DeePore: a deep learning workflow for rapid and comprehensive characterization of porous materials

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Abstract

DeePore is a deep learning workflow for rapid estimation of a wide range of porous material properties based on the binarized micro–tomography images. We generated 17,700 semi–real 3–D micro–structures of porous geo–materials and 30 physical properties of each sample are calculated using physical simulations on the corresponding pore network models. The dataset of porous material images obtained and physical features of them are unprecedented in terms of the number of samples and variety of the extracted features. Next, a re–designed feed–forward convolutional neural network is trained based on the dataset to estimate several morphological, hydraulic, electrical, and mechanical characteristics of porous material in a fraction of a second. The average coefficient of determination ($R^2$) for 3,173 testing samples is 0.9385 which is very reasonable considering the wide range of micro–structure textures and extracted features. This workflow is compatible with any physical size of the images due to its dimensionless approach.

Keywords: Deep Learning, Physical Properties of Porous Media, Convolutional Neural Networks, Porous Material dataset, Pore Network Modeling

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1. Introduction

1.1. Classic porous material characterization

Data science is becoming an essential tool to analyze the structural features of porous materials based on the tomography images [1, 2, 3]. The behavior and performance of porous material are strongly related to the characteristics of its internal micro-structure. In order to discover the descriptive features and the processstructureproperty relationships in a porous material, we need to achieve a rich representation of the internal structure of the porous materials [1, 4, 5, 6]. Spatial description of such micro-structures have created added-value in diverse fields of studies, from composite material engineering [7, 8, 9] and food processing [10, 11], to the petroleum and petrochemical industries [12, 13]. For instance, during the past two decades, the field of digital rock physics grew rapidly and showed outstanding advances owing to the power of imaging and analysis techniques [12, 14]. Based on the captured images, we are able to build realistic simulation models and run many digital measurements and experiments on porous material such as pore and throat sizes, hydraulic and electric conductance, two-phase displacement, and mechanical deformations [15, 16]. Direct calculation of the aforementioned physical properties based on the tomographic data could be a complicated and computationally expensive task especially in the case of large-size images [17, 18, 19]. In this regards, machine learning approaches can be utilized to make hybrid [20] or full artificially intelligent models [21] which are able to reduce the computational costs significantly while maintaining the level of accuracy.

1.2. Deep learning for porous material studies

Shallow neural networks are powerful tools for modeling moderately complex problems in a timely and efficient manner [22, 23, 24] while they are not very suitable to predict high orders of non-linearity [25]. In contrary, deep learning models are capable of estimating a highly non-linear behaviour if they are trained on an adequately diversified and large set of input and output data [26, 27]. Convolutional neural networks (CNNs) as a particular type of deep neural networks can be used for analyzing data with a recognized grid-like topology, similar to image data [28, 29, 30]. A typical CNN uses several filters to extract higher level features from the input data or images and gradually narrows it down to the specified output features [31]. CNNs have been mostly used for image segmentation, recognition, classification, and regression [28, 30, 32]. In mathematical terms, convolution is a spatial operation to transform an original function or data into a secondary realization using an operating kernel [33]. Convolution on an input image could lead to generating negative values which are not usually favorable considering the physical meaning of the output layer in that specific problem. As a post-processing technique, Rectified Linear Units (ReLU) layer can be used to change the negative values into zero [34, 35, 36]. At each level of convolution, we can use a down-sampling method such as maximum or average pooling to condense the volume of data without loosing noticeable amount of information [37]. In many cases CNNs can be followed by some fully-connected dense layers of nodes to give more flexibility to the model [38]. CNNs have been used in many recent porous material studies for...
different purposes including segmentation of porous media images [39, 40], image quality improvement [41], super resolution, reconstruction [42, 43], classification [44], and regression [45, 46]. Here we briefly describe a background of these applications and narrow the topic down to the specific approach of the present study.

1.2.1. Image improvement and reconstruction

Considering the multi-scale nature of many of the porous micro-structures, it is necessary to have plenty of details in images while covering a large volume of the object at the same time. In this regards, super resolution techniques powered by CNNs are valuable tools to be trained on pairs of low and high resolution images. There are plenty of recent studies that have presented quantitative methods to obtain a high resolution tomography image of porous material using images with lower spatial resolution [43, 47, 48, 49, 50, 51]. As a recent example, Kamrava et al. [41] have used a cross-correlation-based simulation to generate an augmented dataset of porous shale images and make a CNN that is able to improve the image quality of similar porous textures.

The resolution enhancement can go further to a level that we are able to generate a detailed realization of the porous material based on the simple input of noise maps through a specific type of CNNs known as Generative Adversarial Networks (GAN) [52, 53, 54, 55]. As an example, Mosser et al. [52] presented a workflow to train a GAN based on the available 3-D tomography images and to reconstruct similar realizations of the original images, while not making an exact copy of them. Then by looking at the hydrodynamic properties of the constructed porous material, they have evaluated the similarity of the realizations.

1.2.2. Classification of porous materials

CNNs are good tools to classify images based on texture, visible elements, or objects [30]. This texture recognition has several applications in material and geological sciences to classify or cluster a dataset of porous material images. Additionally, some other researchers utilized the CNN framework for recognition of the materials texture [56, 44]. For instance, in geoscience, classifying different types of rocks in terms of mineralogy and micro-structure could be a time consuming and biased task if done by hand, while CNNs have widely been used in the past three years to automate these processes in a timely and efficient manner [57].

1.2.3. Image-based regression models

Many diverse physical properties of porous materials have been estimated using CNNs in recent years; from thermal to hydraulic and mechanical features. Wei et al. [58] proposed a CNN to predict the effective thermal conductivities of composite materials and porous media with more than 0.98 accuracy ($R^2$) on 100 testing image samples while training on 1400 samples. Additionally, permeability and porosity have been heavily investigated through CNNs [59, 60, 61, 62]. CNNs are able to take both binary or gray-scale images of porous materials to estimate porosity and permeability with an acceptable error. Alqahtani et al. [46] used CNNs to estimate porosity, average pore size and specific surface of the porous rocks based on both types
of 2–D tomography images and found that binary images could give a more accurate estimation of porous material characteristics compared to the gray–scale ones. However, the morphology of the binarized images is highly dependent on the thresholding technique and it suffers from an inherent uncertainty [63]. In another attempt, Cang et al. [64] designed a CNN for prediction of physical properties of heterogeneous materials and successfully predicted the Young modulus, diffusion and permeability of the porous material with more than 90% of certainty on their testing data. Recently, Karimpouli and Tahmasebi [65] developed a CNN model to estimate P-wave/S-wave velocities based on the cross-sectional images of porous material. They were able to estimate these parameters with coefficients of determination around 0.65, and 0.74, respectively.

1.3. Highlights of the present study

Considering the above-mentioned categories of CNN applications in porous material research, the present study can be considered as an image–based regression model. Compared to the previous efforts and studies to estimate porous material properties via deep learning, the present work is more comprehensive and generalized considering the following aspects:

- Input and output data are obtained from 3–D micro–structures while most of the recent studies have analyzed 2–D image data [46, 65, 58].
- The number of semi–real samples of the input data in this study is relatively large compared to the previous studies (Karimpouli et al. [65] used 256 samples, Alqahtani et al. [46] used 7262 samples, while the present study uses 17700 samples).
- The number of extracted features is substantially higher than recent comparable studies (Karimpouli et al. [65] 2 features, Alqahtani et al. [46] 3 features, the present study 30 features including 15 curves each of which with 100 data points).
- A dimensionless and size–independent approach is introduced to calculate porous material features that enables us to analyze images with any spatial resolution, while in many of past studies input images have a fixed spatial resolution such as [64, 61, 103, 65].

2. Methodology

In this study, we use an augmented set of semi–realistic tomography images of geological porous material to train a convolutional neural network (CNN). The aim of this artificial intelligence model is to predict multiple physical properties of a porous material based on pore scale images of it. We call this deep learning model of porous material characterization as DeePore. To the best of our knowledge, the generated dataset of this study is unprecedented in terms of comprehensiveness and a wide range of variables.
2.1. Input data augmentation

The original core of the image dataset is composed of 60 real micro-tomography images which their detailed information and corresponding references are available in Appendix A. Considering the fact that it is critical for CNNs to be trained on a large-size dataset of images, and due to the limited availability of the diverse and realistic tomography data of porous material, we have adopted a previously developed algorithm to generate more realizations of such data by transforming the existing ones [66]. To do this, we select two different images out of the 60 samples and interpolate a hybrid texture among them by weighted averaging of the normalized distance maps. A simplified example of the interpolation technique is illustrated in Fig. 1. In this example, two initial grayscale images with different textures (Fig. 1-a and h) are binarized using a locally adaptive Otsu algorithm [67] (Fig. 1-b and i). Then, normalized maps of the Euclidean distances are calculated (Fig. 1-c and j) and combined by weighted averaging to mimic an interpolated texture (Fig. 1-e). Finally, we can set the threshold level on the obtained hybrid map to reach any desired amount of porosity (Fig. 1-d, g and k).

As a more realistic example, Fig. 2 illustrates the data augmentation technique over only two real tomography images (Fig. 2-c and w). In this figure, by going from top to the bottom rows, texture is gradually changing from sample #1 to #2. Meanwhile, by moving from left to right side of the matrix, porosity is increasing by manipulating the threshold level mentioned above.

It is noteworthy to highlight that the distance maps should be normalized prior to averaging in order to avoid large elements of one image from cloaking the smaller ones in the other image. In order to generate the hybrid realizations of each pair of the real images, we have assumed 10 uniform random numbers between 0 to 1 as interpolation weights, as well as 10 uniform random numbers between 0.1 to 0.45 as final porosity fractions. Consequently, the total number of the images in the dataset would be \( \binom{60}{2} \times 10 \) that yields 17700. However, considering that we aim to calculate several physical properties of these materials, it is expected to filter out outlayer geometries with non-physical or null properties that cannot be modelled through the regression techniques. For example, in the case that there is no percolating pathway from one side to the other side of the sample, hydraulic permeability, will be zero and formation factor which indicates electrical resistivity of the void space approaches to infinity. Also, tortuosity will have a null value in such cases.
Figure 1: Texture interpolation by weighted averaging of the normalized distance maps, (a and h) original gray maps, (b and i) binarized geometries, (c and j) normalized distance maps of the solid space, (e) equally-weighted average of the distance maps, (d, g and k) three realizations made by changing the threshold level that controls the porosity
Figure 2: Data augmentation based on two real tomography images with a wide range of porosity and texture distributed between two original samples (d and w), porosity of the samples increases from left to right and texture is transforming from c to w when moving downwards.

2.2. Building the ground truth data

After construction of the augmented set of image data, we use a series of in–house codes developed based on the available literature to analyze the micro–structures of the porous material. In this regards,
pore network modeling techniques [68] are used to simulate different physics and processes on the 3–D porous samples and the results obtained are assumed to be the ground truth for training the DeePore CNN. In addition to pore network modeling, solid network models are also used to characterize the mechanical behaviour of the studied material similar to networks presented by Herman in 2013 [69] but in 3–D. A sample realization of the solid and pore networks of a porous material are visualized in Figure 3–d and g. In order to construct these networks, initially we need a 3–D binarized image (Fig. 3–a) that is segmented to the void and solid spaces which are respectively shown in Figure 3–b and e. Then using watershed segmentation algorithm we break down an interconnected micro–structure into a separately labelled map of nodes as can be seen in Figure 3–c and f. The color gradient in these illustrations indicate the relative equivalent radius of the nodes extracted for both void (pore) and solid networks. When we have detected location and boundaries of each node, then by analyzing the node map connectivities, two networks can be extracted for both void and solid spaces (Fig. 3–d and g). Watershed segmentation algorithm which is used to break down the micro–structures into a mathematically describable 3–D network, has been widely employed for porous material characterization from tomography images [70, 71, 72]. This algorithm uses the Euclidean distance transform of a binary object to detect the narrowest parts of the connections between different nodes. More details on the methodology and validation of watershed segmentation algorithm can be found in [71, 72].

Now in order to build the ground truth data for training DeePore CNN, we investigate the constructed pore and solid networks by measuring several morphological features and running physical simulations (Fig. 3–h). In this section, we briefly describe the simulation techniques employed and some assumptions made to generalize the analysis of outcomes. As an example, we have illustrated 3 simulation results on a sample pore network model in Fig. 3–g. These simulation results are fluid saturation in a 2–phase drainage process, electricity flow through the saturated pore–space, and pore pressure of the single–phase fluid flow, respectively depicted in Fig. 3–h1 to h3 to give some insight on the ground truth generation.

The list of the physical properties and features that have been obtained for each of the samples within the dataset is provided in Table 1. As can be seen, we have reported 15 single–value features that comprehensively describe the morphological, hydraulic, mechanical and electrical properties of porous material. Additionally, 4 functions and 11 distribution curves are extracted for each porous sample to describe its characteristics (Fig. 3–i). Here is a brief introduction to the calculated set of properties and more details regarding the methodology of extracting each of the features is available in the corresponding references in Table 1.

2.2.1. Morphological properties

Based on the extracted network models, probability distribution in addition to the average values are reported for pore body radius, pore throat radius, throat length, grain radius, and pore connectivity [72] which is also known as the network coordination number [12]. In addition, pore density that indicates the number of pores per unit volume of the geometry, pore sphericity [73], grain sphericity [74], and specific surface are calculated for each of the 3–D images in the dataset. Furthermore, we have used Dijkstra’s algorithm [75]–[76] to find the shortest path from one face to the other face of the pore networks and calculate
tortuosity. In this regards, the shortest path between each two random pairs of the pores from inlet to the outlet of the pore network is calculated for several times and average value of all shortest paths is reported as tortuosity. Finally, as a morphological property of porous material we have calculated the two–point correlation function of the binarized images which shows how well–correlated are the porosity of two random points selected with a specified distance between them [77]. For more details regarding the calculation methodology for each of the properties please refer to references provided in Table 1.

2.2.2. Hydraulic properties

Absolute and relative permeabilities are calculated based on the extracted pore networks. For calculating the fluid conductance in each pore throat, realistic cross-sectional shapes of the throats are used to provide better results [20]. Additionally, for calculation of the two–phase flow functions, we have assumed zero contact angle in the case that two immiscible fluids are present within the porous media. The procedure we use to model two–phase displacement in a pore network is a quasi–static approach with stepwise increment of the non–wetting phase pressure and domination of the capillary forces over the viscous forces. This approach is fully described by Valvatne and Blunt [78]. The capillary pressure curve is another important hydraulic property of the porous material and as discussed, we require a technique to remove the pressure unit of this parameter. To this end, we have used the concept of Leverett J-function curve [79] which is a dimensionless version of the capillary pressure normalized for different porosities, permeabilities, contact angle and interfacial tension between the two displacing fluids in porous media.

2.2.3. Electrical properties

Formation and cementation factors are two electrical properties of porous material that have been calculated using the extracted pore network models [80, 81]. These parameters are critical in Archie’s equation [82] and helps to describe the electrical behaviour of a porous medium saturated with a conductive fluid. Formation factor is the ratio of the electrical resistance of the fully saturated porous media to the electrical resistance of the pure fluid [83]. Also, with a similar approach, this value remains the same when we are measuring the ratio of the mass diffusivity of a component in a bulk fluid relative to its diffusivity through the fully–saturated porous media [84, 85].

2.2.4. Mechanical property

In addition to many pore–dependent properties, we have modelled relative Young modulus of the material which is a solid phase feature. For this purpose, we assume that the extracted solid network is a truss–like structure and by applying normal compressional force on each side of the geometry, the directional Young modulus is calculated by dividing the normal stress over the strain ratio [86, 87]. Then arithmetic average of the directional values is calculated and divided by the Young modulus of the pure non–porous material to obtain the relative Young modulus which is a dimensionless number [88].
2.2.5. Dimensionless approach

It is noteworthy that we have removed the original spatial resolution of the data and defined a unified unit of length which is equal to the physical size of each voxel. For example, the unit of absolute permeability which is area has become \( px^2 \) which means that we need to multiply the resulted permeability by the spatial resolution to the power of two in order to retrieve the re-scaled permeability value. In the same manner, all other reported features are dimensionless or described only in length unit which is convertible to voxel size. The list of all alternative units is presented in Table I. For features that can be calculated directionally such as permeability, we have assumed an isotropic structure and reported the arithmetic average of the values in \( x, y, \) and \( z \) directions. Although in some cases this averaging does not have explicit physical meaning, but it is used to cover directional non-conformities in the porous structures that can affect the extensibility of the model.
Table 1: List of the physical features of porous material which are considered to be the outputs of the model in addition to the corresponding units and references that describe the methodologies in detail.

2.3. Deep learning method

In the previous sections, we have generated a large dataset of semi-realistic micro-structures of porous material and a wide range of 30 physical properties are calculated for each of the samples. Now we aim to build a machine learning model that is able to estimate these properties purely by analyzing input images and with no explicit knowledge of the underlying physics. As discussed, CNNs have proved to be efficient in image classification, segmentation, and regression. So, we have designed a CNN structure combined with two dense layers of neurons to make a regression model that is able to estimate all physical properties of porous material mentioned above in a supervised manner. Data workflow and CNN structure are presented in Fig. 3 and Table 2. Here, we are providing more details regarding the structure of the network and the
training process.

2.3.1. Network input layer

Initially, we take a 3-D image from the dataset with the size of 256^3 voxels and extract three perpendicular mid–planes of the volumetric data (Fig. 3k to l). Then, the distance transform of the solid space is calculated for each of the images and they are normalized based on the maximum values of each of them (Fig. 3m). Distance maps are not only able to deliver information about the original binary map, but also, describe the Euclidean distances between each point of that binary map to the nearest boundary. This additional information enriches the model input layer with more data compared to passing a simple binary array.

Now, based on the three normalized distance maps, we generate a fictitious RGB image by stacking them into each other and generate an initial feature map to be used as the input for the CNN (Fig. 3n). The reason to mimic an RGB image is the common use of these image formats as input of a CNN. In addition, RGB images are easy to store and read from hard disk and there are plenty of lossless compression methods invented to minimize their size when stored on disk [99]. Usage of the whole 3-D data as the input of the CNN instead of the perpendicular mid–planes could increase the accuracy of the results, while it can significantly increase the computational expenses which is not desirable due to the general purpose of this research to propose an efficient and adequately accurate model.

2.3.2. Network hidden layers

At the first layer of CNN, we initially run a 2 by 2 max–pooling filter to reduce the size of the input data without loosing too much information (Fig. 3-o2). Then, 3 convolutional layers are designed to gradually decrease the size of the information while maintaining the main geometrical features by applying different sequential filters on the input images (Fig. 3-o3 to o5). Each convolutional layer is followed by a 2 × 2 max–pooling filter to finally make data small enough to be fitted into a fully–connected dense layer. The first dense layer is activated by ReLU, while the second one uses sigmoid (Fig. 3-o6 and o7). This network architecture is designed by manually testing a range of different structures and monitoring the performance of the model in terms of the learning speed and accuracy. It is noted that the sizes of the convolution kernels are 8 × 8, 4 × 4, and 2 × 2, respectively, for the aforementioned three convolutional layers and stride is equal to 1 × 1 for all three kernels. More details on the structure of the proposed CNN is provided in Table 2.

2.3.3. Network output layer

As it can be seen in Table 2 the output layer of the network is a one dimensional array of 1515 elements (Fig. 3-o8). The first 15 elements of the array are 15 single–value features calculated for each of the porous samples as described in Table 1 rows 1 to 15. The next 1500 elements of the output array describe 4 functions and 11 distribution curves each of which occupies 100 elements of the array. The range of the array indices for each of the output parameters is described in Table 1. In order to fit the wide range of variables and functions into an array of 1515 elements, certain reshaping and interpolation operations are
required for the raw results of pore scale modelling. The four functions that occupy indices from 16 to 415, are Leverett J-function, wetting relative permeability, non–wetting relative permeability and two–point correlation function. The first three are functions of wetting phase saturation which is a fraction between 0 to 1. So, in order to summarize each of these three curves into 100 elements, we have divided the whole curve into 100 pieces each of which with 0.01 distance from each other in terms of wetting phase saturation. Similarly, for two–point correlation function, we have split the curve into 100 segments each of which with 0.5 voxel distance to the next one, in order to cover a total lag distance of 50 voxels in 100 elements. For more details regarding this function please refer to [77]. Next, in order to fit each of the 11 distribution curves into 100 elements, we are using the cumulative format of the probability distributions (CDF) that pack a full range of variable changes into a sigmoid–like curve between 0 and 1. Consequently, we have divided the CDF curve into 100 pieces with 0.01 distance between every two consecutive points in Y axis and embedded the corresponding values of X axis into the output array. For more clarification, a sample set of the described functions and distribution curves will be presented in the Results and Discussion section (Table 3 and Fig. 6).

2.3.4. Model training

Development and training of the DeePore CNN is implemented in Python using Keras with TensorFlow backend [100]. Additionally SciPy, Numpy and Matplotlib [101] as open–source packages of Python are used for data pre– and post–processing. Back–Propagation RMSprop algorithm [102] with the learning rate of $10^{-5}$ is used for training the CNN by minimizing the prediction loss in terms of mean squared error. We have used 64 % of the data samples for training the network, 16 % for evaluation and 20 % are kept outside of the workflow for independent and un–biased testing of the results obtained. We have trained the model for 200 epochs with batch size of 100 samples per each updating of the model gradient. The input and output data are fed into the model using large size Hierarchical Data Format (HDF) files. A Python Generator method, reads the data batch by batch from the HDF file to avoid occupying a large amount of machine memory.
Figure 3: DeePore data workflow for generating the ground truth data and training the CNN based on that, original binary geometry (a), solid and void spaces (b and e), labeld map of nodes (c and f), solid and pore network models (d and g), some of physical simulations on the pore network (h1 to h3), calculated single-value features, as well as the functions and distributions (i), flatten array of ground truth data (j), three perpendicular mid-planes out of the 3-D volumetric data (k), structure of three selected planes with one as solid and zero as void space (l), normalized three distance maps of the solid space which mimics red, green, and blue channels of a synthetic RGB image (m), input feature map of the porous media as a fictitious RGB image (n), (o) structure of the designed CNN with 8 layers each of which described in Table 2.
| Layers | Type           | Input size     | Kernel | Options          | Trainable parameters |
|--------|----------------|----------------|--------|------------------|----------------------|
| 1      | Input          | 256×256×3      | -      | Normalization    | 0                    |
| 2      | Pooling        | 128×128×3      | -      | Max Pool 2×2     | 0                    |
| 3      | Convolutional  | 64×64×6        | 8×8    | Max Pool 2×2     | 1158                 |
| 4      | Convolutional  | 32×32×12       | 4×4    | Max Pool 2×2     | 1164                 |
| 5      | Convolutional  | 16×16×21       | 2×2    | Max Pool 2×2     | 882                  |
| 6      | Fully-connected| 1×1×4608       | -      | ReLU Activation  | 4609×1515            |
| 7      | Fully-connected| 1×1×1515       | -      | Sigmoid Activation| 1516×1515           |
| 8      | Output         | 1×1×1515       | -      | Denormalization  | 0                    |
| Total  | -              | -              | -      | -                | 9,282,579            |

Table 2: Structure of the designed CNN including type, size, option, kernel and trainable parameters of each layer.

3. Results and Discussions

In this section, three main outcomes of this study are discussed. Initially we describe the significance and applications of the present dataset of the porous material and then we focus on the statistical lessons learned by examining cross–correlations of the dataset features. Finally, the accuracy of the features estimated by the model will be checked on the testing samples to demonstrate the capability of DeePore workflow for rapid characterization of the porous material.

3.1. Comprehensive Porous Material Dataset

In this research we have generated a comprehensive dataset of semi–real micro–porous structures with 17,700 samples and a wide range of morphological, hydraulic, electrical and mechanical features are calculated for each of the samples. The presented dataset is unprecedented in terms of the number of the samples and variety of the extracted features. The main application of this dataset is to be used as the raw material for more advanced machine learning studies on porous material. In addition to the raw 3-D geometries, Python codes, extracted pore networks and all calculated characteristics are available in the public domain for replication and improvements in future studies.  

3.2. Statistical Lessons Learned

Considering the large number of analyzed samples of porous material, we have created a rich dataset to investigate the existing trends and relationships among the calculated features. Binary correlation coefficients of 15 single-value features are visualized in Fig. 4 as a heat map to summarize the statistical significance of cross-parameter relationships. Pure blue color at the intersection of two parameters indicates strong correlation and pure red color shows a strong inverse correlation between them. As an example, absolute permeability of porous media is well correlated with average pore–throat radius which is expected based on the available literature [103], while it does not have a significant relationship with average grain radius and

[1] GitHub Repository: [https://github.com/ArashRabbani/DeePore](https://github.com/ArashRabbani/DeePore)
finally it has an inverse relationship with relative Young module of the porous material. This relationship is physically justifiable considering that large values of relative Young module indicate a tight and consolidated structure of porous material [95] which leads to lower permeability. Although, many of these relationships have been widely investigated in the literature [104, 105, 106], having a diverse range of them in a single map (Fig. 4), could provide a concise but broad insight about porous material characteristics.

Figure 4: Heatmap of the cross–correlations between the physical properties of the porous material, blue color indicates that two variables are highly correlated, white color indicates that variables are not statistically related and red color denotes a strong inverse correlation.
3.3. Model performance

Model training is performed both in CPU and GPU architectures. CPU–based computations are done on a machine with four 3.2 GHz. Intel Xenon processors and 32 GB of memory. This arrangement enables the model to be trained in 3 to 4 minutes per epoch. In addition, prediction of the porous media features based on the trained model takes 9.23 ms per sample on average which is 4 to 6 orders of magnitude faster if the features are to be extracted by physical simulations (Fig. 5-a) [20].

Using GPU to accelerate the training and prediction stages can make this workflow even faster. Using an Nvidia GeForce GTX 1660 Ti with Max-Q Design Graphic Card with Compute Capability of 7.5 and 6 GB of memory, we are able to train the model around 4 times faster, in which each epoch would take around 45 s to finish. Also prediction of test dataset can be performed with the speed of 0.379 ms per sample on average which is 24 times faster than the CPU–based instance (Fig. 5-a) and it is a considerable improvement.

At each epoch of training the validation and training losses are measured in terms of mean square error to ensure that over–fitting is not occurring and training has reached an optimum point (Fig. 5-b). In our case, increasing the number of epochs to more than 100, it hardly reduces the validation loss less than $10^{-3}$. So, we have stopped the training at 100 epochs as visualized in Fig. 5. As presented in Table 2, the total number of parameters to be trained is 9,282,579. On the other hand, considering the filtered outlier data, the total training data points would be 10153 × 1515 which is 65% more than the trainable parameters and this makes it hard for the network to memorize data points instead of learning the trends. Thus, based on the above–mentioned numbers and decreasing trend of the validation loss, it can be stated that over–fitting has not occurred before 100 epochs. If we train the network for more than 100 epochs, training loss curve deviates from the validation loss and its a sign of over–fitting for epochs more than 100 (Fig. 5-b).

Using the trained CNN model we have estimated a wide range of porous material characteristics on 20% of the data which are not used in the training or validation processes. The average determination coefficients ($R^2$) of the reference and estimated features for the test data are 0.9101 and 0.9670, respectively, for single–value features (rows number 1 to 15), and function/distribution features (rows number 16 to 30). Also, the average determination coefficient of all 30 features is 0.9385. This overall level of accuracy is reasonably good considering the wide range of porous structures and variety of the predicted features.
In order to provide an insight into the sample outputs of the model, we have presented Table 3 and Fig. 6 for discussing single-value features and functions, respectively. In Table 3, reference values and estimated values are matching with a low level of average relative error at only 5%. If the real spatial resolution of this sample image is assumed to be 5 microns per voxel, consequently, in order to scale the values with the unit of length (px) we simply multiply them by 5. Similarly for the area (px²), values are multiplied by 5². This approach gives us the flexibility to predict porous material characteristics in a wide range of spatial resolutions without changing or re-training the model. A similar approach is used for functions and distribution curves which are depicted in Fig. 6. The average determination coefficient of all 15 curves shown in this figure for sample #1 is 0.9417.

Additionally we have compared the distribution probability of all single-value features to check the correspondence between the reference and estimated data (Fig. 7). This data has been visualized for 3173 testing samples and in the most of the cases both two distributions follow the same pattern, while for parameters like pore-to-throat aspect ratio, some deviations are observed (Fig. 7-j). Also, in grain size distribution reference curve, a bimodal behavior is observed while the estimated distribution has failed to match that trend accurately (Fig. 7-n). This distributed data are also visualized in the form of scattered plots in Fig. 8. These charts carry the same R² values as the distribution curves in Fig. 7 while unit-slope
lines in Fig. 8 could give better insight regarding the over or under-estimation of the parameters. We have observed a degree of underestimation for larger values especially in tortuosity and average connectivity data (Fig. 8-e and f). This is probably due to the skewness of the distribution of these parameters in which a long but thin tail toward the larger values do not lead the model to sacrifice its accuracy on the middle-range data for better coverage on the whole domain. In other words, during the training process, model prefers to have higher accuracy for the majority of the data points instead of less accuracy but better coverage on the whole set of points.

Finally, we have plotted the predicted functions and distributions versus reference values for 100 randomly selected samples from the testing pool of data (Fig. 9). Also, we have calculated $R^2$ coefficients for each of the plotted lines and the average values are presented in Fig. 9. Similar to the distributions in Fig. 7, we have applied a Gaussian filter with standard deviation of 1 to avoid possible noises in the reference and estimated curves. We have found that the data which are directly calculated from the geometrical features of the porous samples such as pore size distribution (Fig. 9-e) are easier to estimate compared to more complicated functions, such as relative permeability (Fig. 9-b and c) that are obtained from a higher level simulation.

| Num. | Feature                        | Reference Value | Estimated Value | Relative Error |
|------|--------------------------------|-----------------|-----------------|----------------|
| 1    | Absolute permeability (px$^2$) | 0.395           | 0.439           | 0.113          |
| 2    | Formation factor (ratio)       | 5.224           | 4.921           | 0.058          |
| 3    | Cementation factor (ratio)     | 1.583           | 1.571           | 0.008          |
| 4    | pore density (1/px$^3$)        | $1.78 \times 10^{-4}$ | $1.75 \times 10^{-4}$ | 0.016          |
| 5    | Tortuosity (ratio)             | 1.197           | 1.190           | 0.006          |
| 6    | Average coordination number    | 5.653           | 5.820           | 0.030          |
| 7    | Average throat radius (px)     | 4.306           | 3.964           | 0.079          |
| 8    | Average pore radius (px)       | 6.947           | 7.026           | 0.011          |
| 9    | Average throat length (px)     | 18.708          | 19.560          | 0.046          |
| 10   | Pore to throat aspect ratio    | 3.166           | 3.483           | 0.100          |
| 11   | Specific surface (1/px)        | 0.159           | 0.156           | 0.023          |
| 12   | Pore sphericity (ratio)        | 0.770           | 0.743           | 0.035          |
| 13   | Grain sphericity (ratio)       | 0.828           | 0.859           | 0.038          |
| 14   | Average grain radius (ratio)   | 10.413          | 10.663          | 0.024          |
| 15   | Relative Young module (ratio)  | 0.107           | 0.089           | 0.169          |
|      | Average                        | -               | -               | 0.050          |

Table 3: Example comparison of the reference and estimated values of 15 single-value features for one of the image samples in the dataset (sample #1).
Figure 6: Example comparison of the reference and estimated values of 15 functions and distribution for one of the image samples in the dataset (sample #1). The average correlation coefficient of the reference and estimated curves is 0.9616.
Figure 7: Comparison between the reference and estimated distributions of the 15 single-value features, a to o charts correspond to the features inscribed in Table 1 rows from 1 to 15.
Figure 8: Comparison between the reference and estimated values for 15 single–value features and their correlation coefficients, a to o charts correspond to the features inscribed in Table 1 rows from 1 to 15.
Figure 9: Comparison of the reference and estimated curves for 15 functions and distributions that correspond to the rows of 16 to 30 in Table [1].
4. Conclusions

In order to deliver the present DeePore package, we have generated a large dataset of semi–real 3–D images of porous structures with 17700 samples and 30 features which are physical characteristics of porous material. Using a regression CNN coupled with two dense layers, a fast and comprehensive characterization of 3–D porous material images is implemented. In summary, the following conclusions can be drawn based on the findings of this research:

- A physically diverse dataset of micro–porous–structures are generated based on texture transformation and porosity manipulation of 60 original tomography images and a wide range of morphological, hydraulic, electrical and mechanical features are extracted for each sample which is publicly available and can be used for deeper future studies.

- A dimensionless approach has been presented to extract or predict the porous material features without being affected by the spatial resolution of the images.

- A statistically accurate feature estimation is implemented using re–designed feed–forward CNN by training the model for 100 epochs while over–fitting is avoided.

- A cross–correlation heat map of the 15 porous material features are presented that gives a concise but broad insight into the significance of relationships between each pair of the extracted features.

- The average coefficient of determination ($R^2$) for all 30 extracted features is 0.9385 which is significant considering the diverse range of porous morphologies and features.

- Via a GPU–based architecture we are able to predict the above–mentioned features for each $256^3$ voxels binary image of porous material in 0.379 ms on average. This high speed of prediction enable us to tackle larger image sizes in future studies.

Future studies

It is noteworthy that each of the physical simulation methods are subject to uncertainty due to some inherent simplification assumptions in pore network modeling. Consequently, it is recommended to use more accurate simulation methods such as direct numerical models to generate the ground truth dataset based on the current set of 3–D images in the future studies.

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Author Contribution Statement

Arash Rabbani has developed the idea of this research, executed the research by computer code development and written the article. Reza Shams contributed to execution of research through trouble shooting of the computer codes, and Masoud Babaei supervised the research and contributed in writing the article.
## Appendix A

Here we have listed the real tomography images of porous material used to generate the dataset using the data augmentation method. The size and spatial resolutions mentioned in this table are modified by resizing/cropping the original images to fit the purpose of this study.

| Num. | Name                  | Resolution (μm/px) | Modified size (px³) | Type      | DOI                                      |
|------|-----------------------|--------------------|---------------------|-----------|------------------------------------------|
| 1    | Berea #1              | 11.72              | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.003 |
| 2    | Berea #1              | 8.35               | 256³                | Sandstone | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 3    | Berea #2              | 3.25               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.003 |
| 4    | Berea #3              | 3.25               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.003 |
| 5    | Berea #4              | 3.25               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.003 |
| 6    | Berea #5              | 4.33               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.003 |
| 7    | Berea #6              | 4.33               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.003 |
| 8    | Berea #7              | 4.33               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.003 |
| 9    | C1                    | 4.45               | 256³                | Carbonate | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 10   | C2                    | 8.35               | 256³                | Carbonate | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 11   | Doddington #1         | 5.41               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.003 |
| 12   | Doddington #2         | 5.41               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.004 |
| 13   | Doddington #3         | 5.41               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.005 |
| 14   | Doddington #4         | 5.41               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.006 |
| 15   | Estailliades #1       | 10.72              | 256³                | Carbonate | https://doi.org/10.1016/j.physa.2009.12.006  |
| 16   | Fontainebleau #1      | 17.17              | 256³                | Sandstone | https://doi.org/10.1016/j.physa.2009.12.006  |
| 17   | Fontainebleau #2      | 17.17              | 256³                | Sandstone | https://doi.org/10.1016/j.physa.2009.12.006  |
| 18   | Fontainebleau #3      | 17.17              | 256³                | Sandstone | https://doi.org/10.1016/j.physa.2009.12.006  |
| 19   | Fontainebleau #4      | 17.17              | 256³                | Sandstone | https://doi.org/10.1016/j.physa.2009.12.006  |
| 20   | Fontainebleau #5      | 17.17              | 256³                | Sandstone | https://doi.org/10.1016/j.physa.2009.12.006  |
| 21   | Fontainebleau #6      | 17.17              | 256³                | Sandstone | https://doi.org/10.1016/j.physa.2009.12.006  |
| 22   | Ketton                | 10.62              | 256³                | Carbonate | http://dx.doi.org/10.1016/j.advwatres.2012.03.005 |
| 23   | S1                    | 10.18              | 256³                | Sandstone | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 24   | S2                    | 5.81               | 256³                | Sandstone | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 25   | S3                    | 10.66              | 256³                | Sandstone | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 26   | S4                    | 10.50              | 256³                | Sandstone | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 27   | S5                    | 4.68               | 256³                | Sandstone | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 28   | S6                    | 5.98               | 256³                | Sandstone | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 29   | S7                    | 5.63               | 256³                | Sandstone | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 30   | S8                    | 5.73               | 256³                | Sandstone | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 31   | S9                    | 3.98               | 256³                | Sandstone | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 32   | F42A                  | 11.72              | 256³                | Sandpack  | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 33   | F42B                  | 11.72              | 256³                | Sandpack  | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 34   | F42C                  | 11.72              | 256³                | Sandpack  | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 35   | LV60A                 | 11.72              | 256³                | Sandpack  | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 36   | LV60B                 | 11.68              | 256³                | Sandpack  | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 37   | LV60C                 | 11.72              | 256³                | Sandpack  | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 38   | A1                    | 4.51               | 256³                | Sandpack  | http://dx.doi.org/10.1103/PhysRevE.80.036307 |
| 39   | Benthemier #2         | 4.97               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.005 |
| 40   | Benthemier #3         | 4.97               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.005 |
| 41   | Benthemier #4         | 4.97               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.005 |
| 42   | Benthemier #5         | 4.97               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.005 |
| 43   | Benthemier #6         | 4.97               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.005 |
| 44   | Benthemier #7         | 4.97               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2012.03.005 |
| 45   | Berea #8              | 7.11               | 256³                | Sandstone | https://doi.org/10.1016/j.advwatres.2015.07.012 |
|   | Source           | Size     | Material        | DOI                                      |
|---|------------------|----------|-----------------|------------------------------------------|
| 46| Clashach         | 10.15    | Sandstone       | https://doi.org/10.1016/j.advwatres.2015.07.012 |
| 47| Doddington #5    | 9.50     | Sandstone       | https://doi.org/10.1016/j.advwatres.2015.07.012 |
| 48| Estaillades #2   | 10.16    | Carbonate       | https://doi.org/10.1016/j.advwatres.2015.07.012 |
| 49| Indiana          | 10.15    | Carbonate       | https://doi.org/10.1016/j.advwatres.2015.07.012 |
| 50| Ketton #2        | 10.15    | Carbonate       | https://doi.org/10.1016/j.advwatres.2015.07.012 |
| 51| Monte Gamb. #1   | 4.94     | Carbonate       | https://doi.org/10.1016/j.advwatres.2012.03.004 |
| 52| Monte Gamb. #2   | 4.94     | Carbonate       | https://doi.org/10.1016/j.advwatres.2012.03.004 |
| 53| Monte Gamb. #3   | 4.94     | Carbonate       | https://doi.org/10.1016/j.advwatres.2012.03.004 |
| 54| Monte Gamb. #4   | 4.94     | Carbonate       | https://doi.org/10.1016/j.advwatres.2012.03.004 |
| 55| Monte Gamb. #5   | 4.94     | Carbonate       | https://doi.org/10.1016/j.advwatres.2012.03.004 |
| 56| Monte Gamb. #6   | 4.94     | Carbonate       | https://doi.org/10.1016/j.advwatres.2012.03.004 |
| 57| Monte Gamb. #7   | 4.94     | Carbonate       | https://doi.org/10.1016/j.advwatres.2012.03.004 |
| 58| Monte Gamb. #8   | 4.94     | Carbonate       | https://doi.org/10.1016/j.advwatres.2012.03.004 |
| 59| Hollington #1    | 2.17     | Sandstone       | https://doi.org/10.1007/s11242-019-01244-8 |
| 60| Hollington #2    | 2.17     | Sandstone       | https://doi.org/10.1007/s11242-019-01244-8 |

Table 4: Sources of the original tomography data and some specifications including original names, size and spatial resolutions.
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