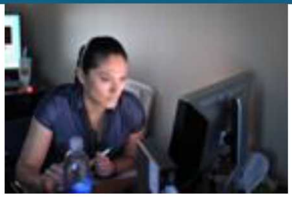
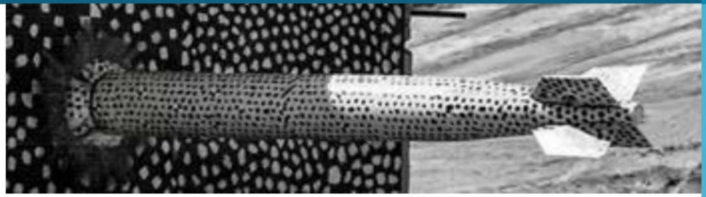
Sandia National Laboratories

SAND2020-3557C

Permeability Prediction of Porous Media using Convolutional Neural Networks with Physical Properties





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Sandia National Laboratories, Albuquerque, NM

AAAI-MLPS, Virtual Conference, March 2020

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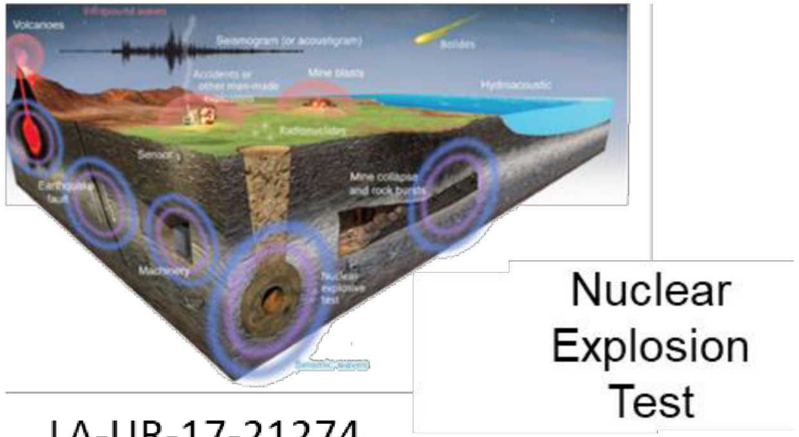
U.S. DEPARTMENT OF ENERGY NNSA

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

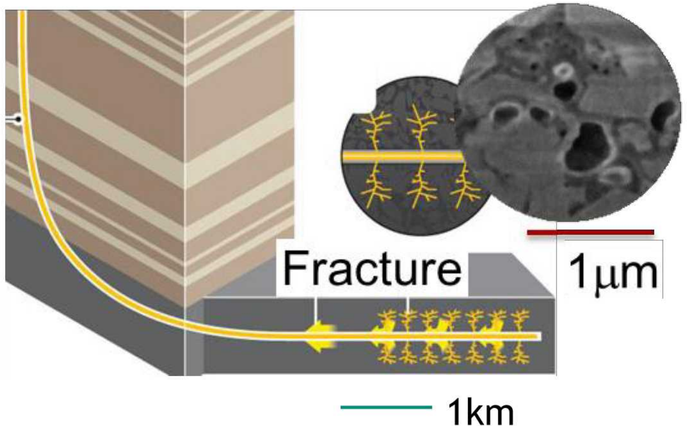
Multiscale, Multiphysics, Big/heterogeneous Data

(Sub-)surface Monitoring

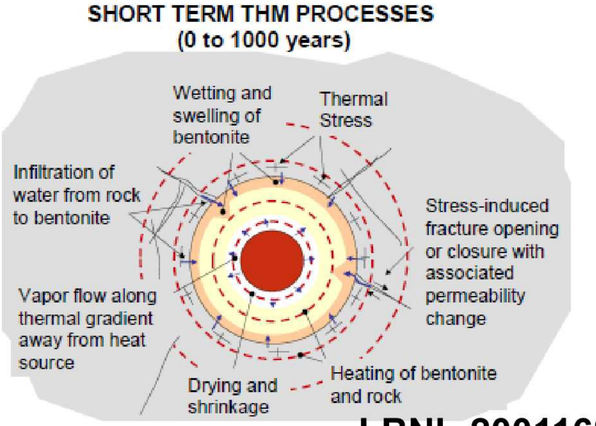


LA-UR-17-21274

Subsurface Energy Security



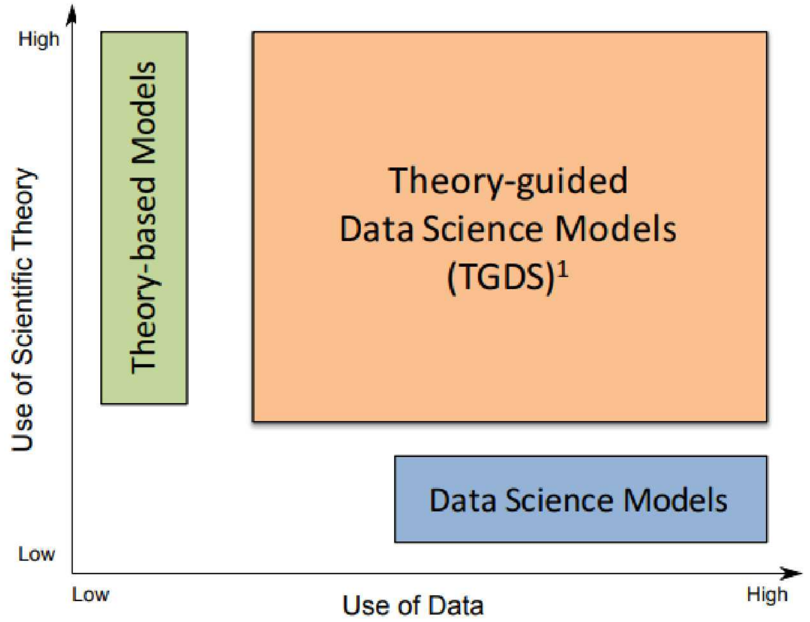
Nuclear Waste Storage



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

BASIC RESEARCH NEEDS FOR

Scientific Machine Learning

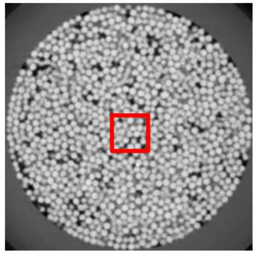
Core Technologies for Artificial Intelligence

DOE BRN report 2018

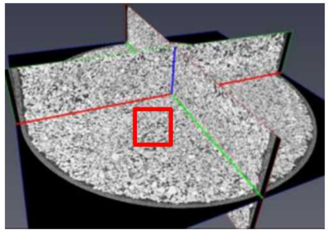
Porous Media and Pore Network (PN) Systems

- Challenge: Complexity in geometry, size, scale, and compositions

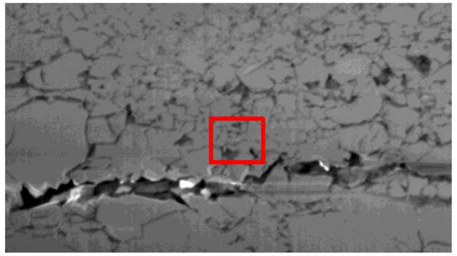
Glass bead pack
(100 μm-1mm)



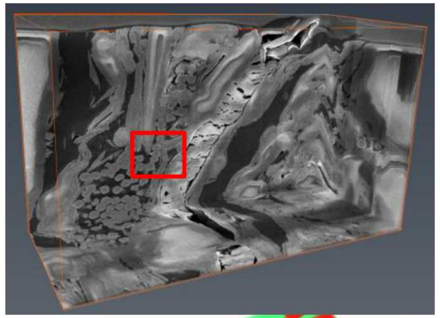
Sandstone
(10's-100's μm)



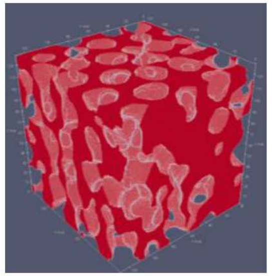
Chalk
(10 nm - 100μm)

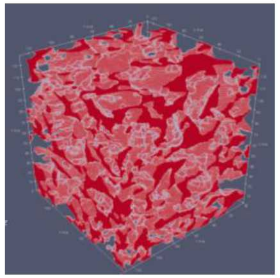


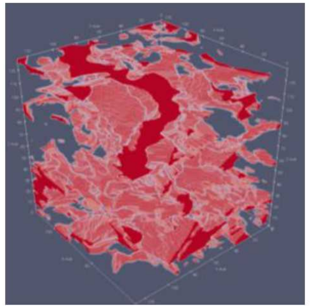
Shale
(1 nm - microns)

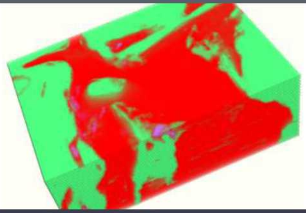


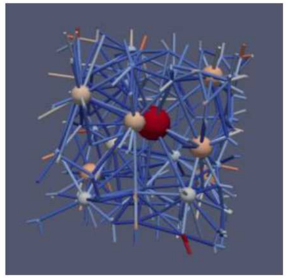
Binary
3D images



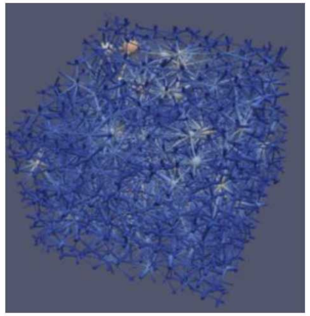




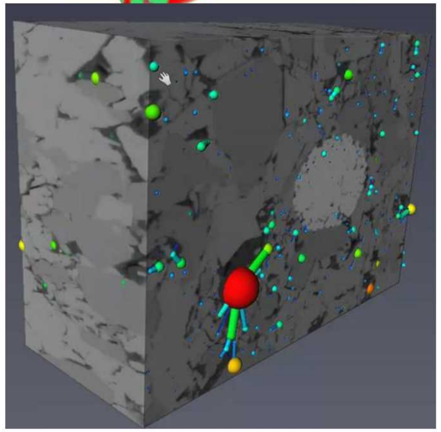




PN from microCT image



PN from microCT image



Xtlas.pergeos.com PN from FIB-SEM image

Semantic Image Segmentation

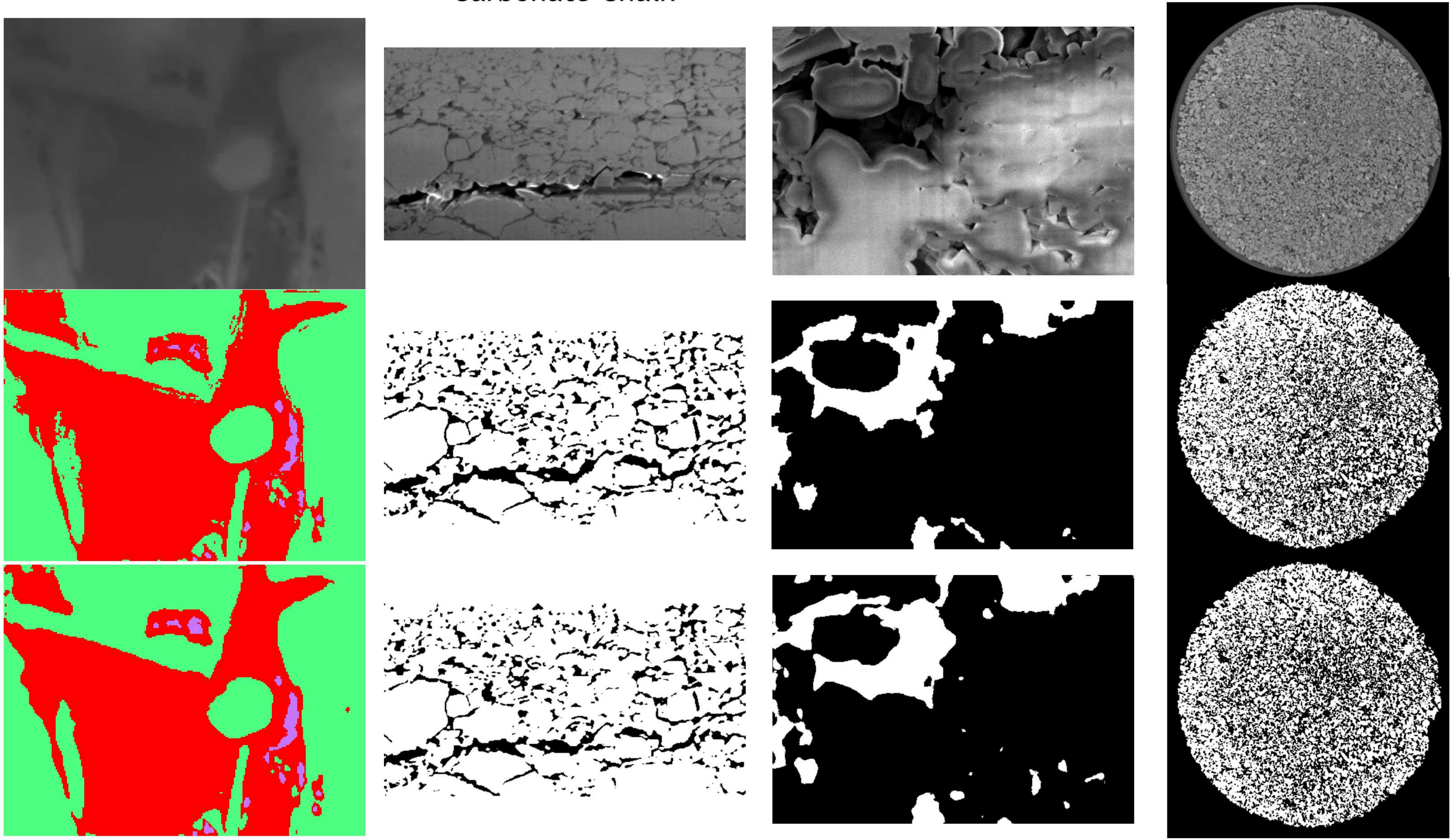
- VGG16+UNET (transfer learning)

Shale | Carbonate Chalk | Carbonate Chalk | Sandstone

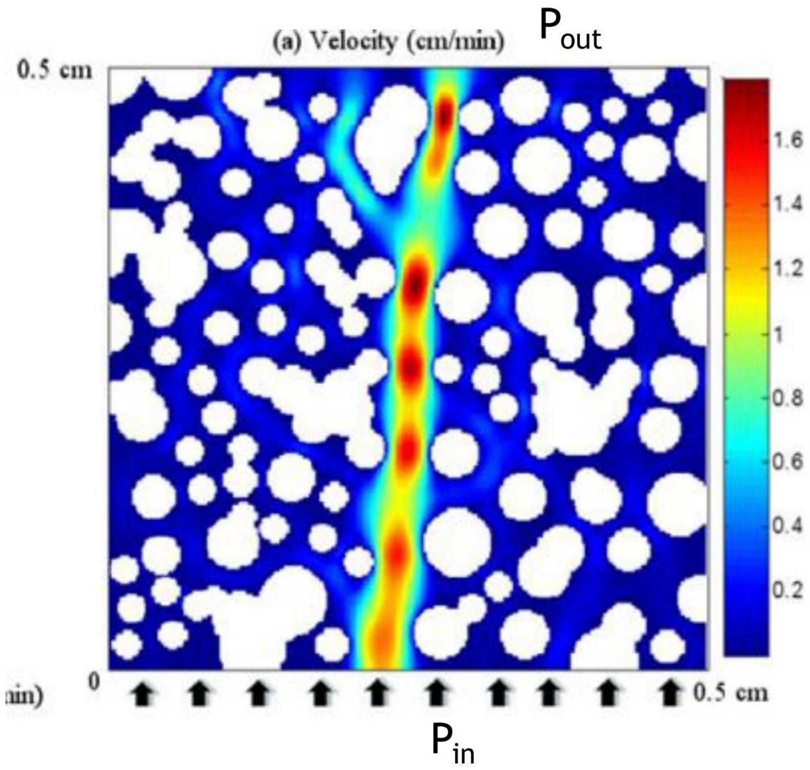
Original Image

Ground Truth

Segmentation



Physics of Interest: Fluid Flow in Porous Media



- Stokes Flow (Low Reynolds number, no slip boundary)

$$\mu \nabla^2 \mathbf{u} - \nabla p = 0$$ The balance of forces in a non-accelerating fluid

$$\nabla \cdot \mathbf{u} = 0$$ The conservation of mass for incompressible fluids

- Darcy's Flow at continuum scale

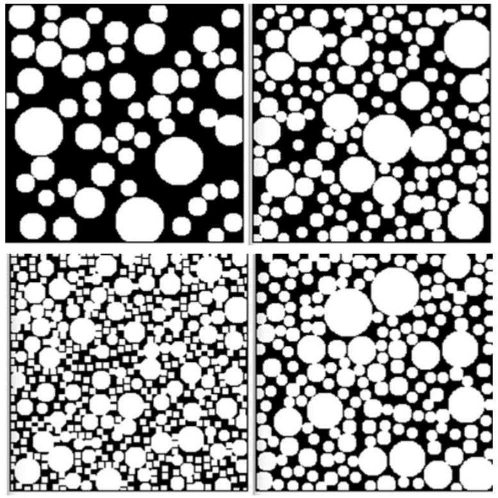
$$\mathbf{v} = -\frac{K}{\mu}\left(\frac{\Delta p}{L} - \rho \mathbf{g}\right)$$ $\Delta P = P_{in} - P_{out}$

- K: Intrinsic permeability (m²) - a measure of the ability of a porous material to allow fluids to pass through it.

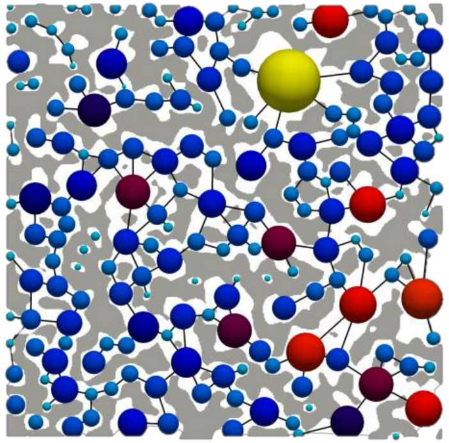
- K: can be estimated using numerical simulations (stokes flow equation, pore network modeling) or empirical relations (Kozeny-Carman equation)

Data Generation (Images, Pore Network, Properties)

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



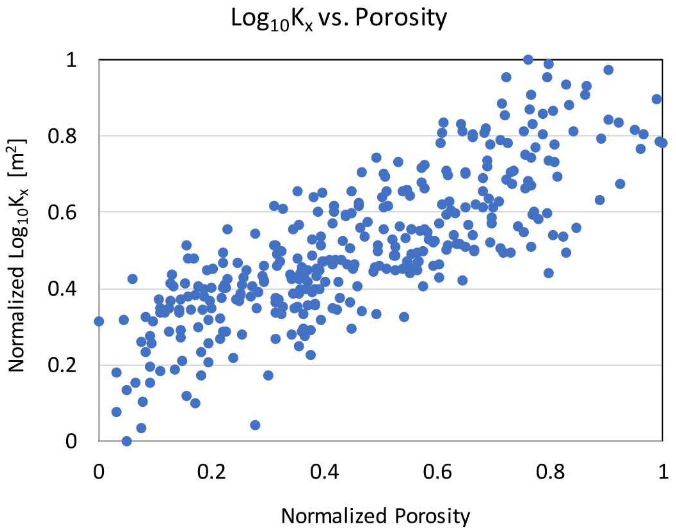
Pore Network Construction

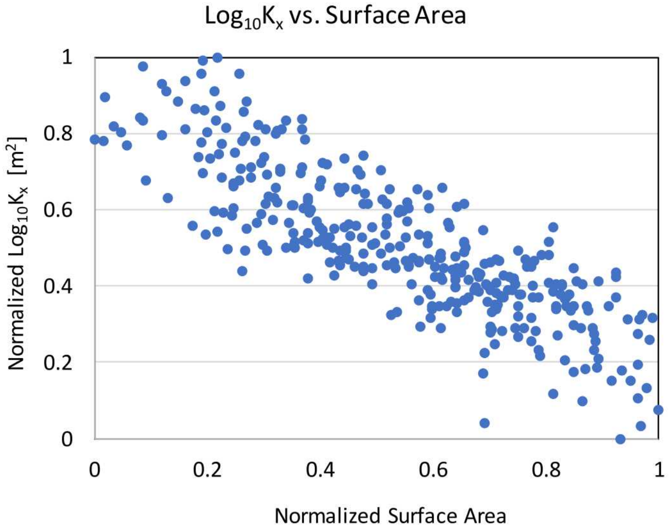
Estimation of properties

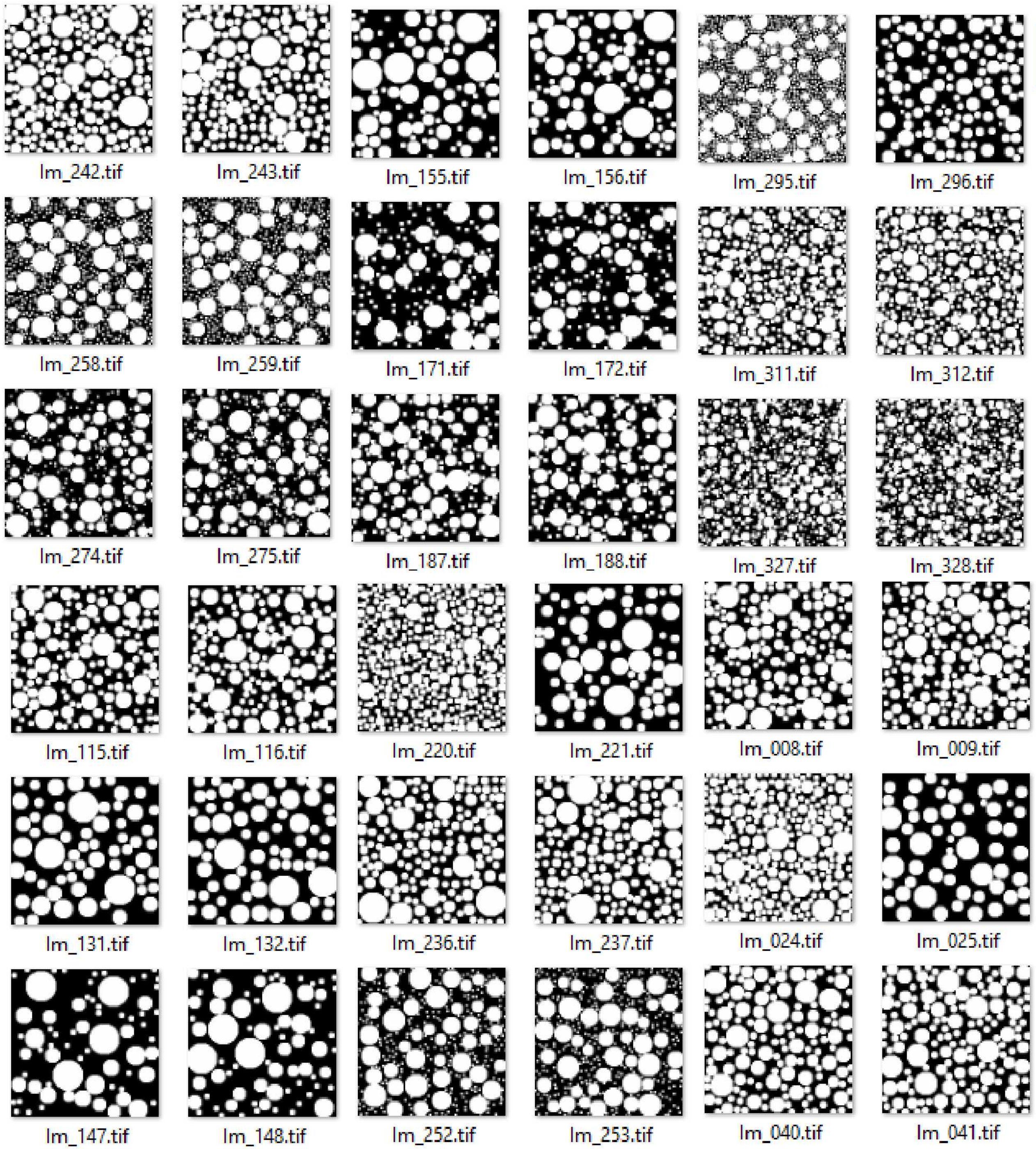
- $K = f$(porosity, surface area)

Porous Media Properties

- $K = f$(porosity, surface area)

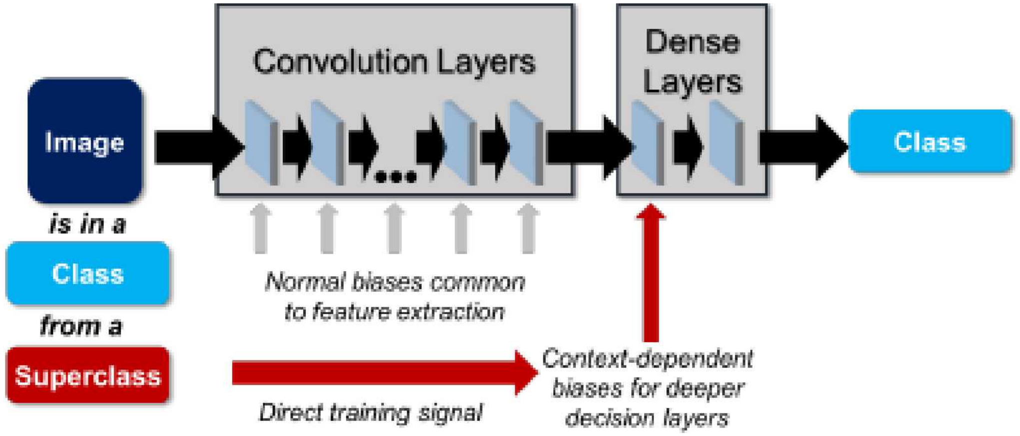






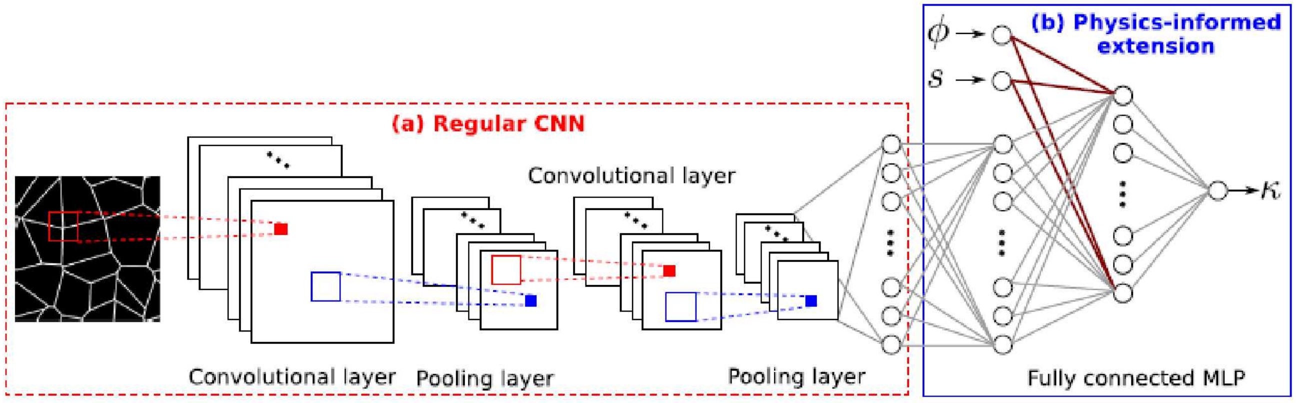
Physics-Informed ML for permeability prediction

Image Classification



Aimone et al., 2018

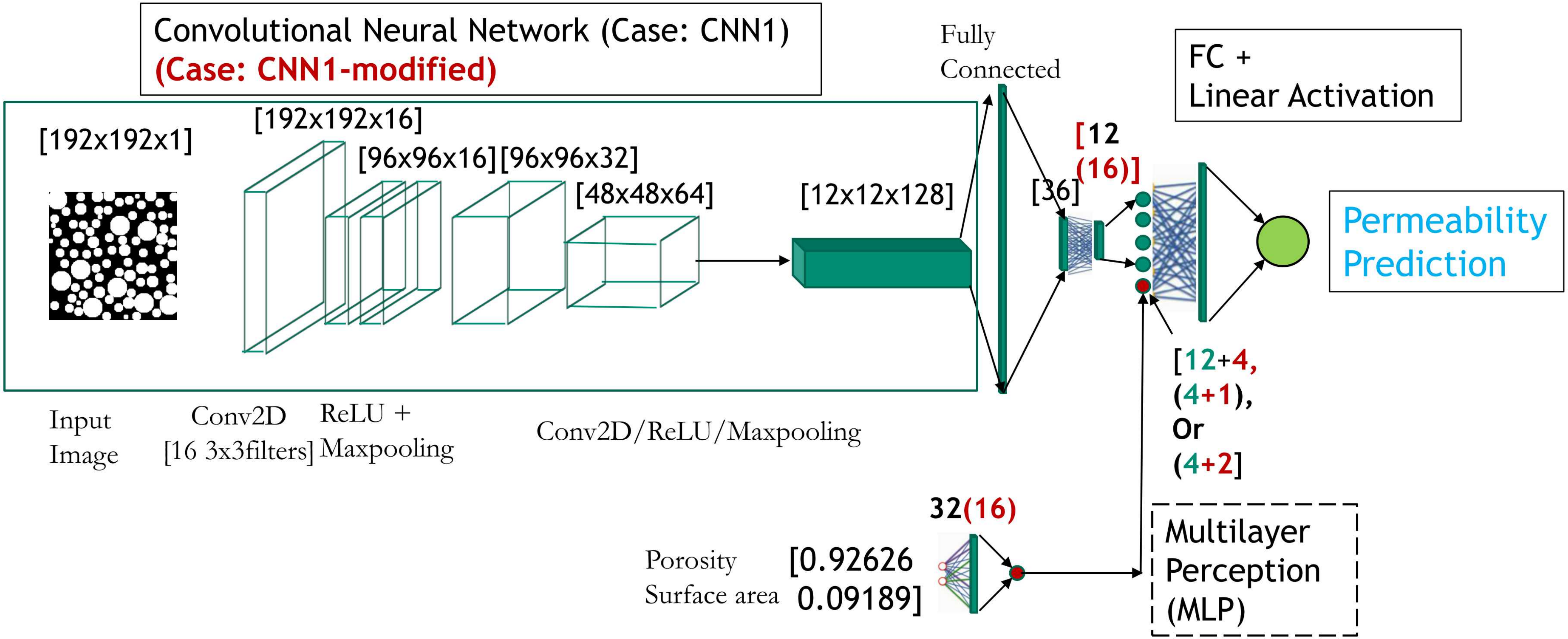
Permeability Prediction



Wu et al., 2018

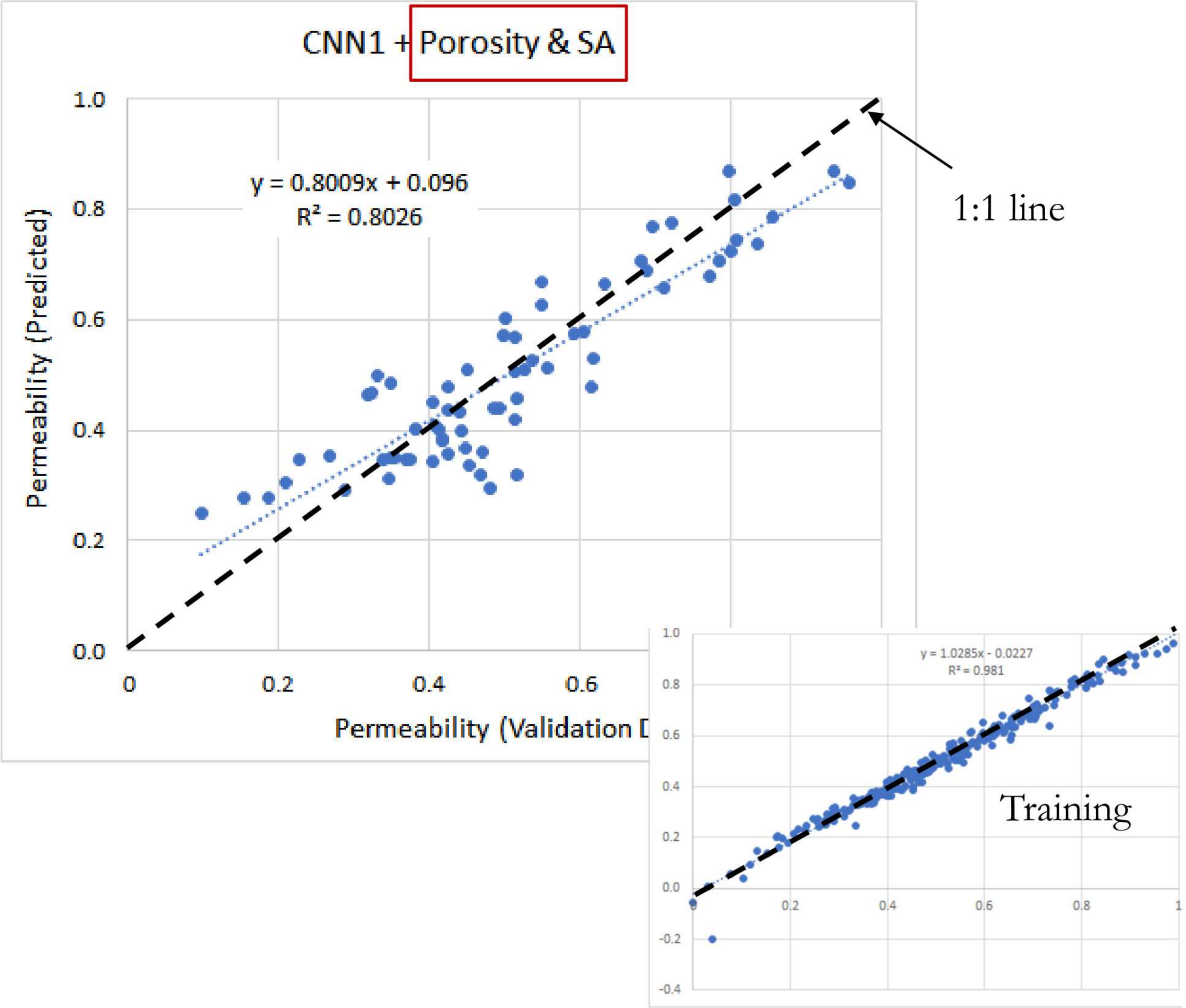
- Effect of CNN architecture
- Methods of how to incorporate physical properties
- Balance between CNN features and physical properties on training

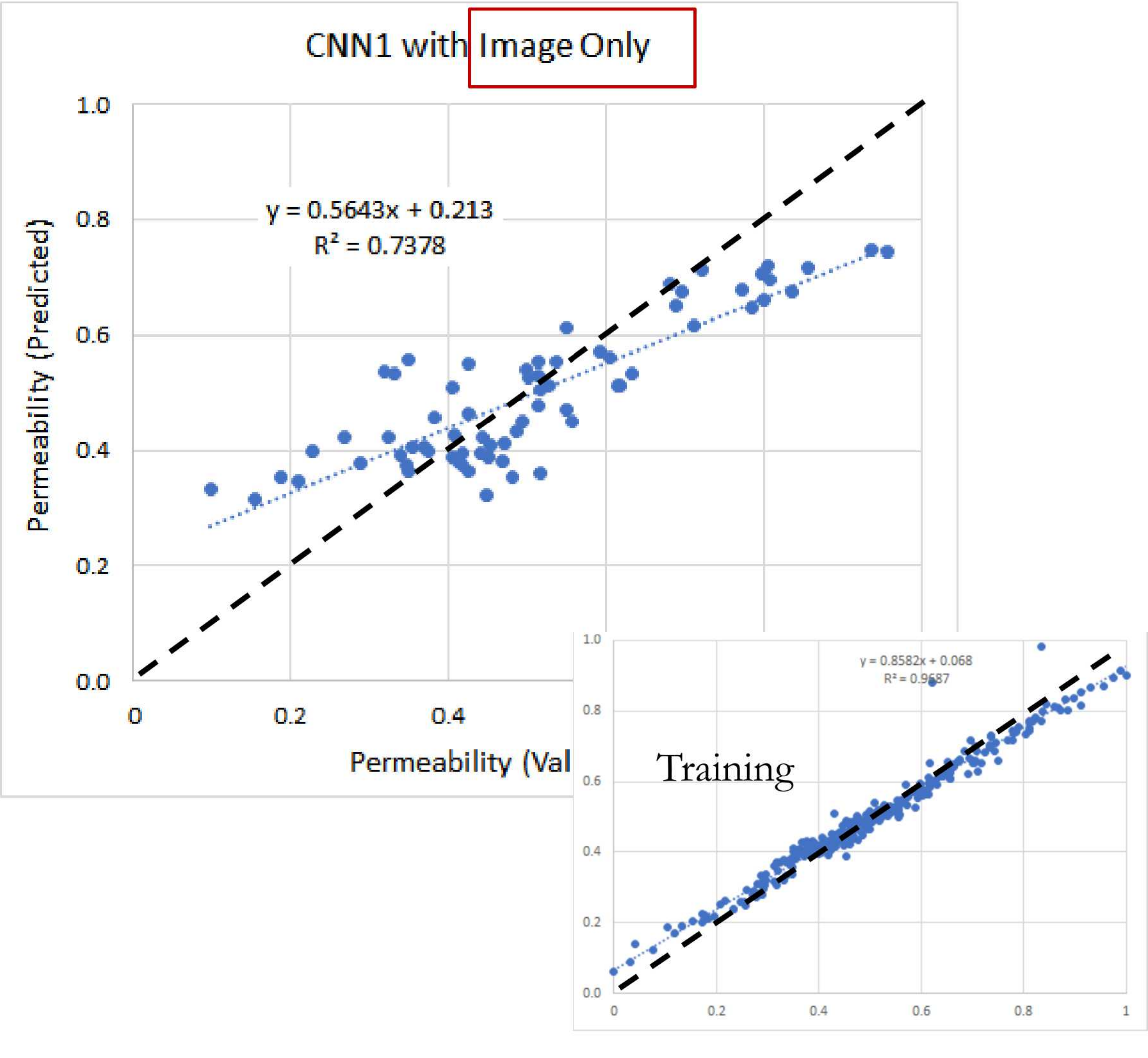
CNN architecture with physical information



- A total of 345 images [276 for training and 69 for testing]
- Porosity and surface area values per each image
- Mean square error as a loss function

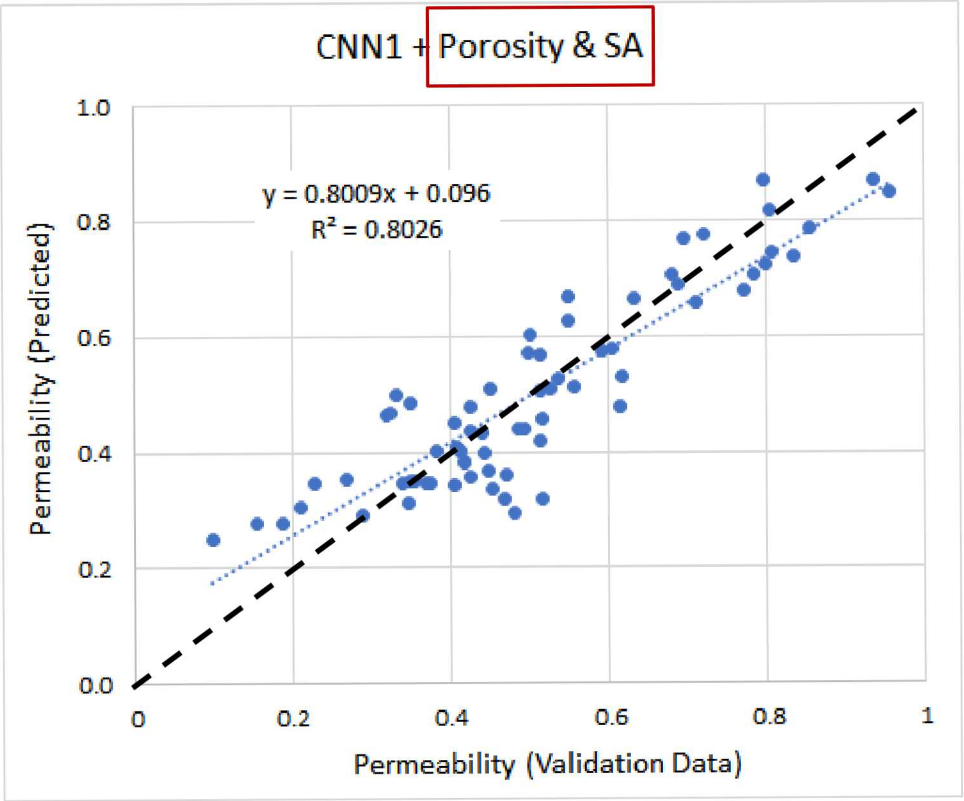
Impact of physical data

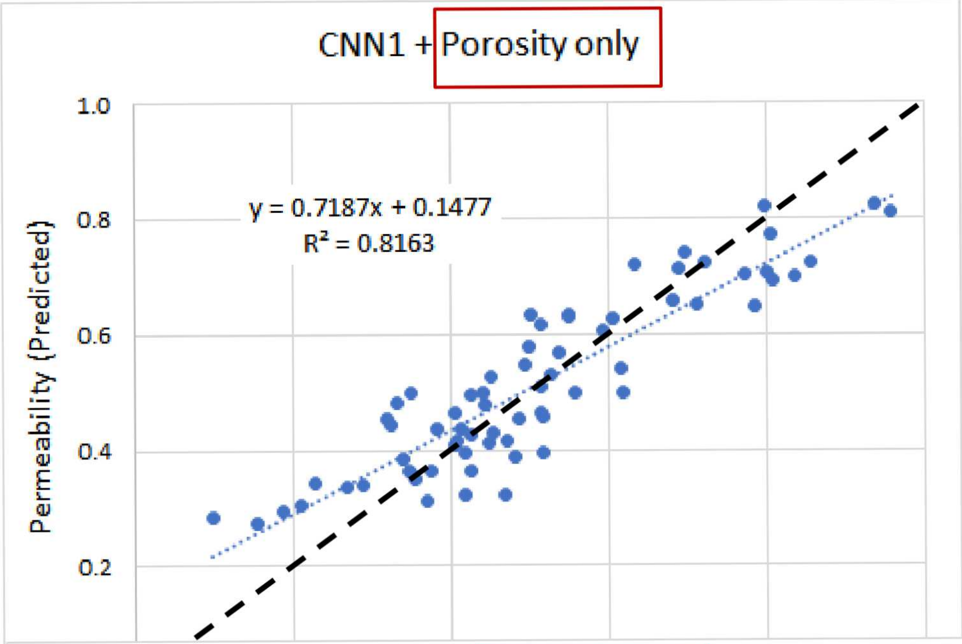


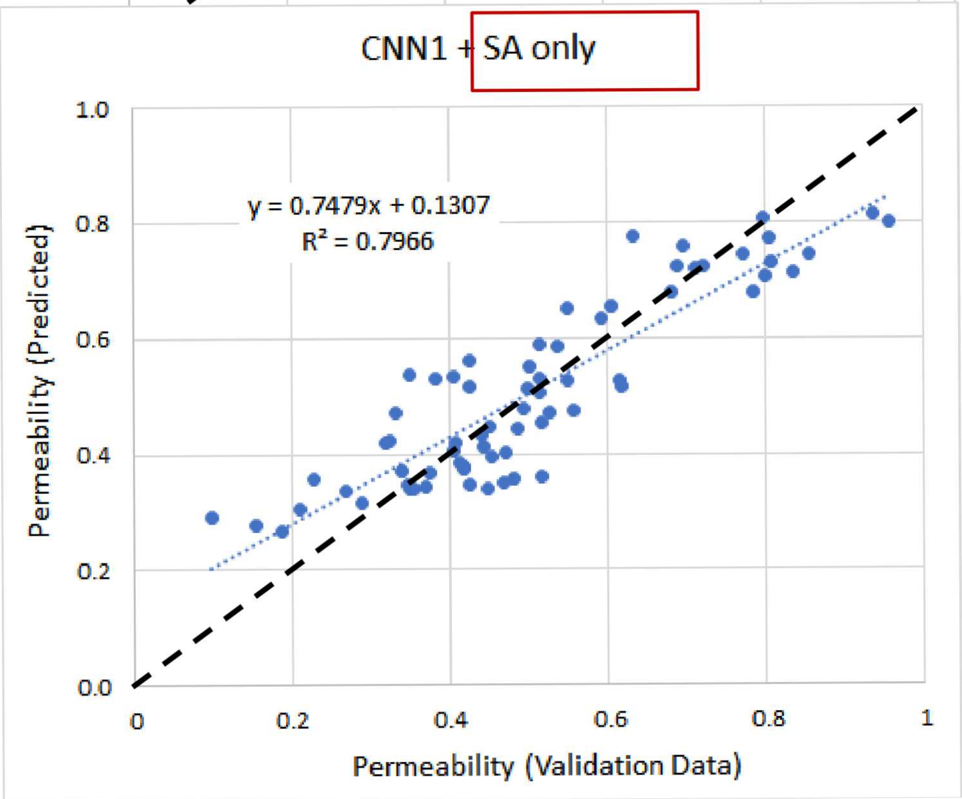


- Addition of physical quantities (porosity and surface area) improves permeability prediction compared to image only case

Impact of physical data



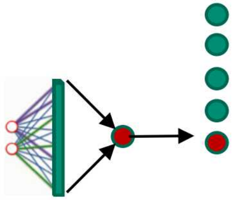




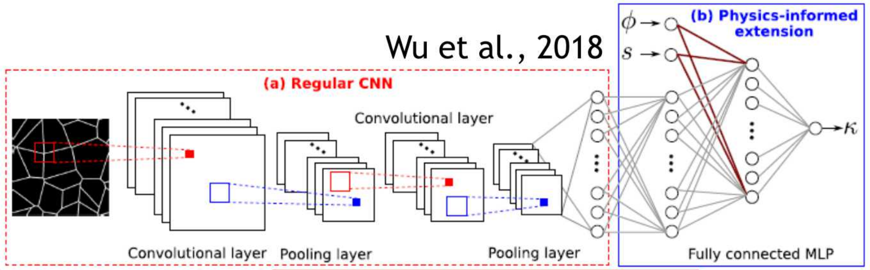
- Two physical quantities improve the prediction better than cases with porosity or SA only
- One physical quantity still better than image only

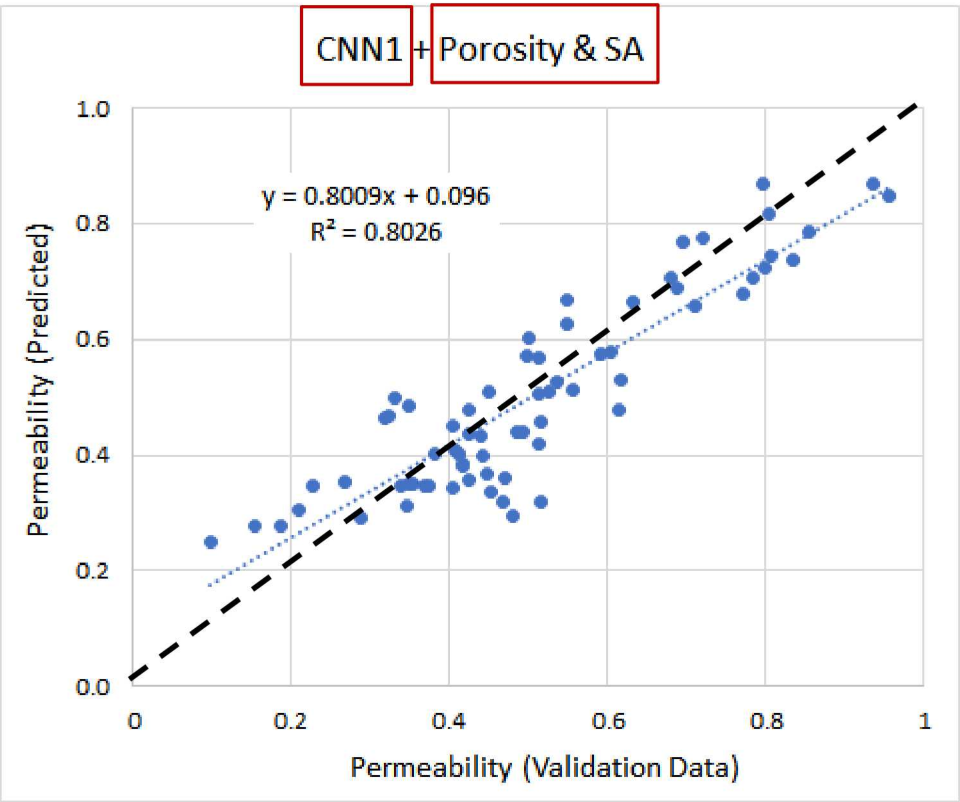
Comparison with a shallow CNN and numeric data input

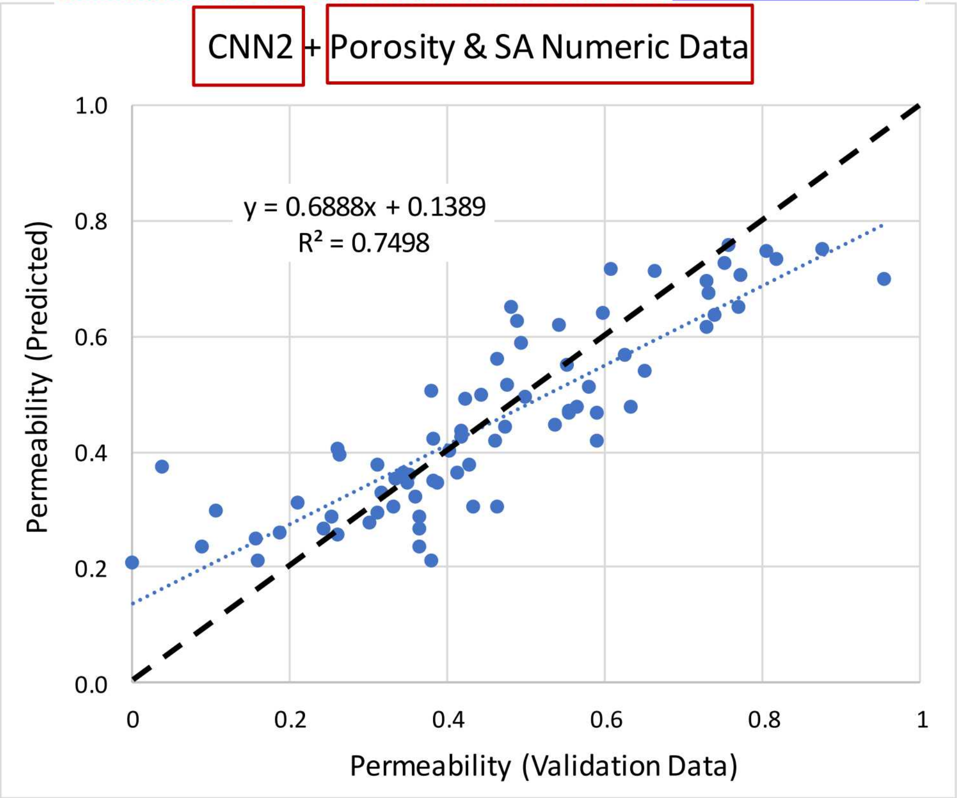
Two physical data processed with multilayer perception, then concatenated with CNN output



Wu et al., 2018



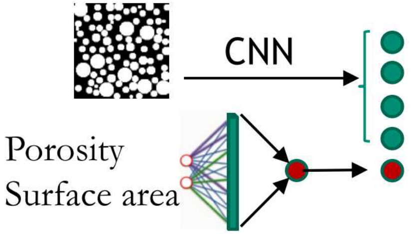




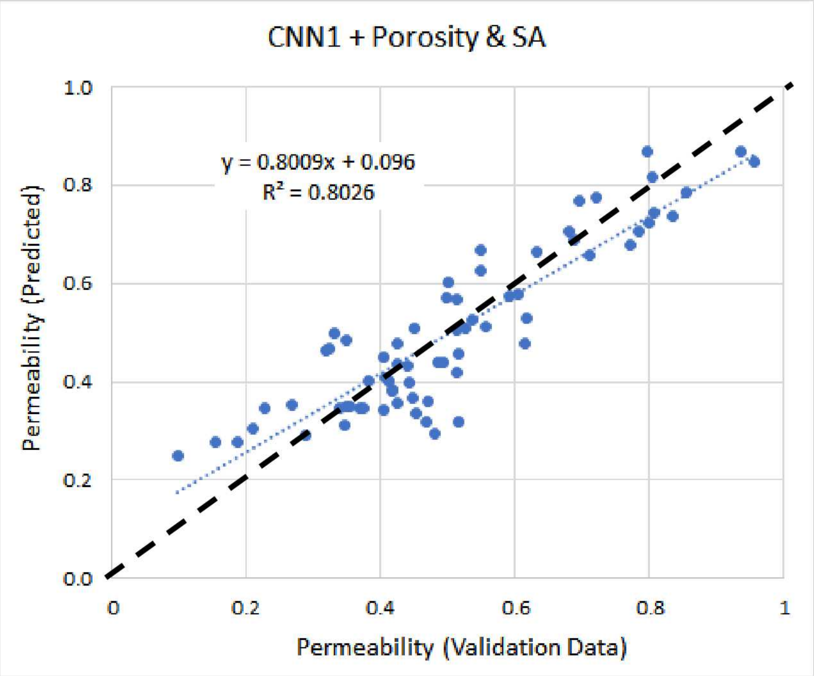
- The method to incorporate physical quantities significantly impacts the prediction

Impact of the Size of MLP output

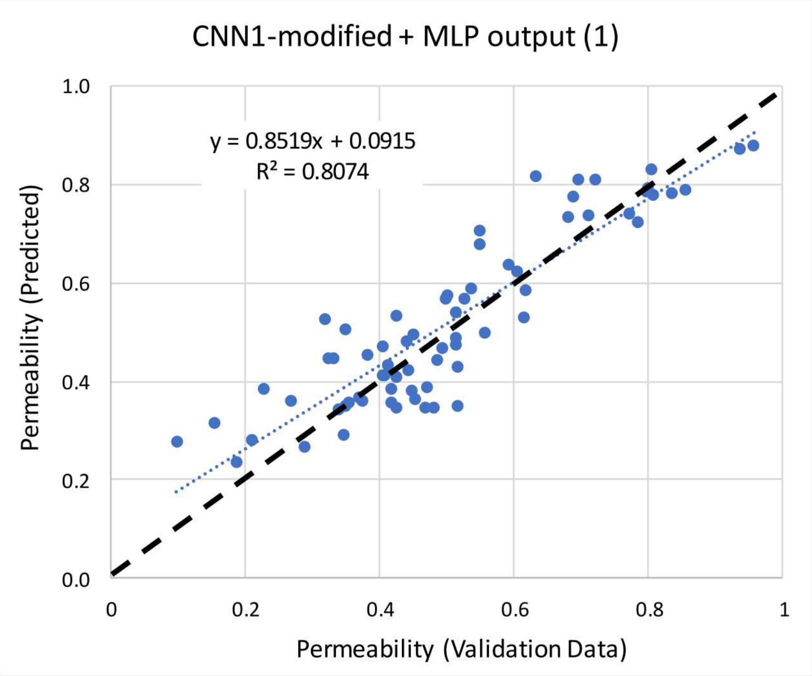
Two physical data processed with multilayer perception, then concatenated with CNN output



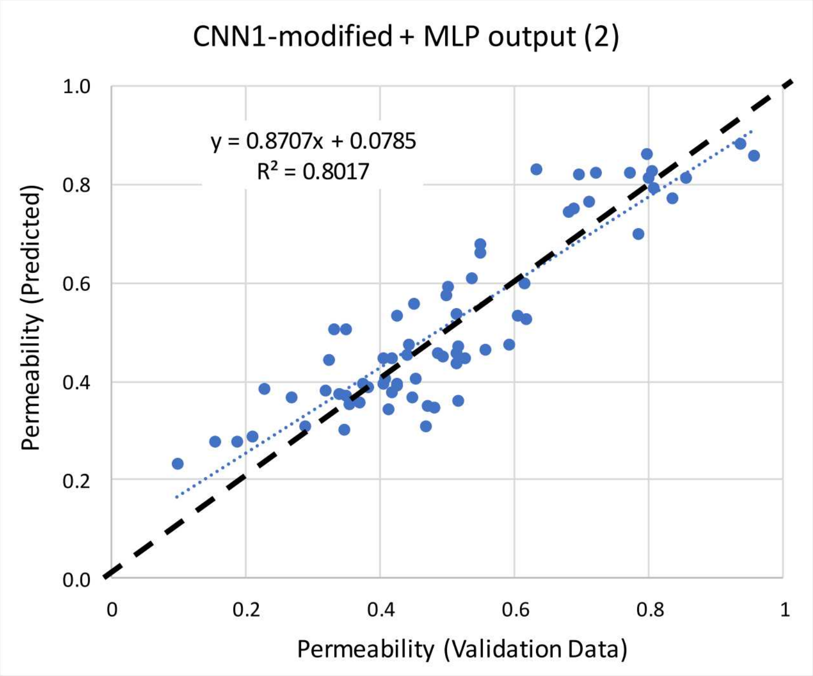
[12+4]



[4+1]



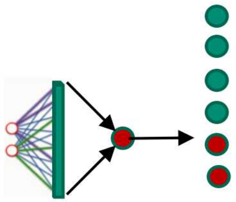
[4+2]



- The balance of information between CNN and physical data impacts the prediction

Impact of combining method of physical data

Two physical data processed with multilayer perception, then concatenated with CNN output



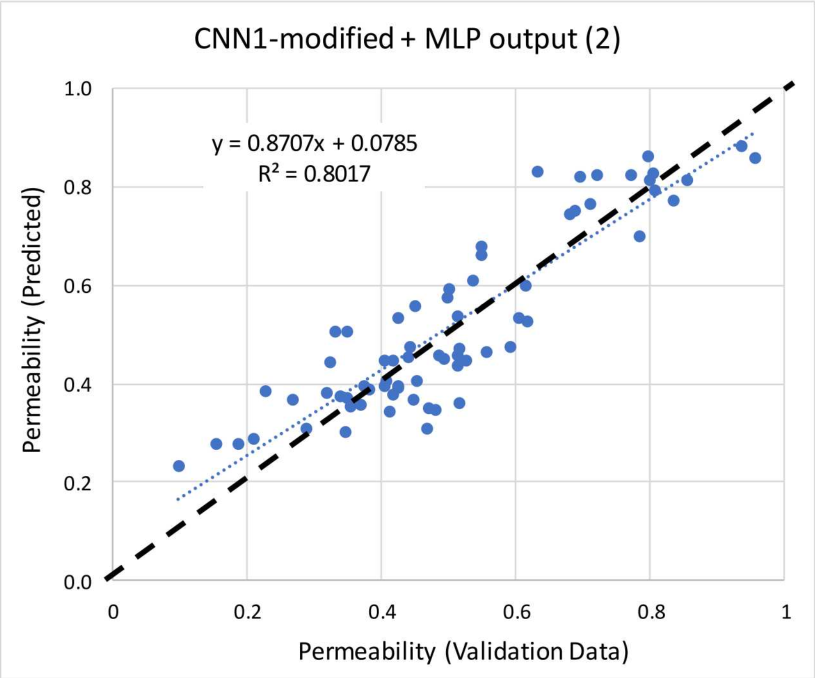
Two physical data directly concatenated with CNN output

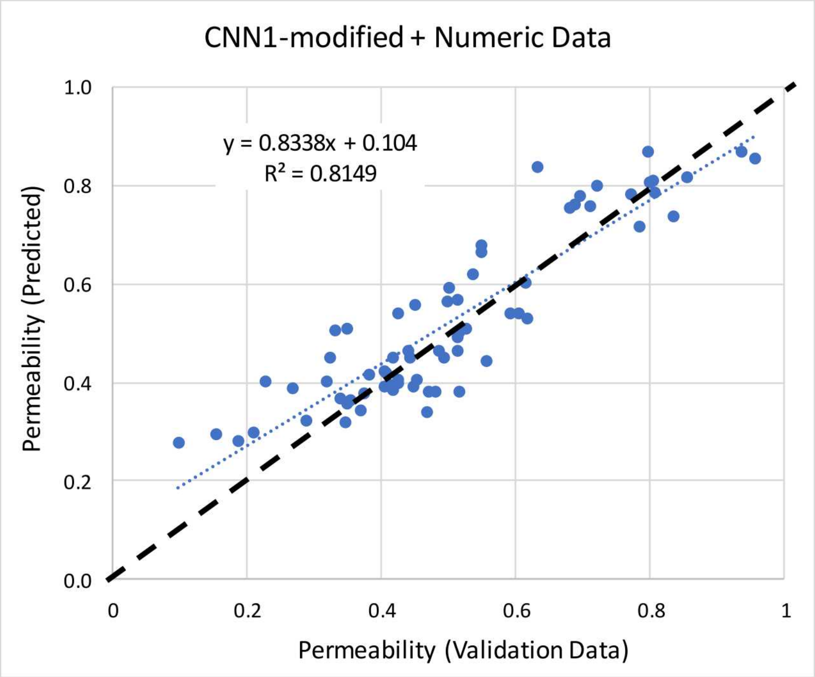
[0.92626
0.09189]

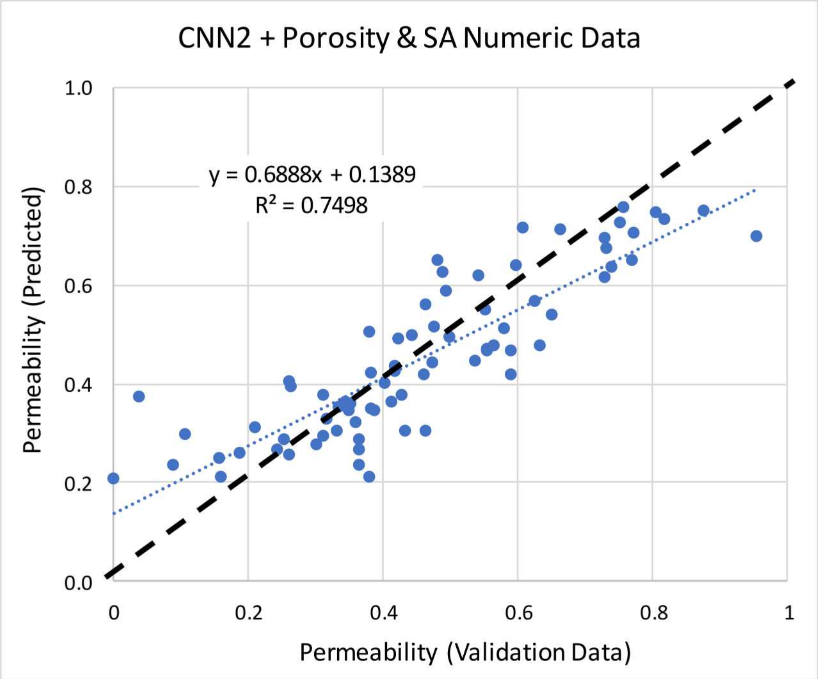
[4+2]

[4+2]

Wu et al., 2018





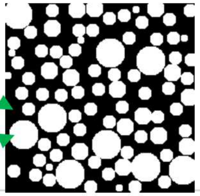


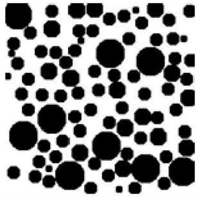
- MLP output rather than direct numerical data improves the prediction

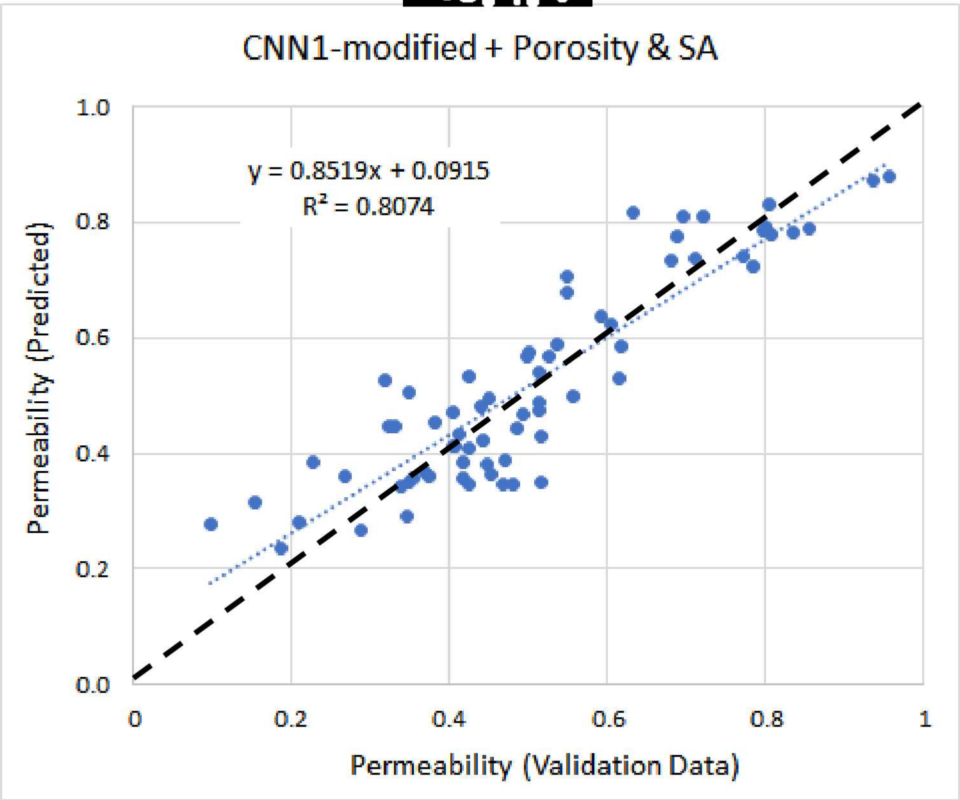
Impact of Binary Image Input

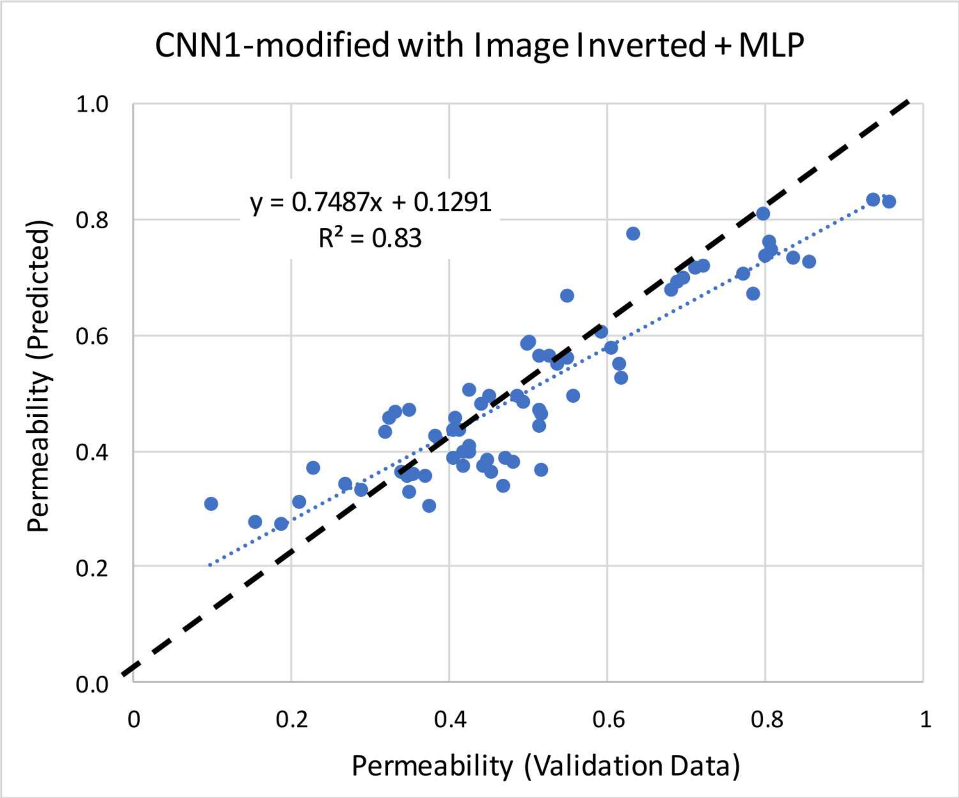
Pore

Grain



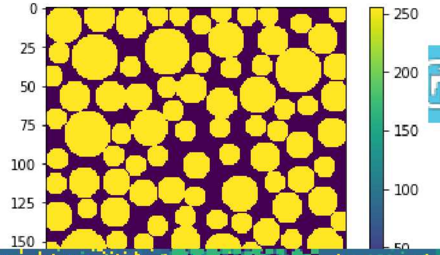




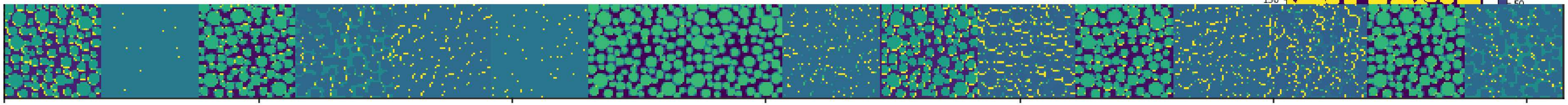


- CNN predicts permeability better with solid phase (obstacles) as true input

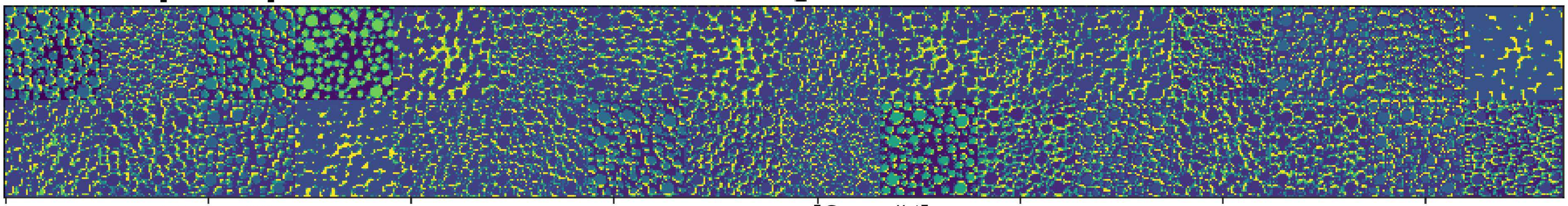
Visualizing Activations



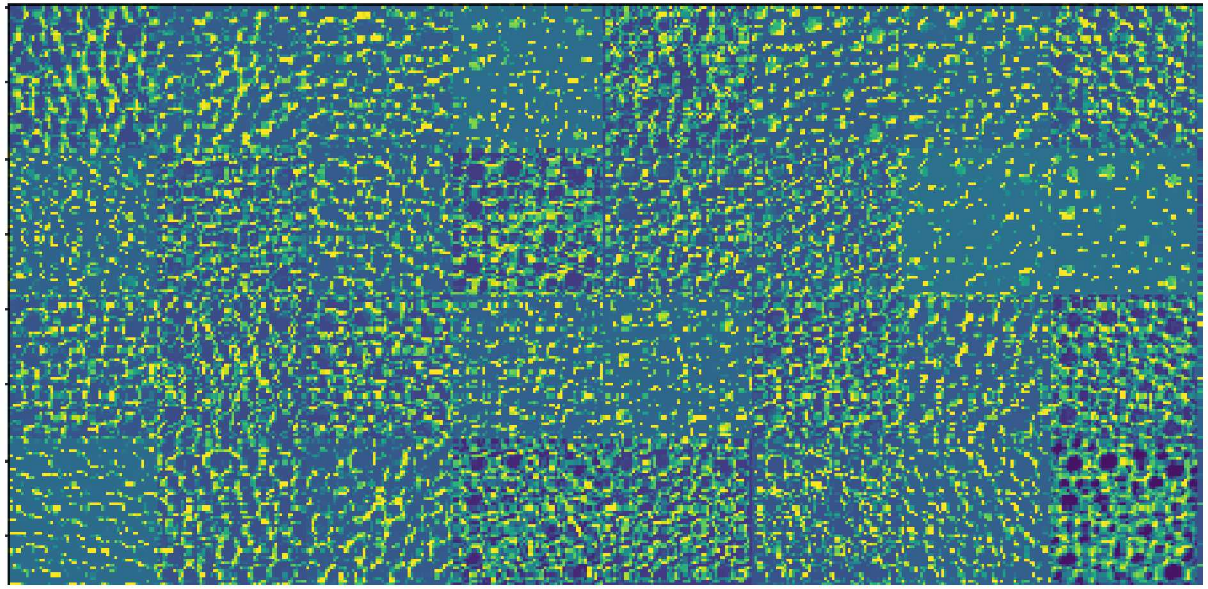
[Conv #1]



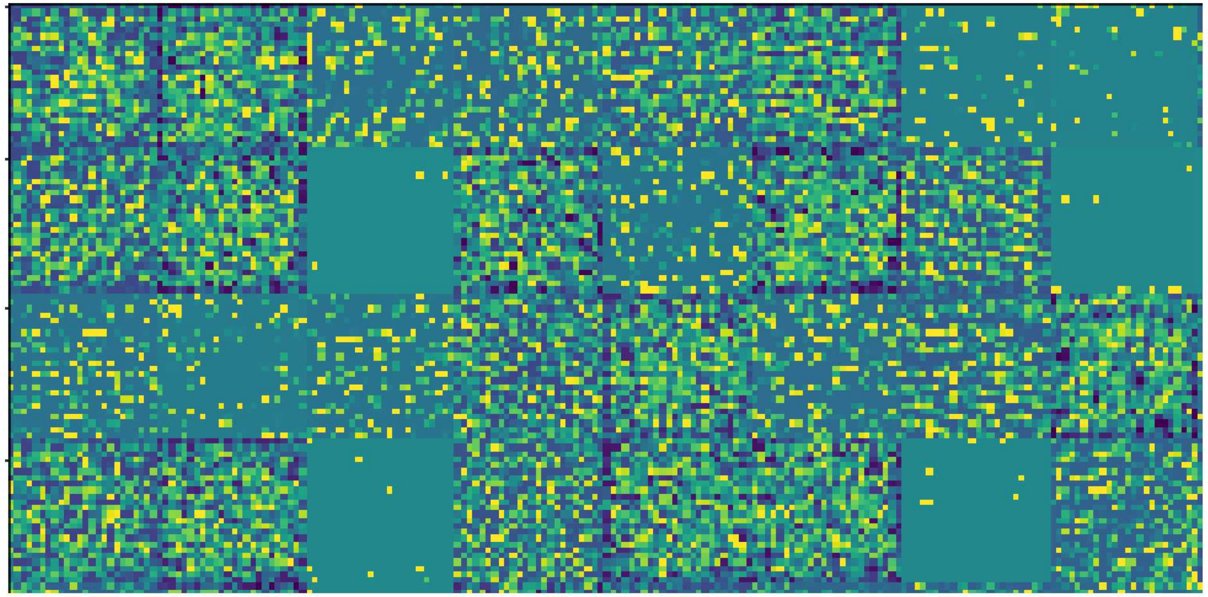
[Conv #2]



[Conv #3]



[Conv #4]



Near Future Works

Incorporation of physical features and data can enhance ML prediction

- Permeability prediction with physical data performed better than the case with image only
- More complex image data with real earth materials will be used with transfer learning using preexisting models (e.g., VGG16) as in semantic image segmentation
- 3D model is under evaluation for 3D permeability prediction
- Incorporation of physical features and equations/residual as physical constraints has a broad implication for PIML