Physics-informed neural networks of moisture diffusion in bio-composites

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Introduction

Bio-composite materials possess excellent degradability, making them environmentally friendly and sustainable [1-2]. Additionally, certain bio-composite materials reinforced with specific biomaterials exhibit corrosion resistance [3]. However, their inherent hydrophilic nature limits their widespread application. Therefore, optimizing material design to enhance water resistance is necessary. However, optimizing through experimental data often requires long cycles. To save time and cost on material design and preparation, numerical simulations provide a more convenient and faster alternative. Due to the naturally multi-scale structure of composite materials, multi-scale simulation techniques that provide detailed information have become a necessary choice.

Method

Coupled multi-scale simulations using finite element (FE) method at both macroscopic and microscopic scales (FE^2) is a very accurate numerical simulation method developed for studying multi-scale problems in materials [4]. However, this method is constrained by the iterative computational efficiency between different scales. In the FE^2 method, after FE discretization, each Gaussian integration point at the macro-scale corresponds to a representative volume element (RVE) model at the micro-scale. The gradient data at the integration point is used to impose boundary conditions on the RVE, which then undergoes finite element computations. The homogenized results are transferred back to the corresponding macroscopic Gaussian integration points, and this process iterates until convergence is achieved at the macroscopic element level, ensuring nodal equilibrium [4]. The microscopic simulation is a time-consuming part of this multi-scale computation. A surrogate model based on deep neural networks (DNN) can serve as an alternative to FE simulations at the micro-scale, significantly improving simulation efficiency while maintaining accuracy [5]. However, data-driven surrogate models typically require large amounts of high-quality labeled data, limiting their applicability in many specific scenarios, especially in complex systems like composite materials.

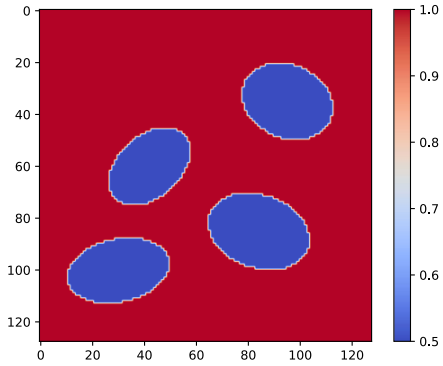

Figure 1: Pixelized distribution of diffusion coefficients as input data

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This work employs a physics-constrained deep learning model based on a convolutional encoder-decoder architecture [6] to generate a microscopic surrogate model. The model uses a functional variation based on a multivariate variation principle as the loss function.

Results

Although this model only requires diffusion coefficients distribution as input data illustrated in Figure 1 instead of labeled data by explicitly solving PDE governing equations in terms of training, as shown in Figure 2, it achieves prediction accuracy comparable to FE simulations.

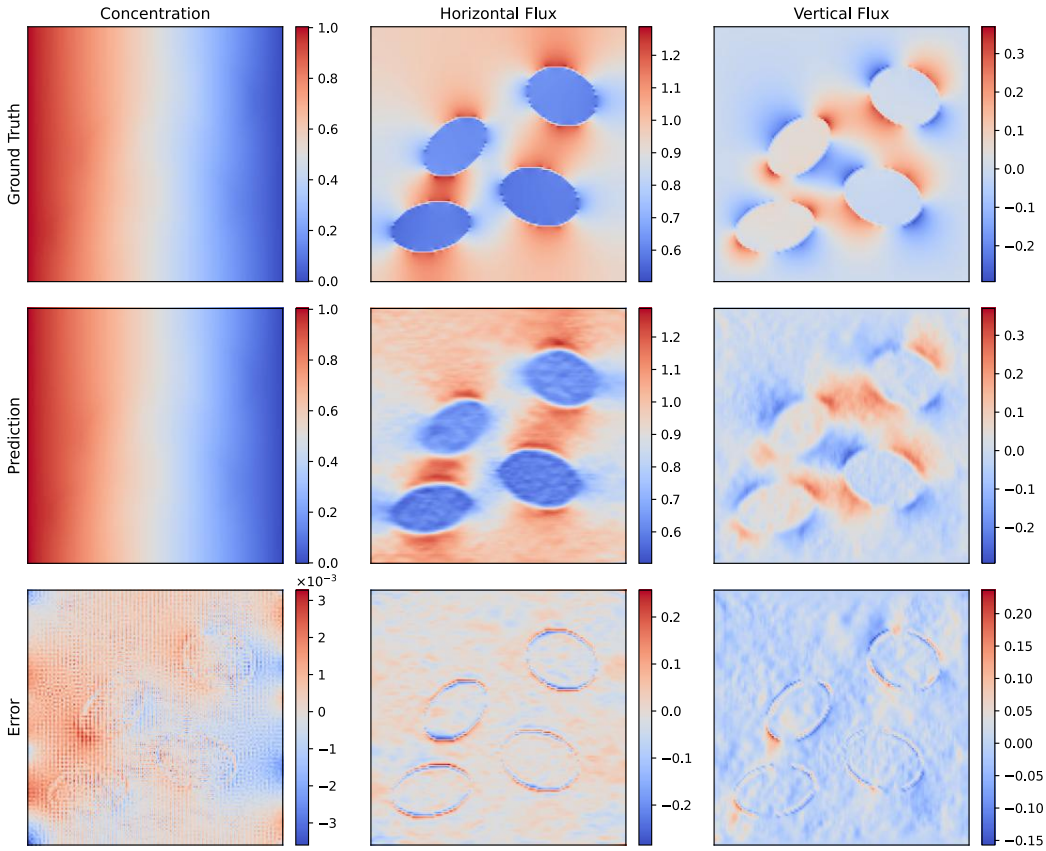

Figure 2: FE simulations, DNN predictions and errors between them.

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