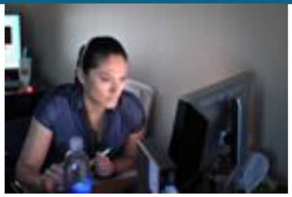
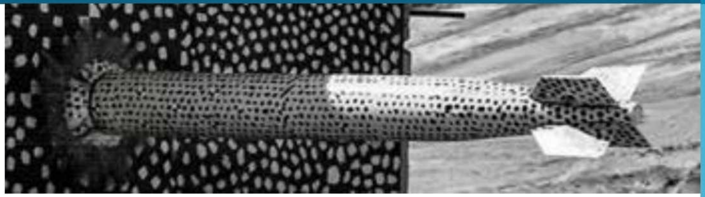
SAND2019-15137C

Physics-informed machine learning of permeability estimation and reactive transport in porous media





Hongkyu Yoon

Sandia National Laboratories

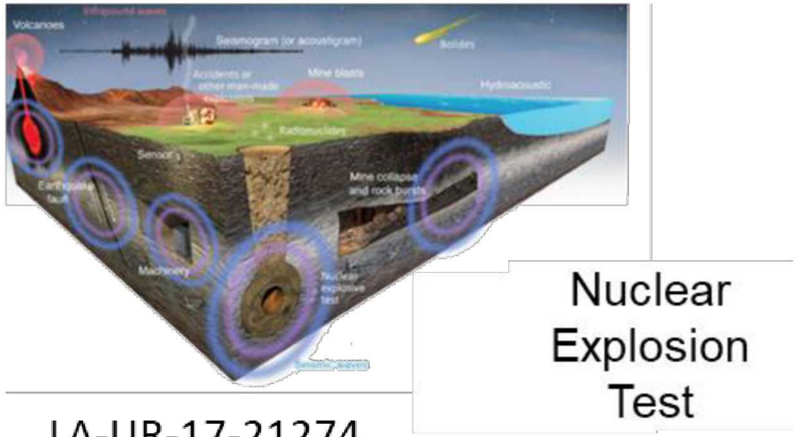
This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories.

Motivation: National Security

- **Multiscale flow, transport, and mechanical deformation** in fractured/porous media
  - Key processes to many security systems: monitoring of nuclear explosion test, subsurface energy resources recovery, and nuclear waste disposal
  - Path-dominant and discontinuous features of fractured media pose significant challenges to understanding and control of physical mechanisms underlying complex behavior in fractured and deformable media
  - Complex, multiscale, multiphysics processes
  - Standard simulation tools lack important physics and coupling, and are too expensive and not flexible

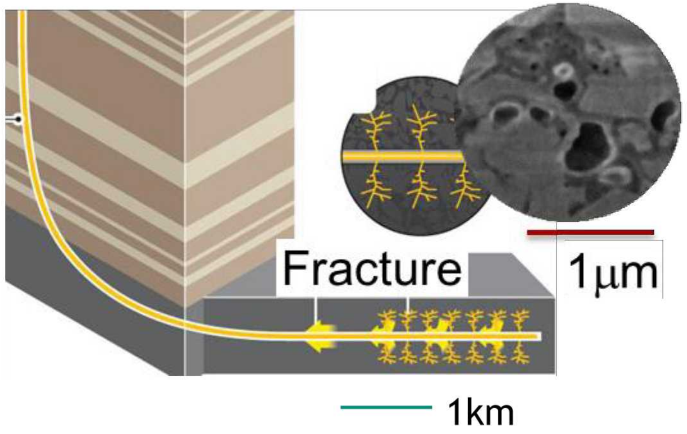
Multiscale, Multiphysics, Big/heterogeneous Data

(Sub-)surface Monitoring

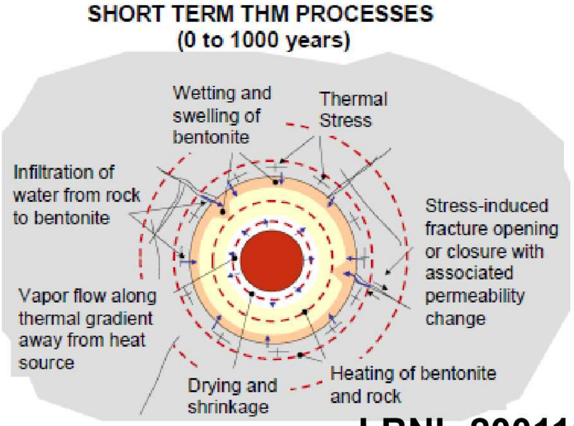


LA-UR-17-21274

Subsurface Energy Security



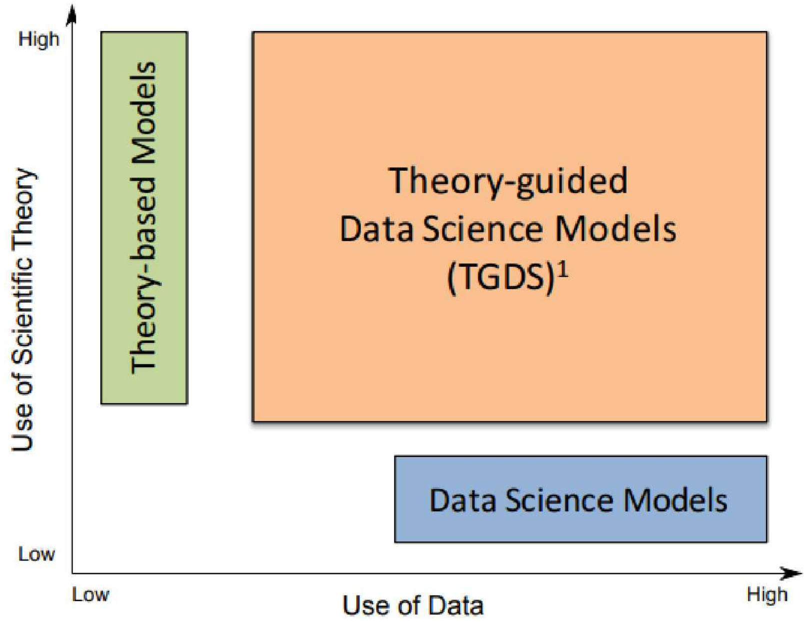
Nuclear Waste Storage



LBNL-2001168

Physics-Informed Machine Learning

- Physics-based ML can overcome the shortcomings of traditional ML methods where data-driven models have faltered beyond the data & physical conditions for training and validation
- Physical constraints, theoretical equations, and relations can be incorporated for data-driven model (e.g., trained model)
- There are many ways to incorporate these principles, but these have not been thoroughly investigated yet
- “This computational technique is transforming science, but physics may yet hold the key to explaining why” (Buchanan, Nature Physics, 2019)

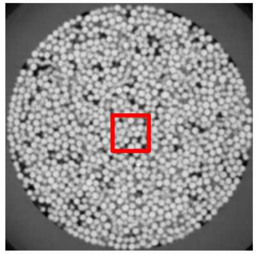


Karpatne et al. “Theory-guided data science: A new paradigm for scientific discovery,” TKDE 2017

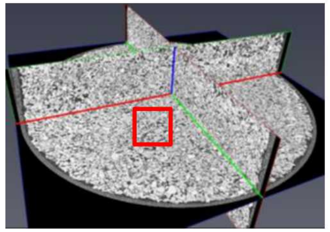
DOE BRN report 2018

Pore Network Systems

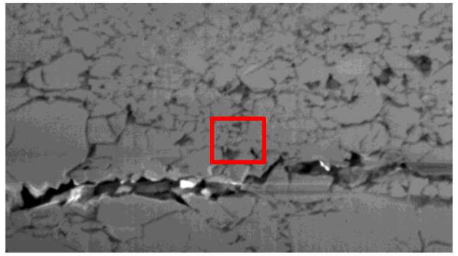
Glass bead pack (1”)



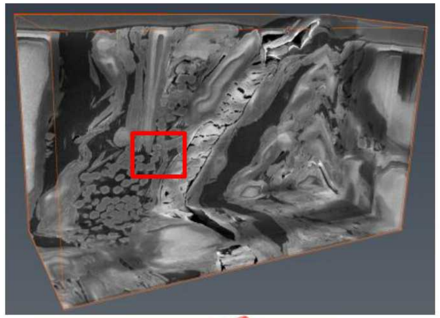
Sandstone (1”)



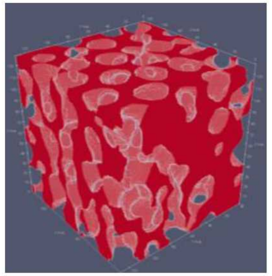
Chalk (10 microns)

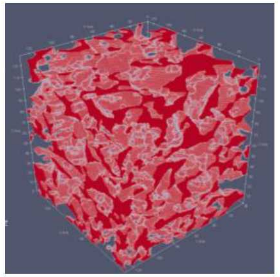


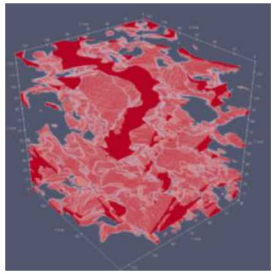
Shale (~1 micron)

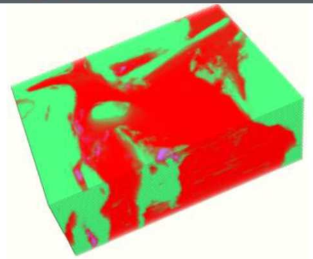


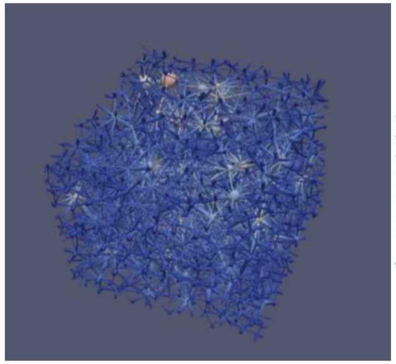
Binary images











PN from microCT image

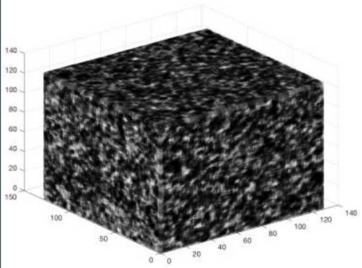
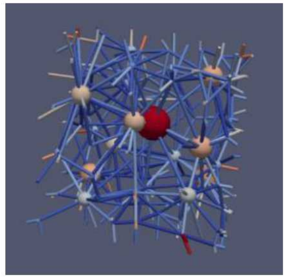
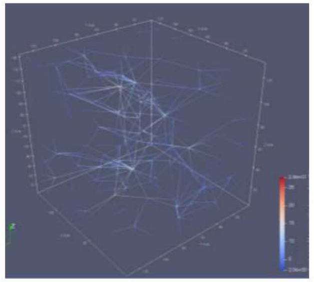


Image generated with GAN



PN from microCT image

Image generated with DCGAN

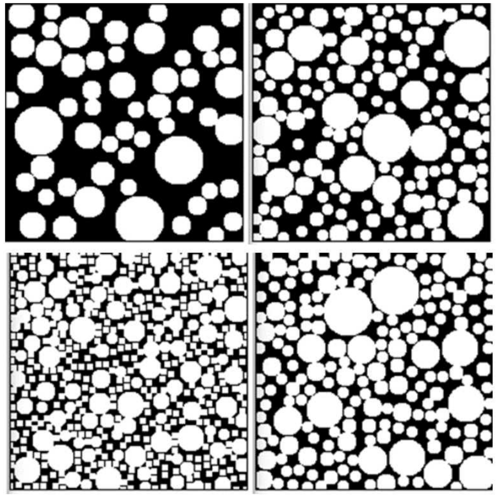


PN from FIB-SEM image

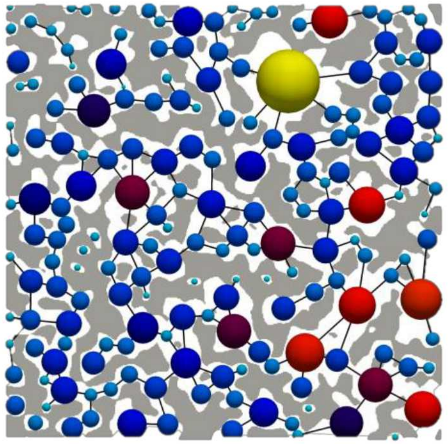
Related posters: H41G-1754, H51I-1595

Images to Pore Network System

1. Image generation (Sphere packing or machine learning methods)
2. Pore network characterization (porosity, surface area, permeability using Open source Porespy/OpenPNM or commercial PerGEOS)
3. Normalization of data

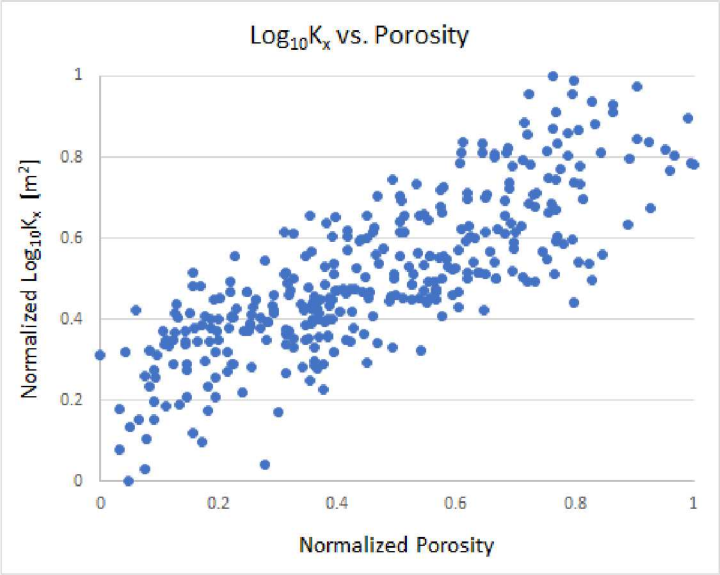


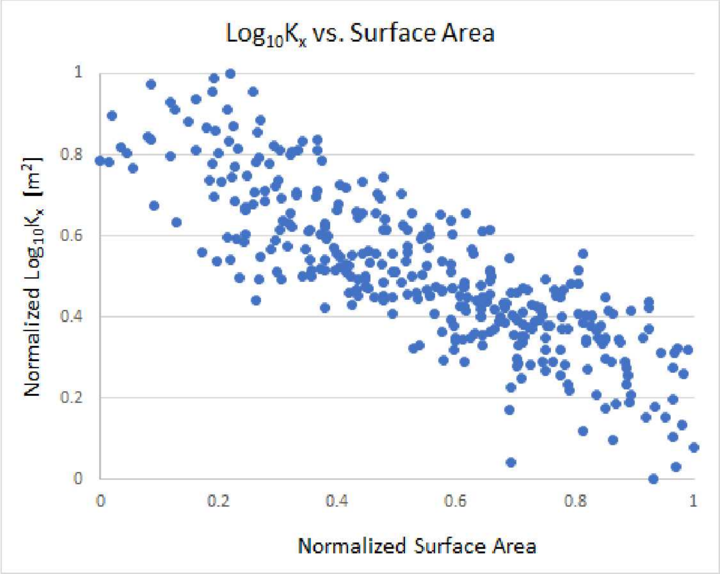
2D Sphere packing



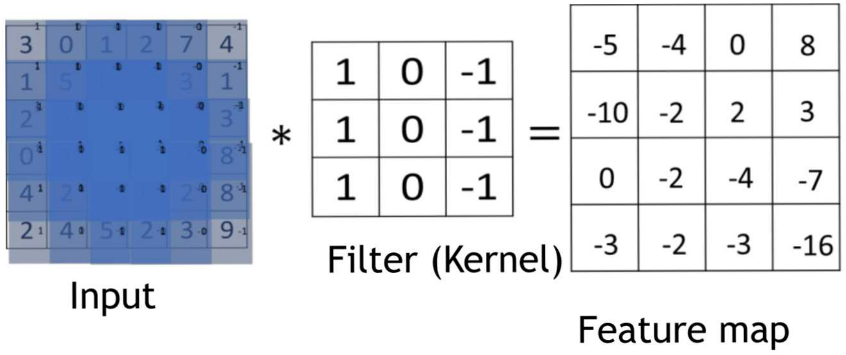
Pore Network Construction

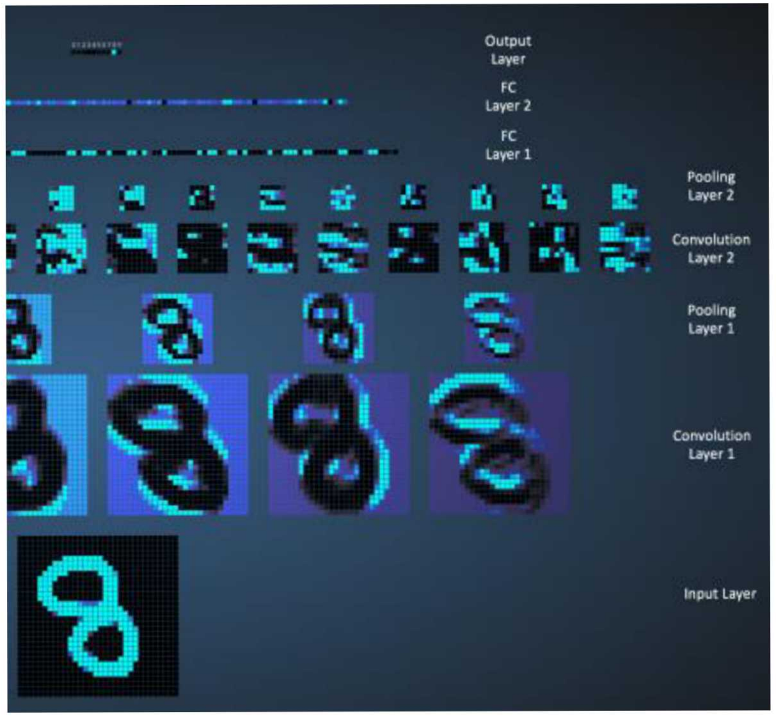
Step 3

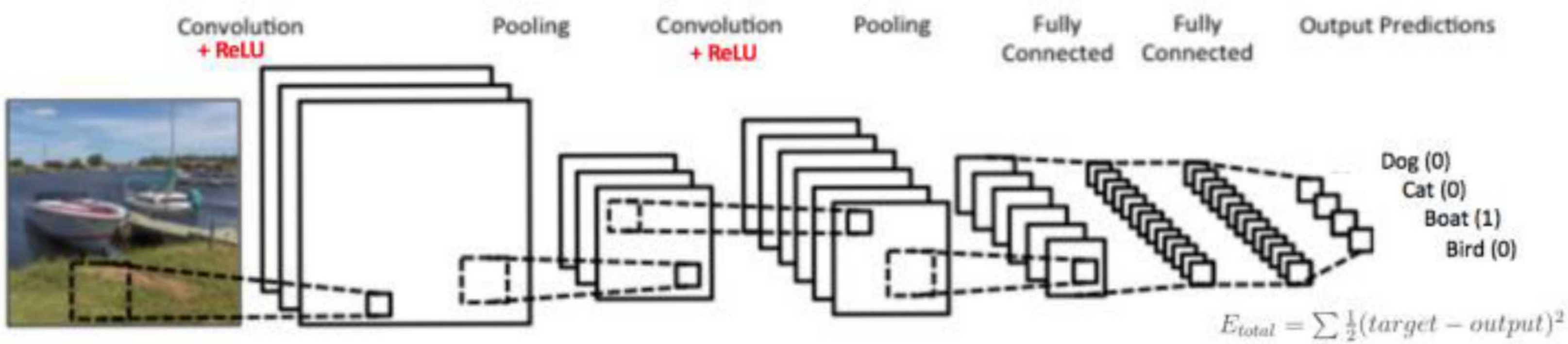




Convolutional Neural Network



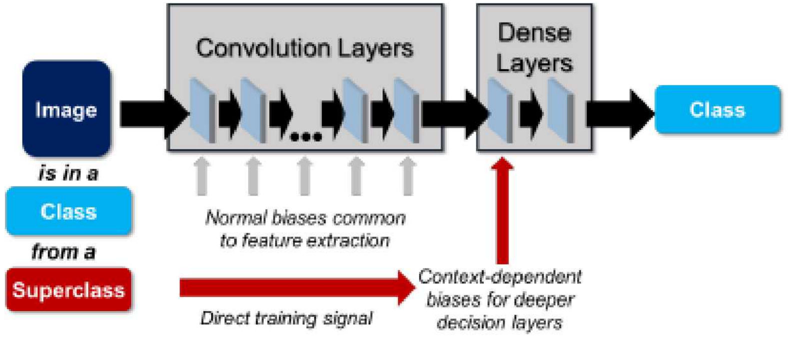




- Convolution + Pooling layers act as Feature Extractors from the input image
- Fully Connected layer acts as a classifier

http://cs231n.github.io/convolutional-networks/
https://ujjwalkarn.me/2016/08/11/intuitive-explanation-convnets/

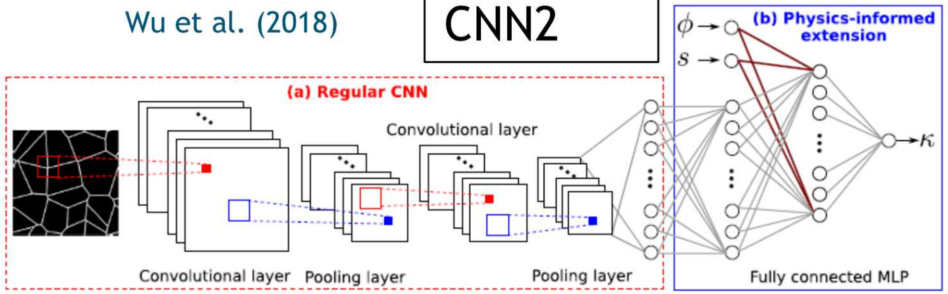
Physics-Informed ML for permeability prediction

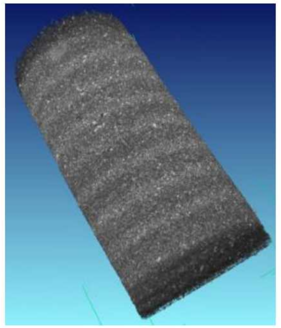


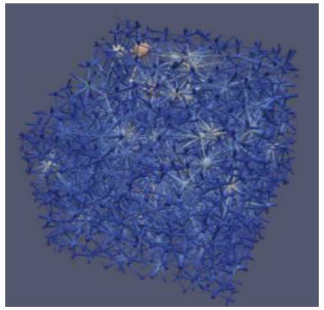
Aimone et al., 2018

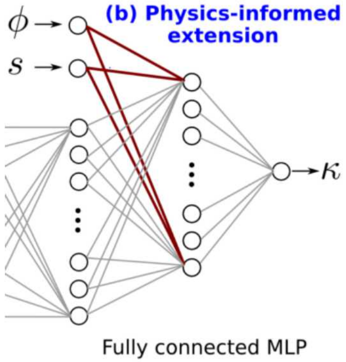
Wu et al. (2018)

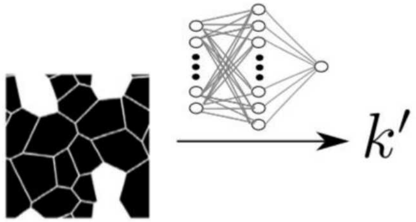
Case: CNN2











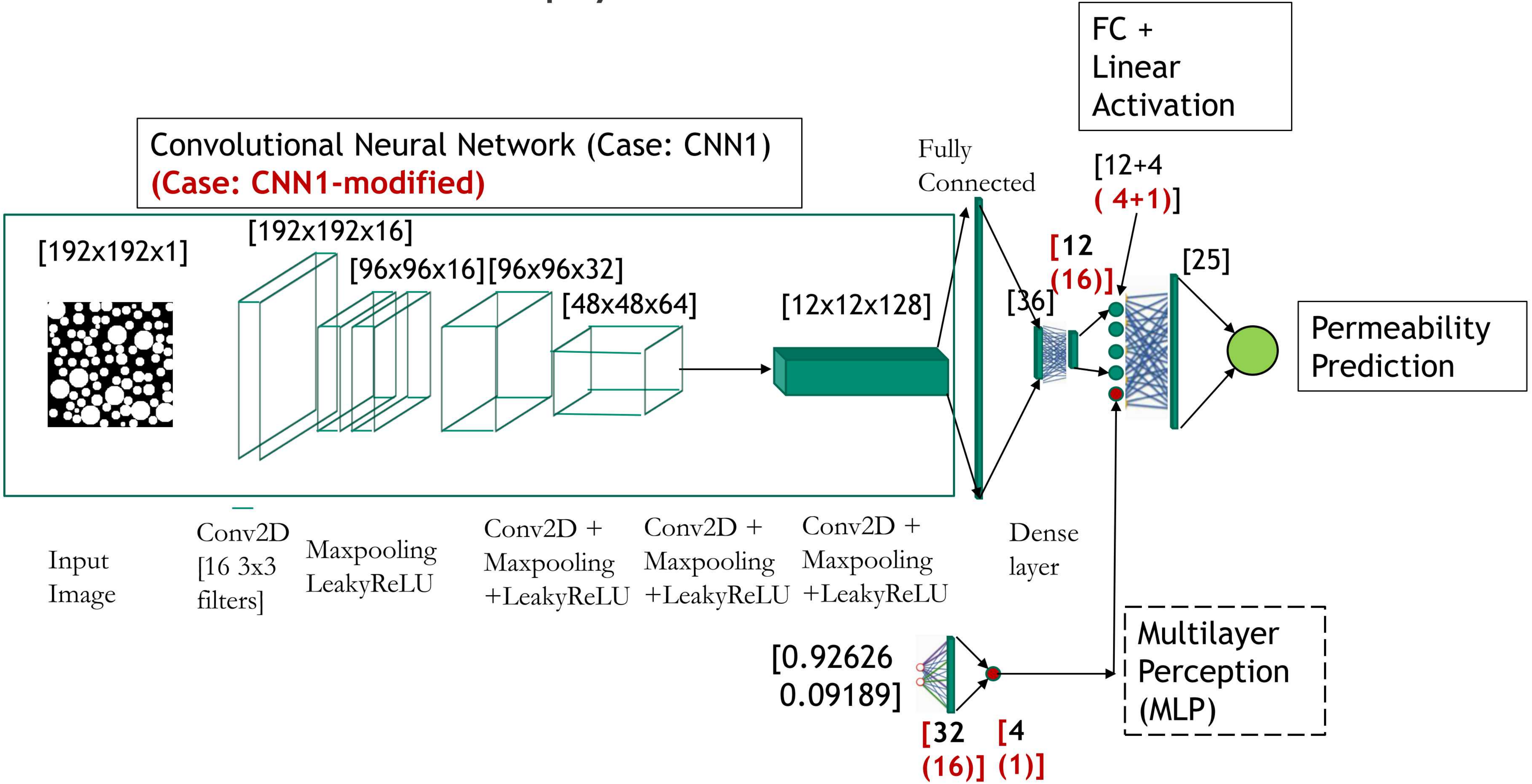
1. Micro-CT image to OpenPNM

2. Building Database

3. Physics-informed Convolutional Neural Network

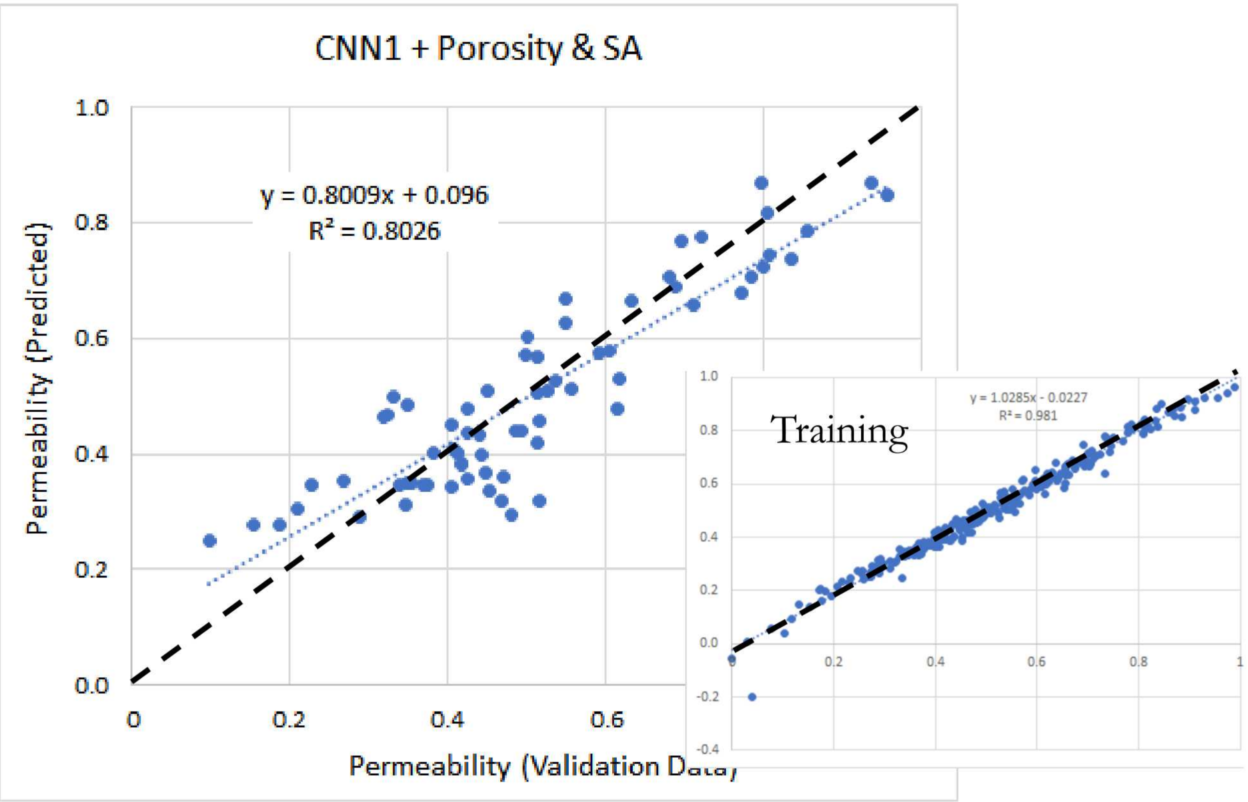
4. Permeability Prediction

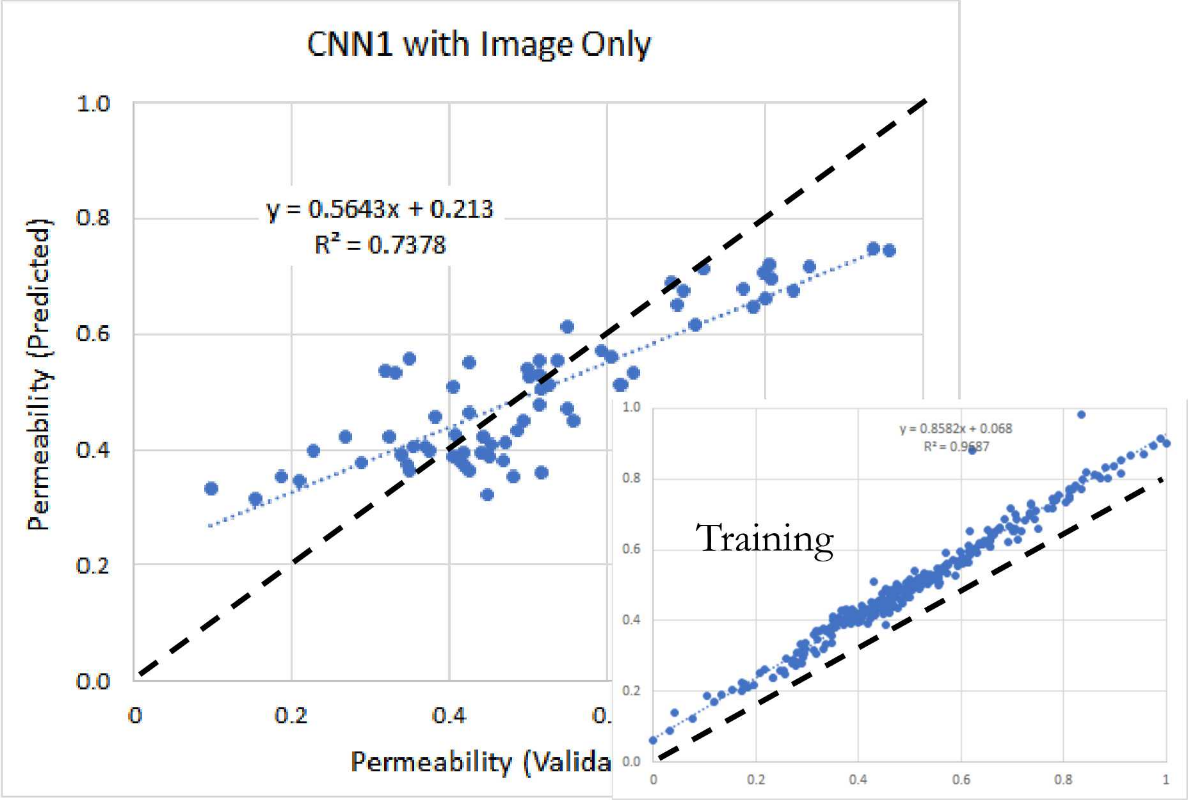
CNN architecture with physical information



Yoon et al. (2020, AAAI workshop)

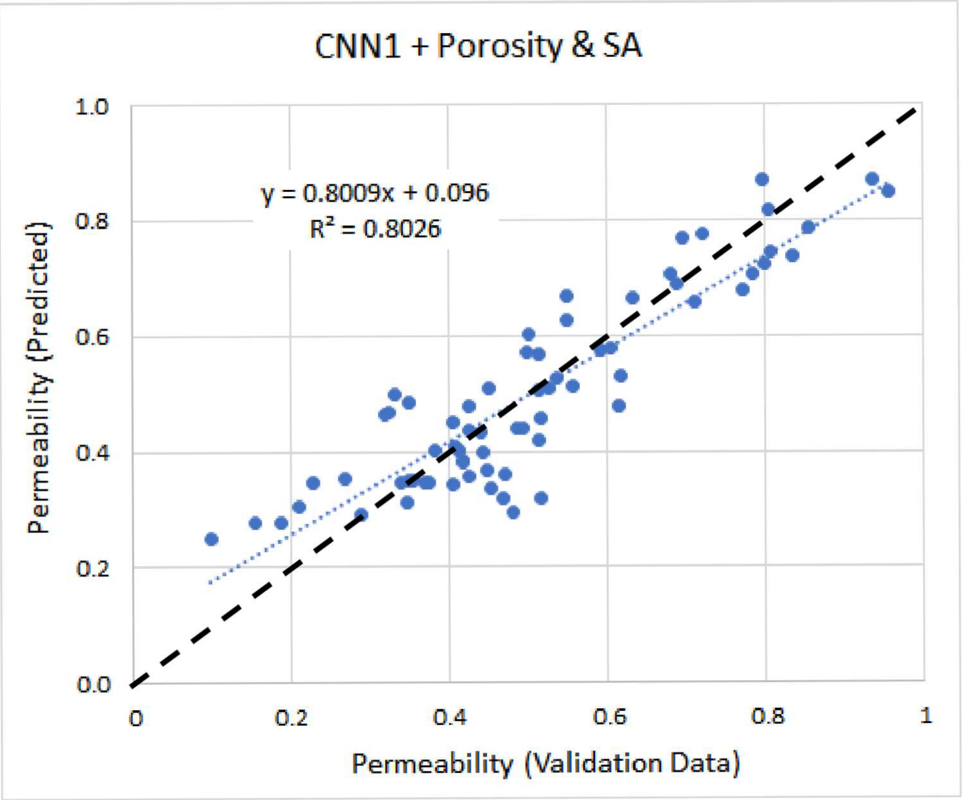
Impact of physical data

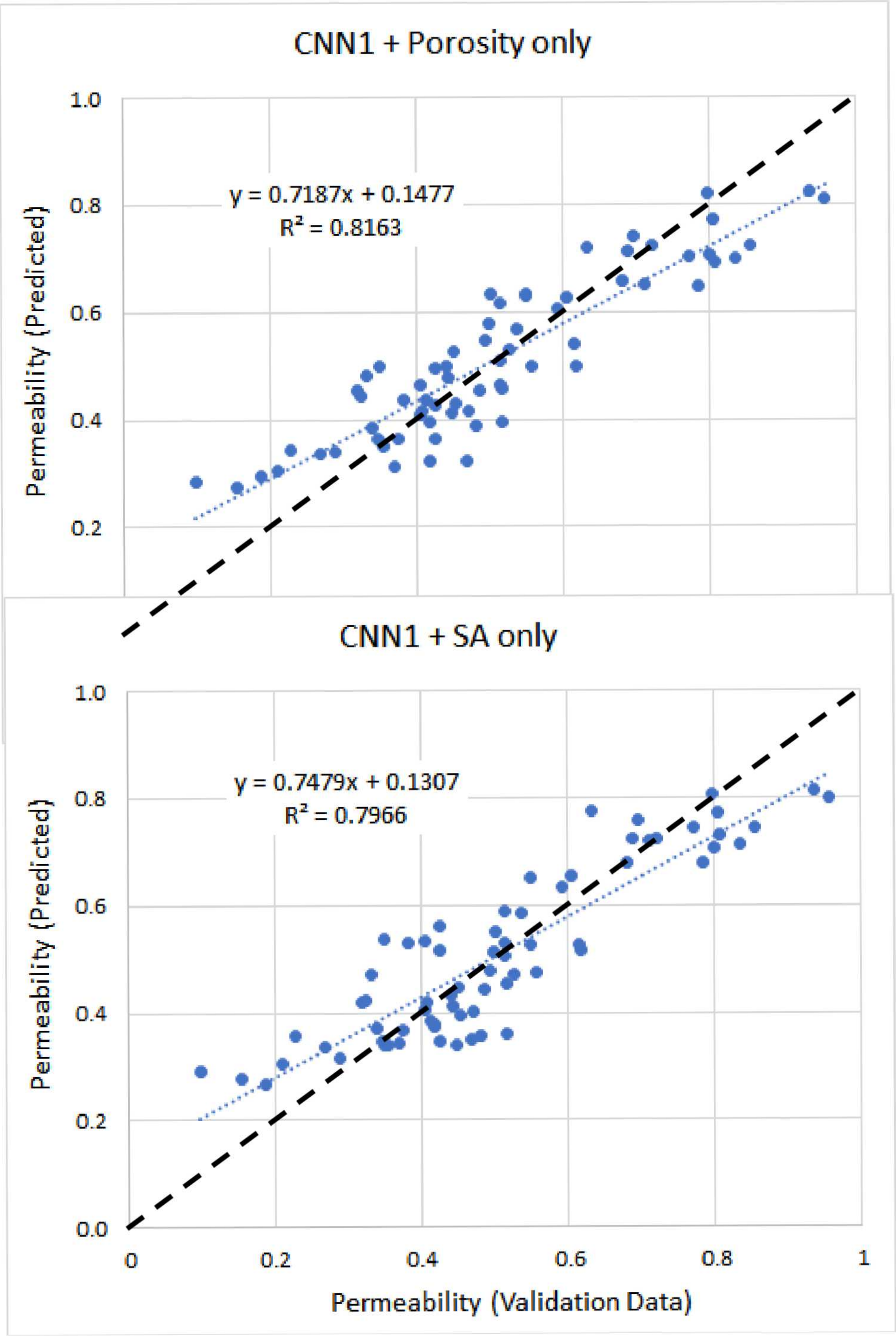




- 345 images [276 for training and 69 for testing]
- Porosity and surface area numeric values per each image
- Addition of physical quantities (porosity and surface area) improves permeability prediction compared to image only case

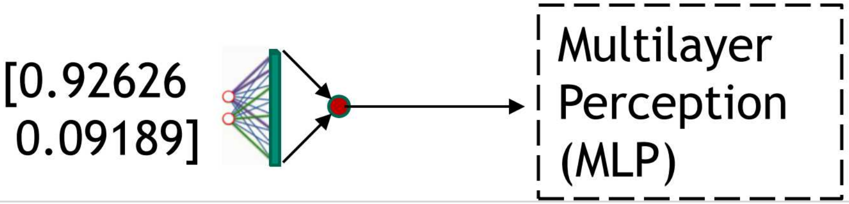
Impact of physical data

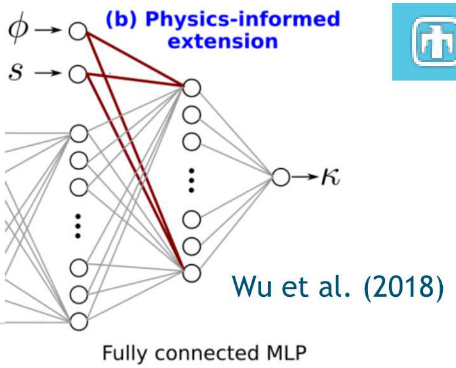


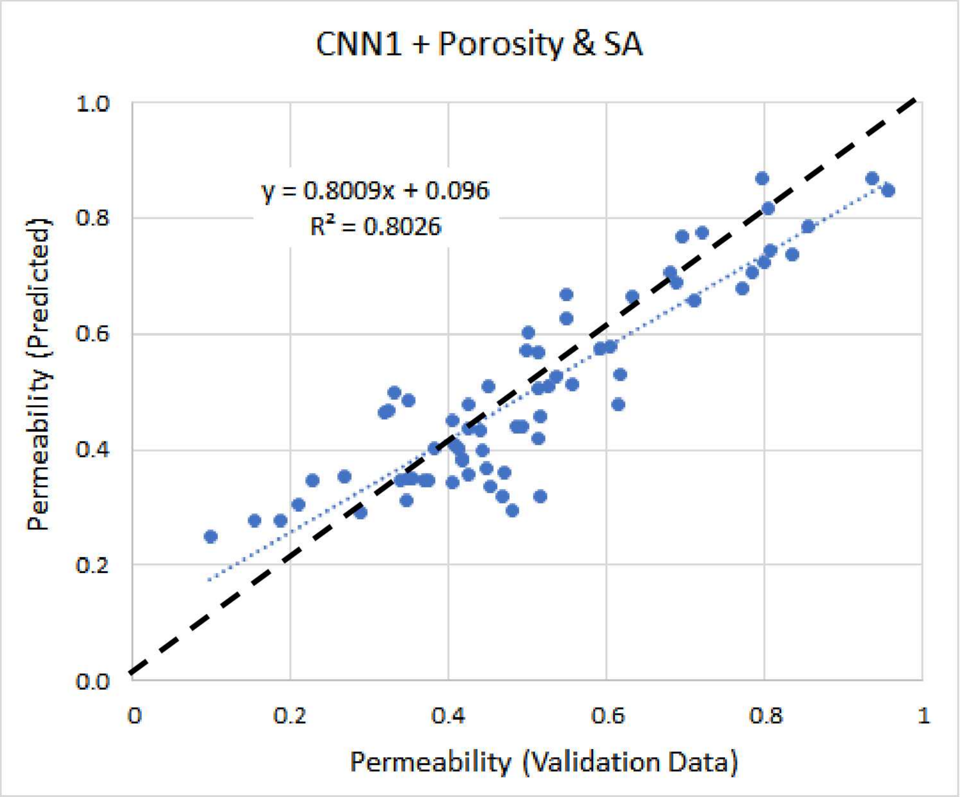


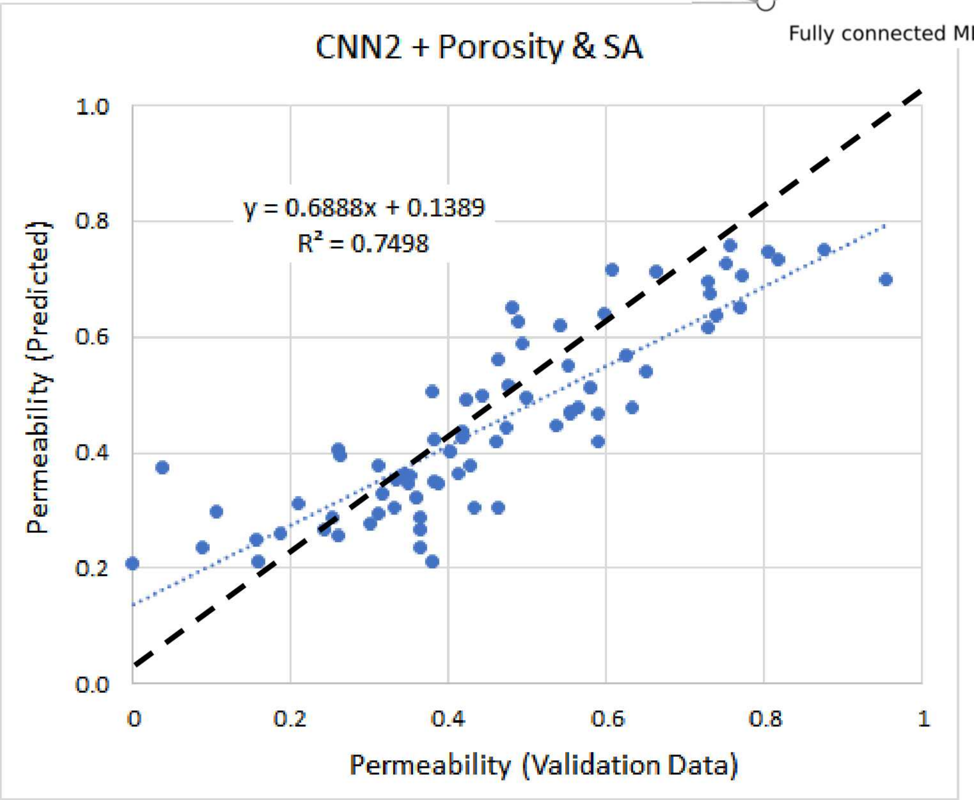
- Two physical quantities improve the prediction better than cases with porosity or SA only

Impact of combining method of physical data



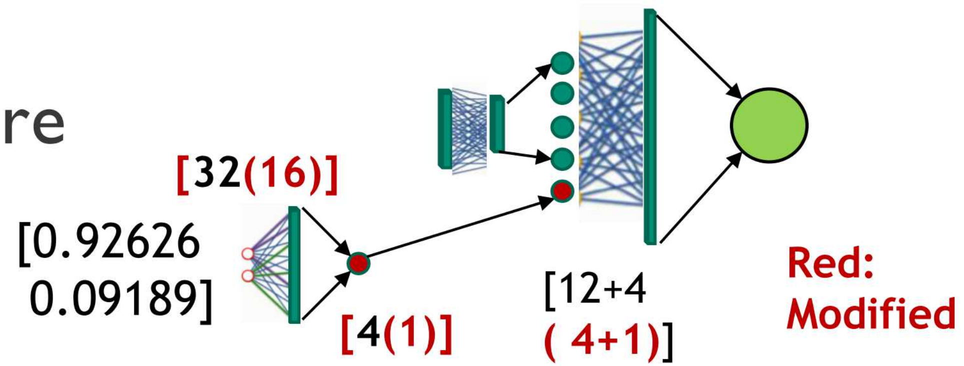


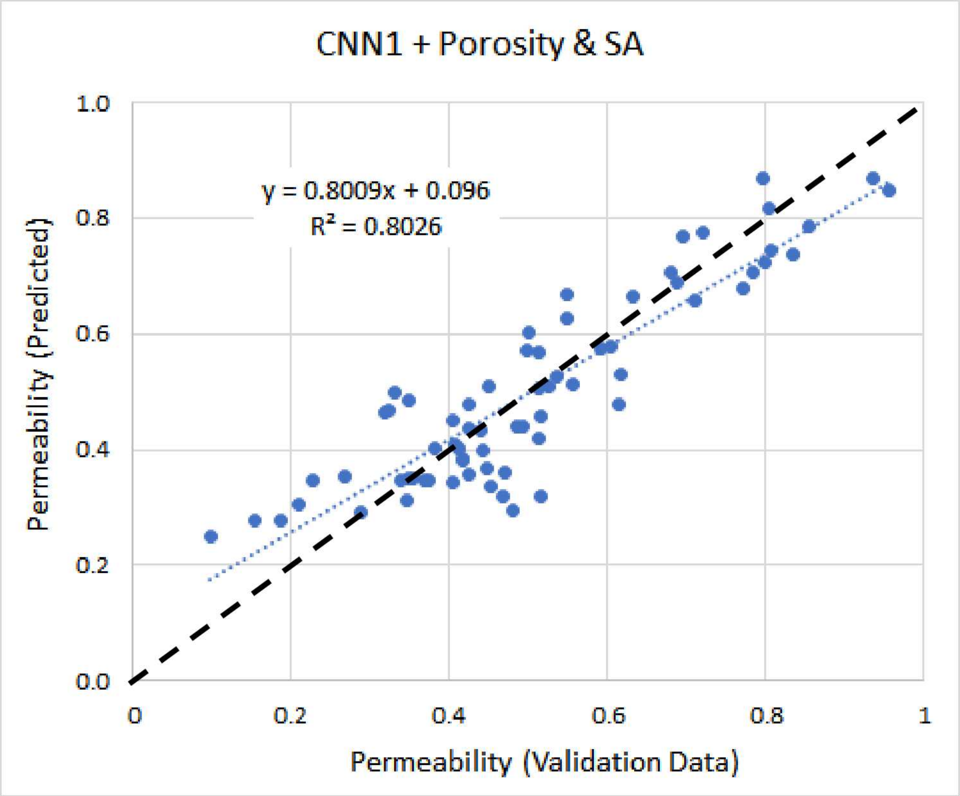


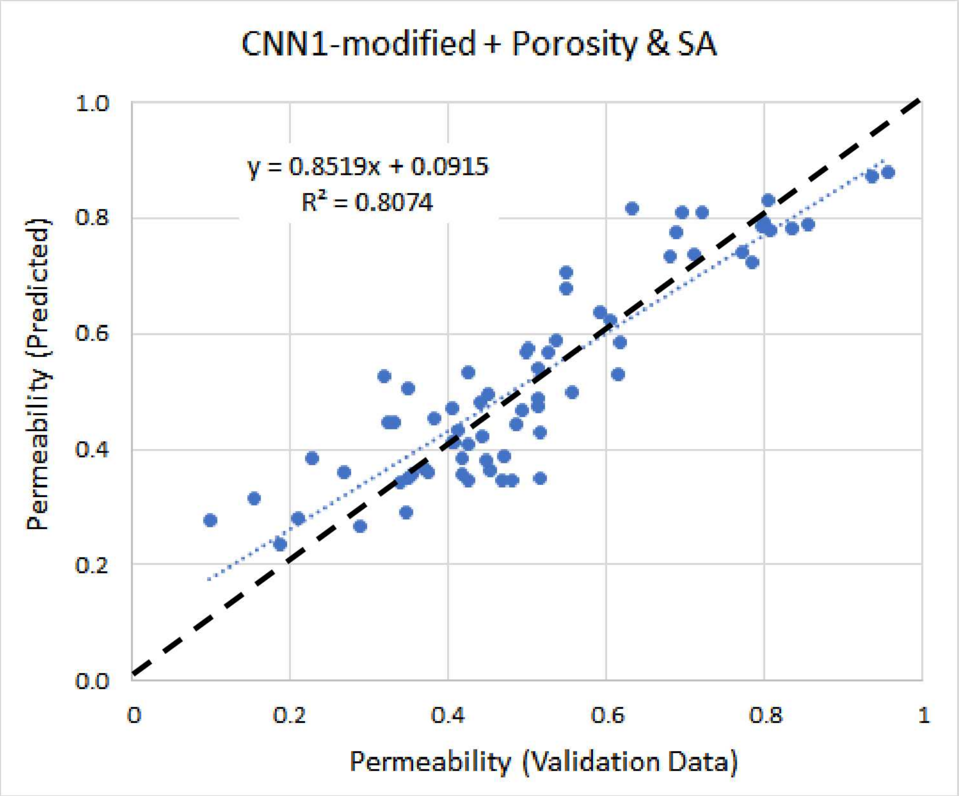


- The method to incorporate physical quantities significantly impact the prediction

Impact of CNN + MLP Architecture



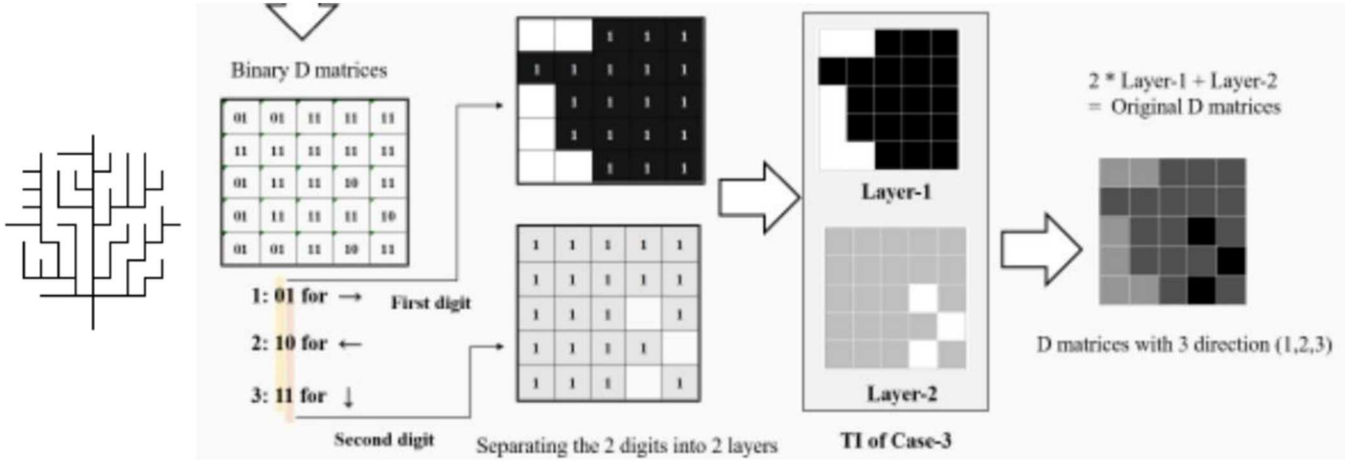


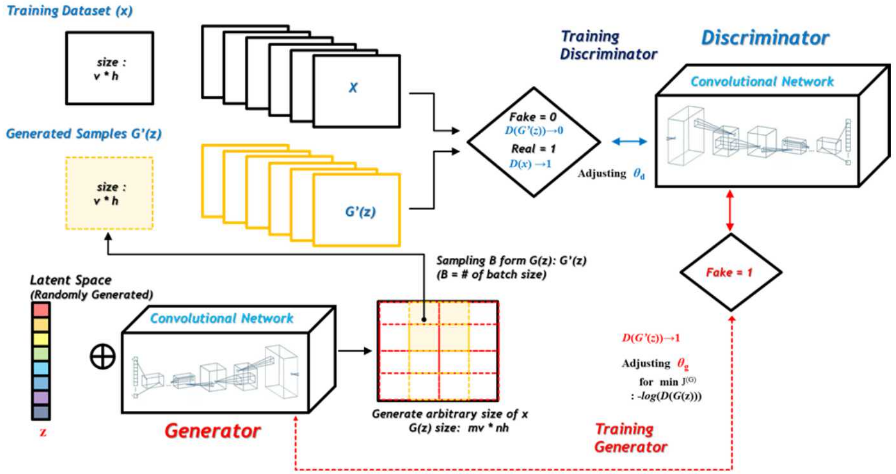


- Combining CNN + MLP also impacts the prediction

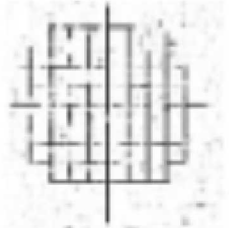
Physics-Informed Deep Convolutional Generative Adversarial Networks (DCGANs)

Physics-informed network generation

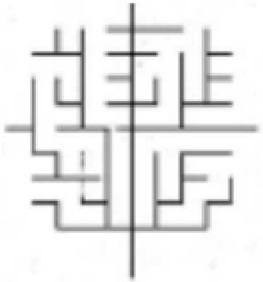




DCGAN

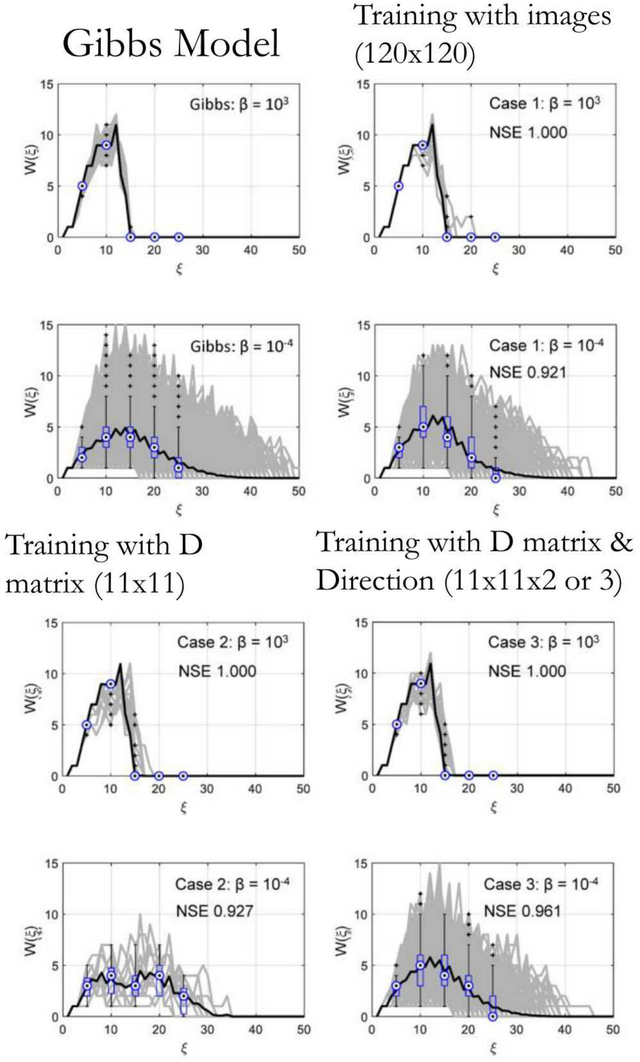


Initial result



Intermediate

Hydrograph Analysis



Kim et al. (Sci. Rep. Under Review)

Summary

Incorporation of physical features and data can enhance ML prediction

- Permeability prediction with physical data performed better than the case with image only
- Deep Convolutional Generative Advesarial Networks was able to produce reliable network systems to improve physical representation and model prediction

Machine learning architecture and combination of different architectures influence the prediction of data-driven models:

- Need to improve our understanding of which features are extracted with different architectures
- Data information extracted from each ML architecture may contain different degree of information, hence it needs to be evaluated more thoroughly
- Hyperparameter optimization will be performed and will apply the methodology for different pore network systems and 3D data