Prediction of Solute Dispersion Coefficient in Porous Media Using Transformer Network

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Microsoft Accor black, Size: 20

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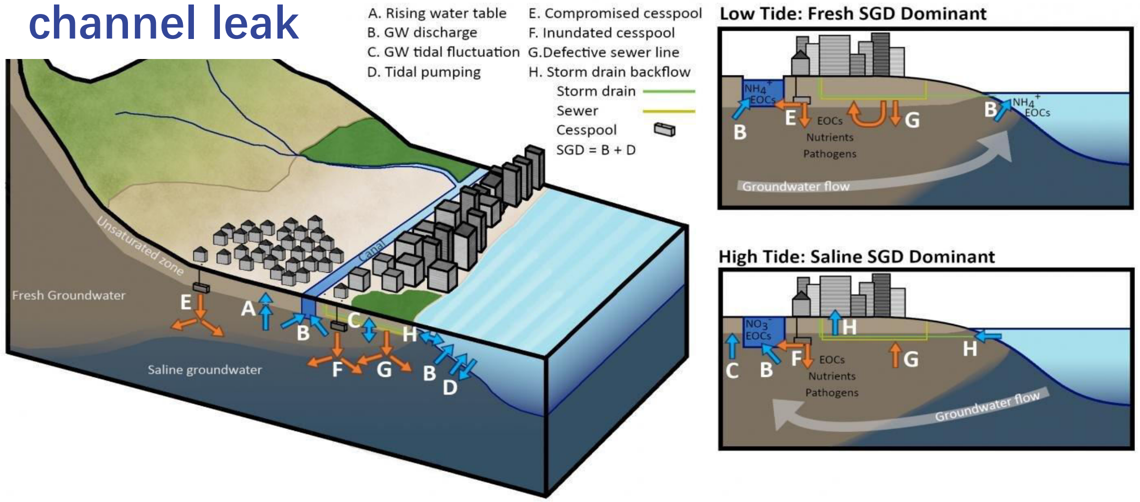
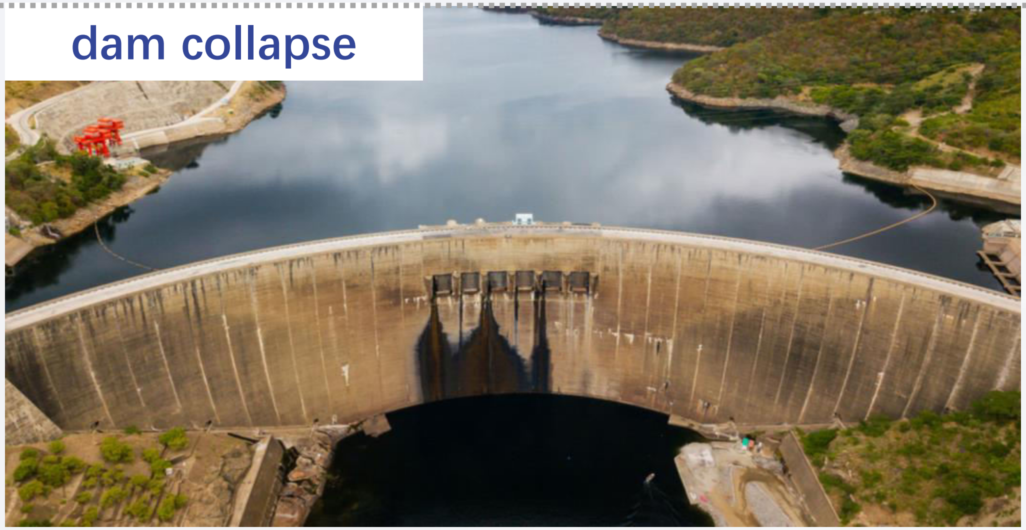
Research Background: Percolation and Solute Transport

The flow of fluids in soil and rocks, as well as the transport of inorganic or organic chemical substances in porous media, belong to the phenomena of percolation and solute transport.

channel leak

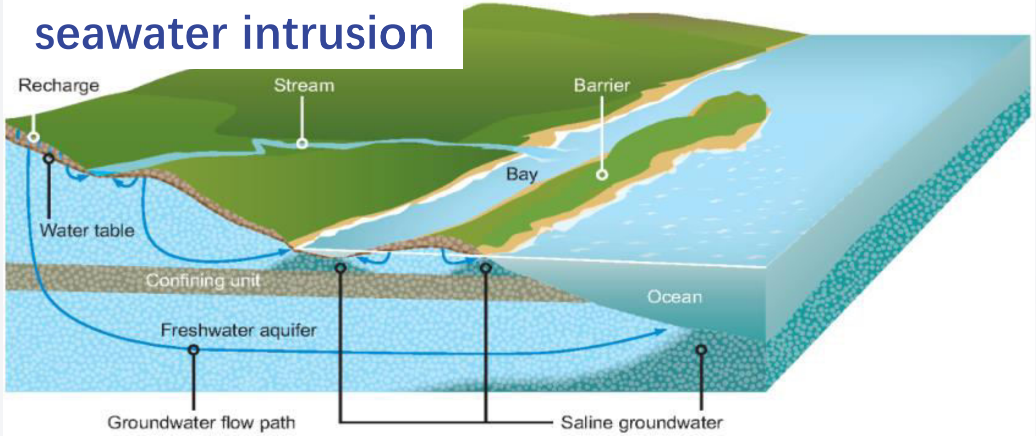


dam collapse



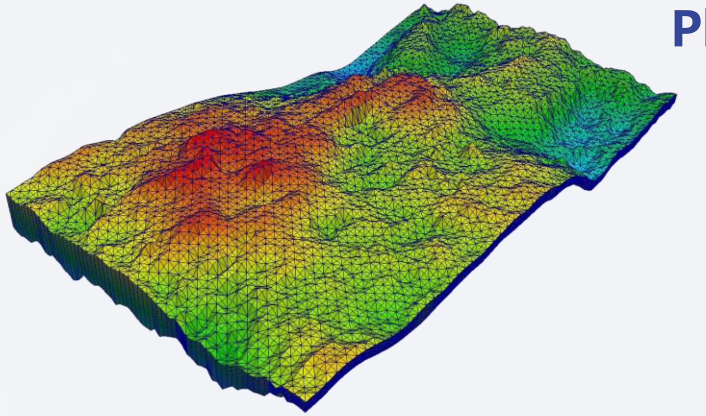
Soil piping

seawater intrusion



Research Background: Percolation and Solute Transport

Darcy's scale model



Groundwater Flow and Solute Transport Model Based on Phenomenological Study: Darcy's Law and Advection-Dispersion Equation.

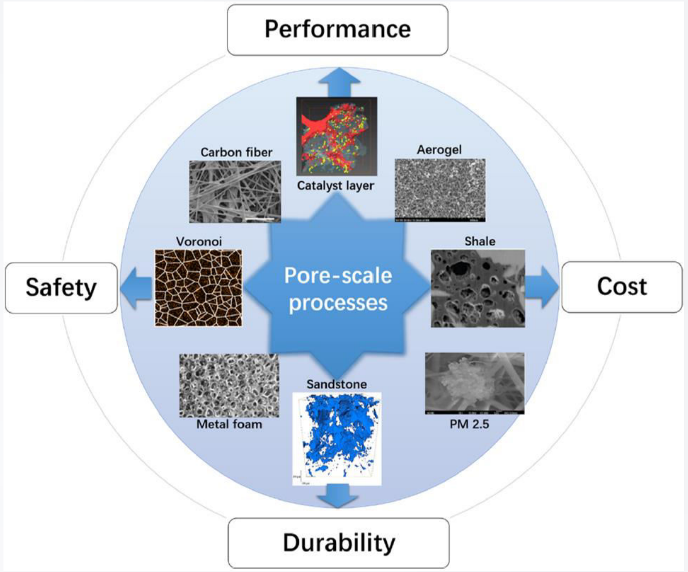
$$\frac{\partial(\varepsilon\rho)}{\partial t} + \nabla \cdot u = 0$$

$$u = -\frac{\boldsymbol{k}}{\mu}(\nabla P - \rho g)$$

$$\frac{\partial(\varepsilon C)}{\partial t} + u \cdot \nabla(C) = \boldsymbol{D}\nabla^2 C + R$$

How to determine the permeability coefficient (k) and the dispersion coefficient (D).

Pore-scale model



The fundamental physical processes at the pore scale: the Navier-Stokes (NS) equation and the advection-diffusion equation.

$$\nabla \cdot u = 0$$

$$\partial_t u + u \cdot \nabla u = -\frac{1}{\rho}\nabla p + \mu \nabla^2 u$$

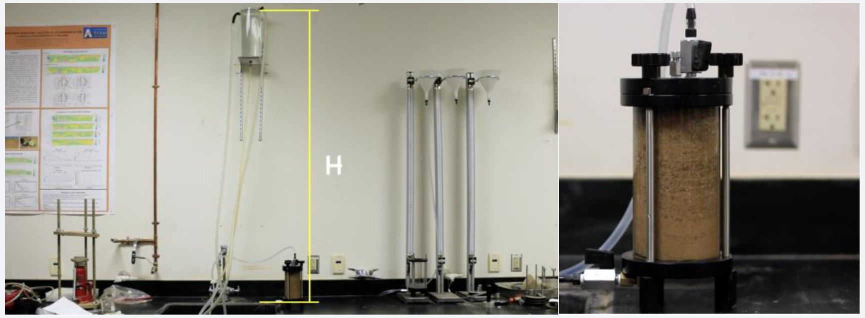
$$\partial_t C + u \cdot \nabla C = D\nabla^2 C + R$$

- ✓ **Accurately describing the microscale processes**
- ✓ **Non-phenomenological theory**

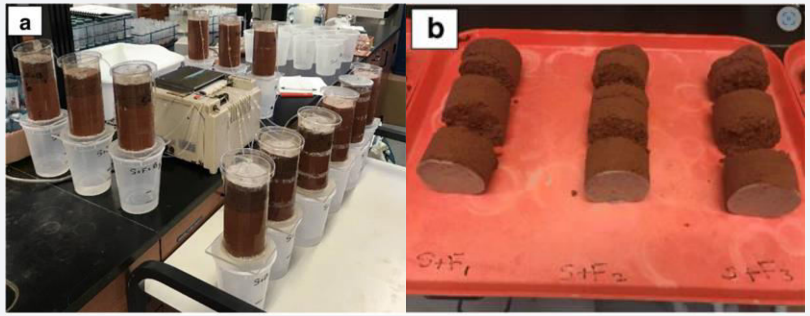
Chen J. et al., *Progress in Energy and Combustion Science*, 2022.

Determining the parameters of the governing equation for solute transport—permeability and dispersion coefficient

Permeability test → k

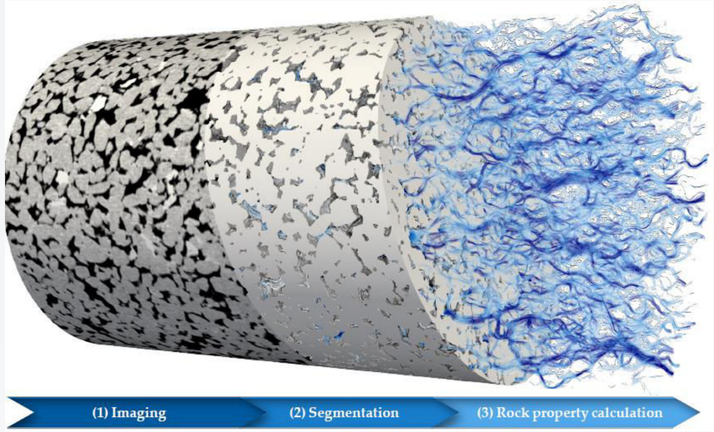


Inverse modeling from data → D

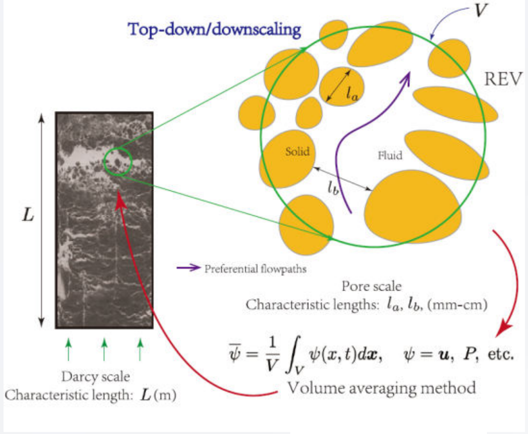


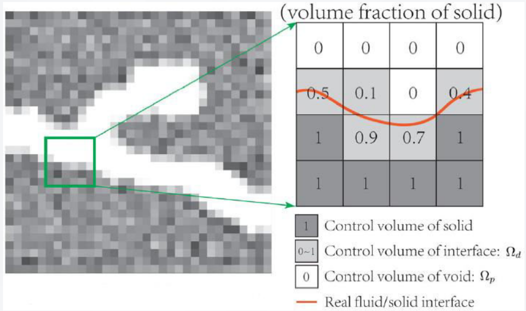
Disadvantages : high experimental costs and time-consuming processes.

Calculate *k* and D from pore-scale process



Upscaling →





Determine the parameters of the Darcy-scale model by accurately simulating pore-scale process: high computational costs

Deep learning methods for predicting permeability

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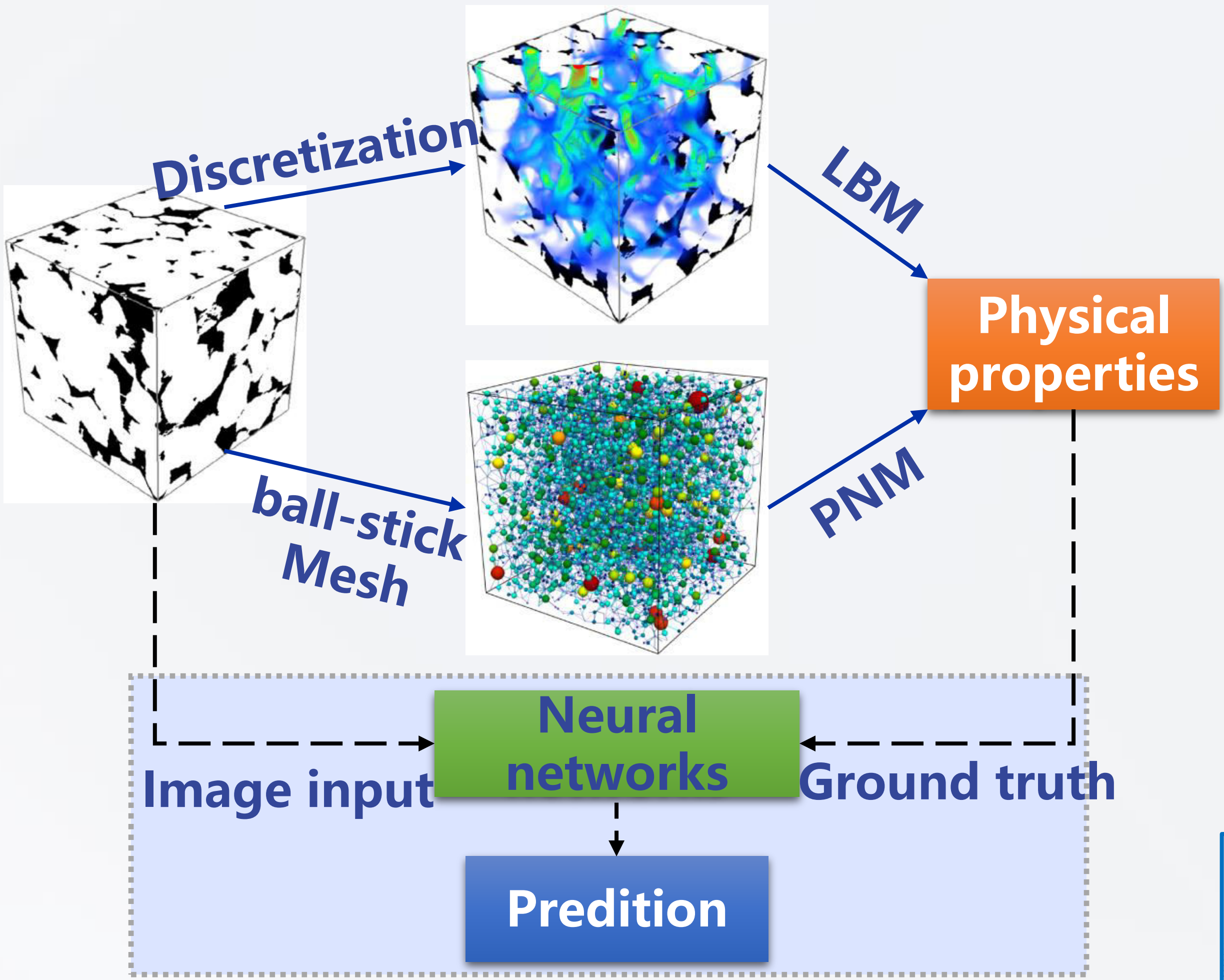
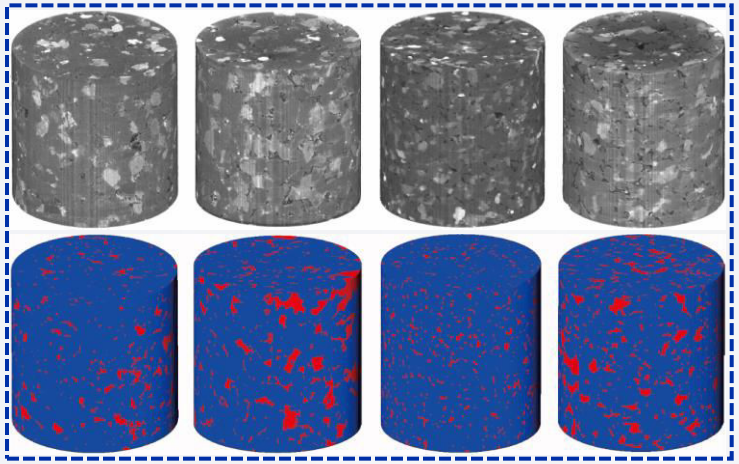
➢ **Build surrogate model based on deep learning neural networks**



✓ **Step1: A large number of 3D rock image samples**



3D reconstruction and threshold segmentation

✓ **Step 2: Determining the deep learning neural network architecture**

Processing 3D images | Regression prediction

- Convolutional Neural Networks for Computer Vision
- Vision Transformer based on self-attention mechanism
- Point cloud neural network for pore structure.

Wu C. et al., *Open Physics*, 2020. Sun H. et al., *Journal of petroleum science and engineering*, 2017.

Shortcomings of common deep learning methods.

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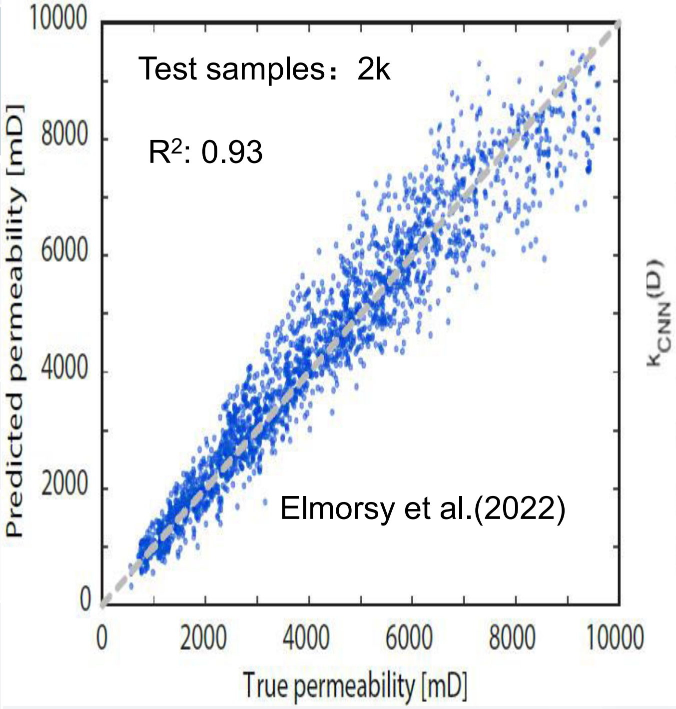
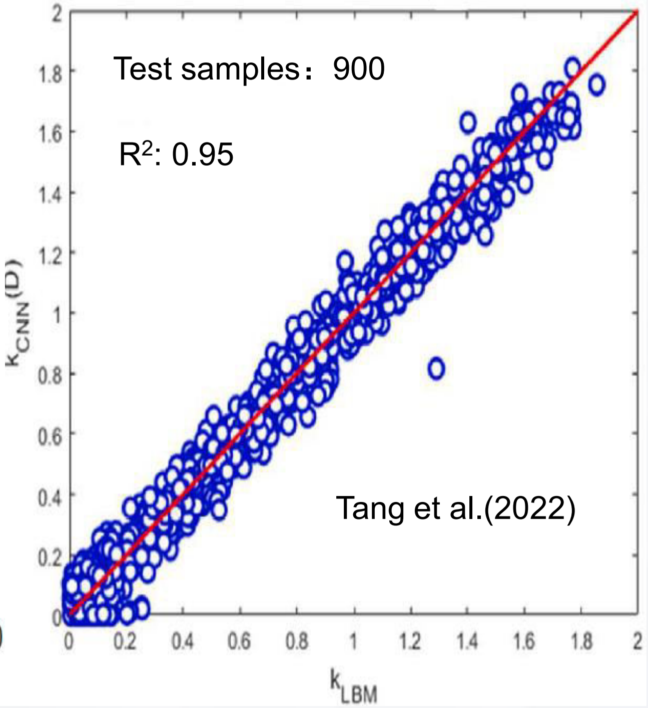
Benchmark:3D Convolutional Neural Network Prediction Results

Reference	Model	Permeability [mD]	Number of training samples	R2
Elmorsy et al.(2022)	3D CNN	200–9,600	>50k	0.95
Hong and Liu (2020)	3D CNN	10–6,000	<4k	0.92
Kamrava et al. (2020)	3D CNN	100–500	>1k	0.91
Tembely et al. (2021)	3D CNN	70–400	<1k	0.87
Alqahtani et al. (2021)	3D CNN	10–1,800	<25k	0.86

Disadvantage: Weak generalization ability





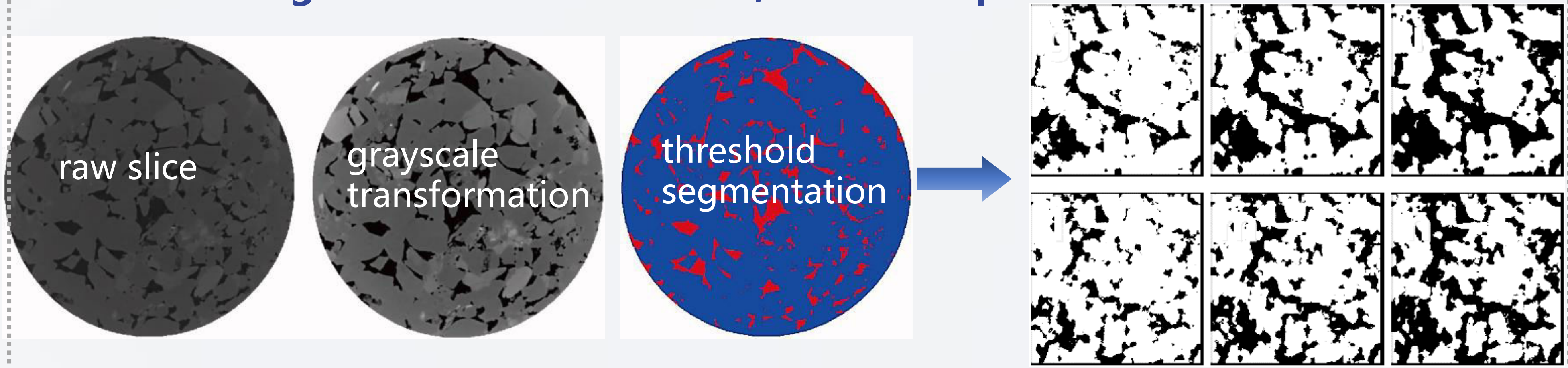
Summary of existing 3D convolutional neural network models for predicting permeability

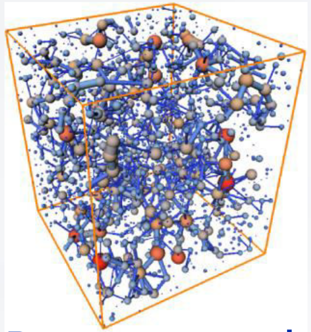
Zhang, F., et al., *Computational Materials Science*, 2021. Shah S. M. et al., *Advances in water resources*, 2016.

A new deep learning framework for predicting the permeability

➢ Generation of porous media sample sets

1. Real CT image + data enhancement， 6250 samples

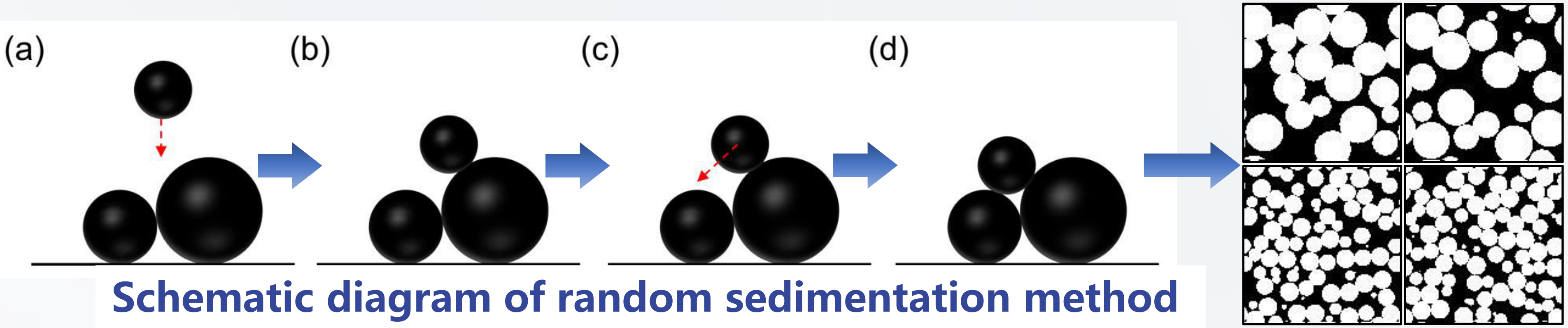




Pore network model

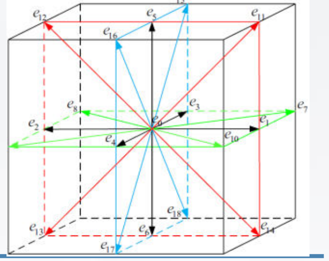
permeability k

2. Samples generated by random sedimentation， 1000 samples



Schematic diagram of random sedimentation method

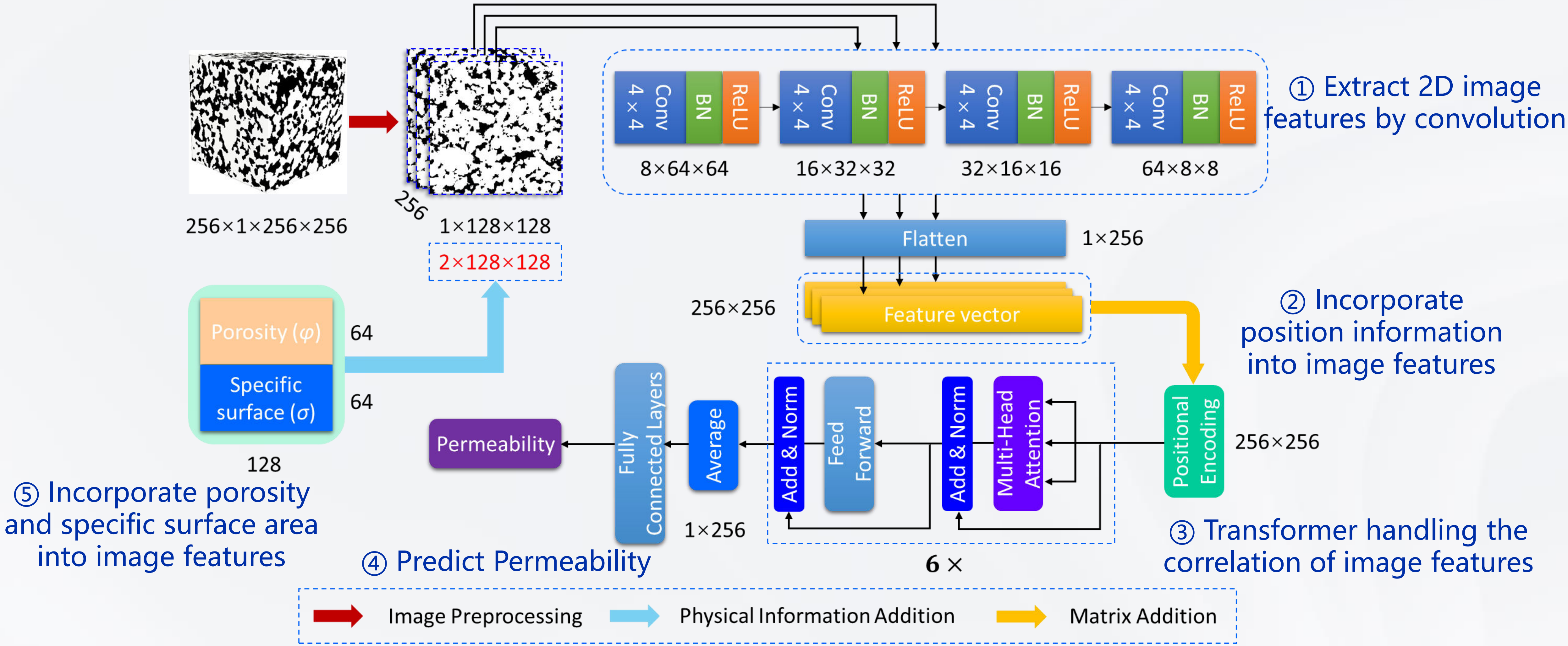
Lattice Boltzmann method



Wu Y. et al., *Journal of Hydrology*, 2019. Tian J. et al., *Engineering with Computers*, 2021. Rabbani A. et al., *Advances in Water Resources*, 2020.

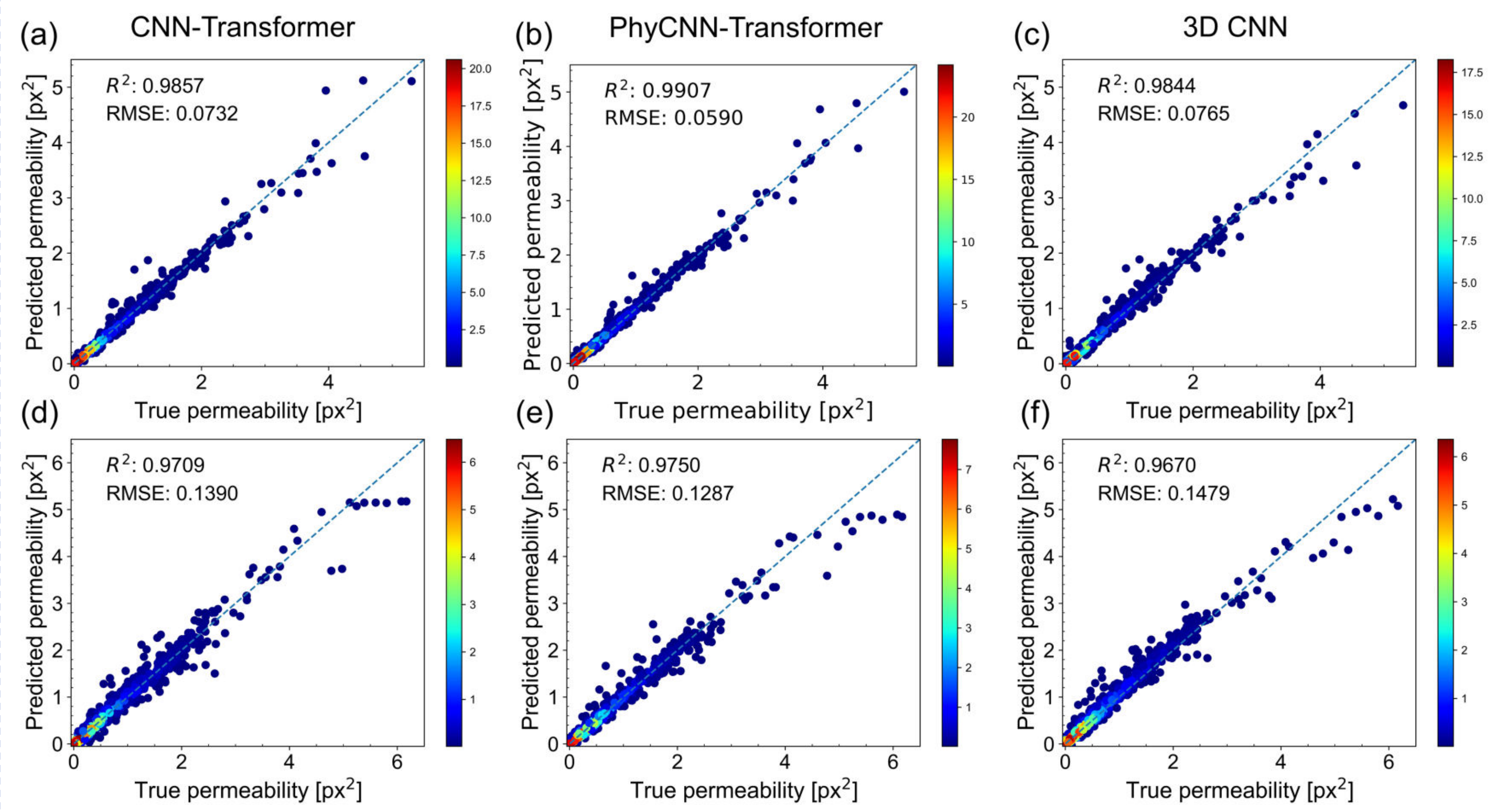
A new deep learning framework for predicting the permeability

- New neural network :CNN-Transformer combined with convolution and self-attention mechanism



A new deep learning framework for predicting the permeability

➢ New Model Prediction Results



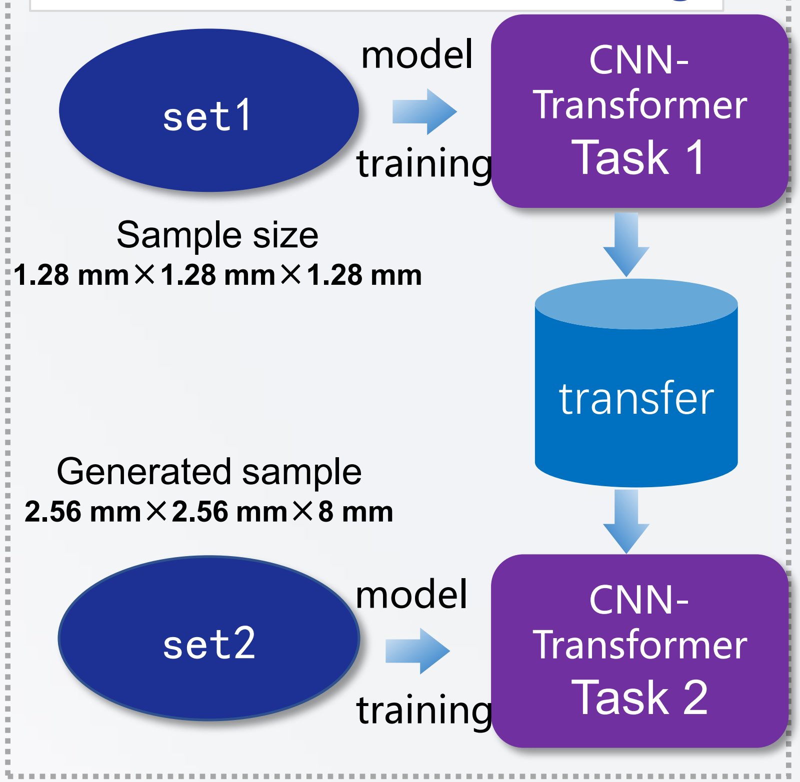
- ✓ **Prediction Performance：3D CNN < CNN-Transformer < PhyCNN-Transformer**
- ✓ **Model training parameters reduced by 57.5%**

3D CNN: 20.2 M parameters，CNN/PhyCNN-Transformer 8.59 M parameters

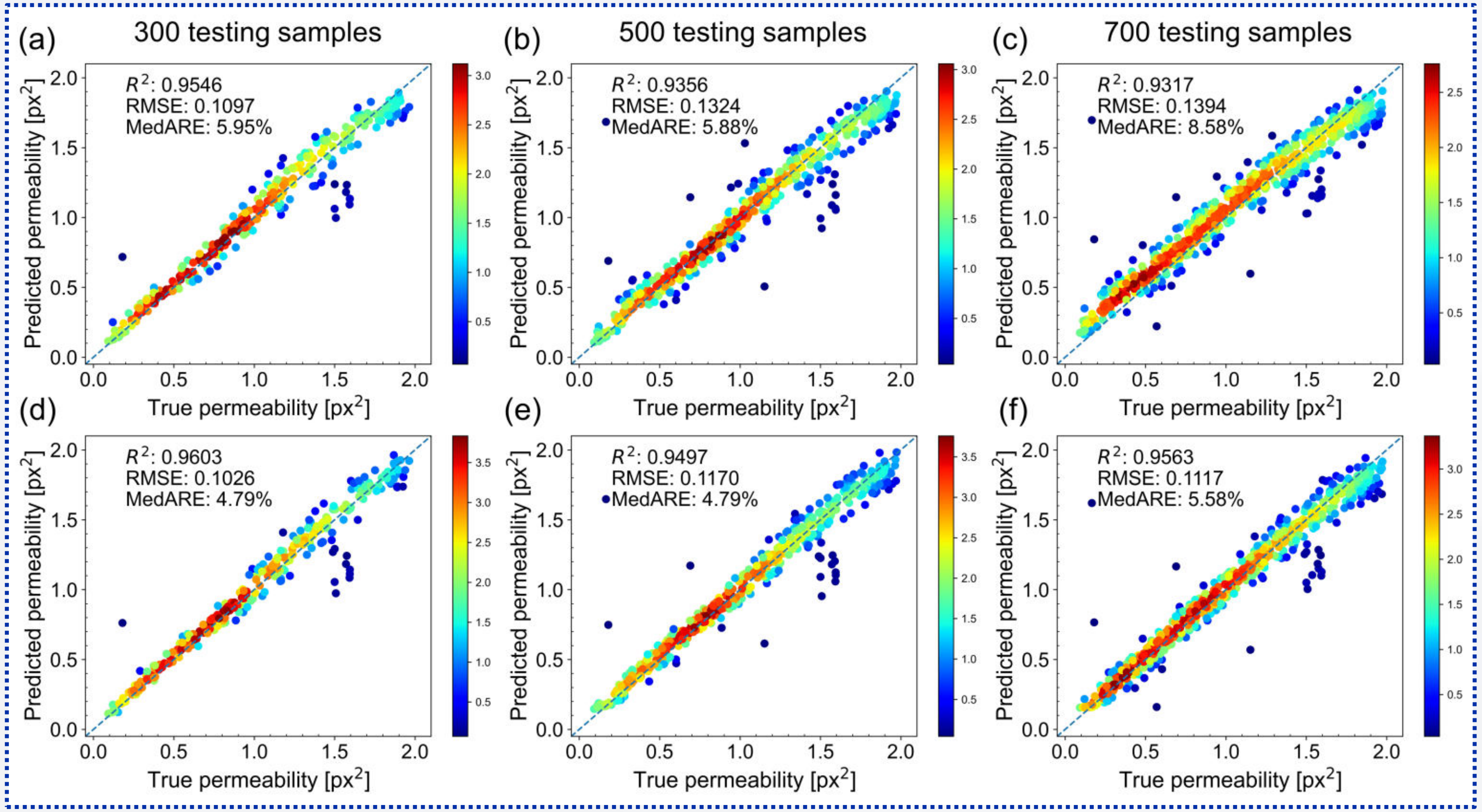
A new deep learning framework for predicting the permeability

➢ Transfer learning: accurately predicting the permeability of porous media with a small sample set

Schematic of transfer learning



Set 2
300-700 samples



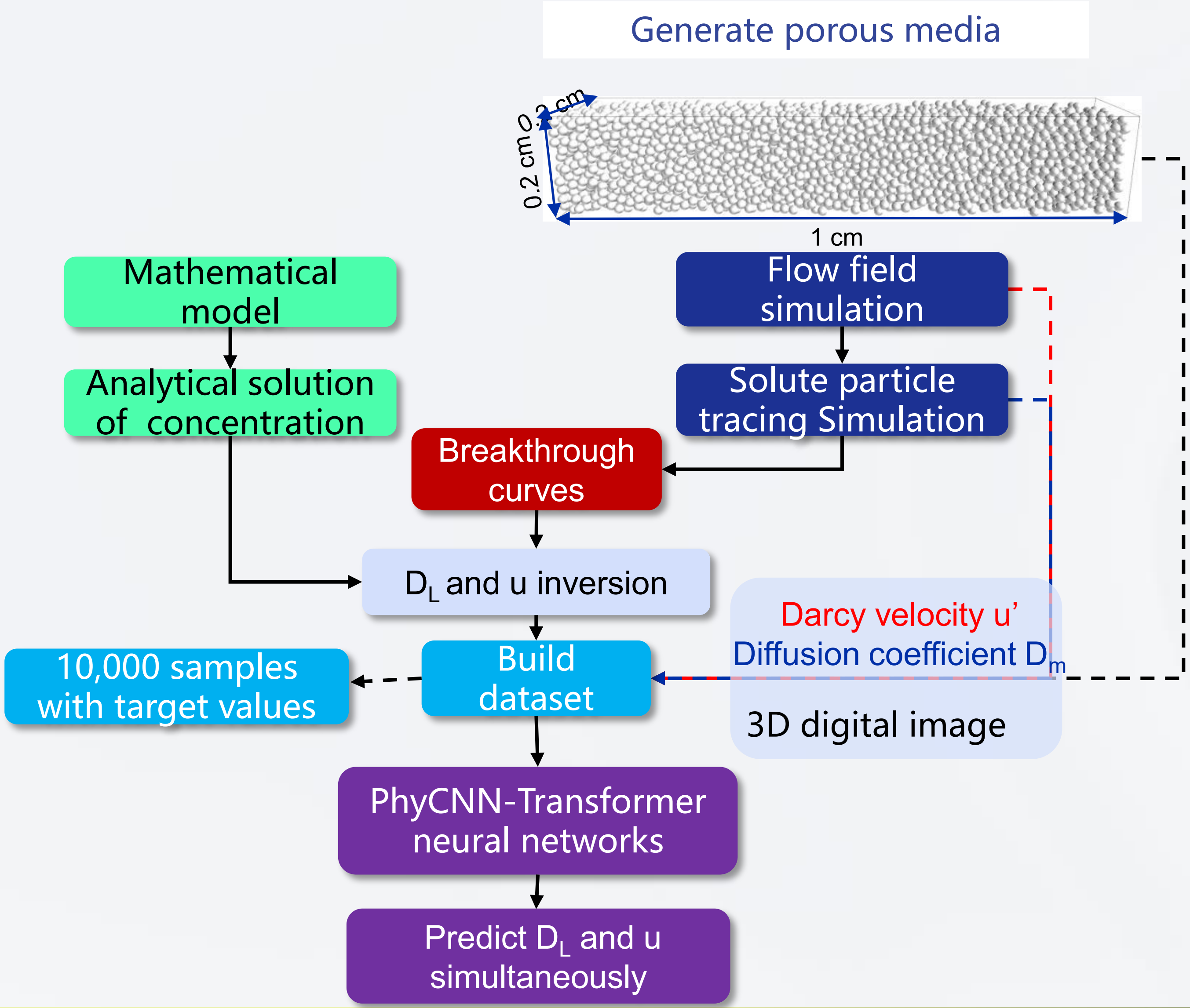
Differences between set 1 and 2:（3D CNN can not handle different sizes）

1. image size of set 1: 256×256×256; set 2: 400×128×128
2. different pore structure
3 different calculation method of permeability

- Same training sample size, PhyCNN-Transformer > CNN-Transformer

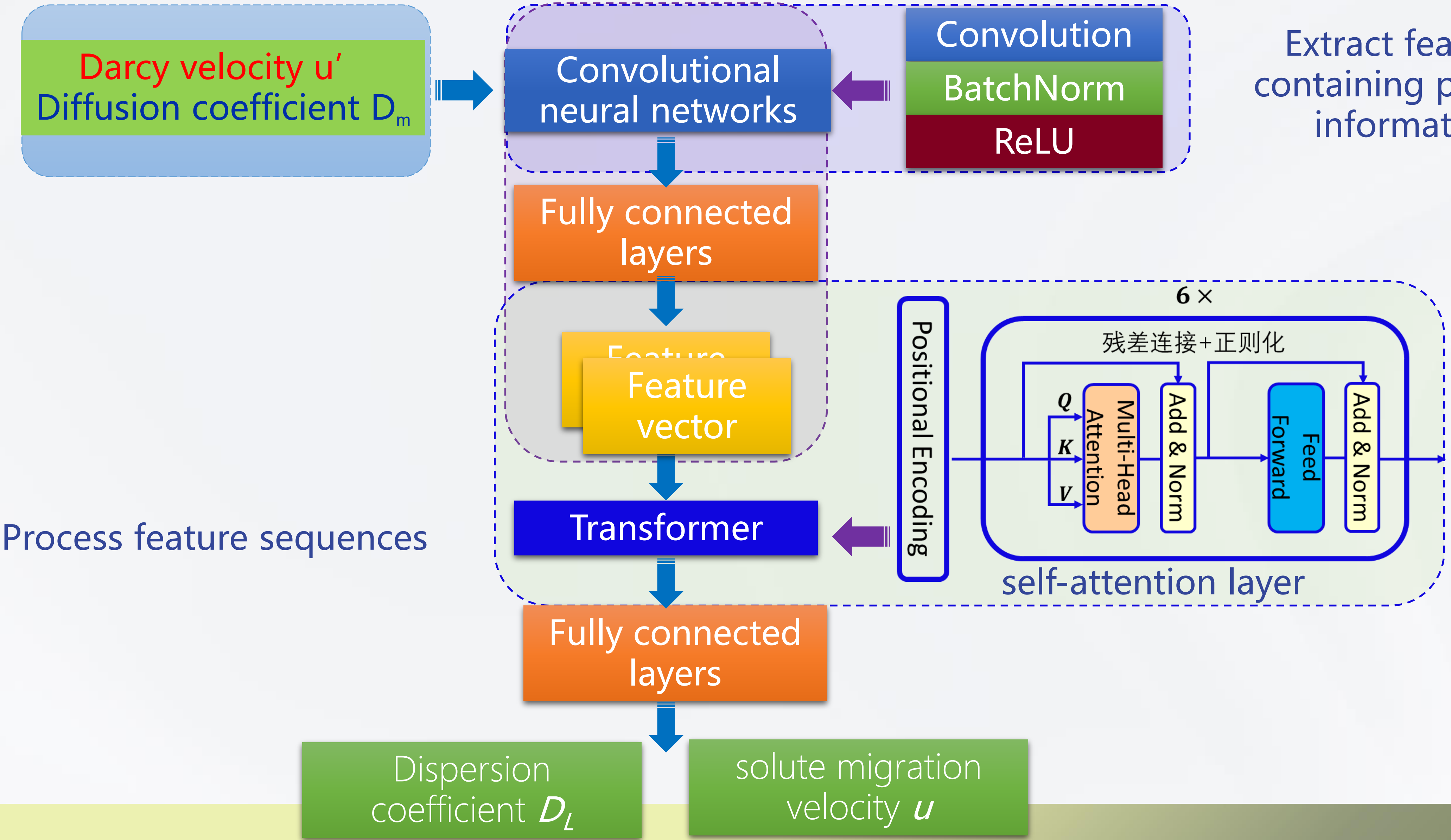
A new deep learning framework for predicting dispersion coefficient

➢ Flowchart for predicting the longitudinal dispersion coefficient



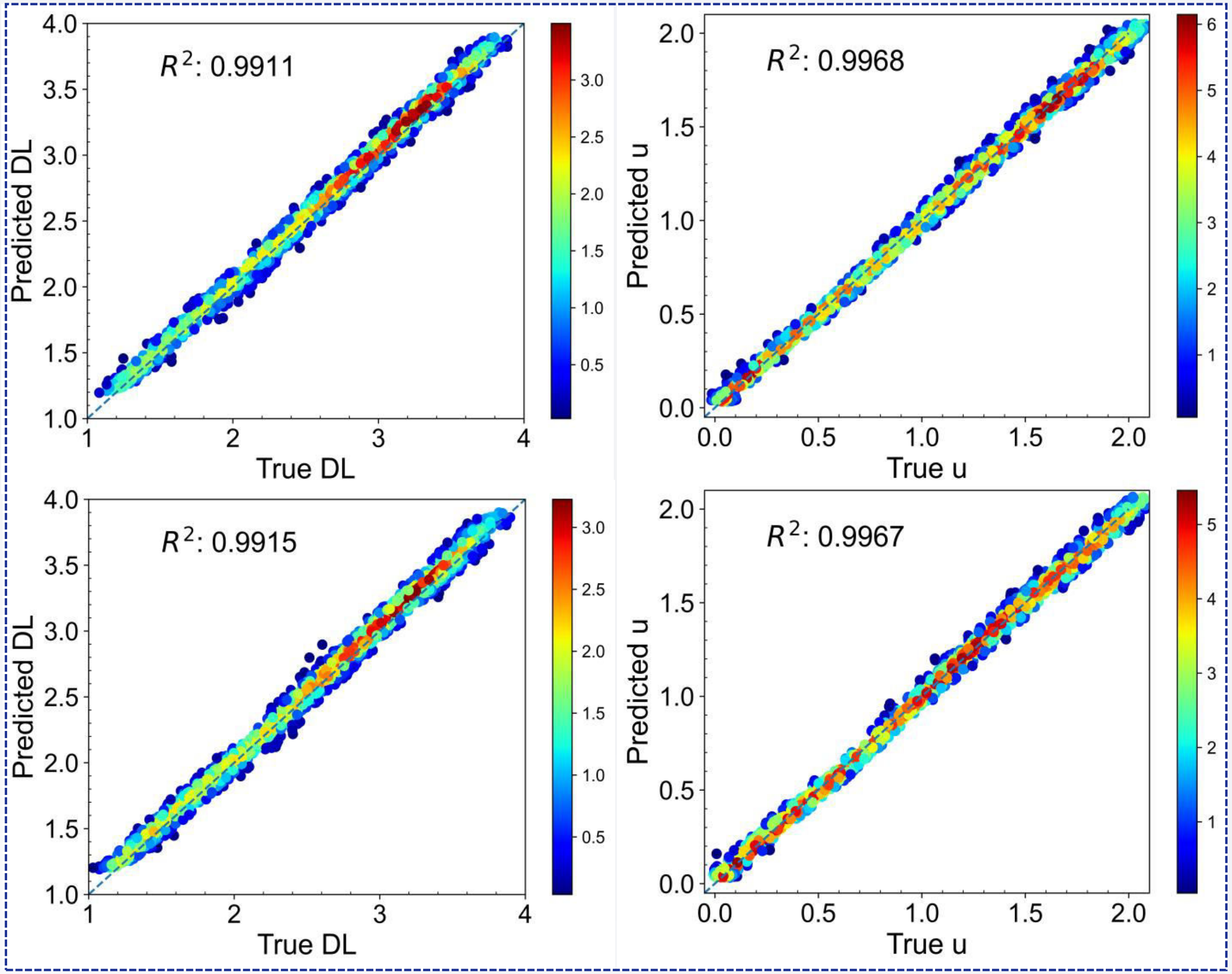
A new deep learning framework for predicting dispersion coefficient

➢ Schematic diagram of neural networks



A new deep learning framework for predicting dispersion coefficient

➢ Performance of neural networks



- ◆ Test set: 2000 samples
  D_L and *u*'s average RMSE = 0.0561

- ◆ Validation set: 1600 samples
  DL and u's average RMSE = 0.0557

Thank you!

诚耀百廿 雄创一流