The Permeability of Gas Diffusion Layers based on Fibrous Micro-Structures using Machine Learning

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Simulation

Darcy's law: $u = \kappa \dfrac{\nabla P}{v} \Rightarrow \kappa = \dfrac{u \cdot v}{\nabla P}$

Through-plane permeability, uncompressed
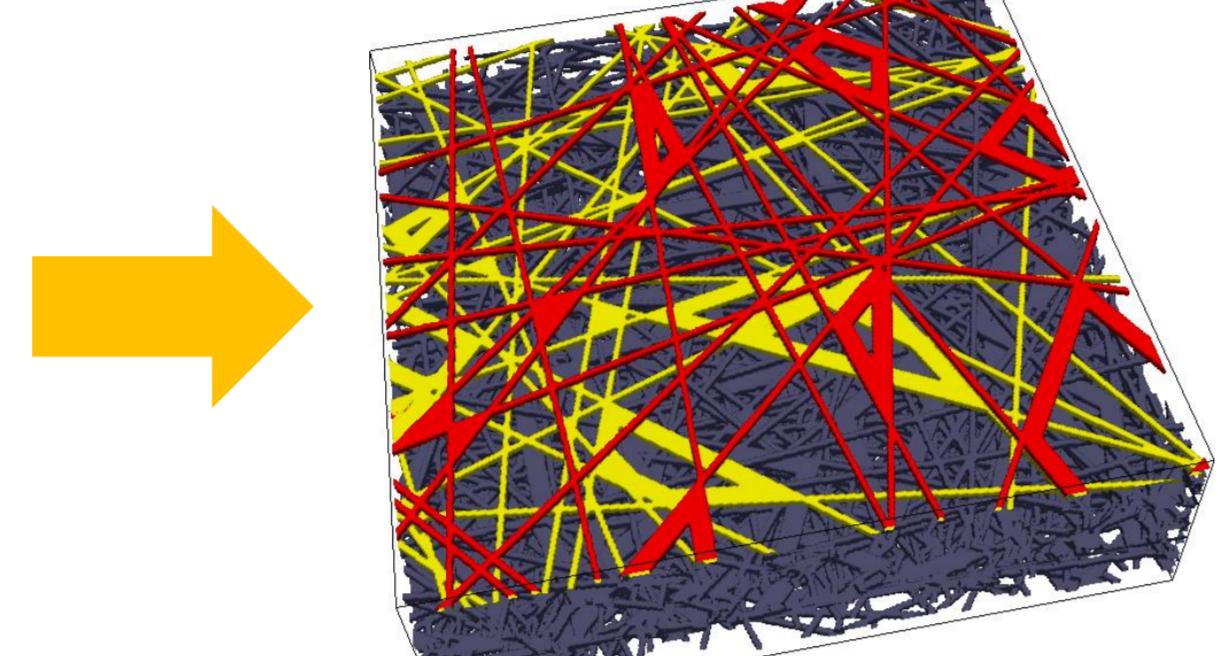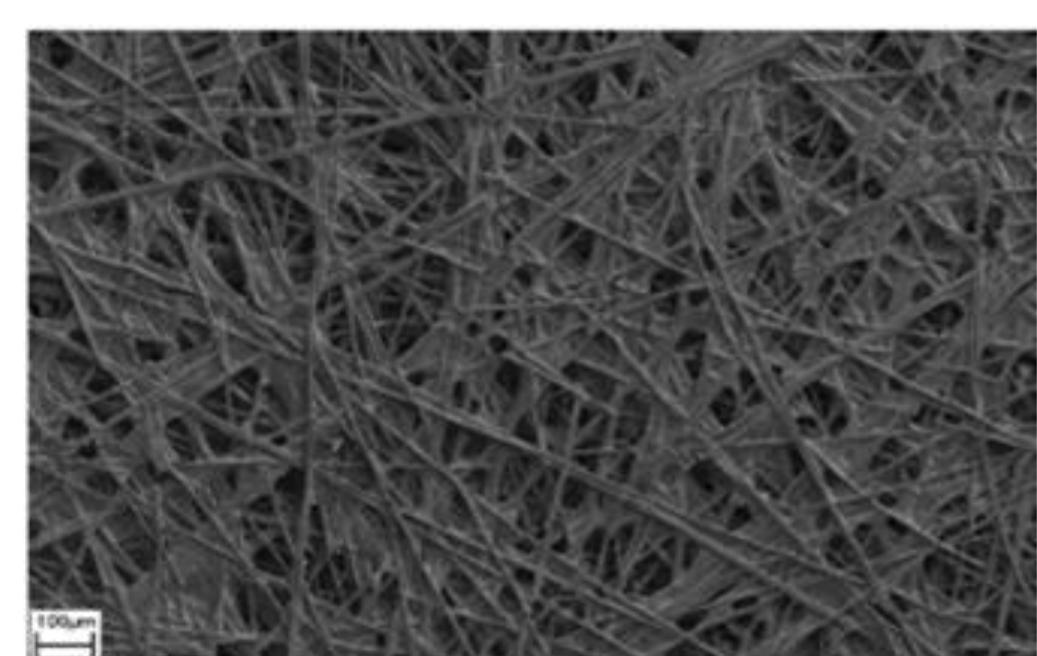
Fig. 1. SEM image of Toray 090 GDL. Fig. 2. Stochastic   geometry model. Fig. 3. JURECA at Forschungszentrum Jülich.   Fig. 4. Results of transport simulations [1].

Training on GPUs
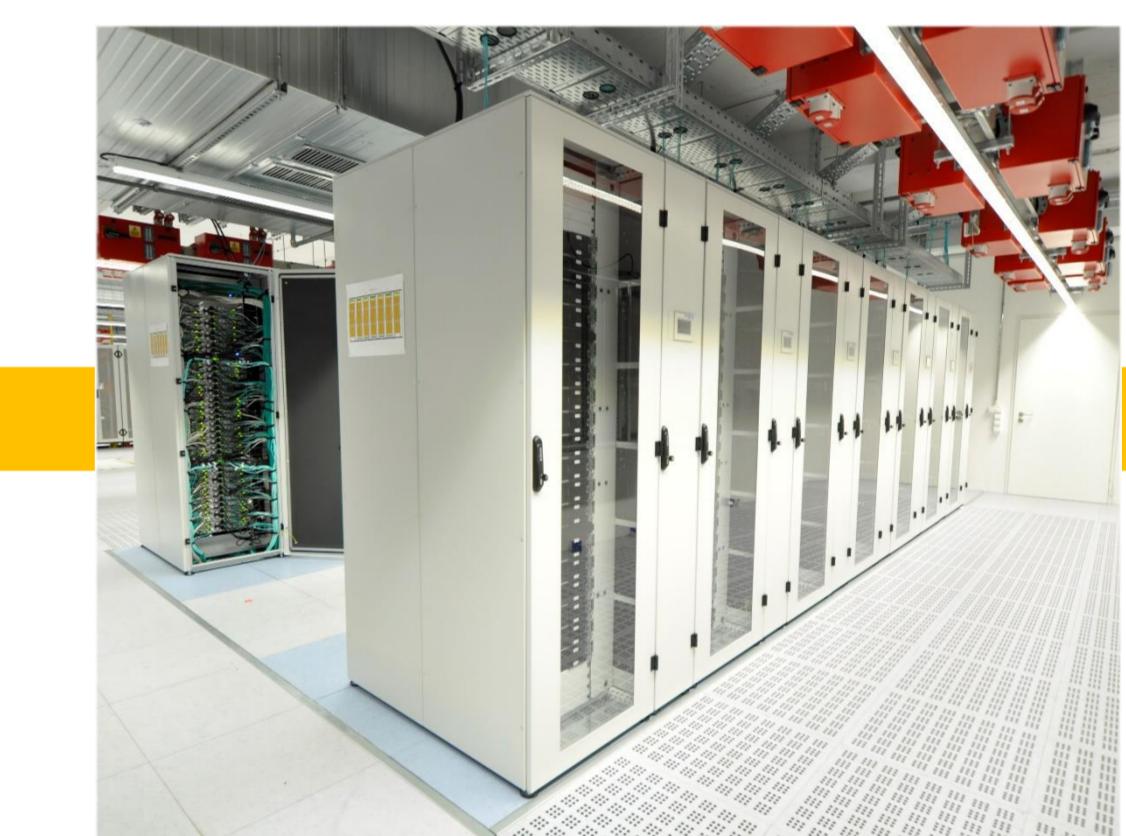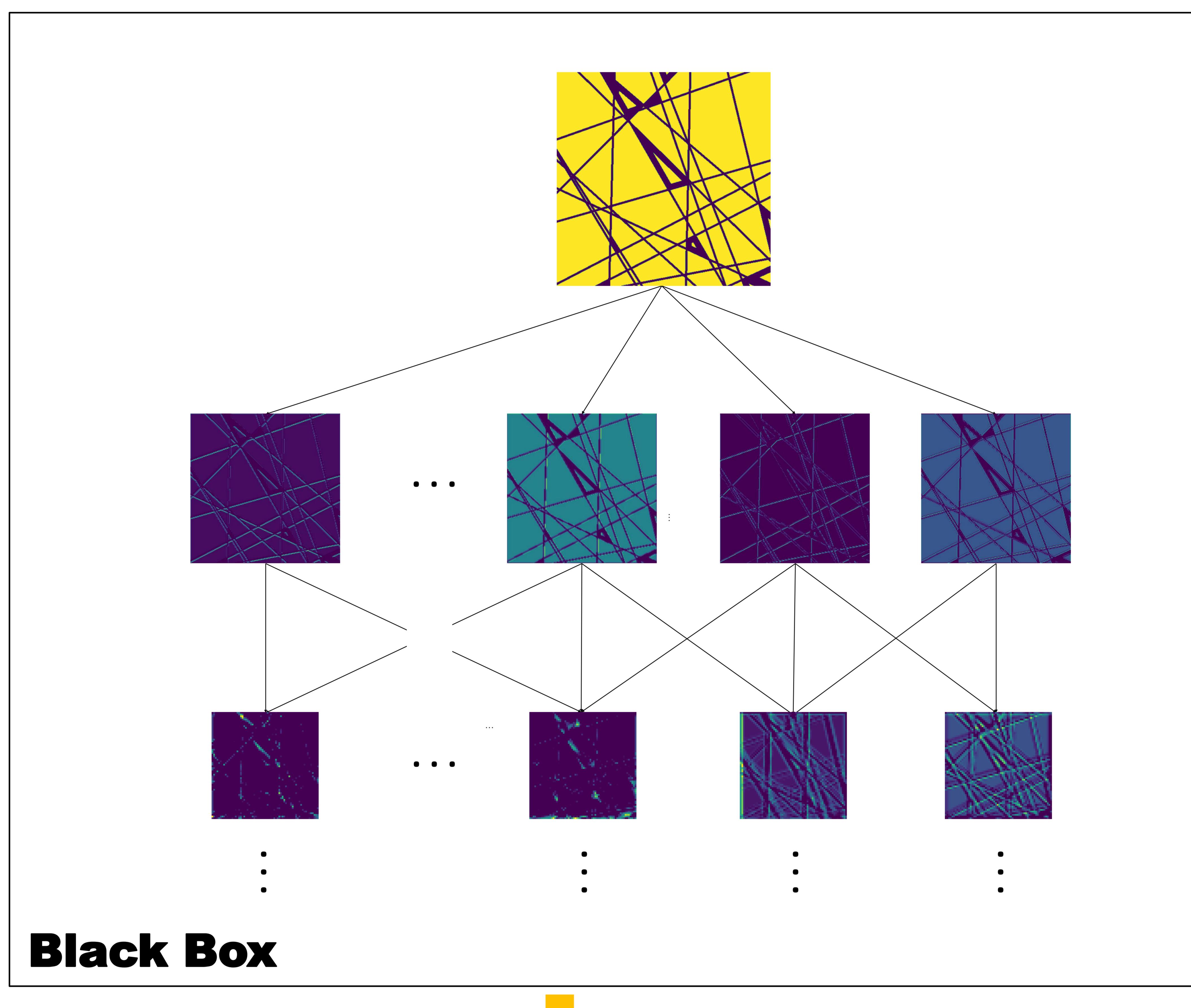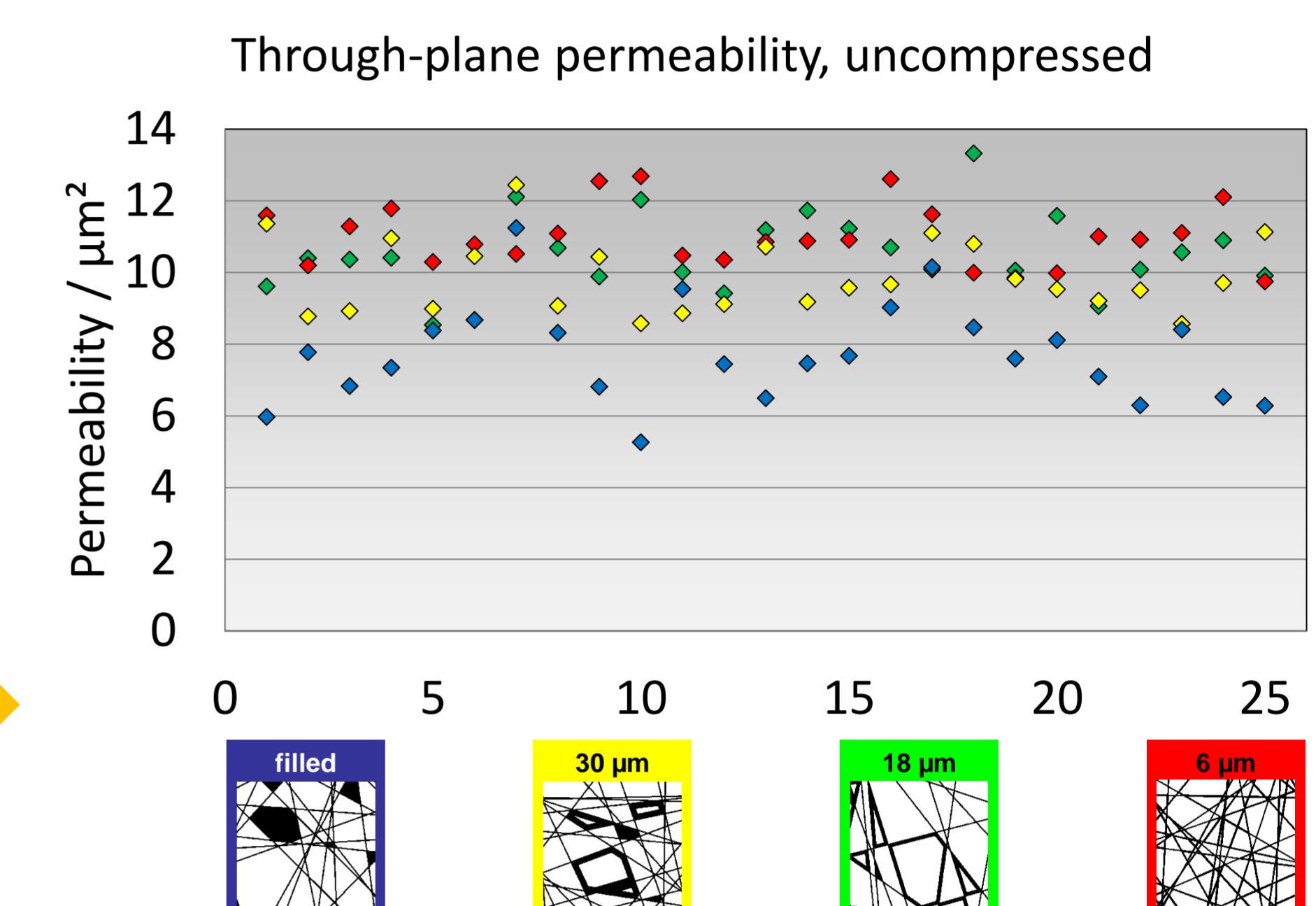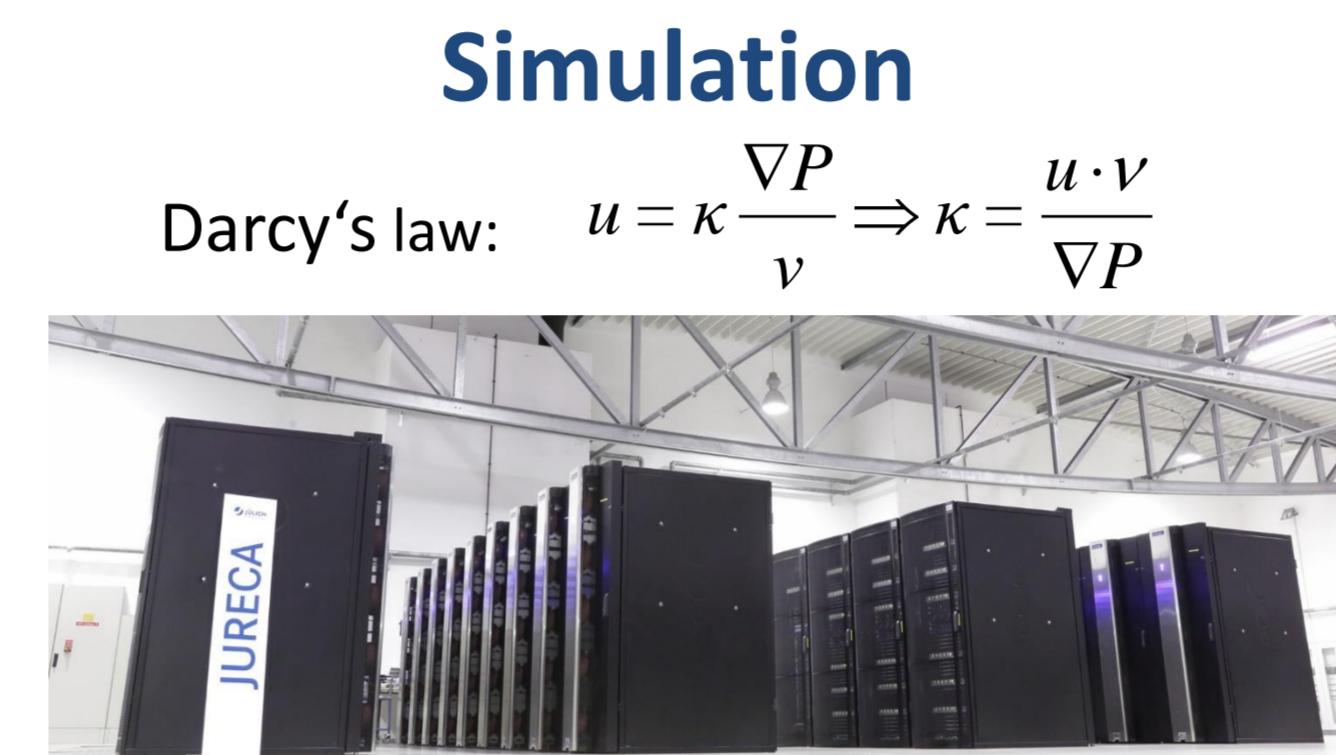
Fig. 5. CLAIX system at the RWTH Aachen.

Black Box

Permeability of gas diffusion layers (GDL) used in fuel cells and electrolyzers

- Historical data [1] for training.

- 541 transport simulations (Fig. 4) on realizations of stochastic geometry model (Fig. 2).

- Uncompressed and compressed material.

- Training on GPU nodes of CLAIX [2] 2x NVIDIA Tesla V100 SXM2 9,700,000 trainable parameters.

- Prediction can run on a standard computer.

- Inlet features (different colors in Fig. 4) are reproduced on prediction [3].

- Green symbols in Fig. 4 are subject of the view into the black box beneath.
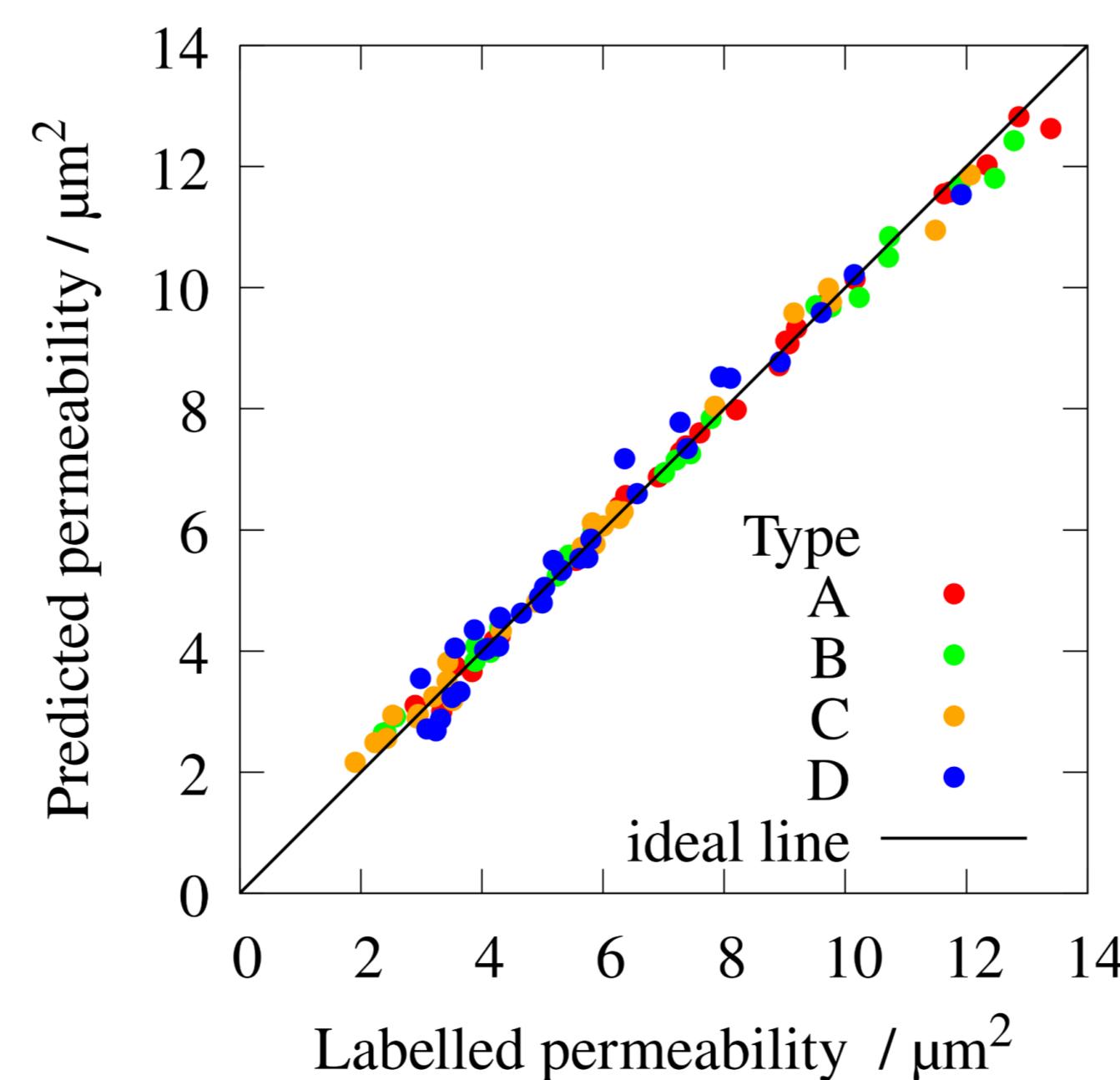

Fig. 6. Permeabilities predicted by the machine learning model, only un-trained data.

References
[1] D. Froning, J. Brinkmann, U. Reimer, V. Schmidt, W. Lehnert, D. Stolten. 3D analysis, modeling and simulation of transport processes in compressed fibrous microstructures, using the Lattice Boltzmann method, Electrochimica Acta 110 (2013) 325-334.
[2] Jannik Wirtz, Untersuchung von neuronalen Architekturen für ein prediktives Modell der Eigenschaften von faserbasierten Gasdiffusionsschichten, Bachelorarbeit, FH Aachen, 2021.
[3] D. Froning, J. Wirtz, E. Hoppe, W. Lehnert. Flow characteristics of fibrous gas diffusion layers identified using machine learning methods, *under review*.