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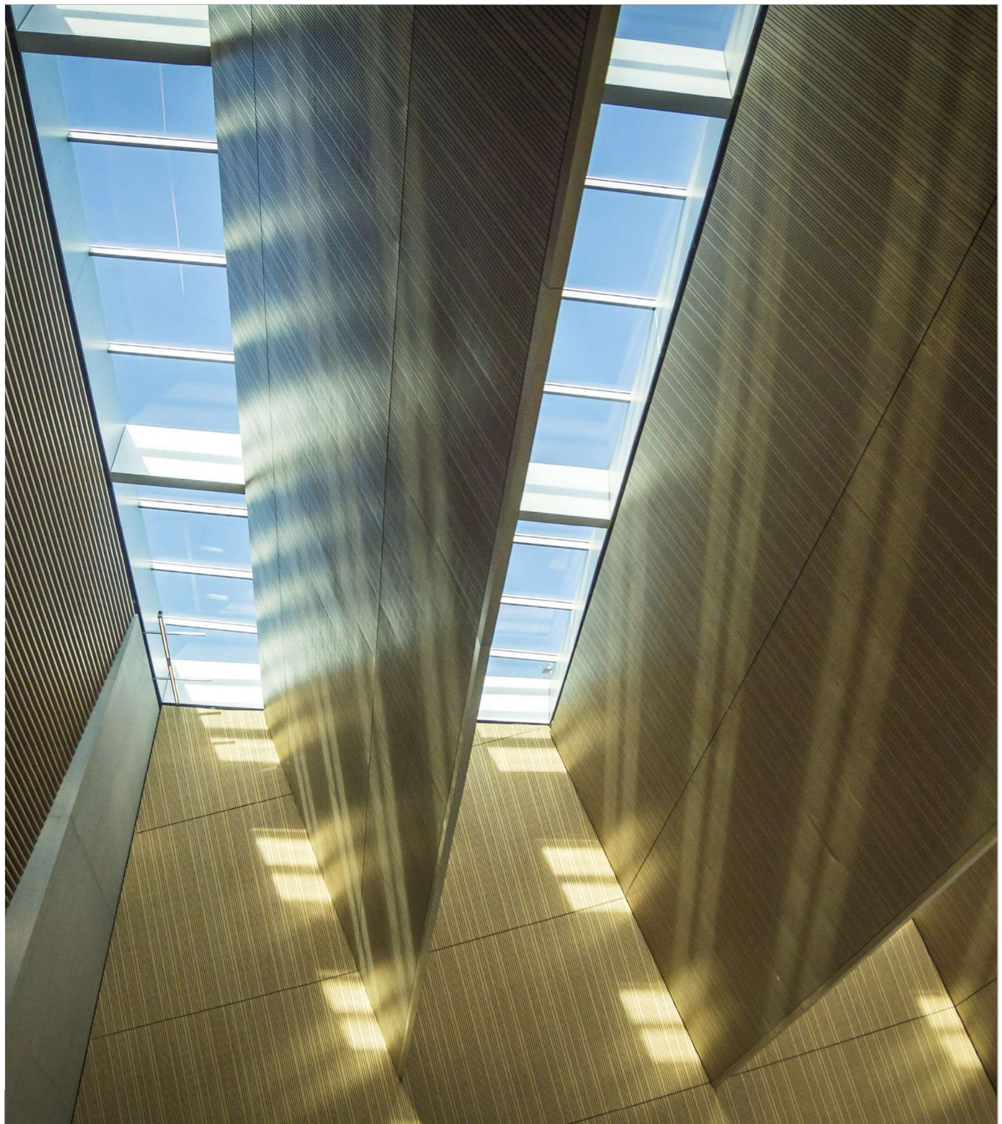

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DEEP LEARNING BASED PREDICTION OF FIBROUS MICROSTRUCTURE PERMEABILITY

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Abstract: *Knowledge of permeability of fibrous microstructures is crucial for predicting the mold fill times and resin flow path in composite manufacturing. Herein we report a method to rapidly predict the permeability of 3D fibrous microstructures. Our method relies on predicting the permeability of 2D cross-sections via deep neural networks and extending this capability to 3D microstructures via circuit analogy as a means of reduced order modeling. Approximately 50% of the permeability predictions of 2D cross-sections have 10% or less deviation from the permeability results obtained via flow simulations in Geodict. Computational time required for predicting the permeability of 3D microstructures is reduced from hours to less than 10 seconds. This framework enables fast and accurate prediction of micro-permeability and serves as the first building block towards prediction of fabric mesostructures' permeability via deep learning based methods.*

Keywords: Deep Learning; Permeability; Microstructures; Numerical analysis

1. Introduction

Permeability, a 3D tensor defined by the pore structure within the fabrics, is a key set of input parameters to predict mold-filling times and filling patterns in Liquid Composite Molding (LCM) [1]. Nowadays, numerical flow simulations in virtual fabric structures is on its way to replace experimental characterization techniques [2,3], and these efforts are further refined owing to X-ray computed microtomography based representation of 3D geometric information within and between individual tows [4,5]. However, the flow simulations in such structures still require substantial computational power and computations typically take hours in parallelized systems. On the other extreme, analytical models provide rapid predictions of permeability and these models range from models based on the isotropic porous media to models that take into account the fiber orientation and tortuosity [6–9]. However, these models are limited in accounting for the local variability in fabric structures.

Convolutional neural networks (CNNs), a type of deep learning algorithm, provide powerful alternatives for detecting patterns in images and linking these features to a property (such as permeability). In materials science, they have been used for many purposes such as for predicting mechanical, thermal and hydraulic properties of material systems [10,11] and also for predicting the permeability of isotropic porous media such as those found in soil sciences [12,13]. This work aims to provide a fast and accurate method for predicting the permeability of

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highly oriented anisotropic media, more specifically the fibrous microstructures encountered in advanced composites. To this end, we propose a method based on the following steps: 1- generate 3D fibrous microstructures, 2- estimate the transverse permeability of individual slices (along the fiber direction) and the full 3D structures using FlowDict module of Geodict software, 3- train a 2D CNN using the simulation results to predict the permeability of 2D slices, 4- predict the 2D permeability in the slices of 3D structures previously unseen by CNN, 5- use the circuit analogy between 2D slices to predict the permeability of 3D structures. The outlined methodology enables us to reduce the computational time from hours required for running 3D flow simulations to estimate the permeability in less than 10 seconds.

2. Methods

2.1 Elementary volume (EV) generation

We generated 400x400 pixels images with 1 μm2/pixel correspondence where fibers had radii, r,: 6, 8, 10, 12, or 14 pixels and fiber volume fraction, vf, was between 0.25 and 0.70, by increments of 0.05. We used a modified version of the Monte-Carlo procedure by Chen and Papathanasiou [14,15], to account for the short-range tortuosity. Figure 1 shows two EVs generated by the modified fiber generator.

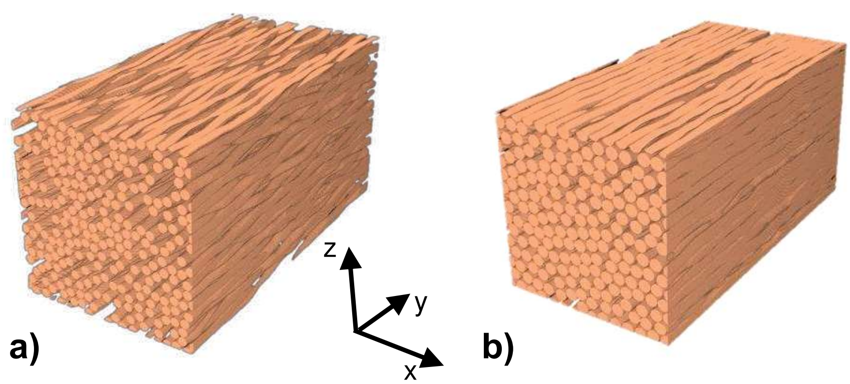

Figure 1. Two examples of generated 3D structures. a) r = 10 pixel, v_f = 0.5, b) r = 14 pixel, v_f = 0.7.

2.2 Flow simulations

We performed flow simulations to extract the transverse permeability (along x- and z-directions) of the generated EVs. These simulations included those where the EVs had a depth of one in y-direction (i.e., on 2D slices) to train the 2D CNN, and simulations on full EVs (which consisted of 800 slices with 400x400 pixels). 3D simulations were used for validating our approach based on combining both the circuit analogy as an upscaling technique.

We used FlowDict module of the Geodict software to perform the flow simulations. The choice was based on Geodict's capability to perform the simulations directly on the binarized images and its suitability for automation as we performed the simulations on thousands of 2D binary images. We defined the boundary conditions as depicted in Figure 2 following the suggestions by Rimmel et al. [16] that were reported for similar simulations using the same software module.

We solved the governing Stokes flow equations (*i.e.*, at negligible or zero-valued Reynolds number) using the Explicit Jump-Stokes solver, as reported in earlier work for permeability characterization [4,5].

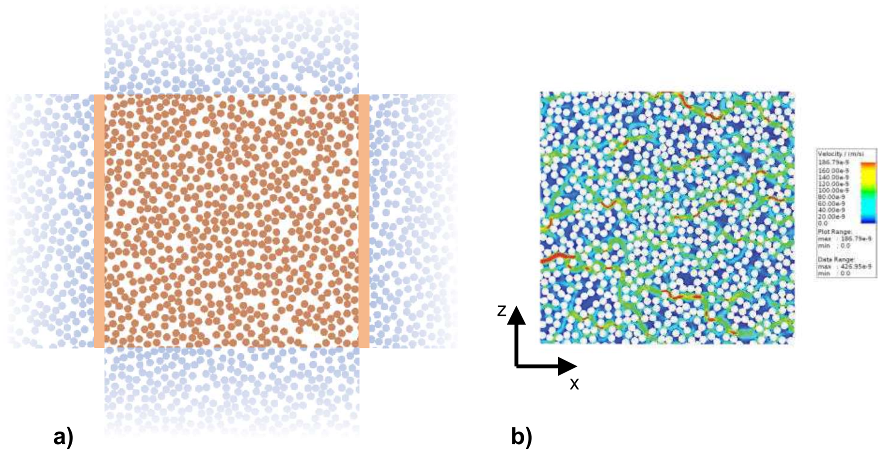

Figure 2. a) Boundary conditions and b) corresponding flow field in x-direction. In a) boundary conditions highlight the implicit inlet/outlet voxels in orange and periodic tangential boundaries in blue.

2.3 CNN architecture and training

We implemented a modified version of AlexNet [17] in Matlab's Deep Learning toolbox. The design of the CNN is outlined in Figure 3. It takes an image with 400×400 pixels as input and outputs the permeability. Each convolutional block in Figure 3 consists of the following: a convolutional layer, followed by an activation via a rectified linear unit (ReLU), followed by batch normalization and max pooling layers. The last block is connected to a dropout layer and a fully connected layer for the regression task. The filters of convolution layers have a size of 7×7, 5×5, and 3×3 respectively. Filters have a stride of 1 and paddings of 3, 2, and 1 and number of filters is 16, 32 and 64 respectively. Max pooling layers' size and stride are as follows: the first two of them have a size of 4×4 and a stride of 4 while the last one has a size of 2×2 and a stride of 1.

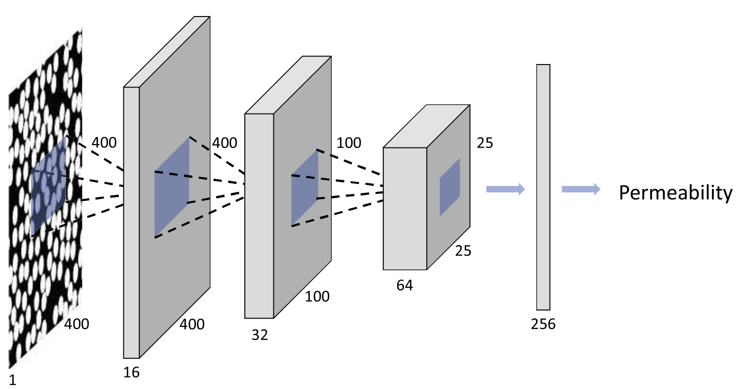

Figure 3. Architecture of the used convolutional neural network where each convolutional block is made up of a convolution, activation, batch normalization and max pooling layers

5 different pixel counts per r and 10 different fiber content combination (v_f) results in 50 unique microstructures, and each microstructure has 1000 slices along the fiber direction. 1280 of the 50000 unique 2D slices are selected randomly and used in the CNN training. 2D microstructure permeability is flip-invariant, and we exploited this characteristic to augment the number of images during CNN training and used the resulting database with a split of 3:1 between training and validation images.

We mapped the logarithm of permeability between -1 and 1 using the minimum and maximum values and used it as the output of the CNN. We trained the CNN for 500 epochs using the ADAM optimizer via Matlab Deep Learning Toolbox on an Nvidia Quadro RTX6000 with 24GB memory; the training lasted approximately 14 hours.

3. Results and Discussion

3.1 2D transverse permeability

3000 randomly selected images' predicted permeability along x-direction and the corresponding simulation results are shown in Figure 4a. CNN predictions seem to be well-aligned with the simulation results in general, some scatter is observed at the low permeability regime - approximately for permeability values lower than 1×10-13 m^2 obtained at high v_f. This is suspected to originate from 0 permeability results returned by the flow simulation at high v_f range. Another trend is the relatively more pronounced scatter in the images where fiber radius is 14 pixels. Figure 4b shows the cumulative distribution of relative deviation of neural network predictions (NN) from the Geodict results (GD), $(GD - NN)/GD$. This is suspected to originate from the disparity between the individual fiber size (and thus the spacing between neighboring fibers) and the filter sizes in the convolutional layers. We note that, even in the case of 14 pixel radius fibers, more than 50% of predictions have 10% or less deviation from the simulation results.

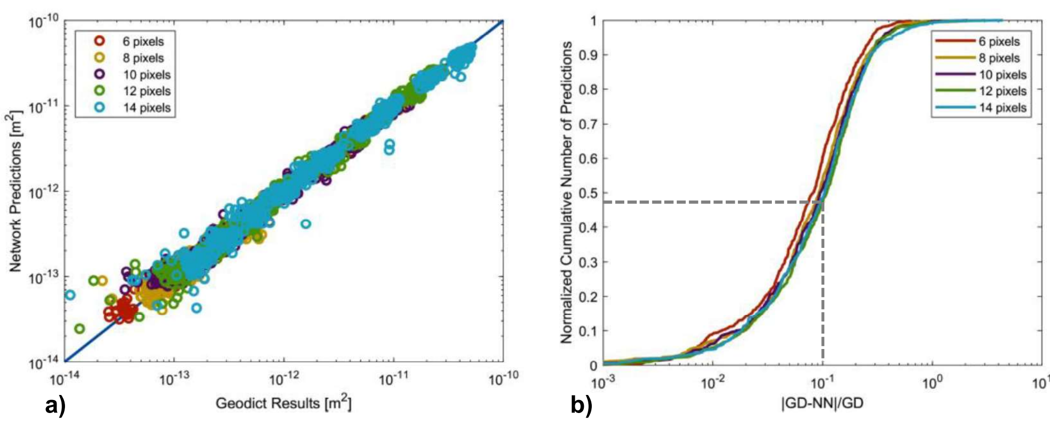

Figure 4. a) Neural network predictions for permeability in x-direction vs. corresponding Geodict results, b) normalized number of predictions as a function of the predictions' deviation from simulation results

3.2 3D permeability: circuit analogy based on 2D predictions

To test the suitability of upscaling the 2D predictions via circuit analogy, we generated 15 new microstructures with 400x800x400 voxel dimensions (800 slices along the fiber direction with 400x400 pixels). These microstructures consisted of images where the fiber radii were represented by 6, 10 or 14 pixels and v_f was 0.3, 0.4, 0.5, 0.6, or 0.7. Flow simulations to obtain the transverse permeability values took between 1675 seconds and 8118 seconds with an average of 4305±1839 seconds. The equivalent transverse permeability (in both x- and z-directions) is calculated via circuit analogy of 800 resistances ($1/K_x$) in parallel using the arithmetic mean of individual slices' permeability. Complete operation, including the pre-processing and post-processing operations, to predict the permeability of individual slices and the equivalent permeability took 8.56 seconds.

Figure 5 shows the permeability values obtained via 3D flow simulations (GD-3D), as well as the resulting circuit analogy results (NN-circuit) for both x- and z-directions. Results show that most of the GD-3D and NN-circuit results fall in a small range for all the studied pixel per radius correspondence and v_f combinations. Departure of both GD-3D and NN-circuit from Gebart's permeability predictions [6] at high v_f is another distinct characteristic of these results and these are in agreement with the observations reported in literature [18] further validating our approach where we achieve reasonable accuracy with significantly smaller computational effort.

The reader is referred to our paper [19] for more detailed description of the methodologies we relied on and for more detailed validation of the proposed approach, also extended for prediction of longitudinal permeability. The said paper also explores the suitability of pre-processing strategies to enable predicting the permeability of images that have different pixel dimensions than what the CNN expects that can be made up of finer or coarser 2D square slices as well as rectangular slices.

4. Conclusion

This work presents a mixed and fast numerical-analytical strategy to predict the transverse permeability of 3D fibrous microstructures. To that end, we treated the images of 3D microstructures as a series of 2D slices. After generating such microstructures and performing flow simulations on 2D and 3D images, we trained a 2D Convolutional Neural Network for predicting the transverse permeability of individual 2D slices. These highly accurate predictions were then used in a circuit analogy to predict the transverse permeability of full 3D microstructures. Results show that predictions in both 2D and 3D are in good agreement with their counterparts obtained via flow simulations and require only a fraction of the computational effort needed for flow simulations. Our approach serves as the first building block towards accurate and fast prediction of fabric mesostructures' permeability where local fiber volume fraction and dual-scale effects are prominent.

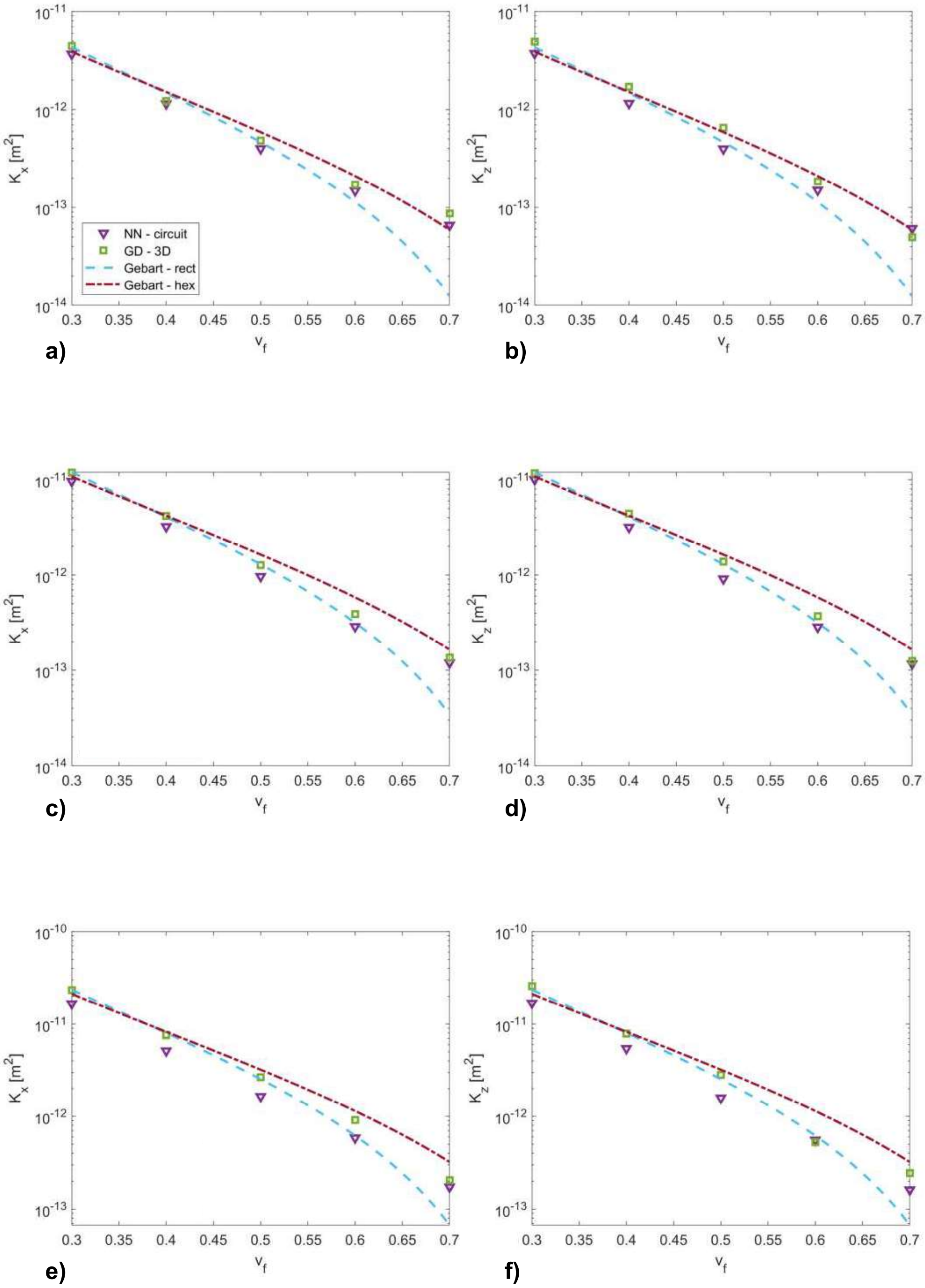

Figure 5. Permeability results obtained via 3D simulations and circuit analogy of the neural network predictions, on images with r = 10 pixel. Top, middle, and bottom rows correspond to the results along the x-, y-, and z-directions, respectively.

Acknowledgements

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