at the surface of domain boundaries are also incorporated. The details of the TgCNN structure are presented in Table 1. To train the TgCNN model, five fine-scale hydraulic conductivity fields are generated with KLE and divided into 500 patches (coarse grid blocks). The 500 patches of hydraulic conductivity are utilized to calculate the equation residuals and impose the physical constraints. It is worth noting that no labeled data are used to train the TgCNN model, and only the physical laws are exploited to provide the valuable information for training.

Therefore, the loss function of the TgCNN model in this case can be rewritten as:

$$L(\theta) = \lambda_{\text{GE}} L_{\text{GE}}(\theta) + \lambda_{\text{BC-H}} L_{\text{BC-H}}(\theta) + \lambda_{\text{BC-v}} L_{\text{BC-v}}(\theta)$$

As previously mentioned, the theory-guidance can assist to alleviate the shortage of labeled datasets for the training of deep learning models, and the label-free TgCNN model in this case can prove this again. The weights of different terms in the loss function are set to be 1 in this case. The learning rate is set to be 0.001 initially, and it decays 10% after each 100 epochs. It takes approximately 158.657 s
to finish the training of the model (1,000 epochs) on an NVIDIA TITAN RTX GPU. It can be seen that it is both convenient and fast to train such a lightweight deep learning model.

The accuracy of the predicted hydraulic heads from the trained TgCNN model can be examined with numerical solutions. For 100 newly generated hydraulic conductivity patches, the $R^2$ scores (also known as coefficients of

Fig. 6 Comparison of fine-scale and upscaled log-transformed hydraulic conductivity field, hydraulic head, velocity, and streamline for the 2D case.
determination) between the predictions and the numerical solutions of hydraulic heads are presented in the histogram in Fig. 4. The scatterplot of hydraulic heads at three different points are shown in Fig. 5. It can be seen that the constructed TgCNN model can predict the hydraulic head solutions accurately for different hydraulic conductivity patches, even when trained without any labeled data.

The TgCNN model can then be used for efficient upscaling of fine-scale geologic models following the workflow presented in Fig. 3. Consider the fine-scale hydraulic conductivity field in Fig. 6 (a) (100 × 100), which is generated with KLE, and the numerical solution of the flow equations for this realization can be implemented with the MATLAB Reservoir Simulation Toolbox (MRST) [19]. Figure 6 (b), (c), and (d) present the fine-scale hydraulic head, velocity in the x-direction, and streamline, respectively. The upscaled hydraulic head and velocity can then be calculated by averaging the fine-scale solutions directly, which can be regarded as the true coarse-scale solutions or benchmarks, as shown in Fig. 6 (e), (f), and (g). Figure 6 (h) illustrates the upscaled hydraulic conductivity field with the numerical method following the workflow in Fig. 1. The upscaled hydraulic head, velocity, and streamline of the numerical method shown in Fig. 6 (i), (j), and (k) can be obtained by inputting Fig. 6 (h) into the MRST solver. Figure 6 (l), (m), (n), and (o) show the upscaled hydraulic conductivity field, hydraulic head,
velocity, and streamline with the proposed deep-learning-based method, respectively. It can be seen that the upscaled conductivity, hydraulic head, velocity and streamline with the deep-learning-based method are almost the same as the numerical results, which demonstrates that the deep learning method can serve as an accurate alternative approach for upscaling. Furthermore, both the results from the deep learning method and the numerical method are similar to the benchmarks (true coarse-scale solutions, Fig. 6 (e), (f), and (g)).

The scattered correlation plots of the upscaled results are presented in Fig. 7. It can be seen that the upscaled hydraulic head and velocity in the x-direction with both the numerical method and the deep learning method can match the true coarse-scale results well. The velocity in the y-direction matches the benchmarks slightly worse, which may be ascribed to the fact that the y-direction is not the principal flow direction ($\Delta H_y = 0$). The upscaled results with the deep learning method are almost identical to those obtained from the numerical method, as shown in Fig. 7, which again demonstrates the effectiveness of the deep-learning-based upscaling method. In order to evaluate the performance of the deep learning method statistically, 1,000 fine-scale hydraulic conductivity realizations are generated with KLE, and upscaled with the numerical method and the deep learning method, respectively. The upscaled results of the 1,000 realizations at a sampled point in the domain are scattered in the correlation plots shown in Fig. 8. It can be
seen that the deep learning method can provide satisfactory upscaling performance statistically. Moreover, the efficiency of the proposed deep learning method can also be assessed. Figure 9 compares the consumed time for upscaling different numbers of fine-scale hydraulic conductivity realizations with different methods. One can see that even though additional time is required to train the TgCNN model, the trained TgCNN model can improve the efficiency of the upscaling process significantly compared to the numerical method, and it takes just several seconds to finish the upscaling of thousands of fine-scale realizations. Therefore, the deep learning method possesses a major advantage in terms of efficiency without the loss of accuracy, and this advantage becomes increasingly obvious as the number of realizations increases.

3.1.2 The effect of training data

The TgCNN model in the former base case is trained in a label-free manner, i.e., trained without labeled training data and only with physical constraints. However, the effect of training data on the upscaling accuracy still needs to be investigated. Several CNN models trained with different amounts of training data and without the physical constraint terms are utilized for upscaling of 300 fine-scale hydraulic conductivity fields, the accuracy comparison of which is presented in Fig. 10. The dashed lines in Fig. 10 show the mean of the 300 $R^2$ scores for the upscaled results with CNN models, and it is obvious that the upscaled results become more accurate as the number of training data increases.
can also be seen that when the labeled training data are ade-
quate, the trained CNN model can also provide satisfactory
upsampling performance, even when trained without physical
constraints. If the labeled training data are limited or com-
putational prohibitive to obtain, however, the guidance of
physical laws in the training process could still be beneficial.

In order to elucidate the effect of physical constraints in the
training process, several TgCNN models are also trained with
different numbers of training data. Similar to the base case in
Sect. 3.1.1, 500 coarse block patches are utilized to calculate the
equation residuals, and to impose the physical constraints. The
comparison of the $R^2$ score average for 300 fine-scale realiza-
tions are presented in Fig. 10. One can see that with the assis-
tance of theory-guidance, the upscaling performance of TgCNN
models is markedly more robust, and the accuracy is higher than
that using the purely data-driven CNN models. Moreover, the
impact of training data is no longer obvious when the physical
equations are utilized to constrain the models, which demon-
strates the effectiveness of the theory-guided training. In addi-
tion, the dependence on the training data volume of the deep-
learning-based upscaling framework can be reduced with the
theory-guidance.

3.1.3 The effect of upscaling ratio

In this subsection, the performance of the deep learn-
ing method with different upscaling ratios is investigated.
Still consider the base case in Sect. 3.1.1. To upscale the
fine-scale conductivity field with upscaling ratios 5 and 20,
two TgCNN models are trained with inputting image size
$5 \times 5$ and $20 \times 20$, respectively. The upsampled results for the
fine-scale realizations in Sect. 3.1.1 with upscaling ratios 5
and 20 are presented in Fig. 11 and Fig. 12, respectively. It
is obvious that the upsampled results become more similar to
the fine-scale results when the upscaling ratio decreased to
5, because more details of the high-resolution conductivity
can be captured as the size of the coarse block decreases. In
addition, the limiting case is that the coarse block size equals
the original fine-scale grids, and thus the ‘coarse results’ and
the fine-scale results would be identical. When the upscaling
ratio increased to 20, the upsampled results become more dif-
ferent from the fine-scale solutions, which is also reasonable,
because more details of the conductivity field are neglected
as the upscaling ratio increases. Furthermore, it can also be
seen that the upsampled results with the deep learning method
can match those from the numerical method well under dif-
ferent upscaling ratios, which demonstrates the ability of the
proposed deep learning method to provide approximately the
same upscaling accuracy as the numerical method.

3.1.4 Extrapolation for different heterogeneity

In this subsection, the extrapolation performance of the
constructed TgCNN model for upscaling geologic models
with different heterogeneity is investigated. Several hydrau-
lic conductivity cases with different correlation length,
rotation angle of major correlation direction, and resolution are generated with KLE (Table 2) to test the upscaling performance of the proposed deep-learning-based upscaling method. It is worth noting that all the hydraulic conductivity cases are upscaled using the TgCNN model constructed in Sect. 3.1.1, which was trained for the 2D base case. That is to say, we do not need to construct the new TgCNN models for each different case separately. Therefore, the extrapolation performance of the proposed method for geologic models with different heterogeneity can be tested. The upscaling results of hydraulic conductivity fields, hydraulic heads, and velocities are presented in Fig. 13 and Table 2.

Cases 1–5 demonstrate that the constructed TgCNN model can be utilized for upscaling of hydraulic conductivity fields with different correlation length. The upscaling of velocity is affected more obviously as the correlation length decreases (Case 1), but the accuracy is still acceptable. Case 6 presents a hydraulic conductivity field with higher resolution, which was generated with higher retained energy using KLE. It can be seen that the upscaling results for this case are also satisfactory, even though this field is finer and less continuous than the base case. Cases 7 and 8 present more anisotropic hydraulic conductivity fields with different rotation angle of major correlation direction. $\theta$ denotes the angle between the major correlation direction and the horizontal axis. It can be seen that the TgCNN model can also upscale those cases well even if it hasn’t seen those anisotropic patterns in the training process.

| Case | $\eta_x$ (L) | $\eta_y$ (L) | $\theta$ (°) | Retained energy | $R^2$ for upscaled $h$ | $R^2$ for upscaled $v_x$ | $R^2$ for upscaled $v_y$ |
|------|--------------|--------------|--------------|-----------------|-----------------|-----------------|-----------------|
| 1    | 10           | 10           | -            | 90%             | 0.99780         | 0.95616         | 0.89901         |
| 2    | 30           | 30           | -            | 90%             | 0.99967         | 0.99398         | 0.98000         |
| 3    | 30           | 10           | -            | 90%             | 0.99978         | 0.99364         | 0.97708         |
| 4    | 10           | 30           | -            | 90%             | 0.99932         | 0.95321         | 0.96303         |
| 5    | 50           | 20           | -            | 90%             | 0.99978         | 0.99919         | 0.99579         |
| 6    | 20           | 20           | -            | 98%             | 0.99707         | 0.96967         | 0.91390         |
| 7    | 40           | 10           | 45           | 90%             | 0.99953         | 0.96629         | 0.92991         |
| 8    | 40           | 10           | 135          | 90%             | 0.99974         | 0.98753         | 0.96600         |

Fig. 12 Upscaled log-transformed hydraulic conductivity field, hydraulic head, velocity, and streamline with an upscaling ratio of 20
Fig. 13  Upscaled log-transformed hydraulic conductivity fields for cases with different heterogeneity
Fig. 13  (continued)
The TgCNN model utilized for upscaling in this subsection was trained for the base case with \( \eta_x = \eta_y = 20 \) [L] and \( \theta = 0 \), but the upscaling accuracy for cases with different statistical characteristics is still satisfactory. These results demonstrate that the constructed TgCNN model has certain extrapolation ability for cases with different heterogeneity. Therefore, there is no need to completely retrain the TgCNN model for those different hydraulic conductivity field patterns, which can help to save computational costs and further improve the efficiency advantage of the deep learning upscaling method.

### 3.2 3D case

In this subsection, the deep learning method is tested in 3D cases, including isotropic and anisotropic scenarios.

#### 3.2.1 Isotropic 3D case

The isotropic scenario of the 3D case is firstly studied in this subsection. The domain size of the fine-scale geologic model is \( 1200 \times 4400 \times 700 \) [L], which can be divided into \( 60 \times 220 \times 35 \) grid blocks with each block’s size being \( 20 \times 20 \times 20 \) [L]. The fine-scale geologic model can be upscaled into \( 12 \times 44 \times 7 \) coarse blocks, with each consisting of \( 5 \times 5 \times 5 \) fine-scale blocks. The correlation length of the stochastic field in the \( x \)-, \( y \)-, and \( z \)-directions is set to be \( \eta_x = 500 \) [L], \( \eta_y = 1000 \) [L], and \( \eta_z = 1000 \) [L], respectively. The mean of the stochastic field \( \ln K \) is set to be \( \langle \ln K \rangle = 0 \), and the variance is set to be \( \sigma^2_{\ln K} = 4.0 \). The exponential covariance function is still utilized:

\[
C_{\ln K}(\mathbf{x}, \mathbf{x}') = \sigma^2_{\ln K} \exp \left( -\frac{|x_1 - x_2|}{\eta_x} - \frac{|y_1 - y_2|}{\eta_y} - \frac{|z_1 - z_2|}{\eta_z} \right)
\]

(26)

The 3D fine-scale hydraulic conductivity realizations can also be generated with KLE [24], and 90% energy is preserved in this case. An example of the generated fine-scale conductivity field is presented in Fig. 14 (a). The hydraulic conductivity field is also assumed to be isotropic in this case, i.e., \( Kx = K_y = K_z \), and the anisotropic scenario is investigated in the next subsection.

In the numerical method, the periodic boundary conditions should be generalized into 3D scenarios as follows:

\[
H(x, y, z)|_{x=0} = H(x, y, z)|_{x=L_x} - \Delta H_1, \quad v_x(x, y, z)|_{x=0} = v_x(x, y, z)|_{x=L_x} + 1
\]

\[
H(x, y, z)|_{y=0} = H(x, y, z)|_{y=L_y} - \Delta H_2, \quad v_y(x, y, z)|_{y=0} = v_y(x, y, z)|_{y=L_y} + 1
\]

\[
H(x, y, z)|_{z=0} = H(x, y, z)|_{z=L_z} - \Delta H_3, \quad v_z(x, y, z)|_{z=0} = v_z(x, y, z)|_{z=L_z} + 1
\]

(27)

and the physical constraints of the periodic boundary conditions should also be revised accordingly:

\[
L_{BC-H}(\theta) = \frac{1}{N^\text{grid-b}_r} \sum_{r=1}^{N_r} \left( \left| \hat{H}|_{x=0} - \hat{H}|_{x=L_x} \right|^2 - \Delta H_1 \right) \]

\[
+ \frac{1}{N^\text{grid-b}_r} \sum_{r=1}^{N_r} \left( \left| \hat{H}|_{y=0} - \hat{H}|_{y=L_y} \right|^2 - \Delta H_2 \right) \]

\[
+ \frac{1}{N^\text{grid-b}_r} \sum_{r=1}^{N_r} \left( \left| \hat{H}|_{z=0} - \hat{H}|_{z=L_z} \right|^2 - \Delta H_3 \right)
\]

(28)

\[
L_{BC-v}(\theta) = \frac{1}{N^\text{grid-b}_r} \sum_{r=1}^{N_r} \left( \left| \hat{v}_x|_{x=0} - \hat{v}_x|_{x=L_x} \right|^2 \right)
\]

\[
+ \frac{1}{N^\text{grid-b}_r} \sum_{r=1}^{N_r} \left( \left| \hat{v}_y|_{y=0} - \hat{v}_y|_{y=L_y} \right|^2 \right)
\]

\[
+ \frac{1}{N^\text{grid-b}_r} \sum_{r=1}^{N_r} \left( \left| \hat{v}_z|_{z=0} - \hat{v}_z|_{z=L_z} \right|^2 \right)
\]

(29)

In this case, the hydraulic head differences in the \( x \)-, \( y \)-, and \( z \)-directions are set to be \( \Delta H_1 = 1 \), \( \Delta H_2 = 0 \), and \( \Delta H_3 = 0 \), respectively. In order to construct TgCNN models for the 3D case, 3D convolution modules are adopted. The inputs of the 3D TgCNN are the 3D blocks of the hydraulic conductivity patches, and the outputs are the corresponding hydraulic head solutions for the conductivity patches. The details of the TgCNN structure are listed in Table 3. To train the TgCNN model, 10 fine-scale conductivity fields are generated with KLE, each of which can be divided into \( 12 \times 44 \times 7 \) coarse blocks. Therefore, 36,960 coarse blocks are utilized to train the TgCNN model. It is worth mentioning that the 3D TgCNN model is also trained in a ‘label-free’ manner in this case, because the 36,960 coarse blocks are not solved with the numerical method to provide the hydraulic head labels, and only used to calculate the residuals of the governing equation. The weights \( \lambda_{GE} \) and \( \lambda_{BC-v} \) are set to be 0.001 in this case, and the rest are still set to be 1. The learning rate is set to be 0.001, and it decays 10% after each 10 epochs. It takes approximately 2128.286 s to train the TgCNN model for 300 training epochs.

The trained 3D TgCNN model can then be used for efficient upscaling of the 3D fine-scale hydraulic conductivity fields following the workflow in Fig. 3. The numerical upscaling method is utilized as a reference. The upscaled results of the fine-scale realization shown in Fig. 14 (a) are presented in Fig. 14 (b) and (c). The fine-scale hydraulic head distribution and upscaling results with different methods are shown in Fig. 15. It can be seen that the upscaled conductivity with the proposed deep learning method is almost the same as that from the numerical method, both of which are similar to the fine-scale conductivity field. The upscaled hydraulic heads with the deep learning method are also similar to those of the numerical references, as well as
the fine-scale results. The scatterplots of the upscaled results are presented in Fig. 16. The deep learning method provides almost identical upscaled results to those of the numerical method. The upscaled velocity in the z-direction with both the deep learning method and the numerical method seems to be worse than those in the x- and y-directions, which may be attributable to the larger heterogeneity in the z-direction. This case demonstrates the feasibility of upscaling for 3D cases with the proposed deep learning method.

### 3.2.2 Extrapolation for SPE10 upper layers

In this subsection, the proposed deep learning upscaling method and the constructed TgCNN model in Sect. 3.2.1 are tested with hydraulic conductivity model of SPE10 benchmark. The SPE10 model has 60 × 220 × 85 grid blocks, and the top 35 layers of the model are extracted to test the proposed method, so the fine-scale model consists of 60 × 220 × 35 grids, which would be the same as the former case. The hydraulic conductivity in the x direction of the original model is considered in this case, as shown in Fig. 17 (a), and the variogram analysis can be performed to estimate the statistics of the log-transformed conductivity field. It can be found that the spherical covariance function can fit the conductivity field best with \( \sigma^2_{\ln k} = 5.0 \), \( \eta_y = 600 \) [L], \( \eta_x = 600 \) [L], and \( \eta_z = 10 \) [L], which are totally different from the statistical information of the case in Sect. 3.2.1. Even though, we didn't retrain a new TgCNN model for this case following these new statistics. Instead, the TgCNN model constructed for the case in Sect. 3.2.1 is utilized directly, to perform upscaling. Therefore, the extrapolation ability of the TgCNN model can also be examined in this case.

The upscaling results of the hydraulic conductivity are presented in Fig. 17. It can be seen that the upscaled conductivity field using the deep learning method is almost the same as that obtained from the numerical method. In addition, the upscaled hydraulic heads and velocities with the deep learning method can also match those upscaled using numerical method well, as shown in Fig. 18. Therefore, the deep learning method shows equivalent upscaling accuracy as numerical method, but with much higher efficiency, only taking approximately 0.5137 s to upscale this case. It is also worth noting that the utilized TgCNN model hasn’t seen the information about the patterns and statistics (covariance function, variance, correlation length) of the SPE10 case in the training process, but it still exhibits satisfactory upscaling performance, which further demonstrates the extrapolation ability of TgCNN model.

### 3.2.3 Anisotropic 3D case

In this subsection, a more complicated 3D case is studied, in which the hydraulic conductivity field is anisotropic. The size of the physical domain is set to be...
3600 [L] × 5000 [L] × 1200 [L], and the correlation length of different directions are set as $\eta_x = 1440$ [L], $\eta_y = 1000$ [L], and $\eta_z = 180$ [L], respectively. The statistics, i.e., mean, variance and covariance function, are set to be the same as those in the former case. The domain can be discretized into $180 \times 250 \times 60$ grid blocks, which is a relatively large-scale model with 2,700,000 grid blocks. The fine-scale model can be coarsened into $36 \times 50 \times 12$ grid blocks with an upscaling ratio of $5 \times 5 \times 5$. Furthermore, the most important difference is that the conductivity in the y-direction and the z-direction are assumed to follow $K_y = 0.8K_x$ and $K_z = 0.3K_x$, respectively. The structure of the TgCNN model would be slightly different for this scenario. Considering the anisotropy of the hydraulic conductivity, the inputs of the TgCNN model include the conductivity of x-, y-, and z-directions, i.e., the inputs have three channels, as shown in Fig. 19.

To train the TgCNN model for this anisotropic case, a fine-scale realization is generated and divided into 21,600 patches (coarse grid blocks) to impose the physical constraints in the training process. In addition, 3,000 patches of conductivity are numerically solved with periodic conditions to provide the labeled training data, which is a relatively small amount of data considering that each fine-scale model can be divided into 21,600 patches. The network was trained for 200 epochs, and it takes approximately 1277 s to finish the training of the TgCNN model. The trained TgCNN model can then be used for efficient upsampling of the anisotropic fine-scale conductivity realizations.

Figure 20 (a) presents one realization of fine-scaled $\ln(K_x)$, and the upscaled results with the numerical method and the deep learning method are presented in Fig. 20 (b) and (c), respectively. It is evident that the upscaled $\ln(K_x)$ with the deep learning method can match the results obtained from the numerical method. Moreover, the general pattern of the true fine-scale $\ln(K_x)$ has also been captured, even in the coarse-scale resolution. The upscaled hydraulic conductivity can then be inputted into the simulator to calculate the coarse-scale hydraulic head.

Figure 21 (a) presents the fine-scale hydraulic head of the realization shown in Fig. 20 (a). The true upscaled hydraulic head obtained by averaging the fine-scale results directly is presented in Fig. 21 (b). Figure 21 (c) and (d) show the hydraulic head obtained by inputting the upscaled conductivity with the numerical method and the deep learning method into the simulator, respectively. It can be seen that the upscaled hydraulic heads with the deep learning method are almost the same as the numerical upscaled results and the benchmark obtained by averaging the fine-scale hydraulic heads. The scatterplots presented in Fig. 22 show the comparison of upscaled results among the benchmark, the numerical method, and the deep learning method. It can be seen that satisfactory accuracy is achieved of the upscaled hydraulic heads and velocity with the deep learning method. Indeed, this case illustrates the effectiveness of the proposed deep learning method for upsampling of anisotropic cases.

The TgCNN model is then utilized for upsampling of 20 fine-scale realizations of hydraulic conductivity fields. The box plots of the $R^2$ score between the upscaled results with the deep learning method and the numerical method are shown in Fig. 23. One can see that the $R^2$ scores are higher than 0.9 and approach 1, which indicates that the deep learning method can provide statistically equivalent upsampling accuracy to the
The scatterplots of the upscaled results at five sampled points of the 20 realizations in Fig. 24 also verify this conclusion. Furthermore, the upscaling efficiency of the deep learning method and the numerical method can also be compared in this case. The consumed time for upscaling the hydraulic conductivity fields and solving the flow equations for the 20 fine-scale realizations with different methods are listed in Table 4. It can be seen that solving large-scale models (2,700,000 grid blocks) directly without any upscaling process is both computationally expensive and time-consuming. For coarsened models with upscaling methods, however, the time consumed to solve the flow equations can be significantly reduced. It only takes approximately 10 s to solve the 20 upscaled models, which illustrates the
effectiveness of the upscaling process. Moreover, the upscaling process can be further accelerated with the deep learning method. It only takes approximately 1 min to upscale the 20 fine-scale models with the trained TgCNN model; whereas, approximately 2 h are required with the numerical method. It is obvious that the deep learning method is superior to the numerical method in terms of efficiency, even when taking training time into account.

Fig. 18 Scatterplots of the upscaled results with different methods for the SPE10 case

Fig. 19 The structure of the TgCNN model for anisotropic scenarios
4 Discussions and conclusions

A deep-learning-based upscaling method for geologic models was proposed in this work. In the traditional numerical upscaling method, the flow equations need to be solved for each coarse grid block, which is time-consuming and cumbersome. In this work, the numerical solver of the flow equations for the coarse blocks can be replaced with a trained deep convolutional neural network, which can accurately approximate the relationship between the patches of hydraulic conductivity fields and the hydraulic heads, and thus improve upscaling efficiency. In order to alleviate the dependence on data volume while training deep learning models, the theory-guidance, e.g., governing equations, periodic boundary conditions, etc., can be introduced as prior knowledge to regulate the deep learning models, which is termed the theory-guided convolutional neural network (TgCNN). With the information provided by the physical equations, the TgCNN models can be trained with limited paired data, or even in a label-free manner.

Several cases are introduced to test the performance of the proposed deep-learning-based upscaling method, including 2D and 3D cases. The trained TgCNN models can provide accurate predictions of the hydraulic heads for different patches of conductivity fields, which can be further used for efficient upscaling of fine-scale geologic models. The numerical method was utilized as a reference. The results demonstrate that the deep learning method can provide equivalent upscaling accuracy to the numerical method, whether in 2D/3D cases, or isotropic/anisotropic cases.
Furthermore, the upscaled hydraulic heads and velocity can match the directly averaged results of the original fine-scale models well. In addition, the extrapolation ability of the constructed deep learning models has also been tested with several cases, in which the trained TgCNN models are utilized to upscale conductivity fields with very different statistical information (correlation length, rotation angle of major correlation direction, and resolution). And satisfactory upscaling results can be obtained, which demonstrates that the trained TgCNN models have certain extrapolation ability to deal with cases that have different patterns from the training conductivity fields. Although only steady cases are introduced to verify the performance of the proposed method, it can be utilized for upscaling of transient cases, because the conductivity fields usually do not change over time.

The efficiency of upscaling can be improved significantly with the deep learning method. With the trained deep learning models, the time-consuming numerical solving process...
can be bypassed, and the forward calculation of deep learning models is much faster than the numerical solvers. Even taking the training time of deep learning models into consideration, the deep learning method still offers more advantages regarding efficiency than the numerical method. Furthermore, for certain large-scale geologic models or tasks that require a large number of realizations (e.g., uncertainty quantification, data assimilation), the superiority of the proposed deep learning upscaling method would be much more obvious. And the extrapolation ability of the trained deep learning models can further improve the efficiency advantage of the deep learning method while dealing with fields having different statistics.

Only single-phase cases were considered in this work, while in future studies, the upscaling framework can be further extended to multiphase flow problems. For multiphase flows (e.g., oil–water flows in oil reservoirs), the proposed method can be firstly utilized to upscale the absolute permeability. Then, the relative permeability also needs to be upscaled by solving the local multiphase flow problems. Therefore, a deep learning surrogate can also be constructed for the local multiphase flow problems to reduce the computational costs of repetitive solution, and the governing equations can be embedded into the training process of the model. In this way, the proposed framework may also be utilized for upscaling multiphase flows.

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Data availability  The datasets generated and analyzed during the current study are available from the corresponding author on reasonable request.

Declarations

Conflict of interest  The authors declare that they have no conflicts of interest to report regarding the publication of this paper.

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