Program MSE
MSE Day 18.11.2022

Machine Learning for Digital Twins in Virtual Materials Design

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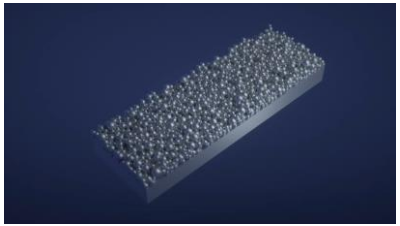
HELMHOLTZ

Ingredients of a Digital Twin

Theory/Model specification

Model implementation

Data



Integration / Validation

Ingredients

Theory/Model specification

noise

simplifications

confounders

Model implementation

simulation code

multiscale

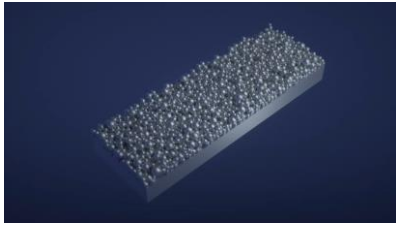
Machine Learning

data from adjacent domains

data with high dimensionality

Integration

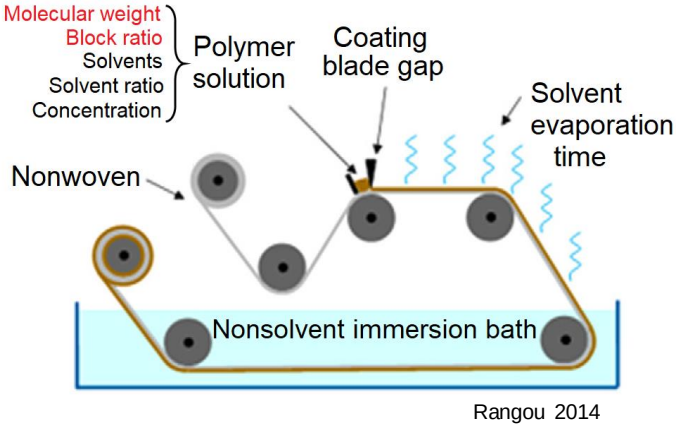
data driven validation



Showcase 1: Machine Learning for optimizing polymer membranes

Motivation

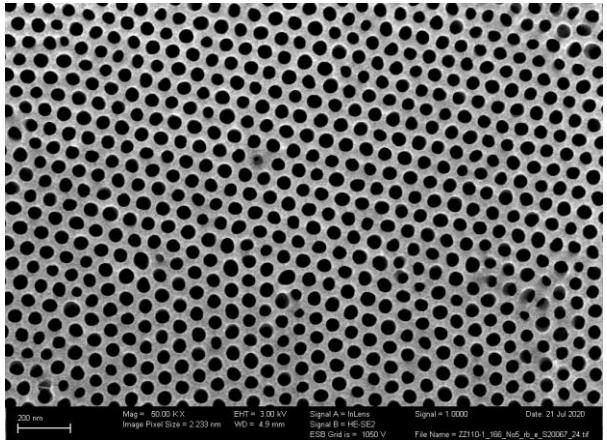
- Machine Learning for functional dependencies (objective functions) which cannot be quantified easily
- Correlate process parameters and the resulting membrane characteristics
  Invert to elicit the optimal process parameters for the intended membrane properties

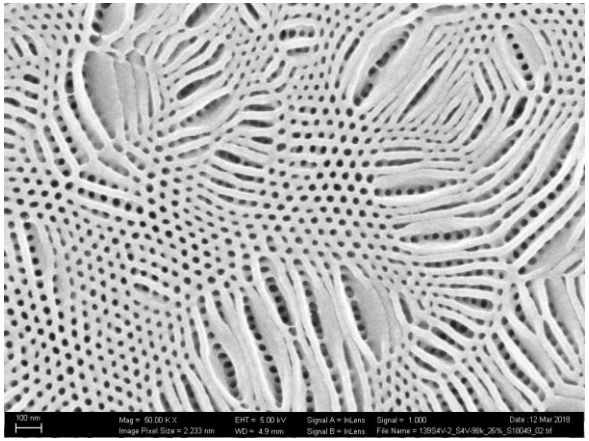


Rangou 2014

Showcase 1: Machine Learning for optimizing polymer membranes

- What if the *optimal* targets are unknown?
  (process parameters → unknown_topology_characteristics)
- What if manual labeling is prohibitively expensive?



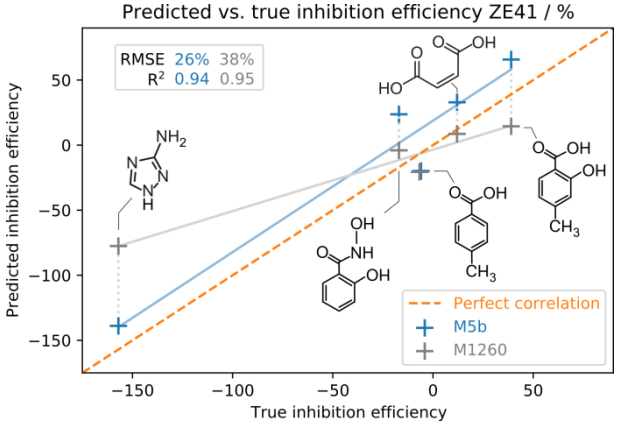


Martin Held & Volker Abetz (Hereon), Fabian Isensee (DKFZ)

Showcase 2: Machine Learning for Mg-Corrosion

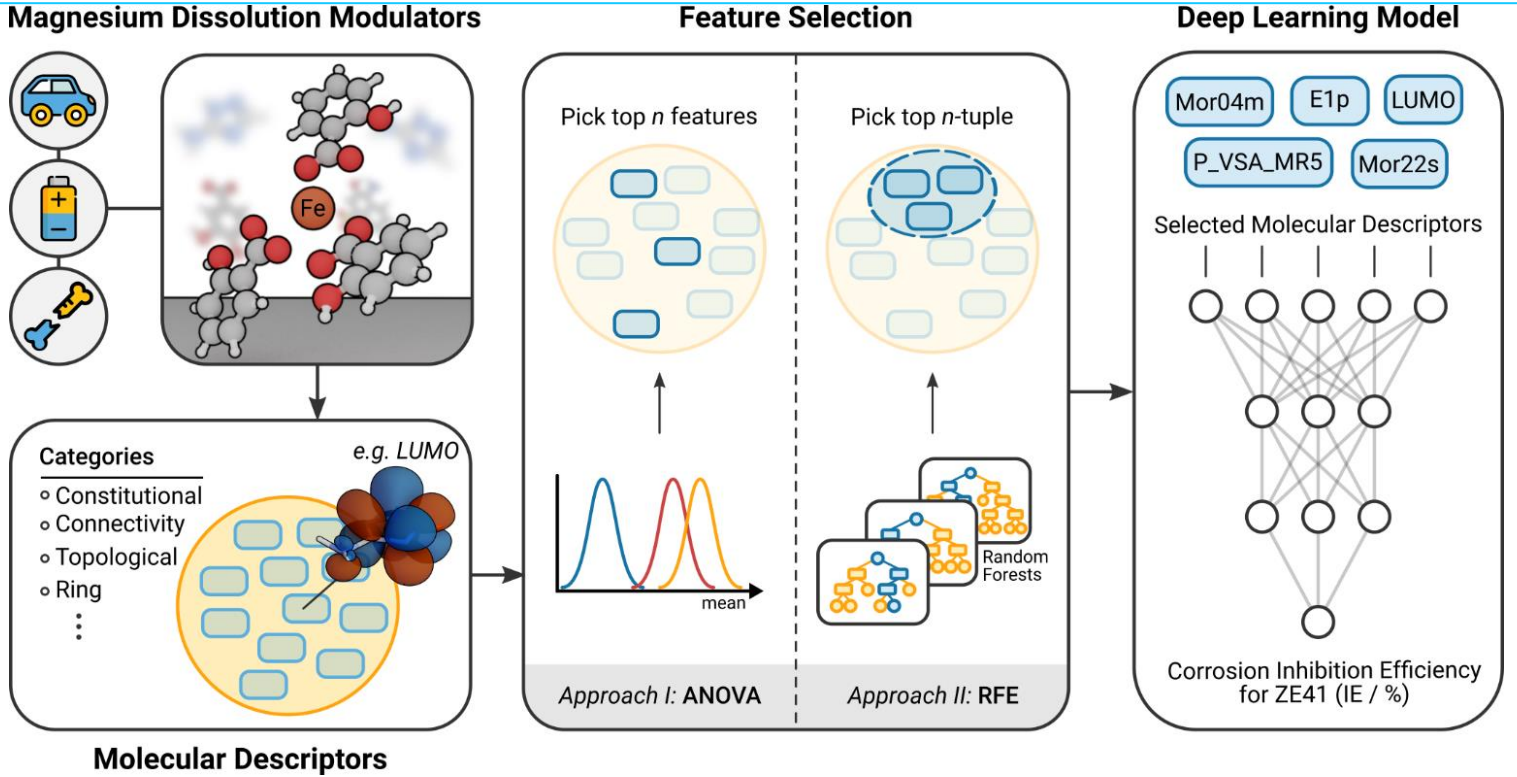
Motivation

- Feature selection:
  - to enable surrogate models
    (by improving the signal/noise ratio)
  - to drive experimental design choices



- Data-driven dimensionality reduction:
  using Machine Learning as an intermediate stage
  to bootstrap analytical understanding

Showcase 2: Machine Learning for Mg-Corrosion

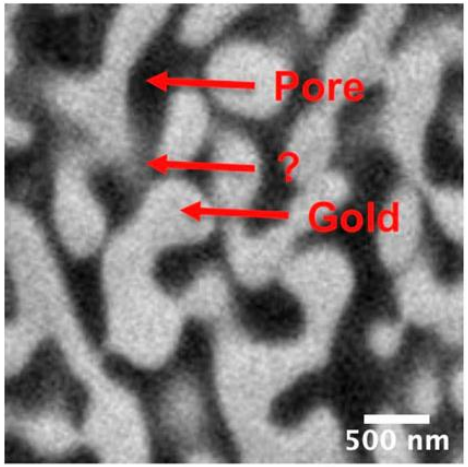


E. Schiessler, T. Würger, S. V. Lamaka, R. H. Meißner, C. Cyron, M. L. Zheludkevich, C. Feiler

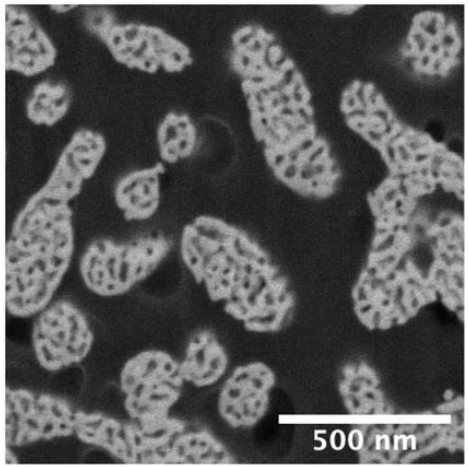
Showcase 3: Synthetic data in electron microscopy

Motivation

- Use case:
  Machine Learning to solve the shine-through effect in FIB data of nanoporous materials
- Use case:
  Machine Learning to correct original data (FIB slice allocation)



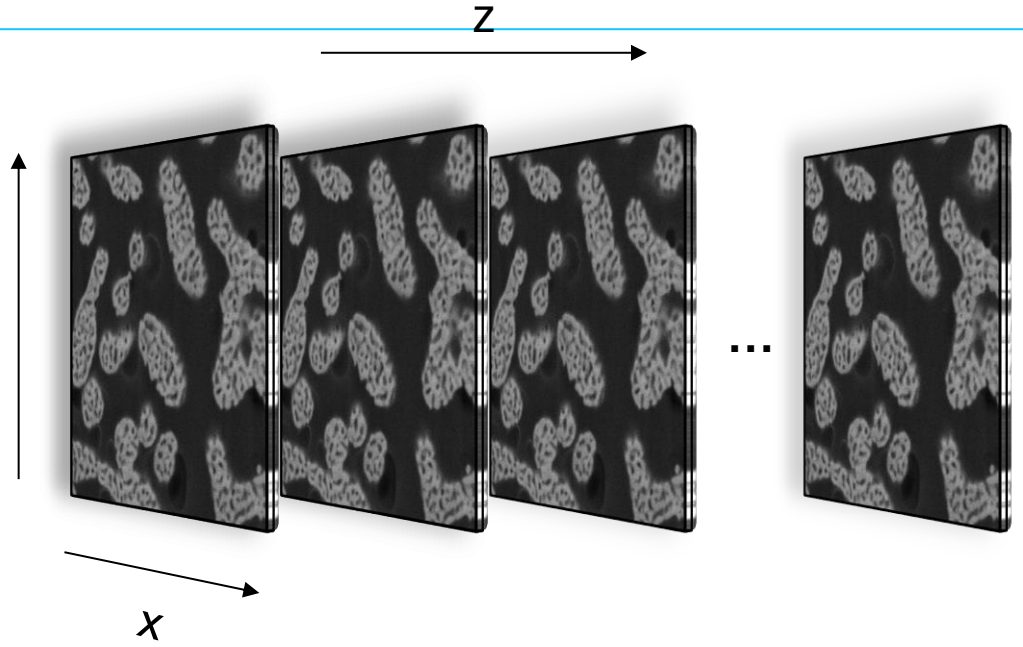
Nanoporous gold



Hierarchical nanoporous gold

Showcase 3: Synthetic data in electron microscopy

Results



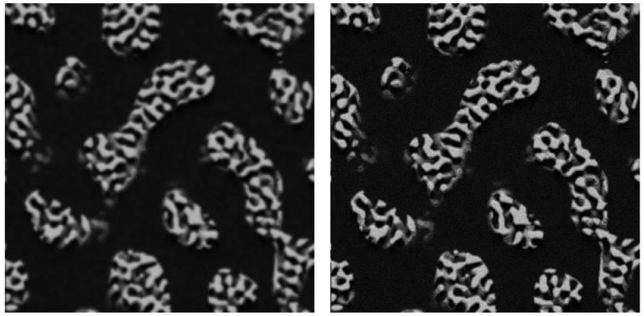
Machine learning for automatic segmentation

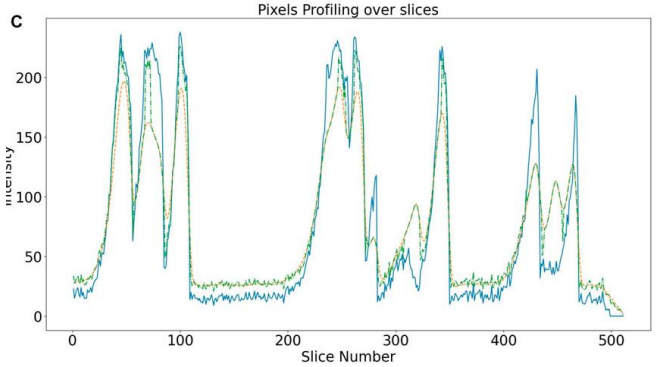
(if sufficient quantities of data are available)

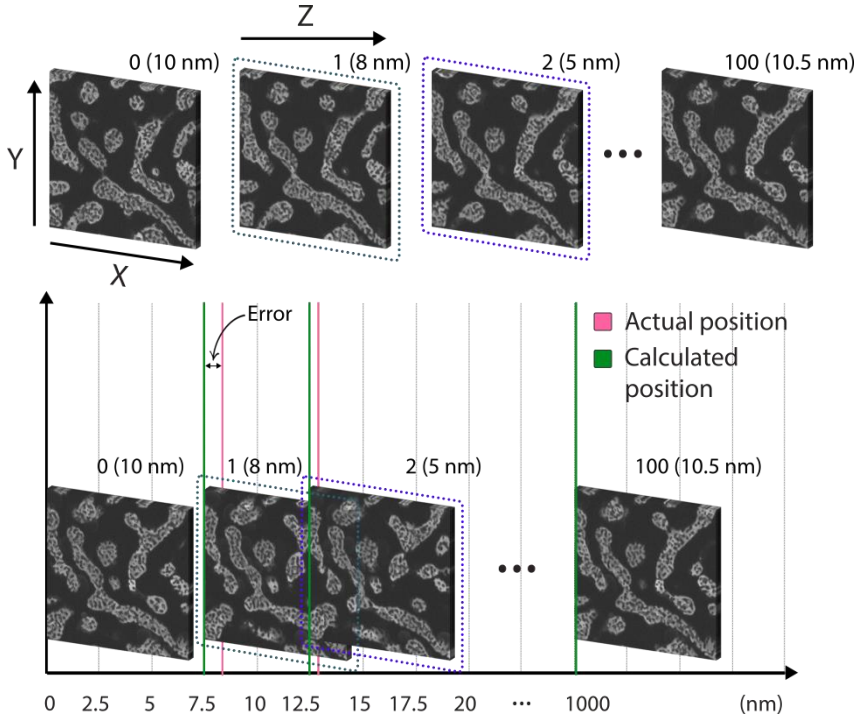
In case of insufficient data to train the Machine Learning model:
construct our own synthetic data in 2 steps:
virtual microstructures → MC simulations → synthetic data usable for supervised learning

Showcase 3: Synthetic data in electron microscopy

Results: Improved segmentation, Correcting original data





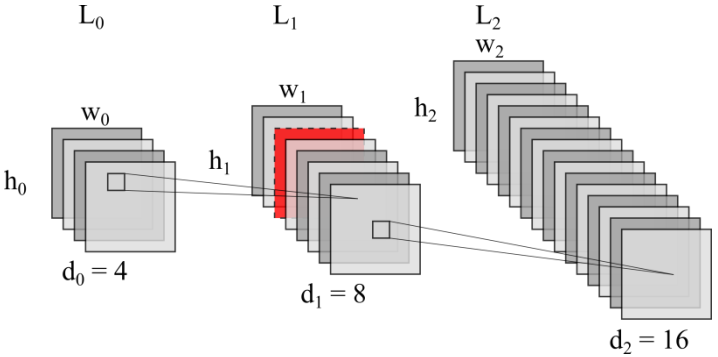


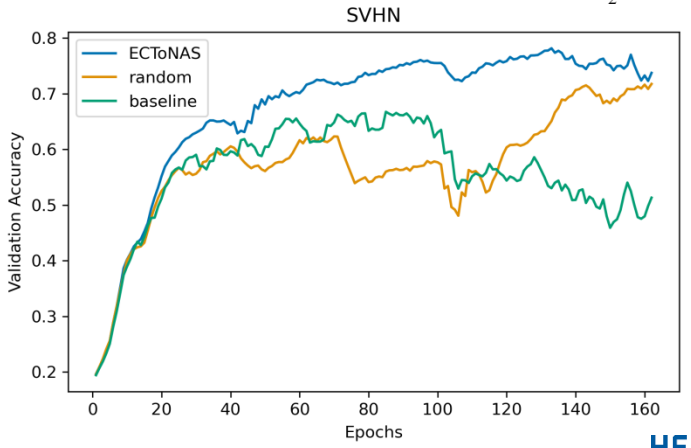
Trushal Sardhara & Martin Ritter & Alexander Shkurmanov & Yong Li & Shan Shi (TUHH), Christian Cyron (Hereon)

Showcase 4: Neural Architecture Search: the „Surgeon“

Motivation

- Machine Learning models have a large number of hyperparameters
  (learning rate, activation function, gd optimizer, batch size, topology choices, etc.)
- Finding the best combination for a given problem is infeasible (combinatorial explosion)
- Network choices have to reflect a deep understanding about the problem domain that is not necessarily present
  (CNN vs. FFNN, LSTM vs. Transformers, best type of autoencoder, etc.)





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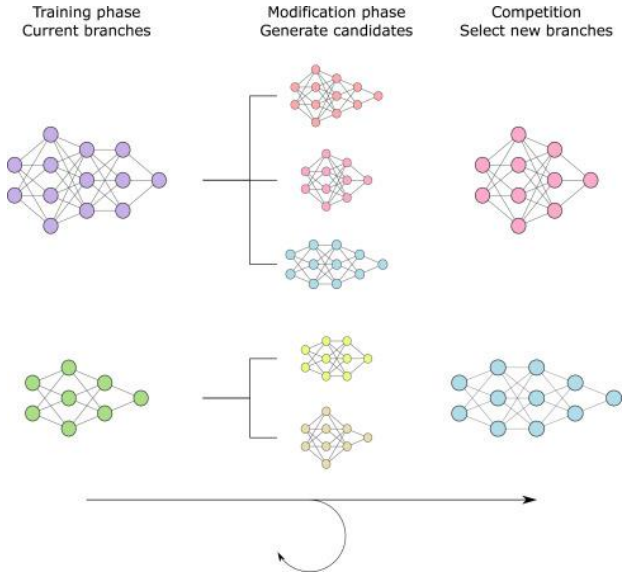
Showcase 4: Neural Architecture Search: the „Surgeon“



Modification choices can also e.g. uphold physical constraints (e.g. Navier-Stokes, PINN alternative); optimize runtime constraints (#weights)

Take-Home Message

- Digital Twin: a *toolkit* rather than a monolithic sibling

- The role(s) of Machine Learning for Digital Twins in VMD
  - Bridging the gaps between the digital twin components
  - (In some cases)
    Building understanding,
    transfer learning for optimizing data acquisition
  - (In rare cases)
    Surrogate models