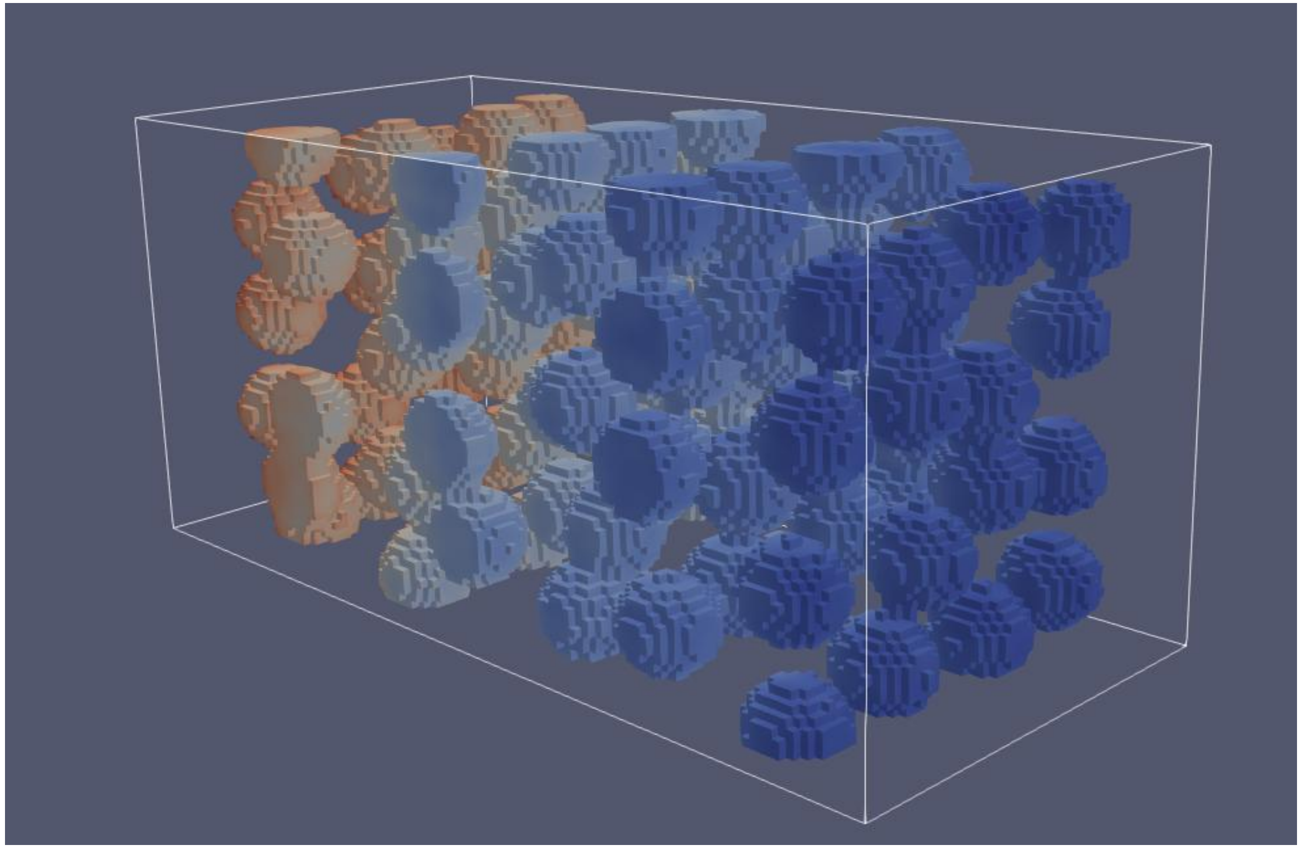
Friedrich-Alexander-Universität
Technische Fakultät

Master Thesis
Estimating Permeability of Porous Media with Fourier Neural Operators

by Lukas Schröder

Agenda

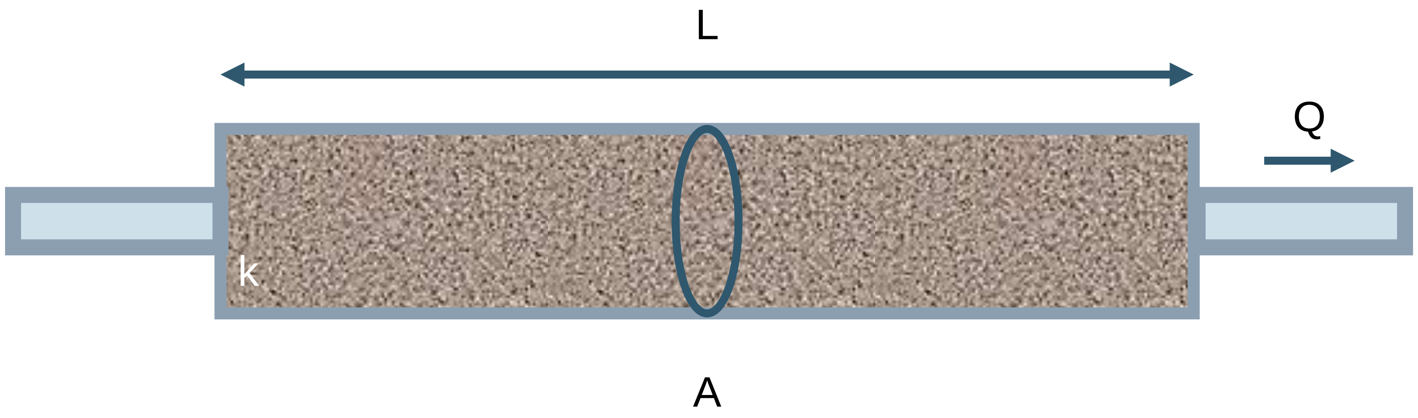


01 Task

01 Task

Goal

- Aim is finding the hydraulic resistance R of provided 3D media
  - Governed by Darcy's law in steady state laminar flows
  - $Q = \frac{\Delta p}{R}$
- Hydraulic resistance can be calculated from a material property called permeability k together with the geometric scales
  - $R = \frac{\mu L}{kA}$



01 Task

Classical way of permeability estimation

Experiments

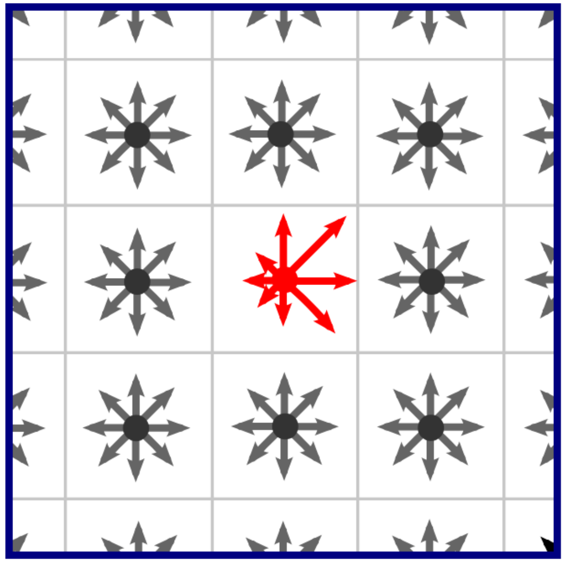
Build a container filled with porous media and measure the pressure difference

Formulas from models

For some geometries, like regular sand and certain rock compositions, there are formulas for permeability from porosity and other properties. Basically, finding correlations with easier to measure parameters.

Numerical Simulation

Derive k from the pressure difference of flow simulations like Lattice Boltzmann methods (LBM) or finite volumes.



01 Task

Thesis approach

Generate sphere geometry in waLBerla → Calculate Flow with LBM in waLBerla/lbmpy → Train machine learning model → Use surrogate model for optimization

Generate sphere geometry in waLBerla

- 3D grid of spheres from different radii and distances, shifted randomly

Calculate Flow with LBM in waLBerla/lbmpy

- Calculate velocities and pressure field

Train machine learning model

- Input: fill flag field
- Output: pressure field
- **Extract: pressure difference**

Use surrogate model for optimization

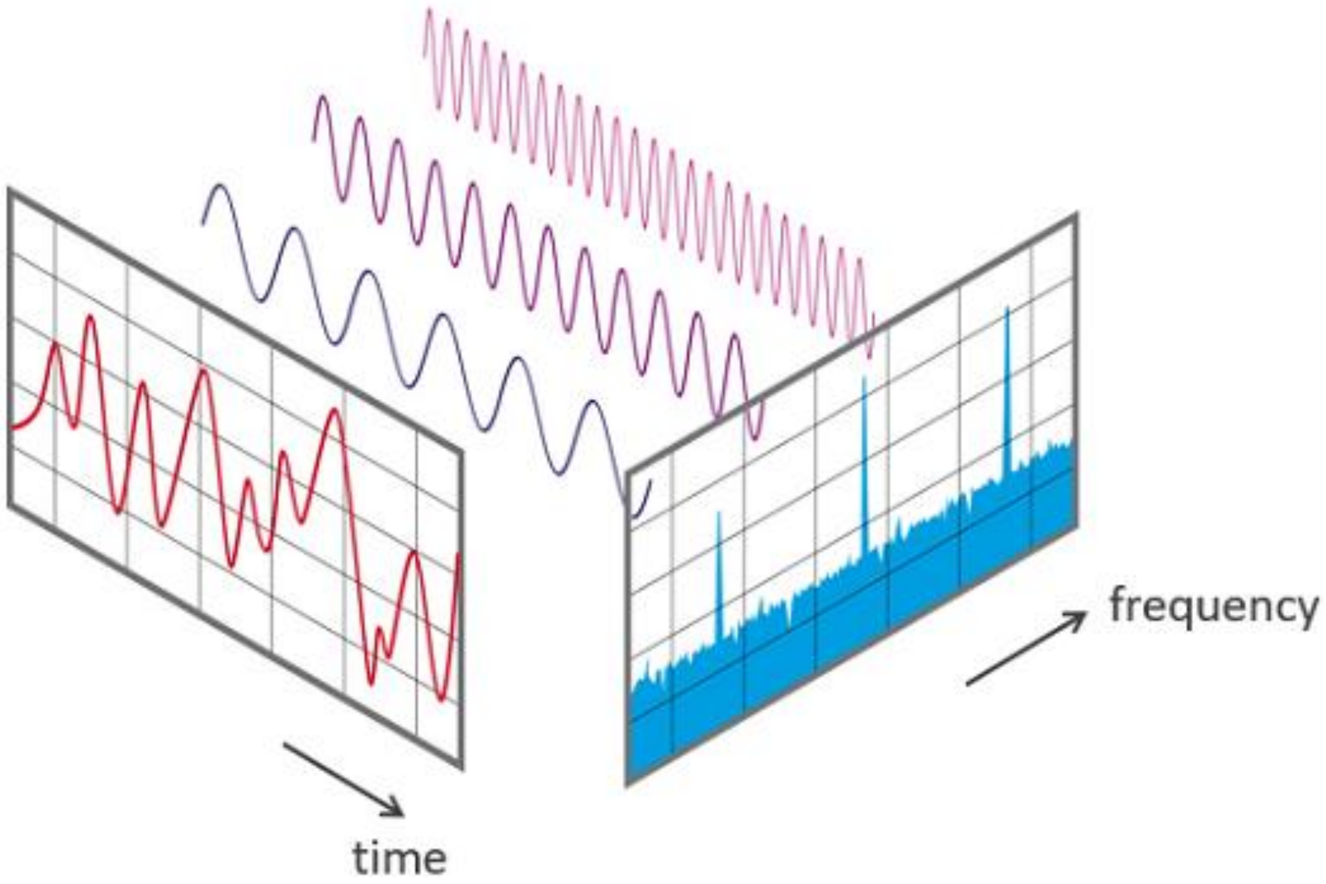
- Inference
- Find geometry with lowest permeability
- Very fast

02 Fourier Neural Operators

Neural Operator

- Idea to learn mapping between infinite function spaces $G: A \to U$
  - Used for example in learning PDEs
- Needs a lifting layer Q to transfer discrete input into higher dimensional codomain
  - Here 3D convolution with kernel size 1
- Projection layer P to transport result back into discrete structures
  - *SIREN* or 2 linear layers
  - This allows for different resolutions of the same problem with the same network

Fourier Transformation

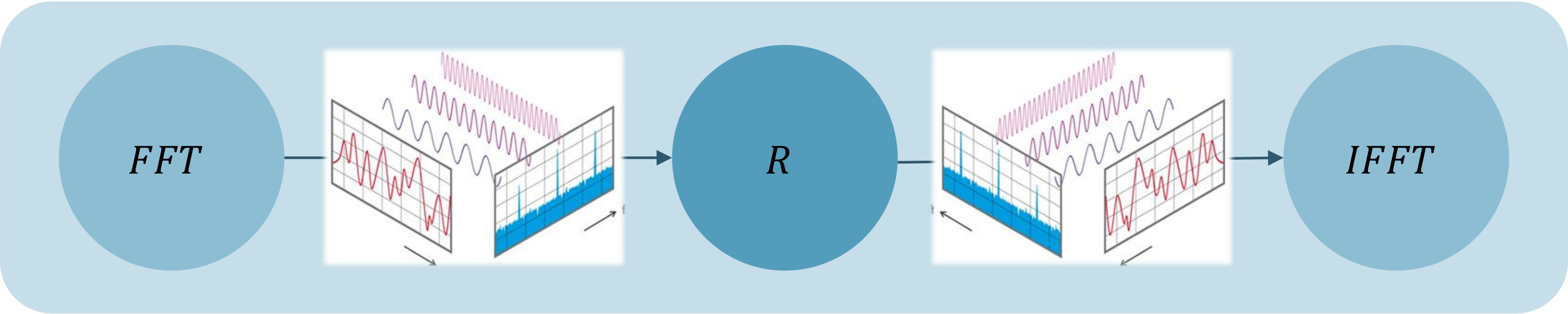


FFT (nti-audio.com)

02 Fourier Neural Operators

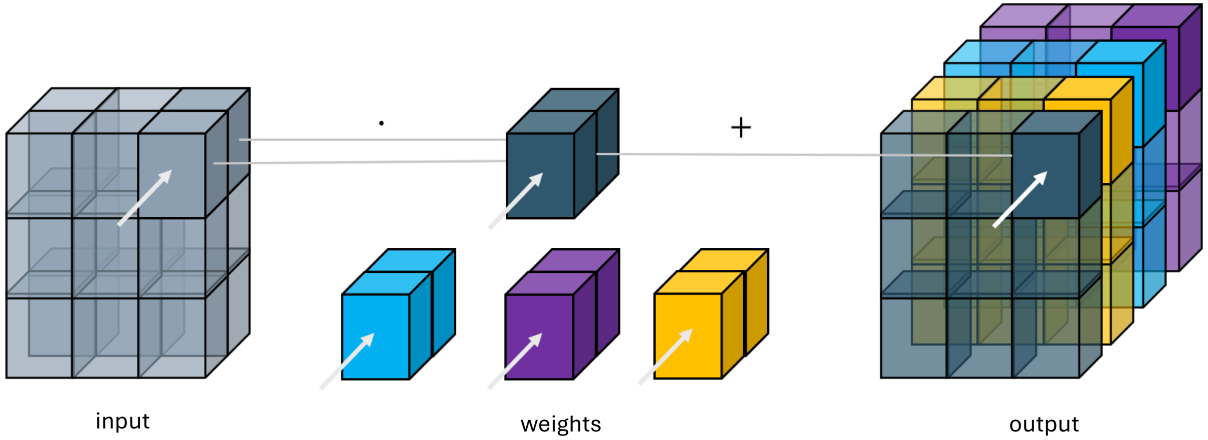
Fourier Neural Operator

- With the kernel integral operator
  - $K(x) = IFFT\big(R \cdot FFT(x)\big)$



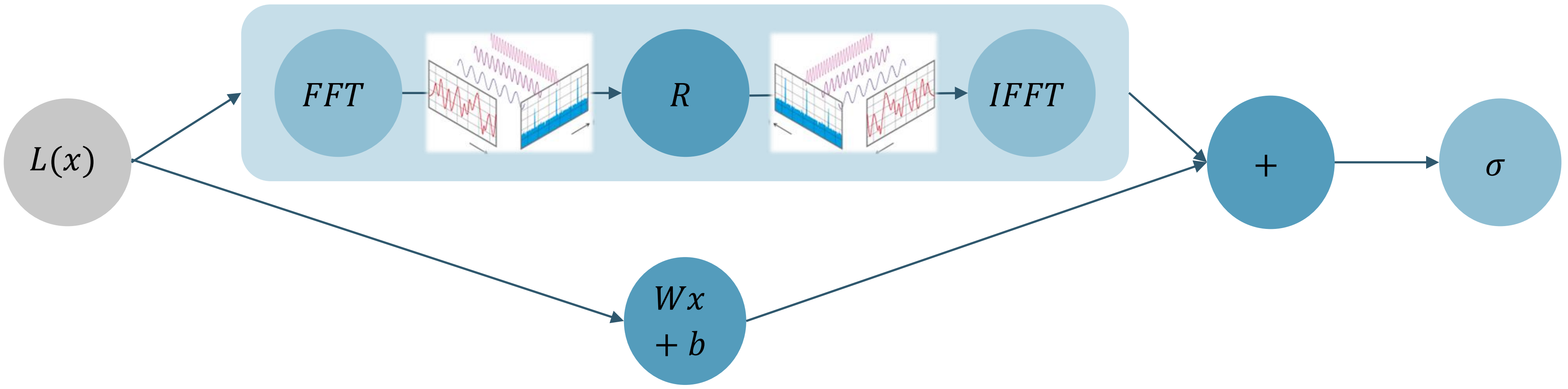
Fourier Neural Operator

- With the kernel integral operator
  - $K(x) = IFFT\big(R \cdot FFT(x)\big)$
- And with 1x1 convolutions as weight application ($Wx + b$)

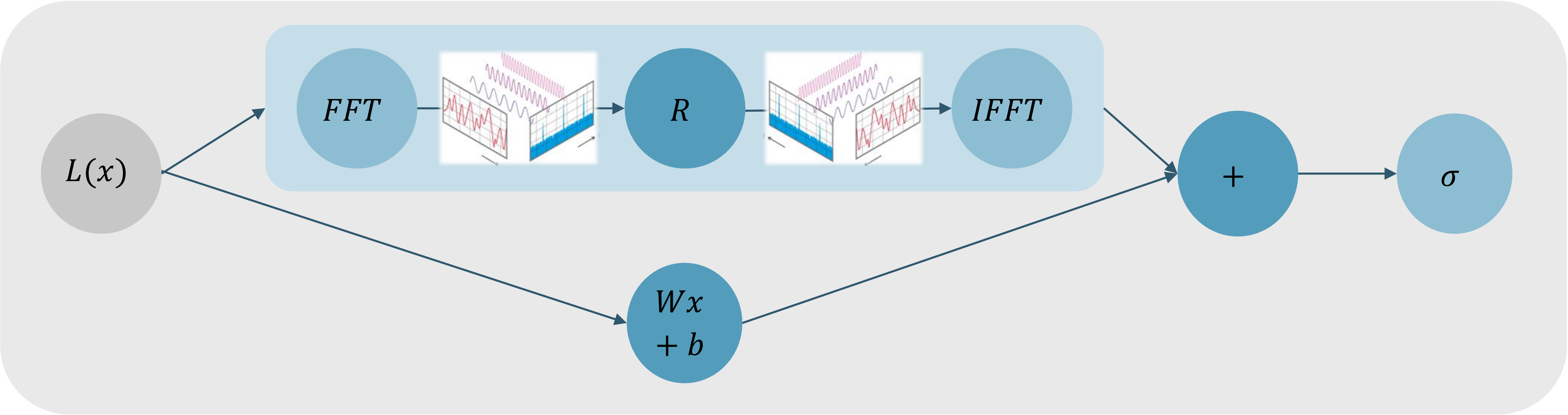


Fourier Neural Operator

- With the kernel integral operator
  - $K(x) = IFFT\big(R \cdot FFT(x)\big)$
- And with 1x1 convolutions as weight application ($Wx + b$)
- Fourier neural operator apply linear transformation in the frequency space in layer L
  - $L(x) = \sigma(Wx + b + K(x))$

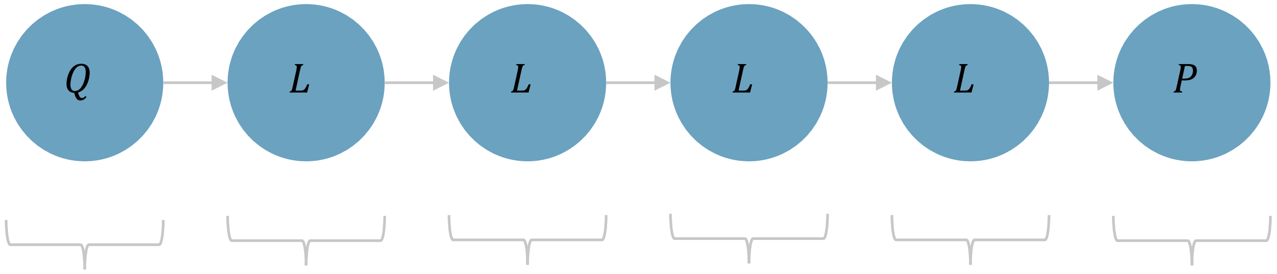


- Fourier neural operator apply linear transformation in the frequency space in layer L
  - $L(x) = \sigma(Wx + b + IFFT(R * FFT(x))$



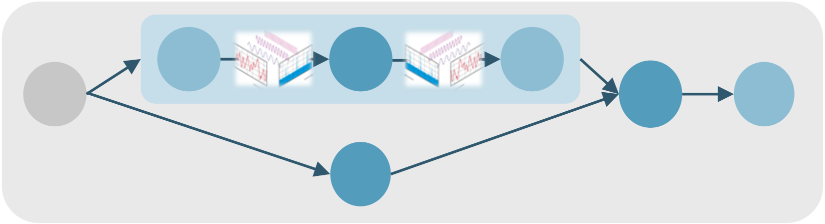
Fourier Neural Operator

- Fourier neural operator apply linear transformation in the frequency space in layer L
  - $L(x) = \sigma(Wx + b + IFFT(R * FFT(x))$
- Resulting model: $G: Q \circ \sigma(L^{(1)} \circ L^{(2)} \circ L^{(3)} \circ L^{(4)}) \circ P$



Lifting:

2x Linear Layer



Projection:

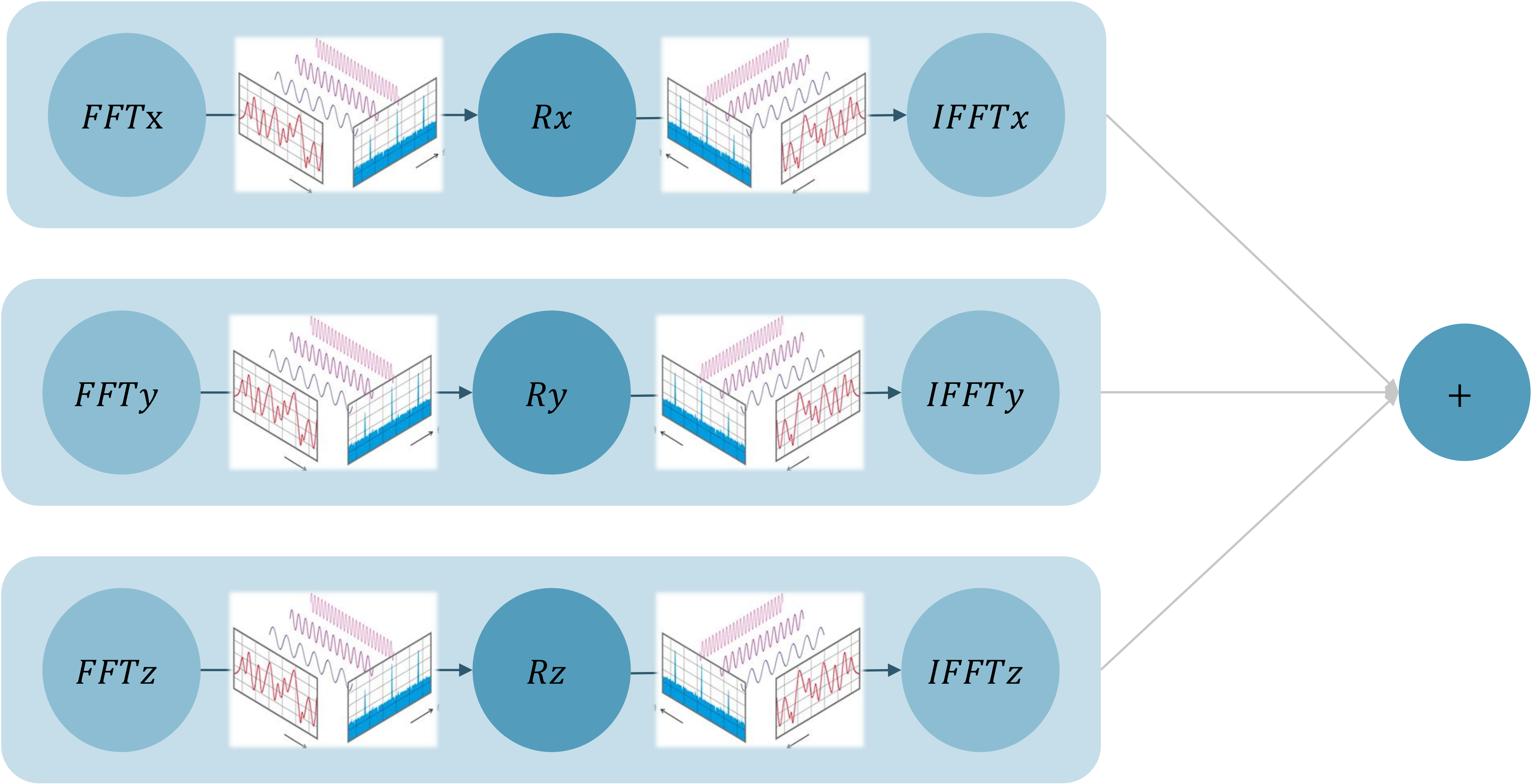
SIREN

02 Fourier Neural Operators

Factorized Fourier Neural Operator

- *Factorized Fourier Neural Operator* for deeper networks
- Splits the Fourier kernel in the three dimension

Factorized Fourier Neural Operator



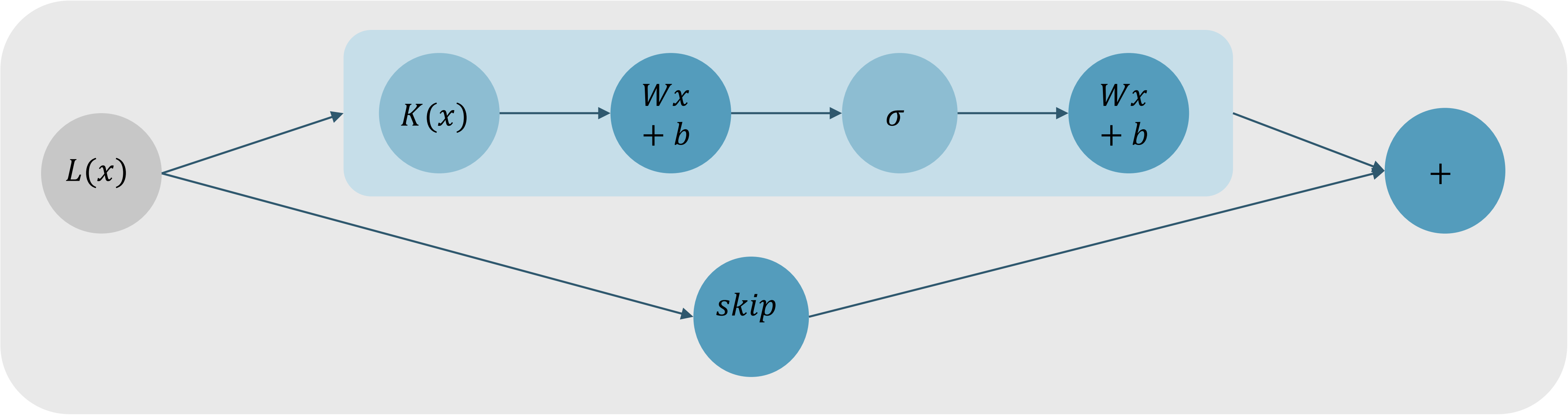
Factorized Fourier Neural Operator

- *Factorized Fourier Neural Operator* for deeper networks
- Splits the Fourier kernel in the three dimension
  - Reduction of model complexity

02 Fourier Neural Operators

Factorized Fourier Neural Operator

- *Factorized Fourier Neural Operator* for deeper networks
- Splits the Fourier kernel in the three dimension
- Borrows concepts from transformer and classical deeper networks
  - Feed forward block with two linear layers per Fourier block with weight normalization
  - Residual connections



02 Fourier Neural Operators

Factorized Fourier Neural Operator

- *Factorized Fourier Neural Operator* for deeper networks
- Splits the Fourier kernel in the three dimension
- Borrows concepts from transformer and classical deeper networks
  - Feed forward block with two linear layers per Fourier block with weight normalization
  - Residual connections
  - Added weight normalization
  - Cosine learning rate scheduling with warmups
- Deeper networks mean more layers that result in more calculation per epoch

03 Experiments & Results

03 Experiments & Results

Overview

Packed Spheres

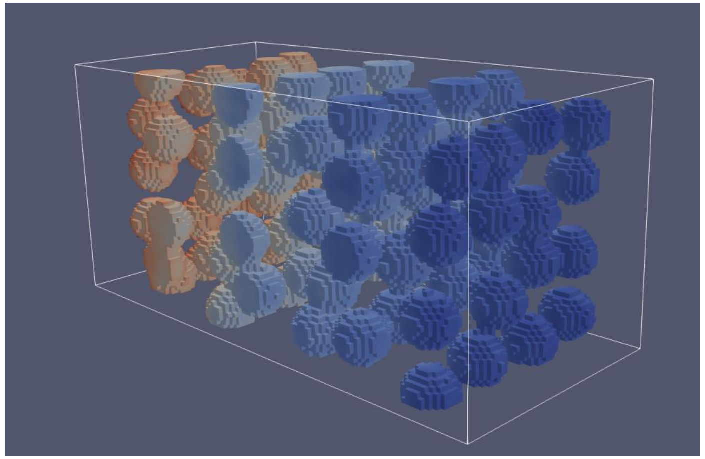
- Used for proving realizability
- Created from a waLBerla performance test setup with random shifts

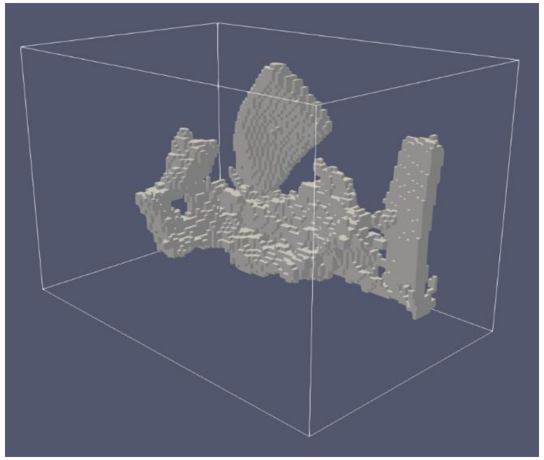
Digital Rock Project Dataset

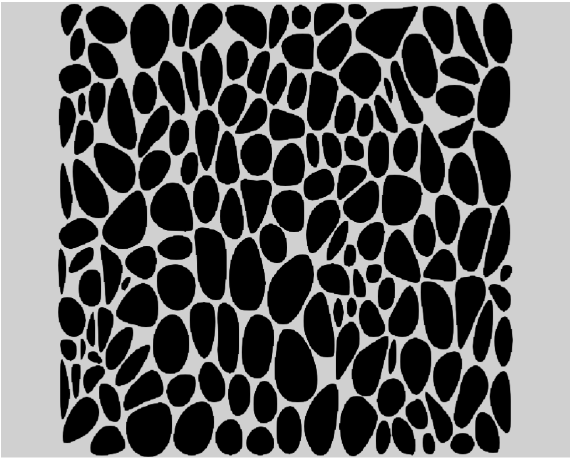
- Small, complex diverse dataset for limit testing
- Overview set of 133 real and synthetic porous media

2D

- From original paper used *in Impana Somashekars* thesis
- Used for comparison with Swin transformers performance





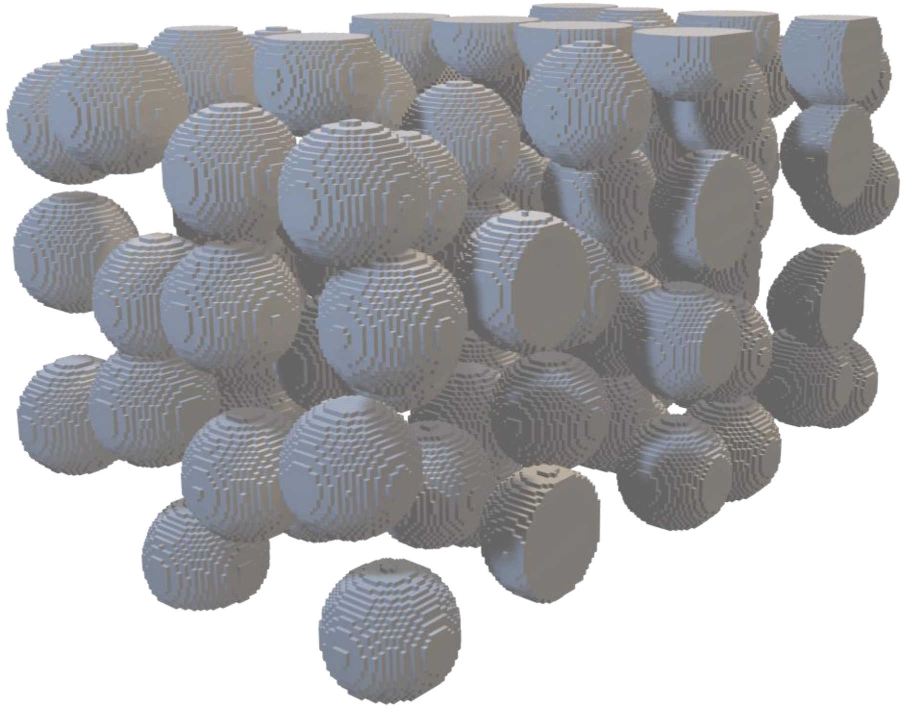


03 Experiments & Results

Realizability with Packed Spheres

Packed Spheres

- Used for proving realizability
- Created from a waLBerla performance test setup with random shifts
- $256x128x128$ domain filled with spheres of diameter $[15, 30]$ and distances $[\text{diameter} + 1, \text{diameter} + 8]$
- Setup
  - Input as $128x64x64$
  - $[32, 16, 16]$ modes in spectral kernel
  - AdamW as optimizer
  - Learning rate in $[0.0025, 0.000125]$



03 Experiments & Results

Realizability with Packed Spheres

Results

- All reach an R^2 score > 98
- No performance increase for original model after 4 layers
- Factorized version better overall
- Proximity of the results
- Factorized models take longer than their original counterpart

Factorized	Layers	MSE field (10^{-2})	MAE (10^{-2})	MAPE	% R^2 Score	Max AE (10^{-2})	Time per epoch in s
False	2	0.039	1.20	4.04	99.18	6.86	**24.28**
False	4	0.017	1.11	3.80	99.35	5.93	44.66
False	6	0.040	1.46	4.80	98.84	7.01	54.75
False	8	0.021	1.34	5.26	99.17	5.56	74.12
True	2	0.054	1.25	5.28	99.42	4.10	48.23
True	4	**0.006**	**0.51**	**2.02**	**99.91**	**1.44**	102.32
True	6	0.009	0.73	3.23	99.80	2.29	131.28
True	8	0.008	0.56	2.66	99.88	1.98	171.56

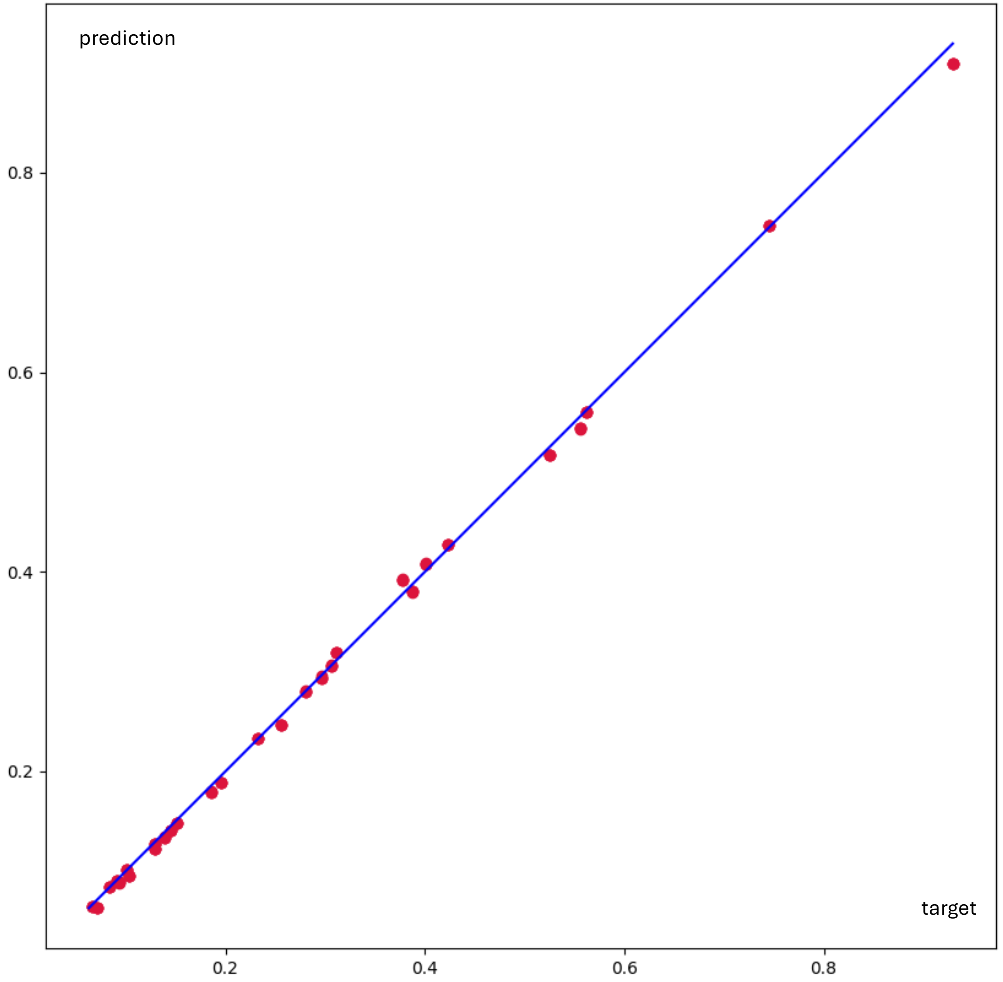
03 Experiments & Results

Realizability with Packed Spheres

Results

- All reach an R^2 score > 98
- No performance increase for original model after 4 layers
- Factorized version better overall
- Proximity of the results
- Factorized models take longer than their original counterpart
- Best configuration: Factorized 4 layer

Factorized	Layers	MSE field (10^{-2})	MAE (10^{-2})	MAPE	% R^2 Score	Max AE (10^{-2})
True	4	**0.006**	**0.51**	**2.02**	**99.91**	**1.44**



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Overview

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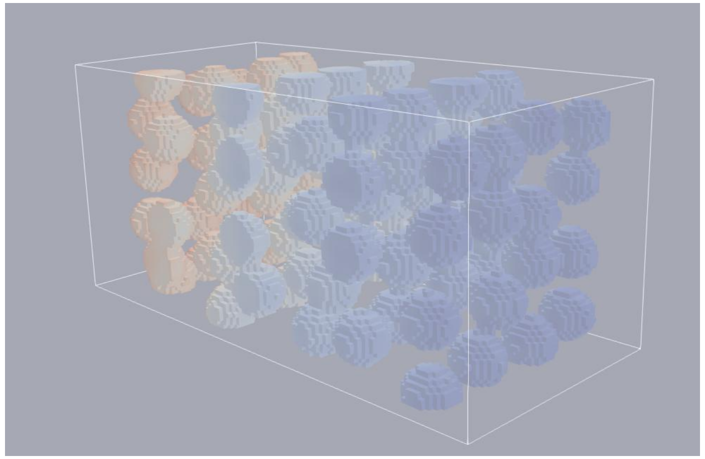
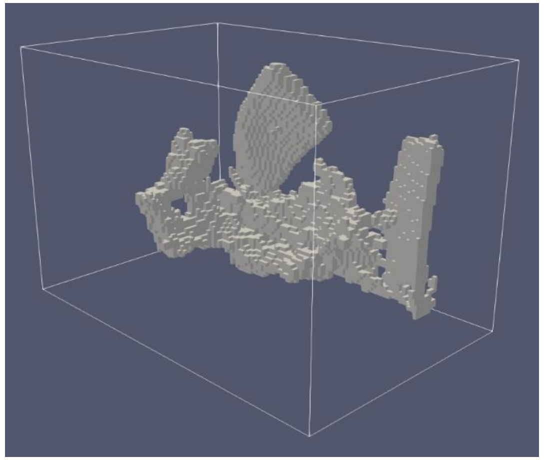


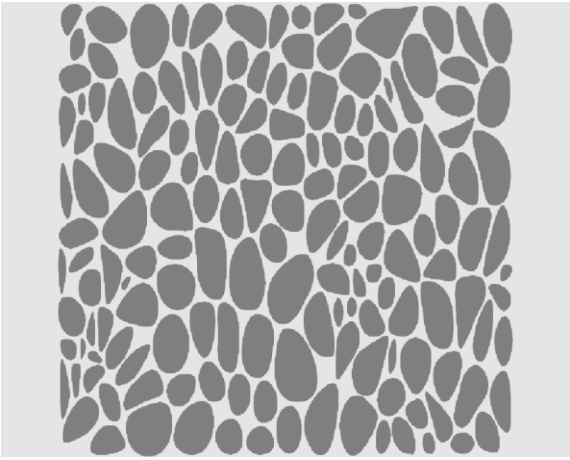
Digital Rock Project Dataset

- Small, complex diverse dataset for limit testing
- Overview set of 133 real and synthetic porous media



2D

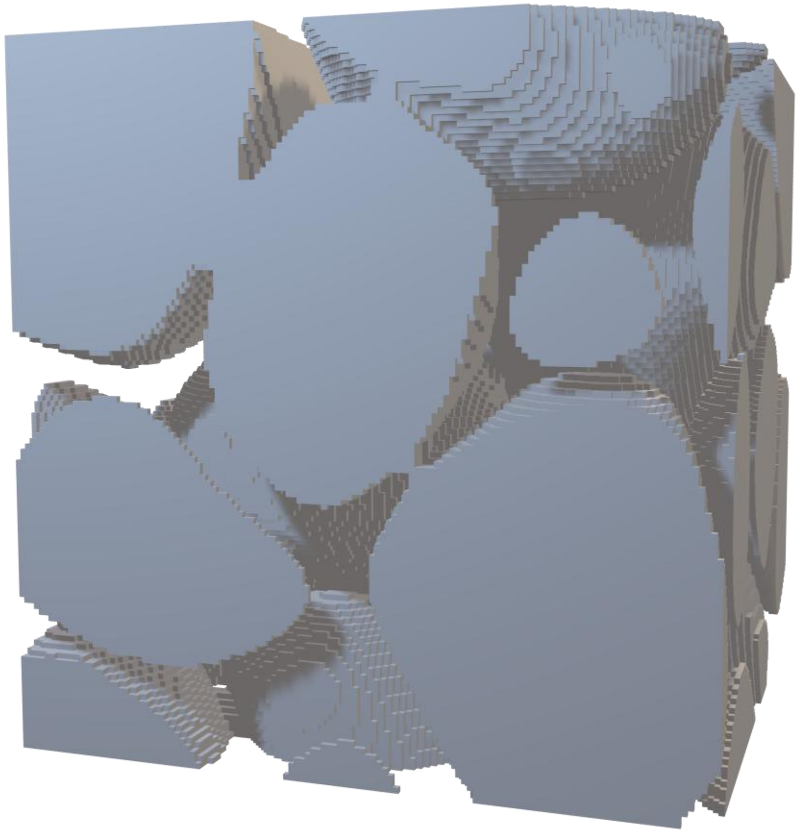
- From original paper used *in Impana Somashekars* thesis
- Used for comparison with Swin transformers performance



Challenging DRP Dataset

Digital Rock Project Dataset

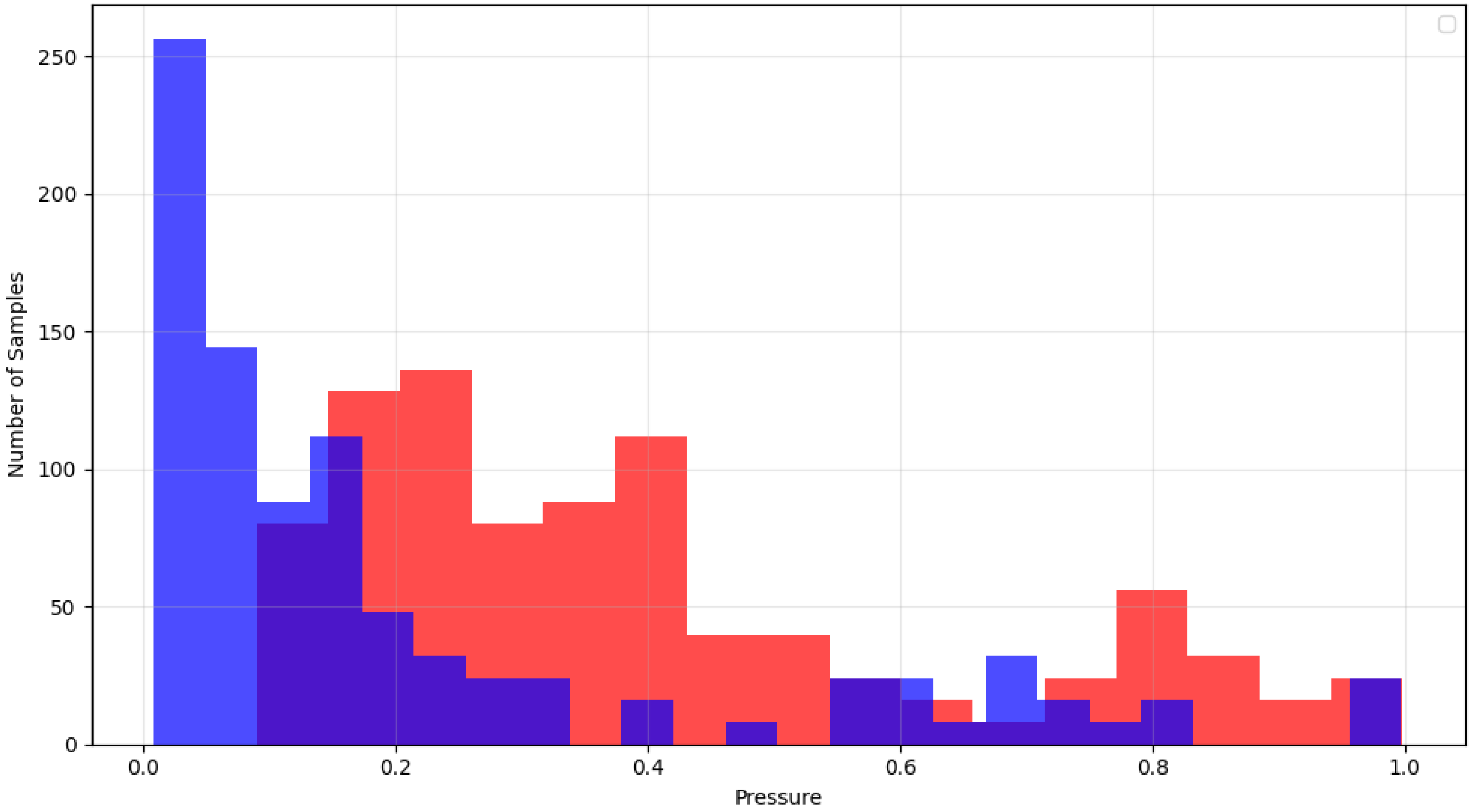
- Small, complex diverse dataset for limit testing
- Overview set of 133 real and synthetic porous media
- Simulated with lbmpy



Challenging DRP Dataset

Digital Rock Project Dataset

- Small, complex diverse dataset for limit testing
- Overview set of 133 real and synthetic porous media
- Simulated with lbmpy
- Data transformed with $x_{\text{trans}} = \sqrt{x}$
- Setup
  - Input as $96x64x64$
  - $[24, 16, 16]$ modes in spectral kernel



03 Experiments & Results

Challenging DRP Dataset

Results

- Hard to achieve R^2 Score > 80
- High maximum absolute errors > 0.4
- High inter-model score fluctuations

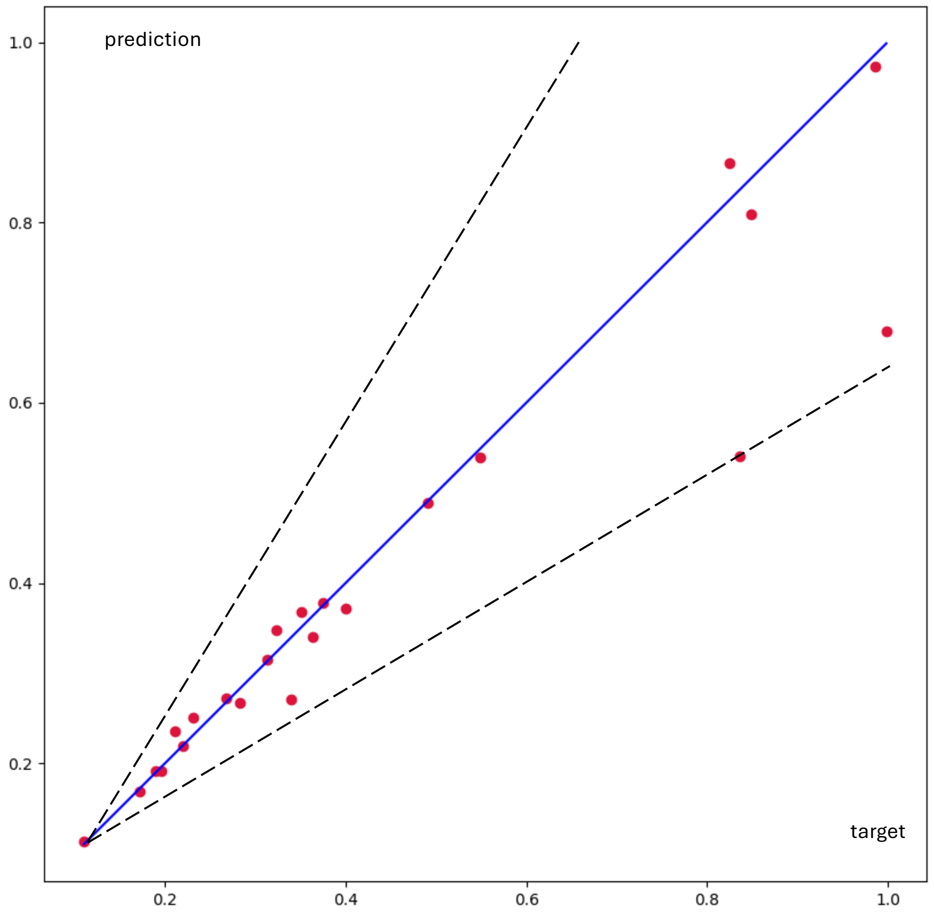
Factorized	Layers	MSE field (10^{-2})	MAE (10^{-2})	MAPE	% R^2 Score	Max AE (10^{-2})	Time per epoch in s
False	2	0.815	6.28	20.83	79.19	46.26	**15.15**
False	4	0.902	6.56	29.25	79.85	52.77	24.97
False	8	0.877	5.98	16.86	76.43	51.40	45.09
True	2	1.249	7.46	31.86	73.11	59.94	27.21
True	4	1.061	6.00	13.68	68.19	70.02	49.50
True	8	**0.862**	**4.42**	**13.17**	**88.54**	**37.48**	102.87
True	12	0.662	5.40	16.79	77.57	65.52	139.31

Challenging DRP Dataset

Results

- Hard to achieve R^2 Score > 80
- High maximum absolute errors > 0.4
- High inter-model score fluctuations
- Hard to predict high pressure cases drive errors
  - Idea: Filter highest 10% out

Factorized	Layers	MSE field (10^{-2})	MAE (10^{-2})	MAPE	% R^2 Score	Max AE (10^{-2})
True	8	0.862	4.42	13.17	88.54	37.48

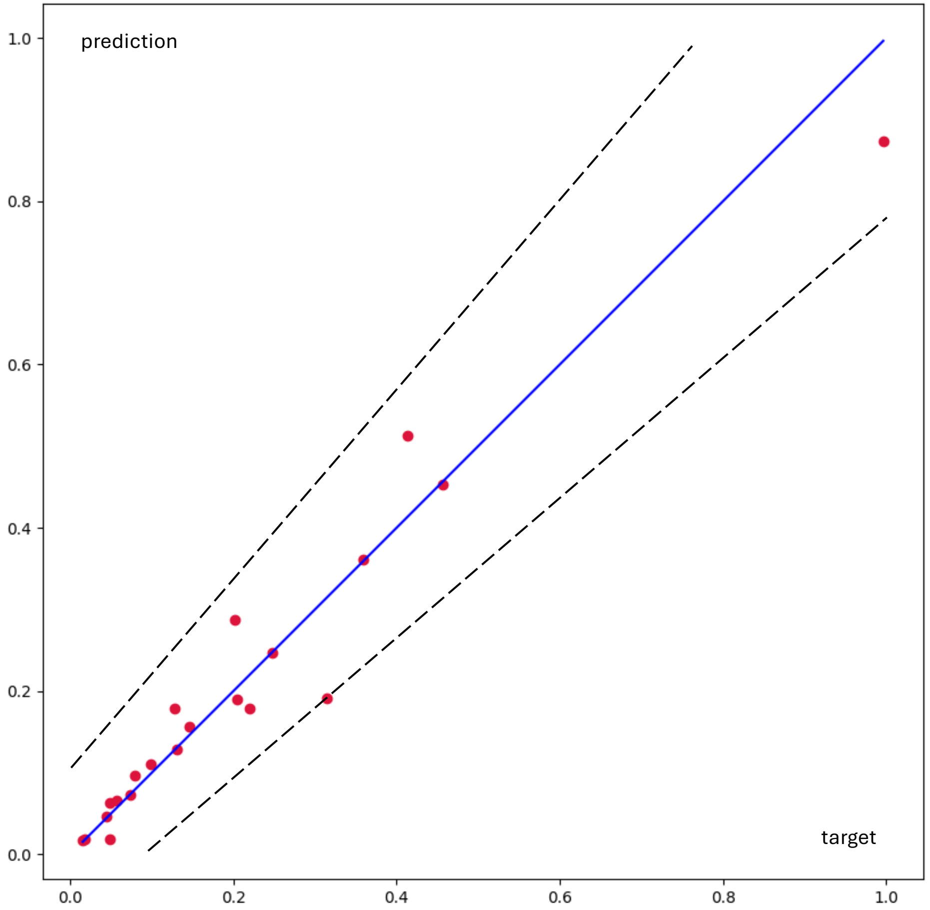


Challenging DRP Dataset

Results

- Hard to achieve R^2 Score > 80
- High maximum absolute errors > 0.4
- High inter-model score fluctuations
- Hard to predict high pressure cases drive errors
  - Idea: Filter highest 10% out

Filtered	MSE field (10^{-2})	MAE (10^{-2})	MAPE	% R^2 Score	Max AE (10^{-2})
False	0.106	3.06	16.60	94.62	12.34
True	**0.862**	**4.42**	**13.17**	**88.54**	**37.48**



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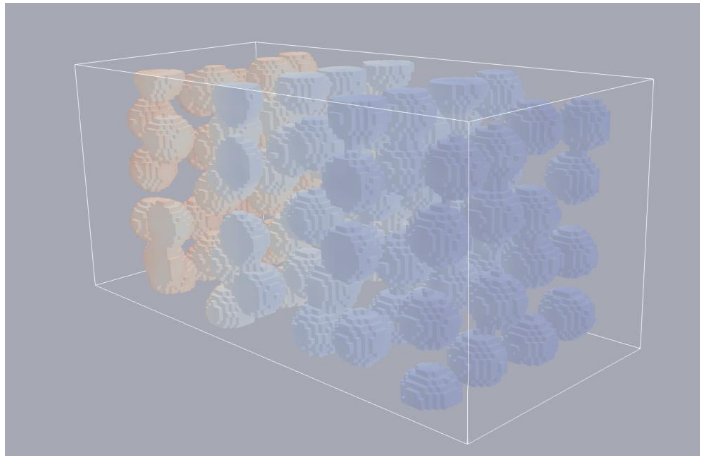
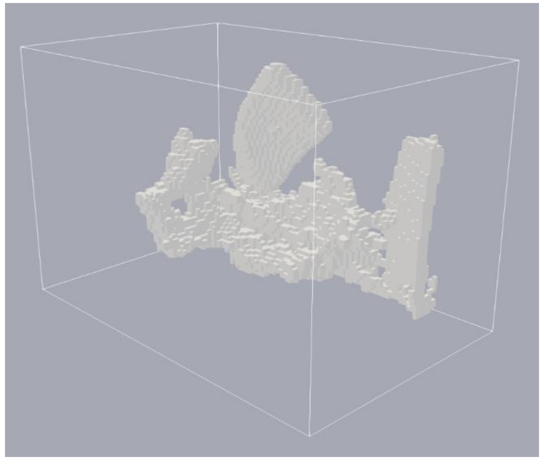
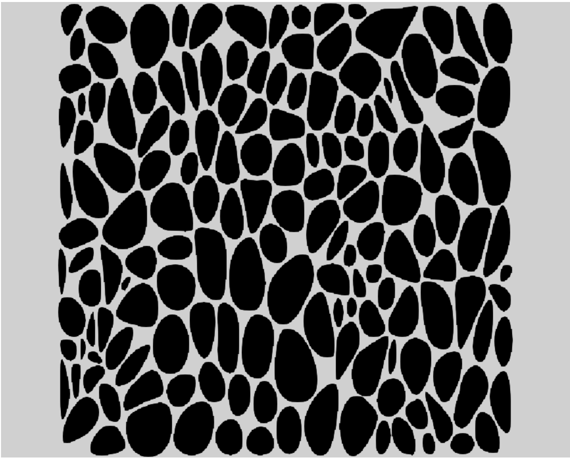
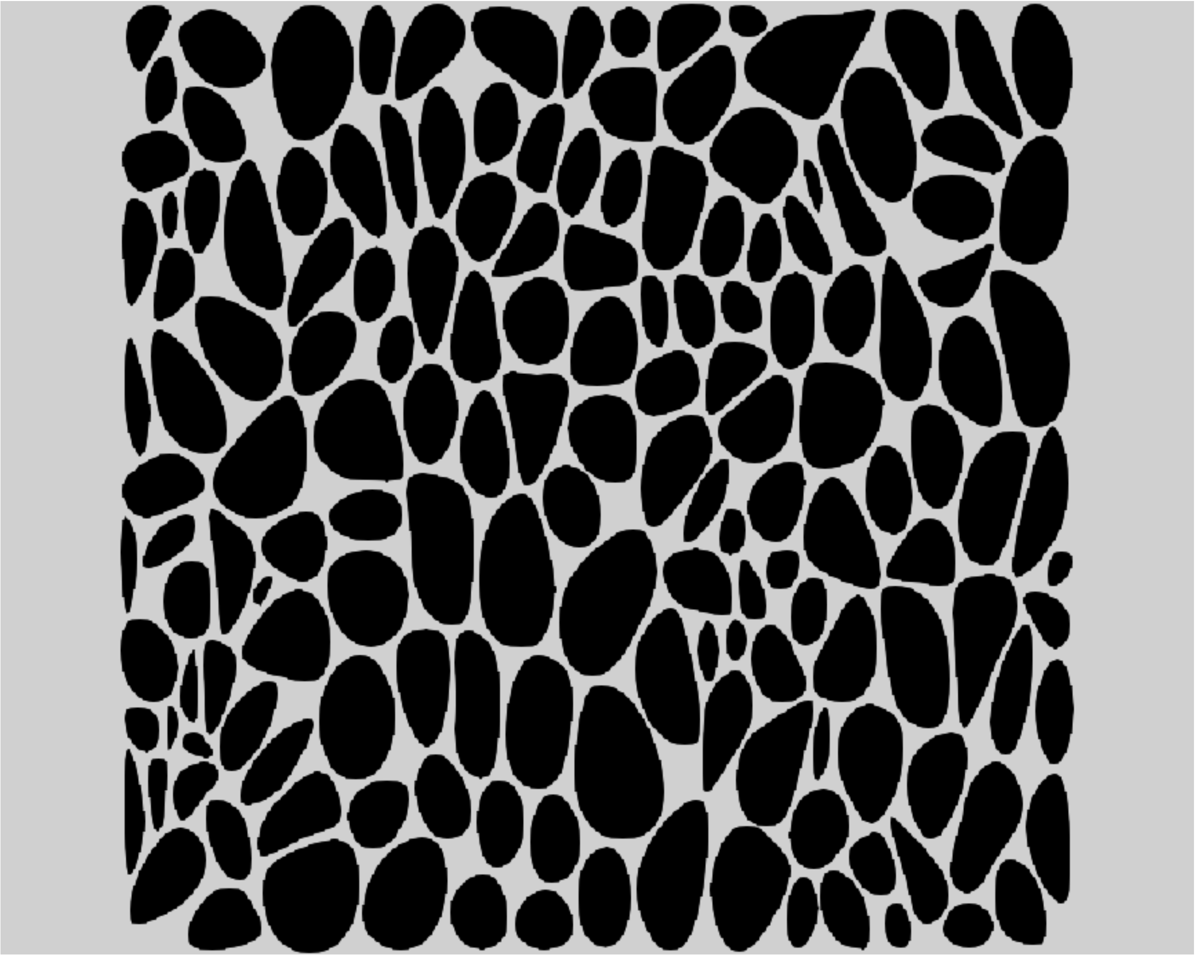






2D

- From original paper used *in Impana Somashekars* thesis
- Used for comparison with Swin transformers performance
- Simulated with lbmpy
- Sets: 1000 generated polynomials, 600 rough sandstone and 200 rocks



2D Comparison

Results

- Good results on standard, full and rock set with R^2 score > 94
- Noisy set fails with R^2 score < 50

Factorized	Layer	Dataset	MSE field (10^{-2})	MAE (10^{-2})	MAPE	R^2 Score	Max AE (10^{-2})	Time per epoch in s
False	4	standard	1.374	1.68	8.44	94.06	28.29	**4.51**
True	4	standard	**0.442**	**0.86**	**5.33**	**98.78**	**10.68**	8.62
True	8	full	0.658	0.70	17.02	94.50	23.00	31.36
True	8	rocks (on full)	5.661	3.46	26.45	93.29	23.00	31.36
True	8	noisy (on full)	0.139	0.60	35.38	47.99	4.69	31.36

2D Comparison

Results

- Good results on standard, full and rock set with R^2 score > 94
- Noisy set fails with R^2 score < 50
- Comparison
  - Slightly improved performance in R^2 scores and maximum AE
  - Training takes only 6% of the transformers time!
  - Noisy set still works with the transformer

Model	Dataset	R^2 Score	Max AE (10^{-2})	Time per epoch in s
FFNO 4-layer	standard	**98.78**	**10.68**	**8.62**
Swin Transformer	standard	98.14	~12	~140
FFNO 8-layer	rocks (on full)	93.29	-	**32.36 (entire set)**
Swin Transformer	rocks	**93.82**	**-**	~80
FFNO 8-layer	noisy (on full)	47.99	-	**32.36 (entire set)**
Swin Transformer	noisy	**92.35**	-	~30

04 Discussion

04 Discussion

Hyperparameter for FNOs

- AdamW, weight normalization and the cosine learning rate scheduling allow for **short training time and stability**

- Original FNO architecture deliver **reliable results in a faster time**
- Original architecture does **not improve for added depth** after 4 layers

- Factorized FNO architecture delivers the **best results** in all tested cases, but not always meaningfully better
- Factorized FNOs **scale better with more layers** until 8 layers (here)

→ 2/4-layer original FNO for efficiency

→ 8-layer factorized FNO for maximum performance

04 Discussion

Use Cases for FNO based Surrogate Models

Comparison with Analytical Solution

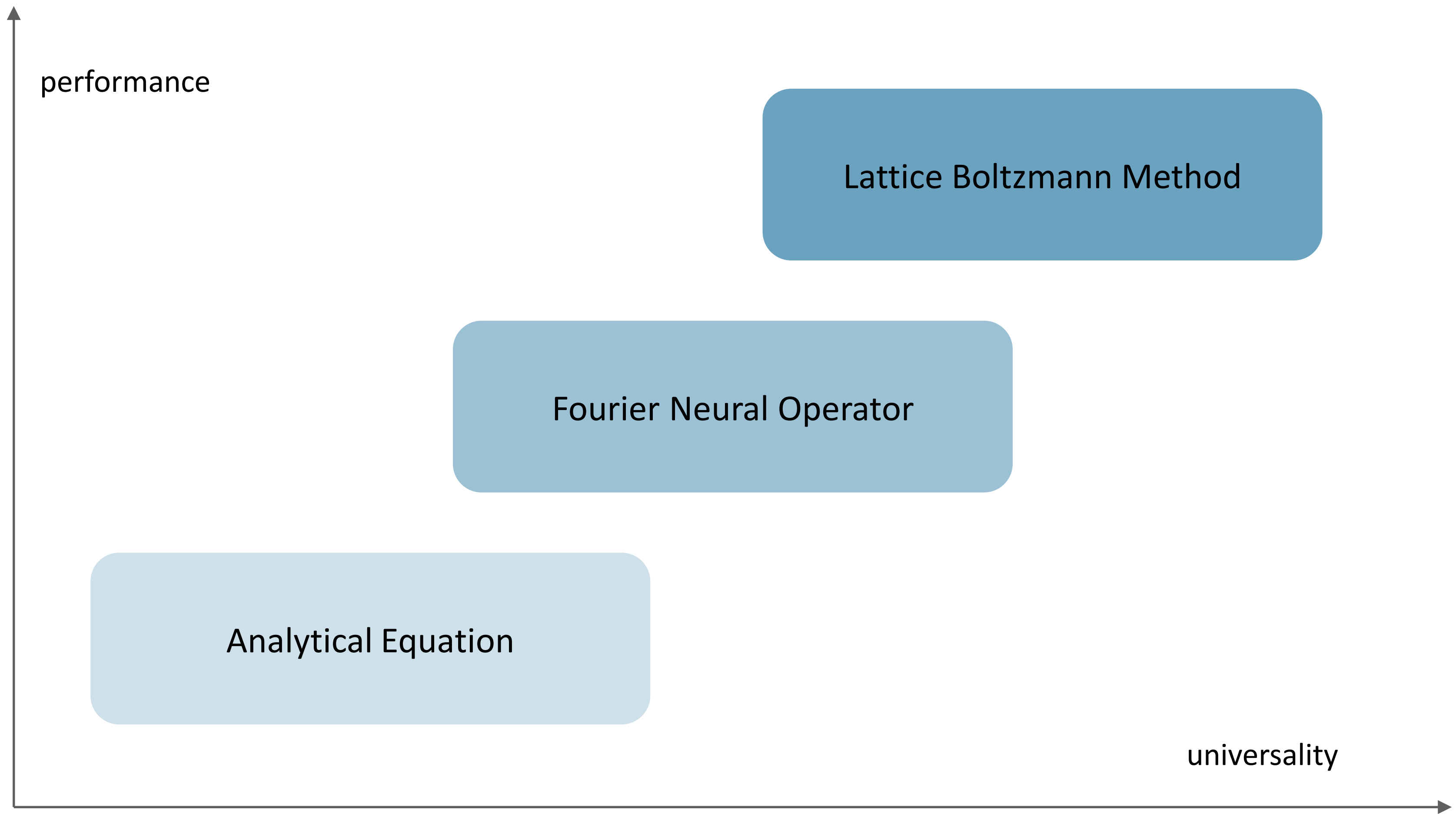
- Formulaic solution are evaluated instantly
- Limited range of applicable geometries
- Performance Example:
  - Shifted spheres with *Kozeny-Carman* equation
  - R^2 score 95.04 (FFNO 4-layer 99.91)

Comparison with LBM

- LBM is more accurate and calculations can be parallelized
- Can be simulated for (nearly) any geometry
- Speed comparison
  - One sample $\sim 207s$ with lbmpy (vs $\sim 0.15s$ inference) on the same GPU
  - Breaking even point with FNO training, simulating training samples and evaluation:
    - ~ 275 evaluation samples
    - when trained on 250 simulated geometries

04 Discussion

Use Cases for FNO based Surrogate Models



05 Conclusion & Outlook

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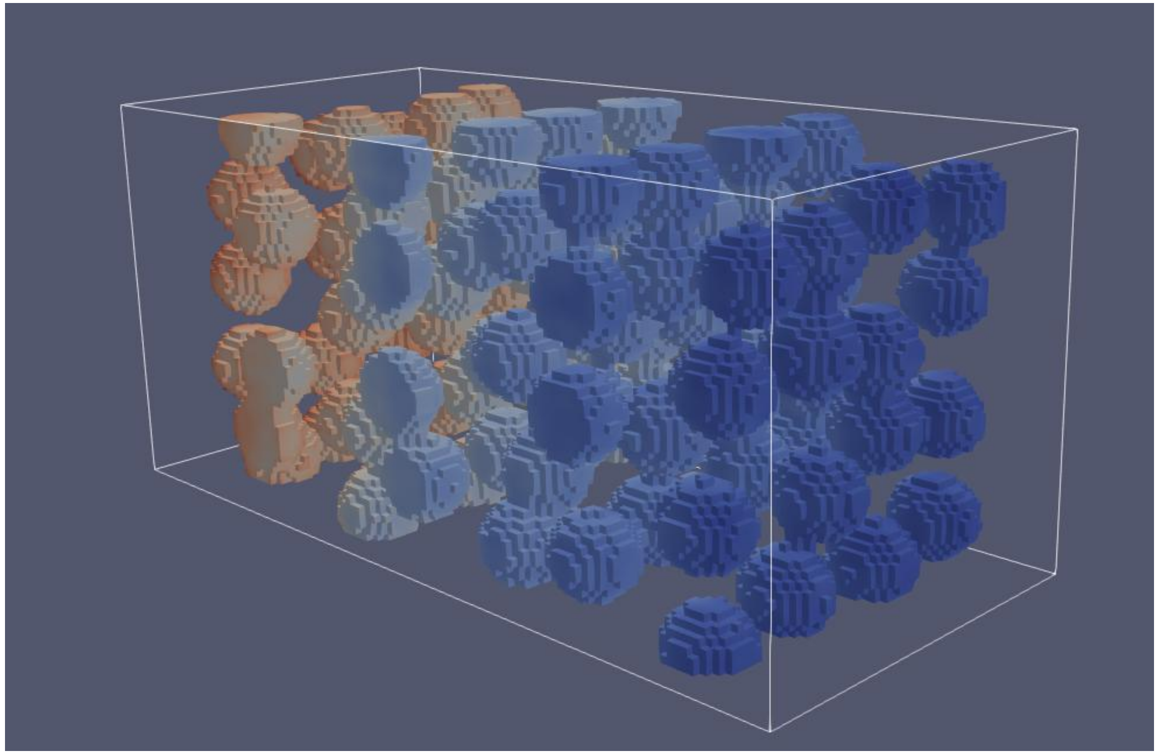
5 Learnings

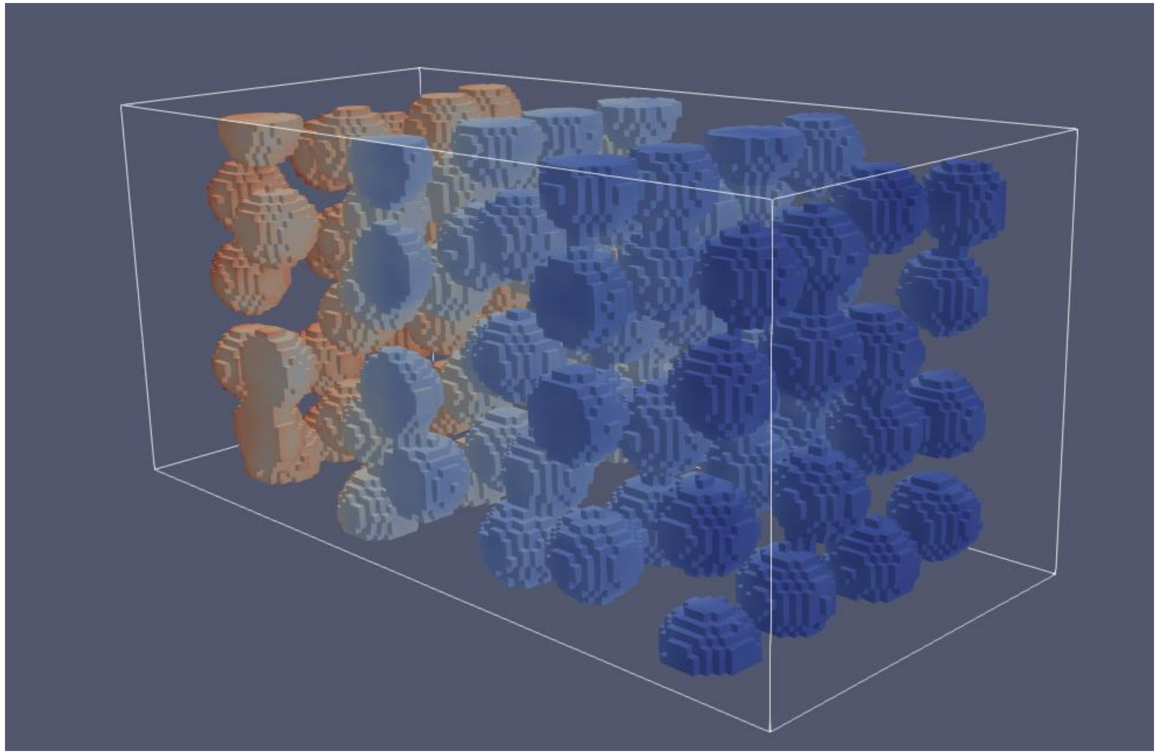
- Fourier neural operators can capture the pressure field to a reliable degree
- When enough geometries are provided of similar cases, wide ranges of cases can be predicted
- Original architecture is best for efficiency, while the factorized performs best
- It can bridge the range of LBM with the speed closer to analytical solutions with a state-of-the-art NN
- Use case is when many similar geometries need to be evaluated quickly



05 Conclusion & Outlook

Outlook

- Test scalability with big and complex databases
- Investigations of physically informed neural networks (PINNs)
- Comparison with more modern and elaborate analytical solution
- Test FNOs on entire flow prediction



Thanks
for Your Attention