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Using Machine Learning to Predict Permeability in Porous Materials

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PRESENTED BY

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Personal Background

- Pursuing Bachelor's in Mechanical Engineering with an additional major in Statistics from Carnegie Mellon University
- Worked in Professor Amir Barati Farimani's Mechanical and Artificial Intelligence Lab (MAIL) on performing molecular dynamics simulations using LAMMPS and VMD at CMU
- Future Plans: Pursuing a focus on Machine Learning and Data Science to solve Mechanical Engineering problems more efficiently

Outline

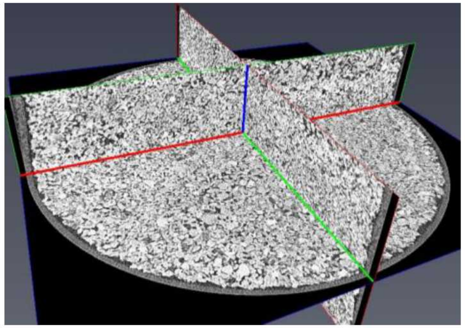
1. Introduction
2. Methodology
3. Results
4. Discussion and Future Plans

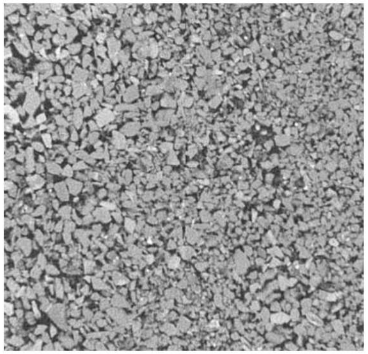
Introduction

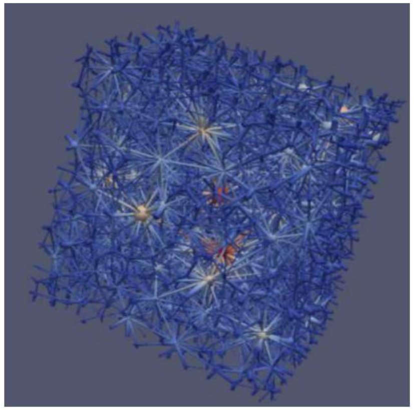
- Project: To apply and advance **machine learning (ML)** techniques to accurately predict **permeabilities** of porous materials (e.g., sandstone, carbonate rocks)

- Importance:
  - 1. Permeability is one of most important parameters to predict flow & transport processes for subsurface energy (oil, gas, thermal) recovery, filters, and underground seepage
  - 2. ML trained model can calculate permeabilities by several orders of magnitude faster than physics-based simulations
  - 3. Can be applied to other porous materials such as batteries and fuel cells

- Programs used:
  - OpenPNM - Open-source Python package of pore network models to compute permeabilities
  - Porespy - Image analysis tool used to convert Micro-CT images into pore networks using a graph network system

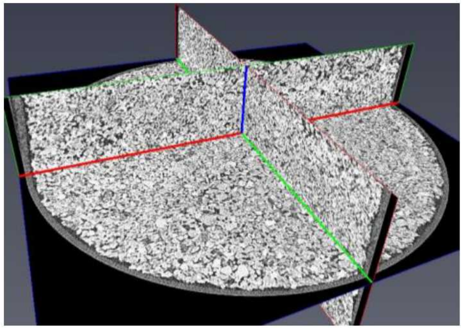


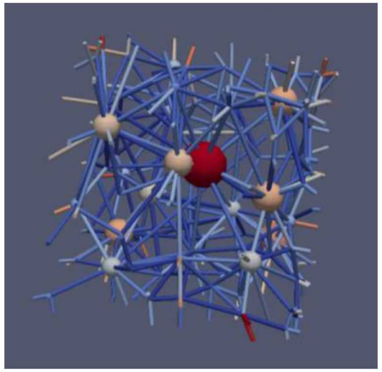




What is a Pore Network Model?

- Pore Network Model (PNM): Approach of modeling void space in porous material as pores and throats for the purpose of **simulating transport** in **porous materials**





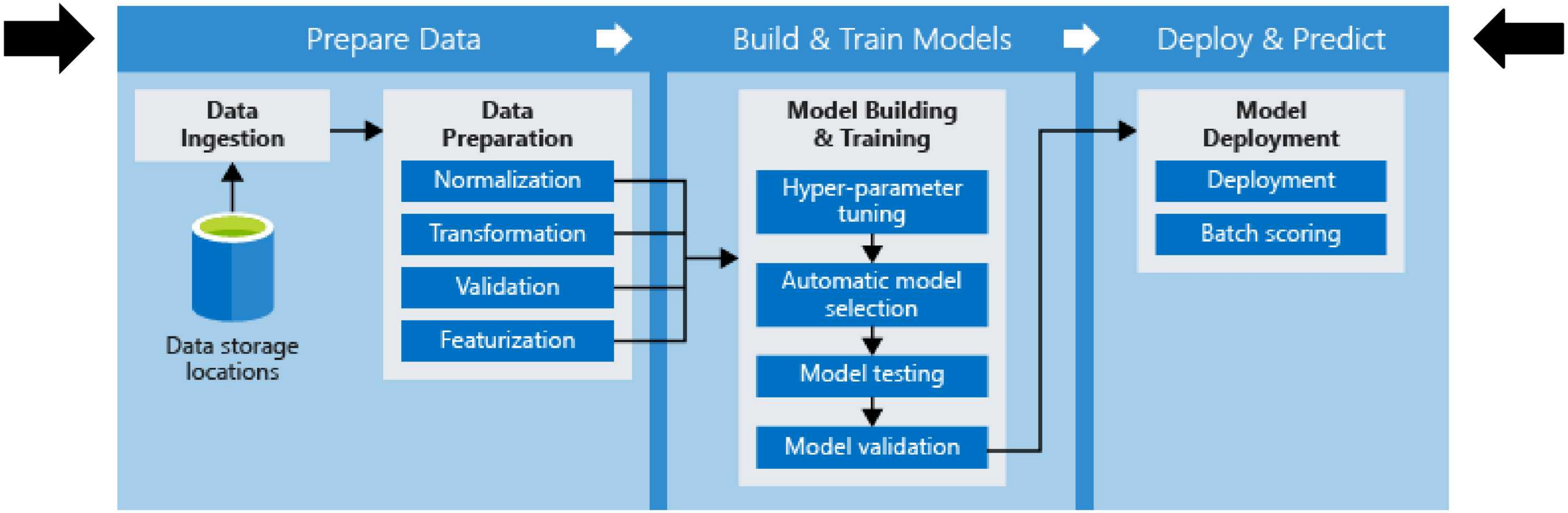
Programs: We use OpenPNM and Porespy to create pore network models

Applications?

- Multiphase flow in Proton-Exchange Membrane (PEM) fuel cells
- Electrodes used in batteries
- Geological formations of interest such as oil recovery and contaminant transport

What is Machine Learning?

- Machine learning is **data analysis** method based on the idea that systems can **learn from data** and **make decisions**



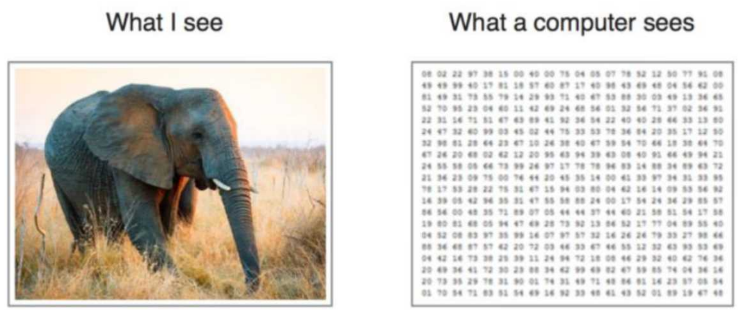
https://docs.microsoft.com/en-us/azure/machine-learning/service/concept-ml-pipelines

- Apps: TV show and movie recommendations, Virtual Assistants, Map Services, Email Spam Filtering

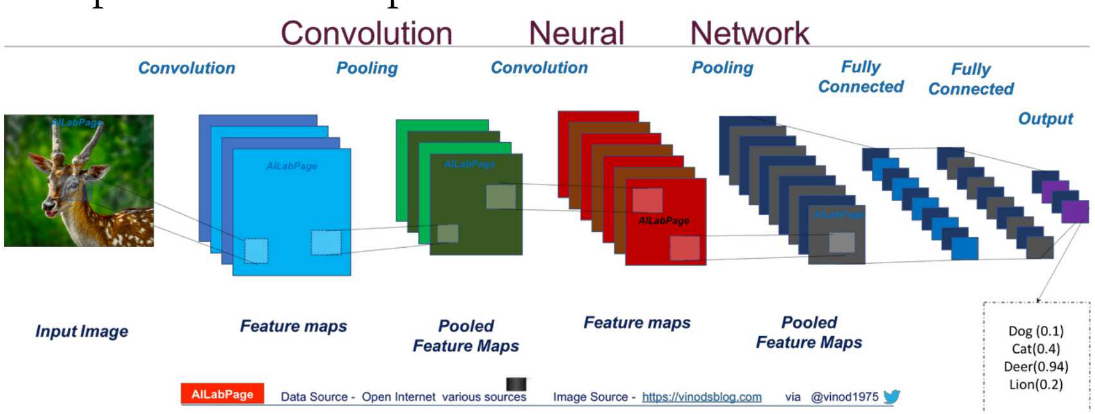
Description of the methodology

What is a Convolutional Neural Network?

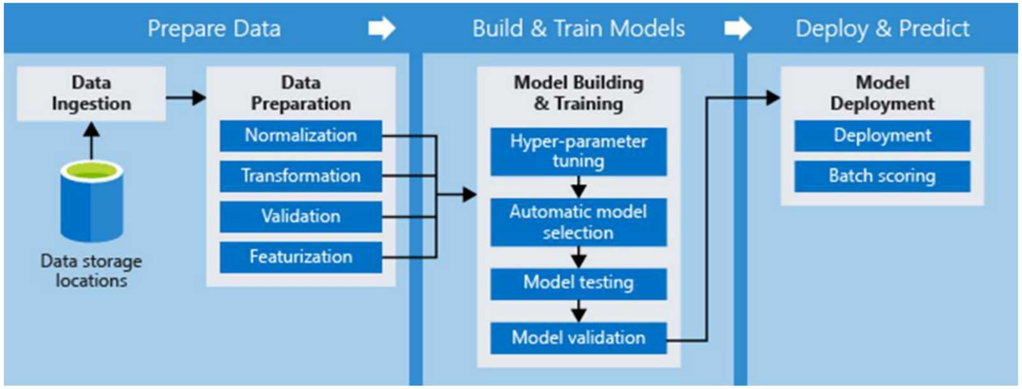
- Convolutional Neural Network (CNN) is a class of deep neural networks commonly used in image recognition and image processing



- **How a human evaluates:** trunk and large ears -> elephant
- **How a computer evaluates:**
  - Uses a series of convolutional, pooling, and fully connected layers to filter characteristics
  - Curves -> eyes, ear, trunk -> head -> entire body -> looks through its database -> makes an assumption it is an elephant



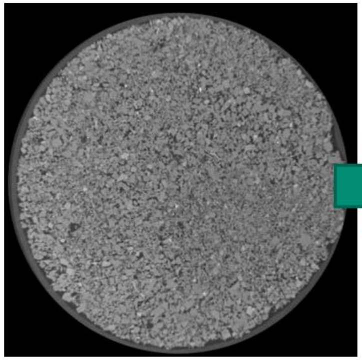
Description of the methodology (cont…)



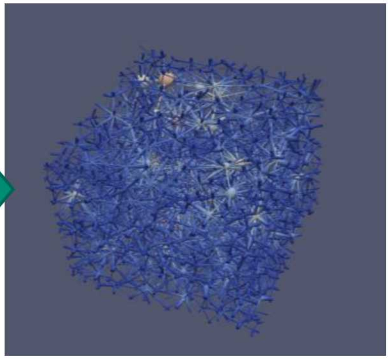
https://docs.microsoft.com/en-us/azure/machine-learning/service/concept-ml-pipelines

Prepare Data

1. **Micro-CT image to OpenPNM:** Convert 3-D Micro-CT images of sandstone and chalk into OpenPNM pore network models
2. **Building Database:** Build a database of permeabilities calculated from many (~1-10K) subsets of 3D images using OpenPNM simulations



1. Micro-CT image to OpenPNM



2. Building Database

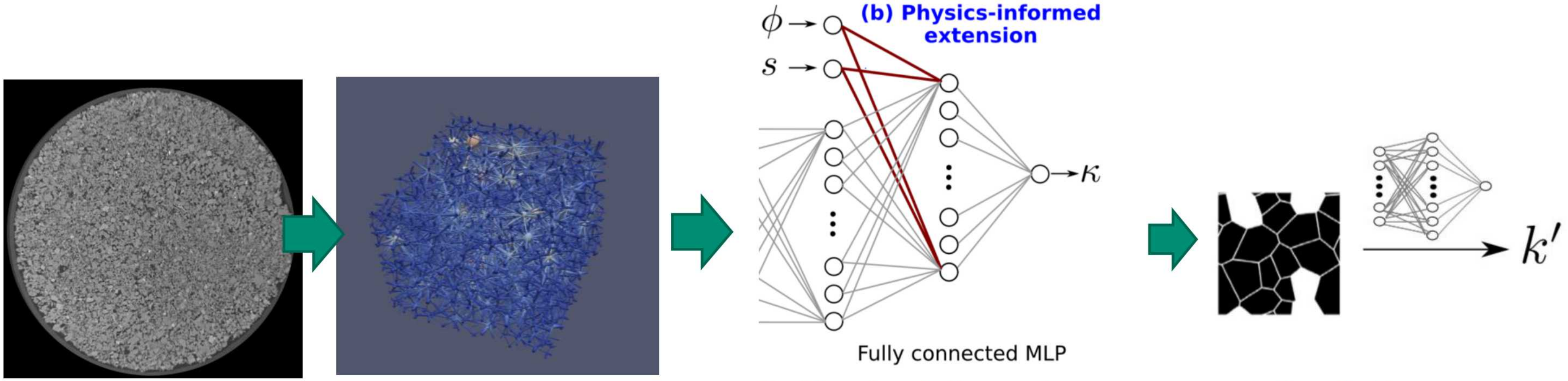
Description of the methodology (cont…)

Build & Train Models

3. **Physics-informed Convolutional Neural Network:** Use the data from the generated database to train a physics-informed Convolutional Neural Network
   - Input: Micro-CT images, Physics-based key physical properties (e.g., porosity, surface area, connectivity)
   - Output: Permeability

Deploy and Predict

4. **Prediction:** The trained CNN model from step 3 will then be used to predict permeability of new images that are not in the training database



1. Micro-CT image to OpenPNM

2. Building Database

3. Physics-informed Convolutional Neural Network

4. Prediction

Wu et al. (2018)

Results

So far I have created a database of the permeabilities and porosities of various dimensions and locations (e.g [X = [790,890], Y = [790,890], Z = [0, 100])

	A	B	C	D	E	F	G	H	I	J	K
1	Xi	Xf	Yi	Yf	Qxx	Qyy	Qzz	Kxx	Kyy	Kzz	Porosity
2	(100	200	600	700	2.48E-05	1.67E-06	2.27E-05	3.48E-11	2.35E-12	1.40E-10	0.31388708133971294)
3	(100	200	700	800	2.72E-05	3.49E-06	2.79E-05	3.82E-11	4.90E-12	1.71E-10	0.2953023923444976)
4	(100	200	800	900	2.57E-05	2.36E-06	2.59E-05	3.62E-11	3.32E-12	1.59E-10	0.2993578947368421)
5	(100	200	900	1000	3.19E-05	4.16E-06	3.13E-05	4.48E-11	5.85E-12	1.92E-10	0.32214306220095695)
6	(100	200	1000	1100	3.49E-05	8.21E-06	3.32E-05	4.90E-11	1.15E-11	2.04E-10	0.34490382775119616)
7	(200	300	400	500	1.42E-05	2.03E-06	1.58E-05	2.00E-11	2.85E-12	9.68E-11	0.2884234449760766)
8	(200	300	500	600	2.03E-05	2.25E-06	2.36E-05	2.86E-11	3.17E-12	1.45E-10	0.29389521531100476)
9	(200	300	600	700	2.69E-05	4.38E-06	2.79E-05	3.79E-11	6.15E-12	1.71E-10	0.3074971291866029)
10	(200	300	700	800	1.88E-05	3.46E-06	2.58E-05	2.64E-11	4.87E-12	1.59E-10	0.31183588516746413)
11	(200	300	800	900	2.53E-05	2.31E-06	2.95E-05	3.55E-11	3.25E-12	1.81E-10	0.29940334928229667)
12	(200	300	900	1000	3.01E-05	1.82E-06	2.59E-05	4.23E-11	2.56E-12	1.59E-10	0.31598373205741626)
13	(200	300	1000	1100	3.35E-05	1.48E-06	1.80E-05	4.71E-11	2.07E-12	1.11E-10	0.30603492822966505)
14	(200	300	1100	1200	1.98E-05	6.00E-08	2.05E-05	2.78E-11	8.43E-14	1.26E-10	0.28536076555023926)
15	(300	400	300	400	8.39E-06	1.05E-07	7.98E-06	1.18E-11	1.47E-13	4.90E-11	0.24285454545454546)
16	(300	400	400	500	1.82E-05	1.52E-06	1.07E-05	2.56E-11	2.13E-12	6.56E-11	0.2906354066985646)
17	(300	400	500	600	3.63E-05	5.09E-06	3.49E-05	5.10E-11	7.16E-12	2.14E-10	0.3328732057416268)
18	(300	400	600	700	3.06E-05	4.60E-06	3.42E-05	4.30E-11	6.46E-12	2.10E-10	0.34153014354066985)
19	(300	400	700	800	2.22E-05	6.13E-06	2.28E-05	3.12E-11	8.63E-12	1.40E-10	0.3092535885167464)
20	(300	400	800	900	3.23E-05	4.09E-06	3.14E-05	4.54E-11	5.75E-12	1.93E-10	0.32602631578947366)
21	(300	400	900	1000	4.04E-05	1.87E-06	3.88E-05	5.68E-11	2.62E-12	2.39E-10	0.32635167464114834)
22	(300	400	1000	1100	3.74E-05	4.44E-06	4.60E-05	5.26E-11	6.24E-12	2.83E-10	0.34013014354066984)
23	(300	400	1100	1200	2.50E-05	2.21E-06	2.80E-05	3.51E-11	3.10E-12	1.72E-10	0.3084043062200957)
24	(300	400	1200	1300	1.42E-05	7.99E-07	1.75E-05	1.99E-11	1.12E-12	1.07E-10	0.2826727272727273)
25	(300	400	1300	1400	8.27E-06	3.96E-07	1.39E-05	1.16E-11	5.57E-13	8.52E-11	0.27734593301435406)
26	(400	500	200	300	1.03E-05	5.62E-07	1.05E-05	1.44E-11	7.90E-13	6.45E-11	0.24569521531100477)
27	(400	500	300	400	2.10E-05	1.61E-06	2.01E-05	2.96E-11	2.26E-12	1.24E-10	0.28184354066985645)
28	(400	500	400	500	1.63E-05	1.32E-06	1.62E-05	2.29E-11	1.85E-12	9.94E-11	0.2920315789473684)
29	(400	500	500	600	3.73E-05	2.39E-06	2.97E-05	5.25E-11	3.36E-12	1.82E-10	0.3178712918660287)
30	(400	500	600	700	2.97E-05	4.79E-06	3.05E-05	4.17E-11	6.74E-12	1.87E-10	0.32728564593301435)
31	(400	500	700	800	2.99E-05	1.44E-06	2.47E-05	4.20E-11	2.02E-12	1.52E-10	0.3306492822966507)
32	(400	500	800	900	3.65E-05	4.02E-06	4.19E-05	5.13E-11	5.66E-12	2.57E-10	0.35093014354066987)
33	(400	500	900	1000	4.06E-05	3.44E-06	4.11E-05	5.71E-11	4.83E-12	2.52E-10	0.3388019138755981)
34	(400	500	1000	1100	3.97E-05	2.69E-06	4.16E-05	5.58E-11	3.79E-12	2.56E-10	0.3328535885167464)
35	(400	500	1100	1200	3.69E-05	1.55E-06	3.00E-05	5.19E-11	2.18E-12	1.85E-10	0.32792775119617223)
36	(400	500	1200	1300	2.42E-05	3.01E-07	2.78E-05	3.40E-11	4.24E-13	1.71E-10	0.32558325358851675)
37	(400	500	1300	1400	1.90E-05	7.48E-07	1.78E-05	2.67E-11	1.05E-12	1.10E-10	0.29650287081339716)
38	(500	600	200	300	1.74E-05	5.05E-07	1.01E-05	2.45E-11	7.10E-13	6.20E-11	0.2585641148325359)

Next, we will train a Convolutional Neural Network using this data with the goal of accurately predicting permeability of new porous materials

Results

Expectations:

- Will have successful performance with CNNs
- Physics-informed CNN will perform better than regular CNNs
- Computational cost and time spent will be at least three orders of magnitude lower than OpenPNM simulations
- If successful, CNN tells us that pore geometry is a critical prerequisite of good prediction

Limitations:

- CNNs are computationally expensive

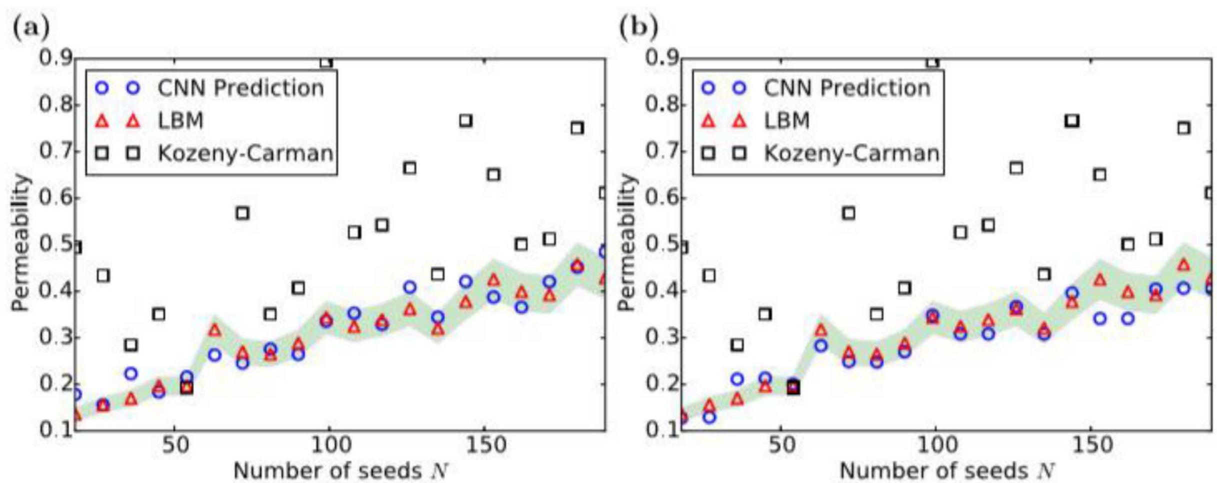


Fig. 6. (Color online) Prediction of permeability for case 2 by using (a) the regular CNN and (b) the physics-informed CNN.

Wu et al. (2018)

Discussion and Future Plans

- First apply CNN to 2D images, then apply to 3D images
  - This will be computationally expensive, especially for a 1680x1680 pixel image
  - Much more coefficients and training data needed
- Optimize computation cost and efficiency of performing 3D CNNs
- Include other geometric properties such as chord length to improve predictions
- Use the model to predict permeabilities of other porous materials such as soil and fuel cells as long as they are governed by geometry

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