

# Leveraging machine learning in porous media

## Supplementary Information I

**Table S1.** List of available online databases for training ML models in the review paper scope.

Name	Information	URL
<b>Heat exchanger and storage</b>		
The National Institute of Standards and Technology (NIST)	Various datasets for thermophysical properties of the materials, including those related to heat transfer in porous media.	<a href="https://www.nist.gov/srd">https://www.nist.gov/srd</a>
MAMBA	Open source (FORTRAN) repository for the porous media chemistry, heat transfer, and fluid flow code, supported by CASL (the Consortium for Advanced Simulation of LWRs).	<a href="https://github.com/shortlab/mamba">https://github.com/shortlab/mamba</a>
Coupled-CFD-and-HAM-Heat-Air-and-Moisture	A numerical model (MATLAB) to characterize the coupled energy and mass transfer that occur during the process of drying a freshly sliced eggplant (porous media).	<a href="https://github.com/Raghul13/Coupled-CFD-and-HAM-Heat-Air-and-Moisture-transport-modeling-in-a-porous-medium">https://github.com/Raghul13/Coupled-CFD-and-HAM-Heat-Air-and-Moisture-transport-modeling-in-a-porous-medium</a>
PINN porous	Linear and nonlinear heat conduction in porous media (Python).	<a href="https://github.com/JoshuaXu7/PINN_porous">https://github.com/JoshuaXu7/PINN_porous</a>
hydrideFoam	Heat transfer and porous media fluid flow solver for hydride beds.	<a href="https://github.com/tgvoskuilen/hydrideFoam">https://github.com/tgvoskuilen/hydrideFoam</a>
<b>Energy storage and combustion</b>		
National Renewable Energy Laboratory (NREL) Data Catalog	NREL provides a wide range of data related to renewable energy and energy storage research.	<a href="https://www.nrel.gov/data.html">https://www.nrel.gov/data.html</a>
Porous Media Group Databases	There are research groups and institutions focused on porous media studies that might have databases or resources related to energy storage and porous media interactions. One example is the "Transport in Porous Media" journal.	<a href="https://www.springer.com/journal/11242">https://www.springer.com/journal/11242</a>
DOE Energy Storage Database	The U.S. Department of Energy (DOE) maintains an Energy Storage Database that covers various energy storage technologies, including electrochemical storage.	<a href="https://www.energystorageexchange.org/">https://www.energystorageexchange.org/</a>
Materials Project	These databases provide materials information relevant to energy storage materials.	<a href="https://materialsproject.org/">https://materialsproject.org/</a>
Open Quantum Materials Database	These databases provide materials information relevant to energy storage materials.	<a href="https://oqmd.org/">https://oqmd.org/</a>
<b>Electrochemical devices</b>		

Battery Library	Microstructure	Li-ion anode and cathode electrode samples with different manufacturing methods. X-ray computed tomography samples	<a href="https://www.nrel.gov/transportation/microstructure.html">https://www.nrel.gov/transportation/microstructure.html</a>
Battery Project – ETH Zurich	Microstructure	3D microstructural and electrochemical data on porous electrodes and separators (NMC, PE separator, Graphite electrodes, commercial anodes)	<a href="https://made.ee.ethz.ch/research/open-source-data-and-software/battery-microstructure-project.html">https://made.ee.ethz.ch/research/open-source-data-and-software/battery-microstructure-project.html</a>
GES-EIS-toolbox		A simple toolbox to analyze electrochemical impedance spectroscopy data using ML	<a href="https://github.com/ppravatto/GES-EIS-toolbox">https://github.com/ppravatto/GES-EIS-toolbox</a>
Porous Generator	Microstructure	Computational reconstruction software for generating existing and novel porous electrode geometries. Can replicate fuel cell, electrolyzer, and battery electrode microstructures.	<a href="https://data.ncl.ac.uk/articles/software/Porous_Microstructure_Generator/20448471">https://data.ncl.ac.uk/articles/software/Porous_Microstructure_Generator/20448471</a>
OpenPNM		Pore network modeling package for predicting electrochemical processes in fuel cells and batteries. Open-source framework.	<a href="https://openpnm.org">https://openpnm.org</a>
DeePore		Morphological properties, Hydrodynamic characterization, Mechanical properties, Thermal properties, Electrical properties	<a href="https://github.com/ArashRabbani/DeePore">https://github.com/ArashRabbani/DeePore</a>
ChemDataExtractor-batteries		Database of battery materials with up to five material properties: capacity, voltage, conductivity, efficiency, and energy. Auto-generated from 229061 papers.	<a href="https://github.com/ShuHuang/batterydatabase/tree/main/chemdataextractor_batteries">https://github.com/ShuHuang/batterydatabase/tree/main/chemdataextractor_batteries</a>
Weka Segmentation		Trainable Weka Segmentation: a machine learning tool for microscopy pixel classification	<a href="https://github.com/fiji/Trainable_Segmentation">https://github.com/fiji/Trainable_Segmentation</a>
ARTISTIC project		ARTISTIC Project: DIGITAL LI-ION BATTERY MANUFACTURING PLATFORM	<a href="https://www.erc-artistic.eu/computational-portal">https://www.erc-artistic.eu/computational-portal</a>
ILASTIK Toolkit		ILASTIK: INTERACTIVE LEARNING AND SEGMENTATION TOOLKIT	<a href="https://www.ilastik.org/">https://www.ilastik.org/</a>
Battery Library	Microstructures	The library features a variety of Li-ion cathode (nickel manganese cobalt [NMC]) and anode (graphite) electrode data samples, calendered and uncalendered with different loadings.	<a href="https://www.nrel.gov/transportation/battery-microstructure-library-data.html">https://www.nrel.gov/transportation/battery-microstructure-library-data.html</a>
StarDist		Object Detection with Star-convex Shapes	<a href="https://github.com/stardist/stardist">https://github.com/stardist/stardist</a>
Vision		U-Net: Convolutional Networks for Biomedical Image Segmentation	<a href="https://lmb.informatik.uni-freiburg.de/people/ronneberger/u-net/">https://lmb.informatik.uni-freiburg.de/people/ronneberger/u-net/</a>
GeoDict		Modeling & simulation of Li-ion batteries Digital Material Development for Fuel Cells	<a href="http://www.geodict.com/geodict-">http://www.geodict.com/geodict-</a>

	Analysis of pore space characteristics	software/geodict-base-modules/simulation/batterydict.html <a href="http://www.geodict.com/industrial-solutions/fuel-cells.html">http://www.geodict.com/industrial-solutions/fuel-cells.html</a> <a href="https://www.geodict.com/geodict-software/geodict-base-modules/analysis/porodict.html">https://www.geodict.com/geodict-software/geodict-base-modules/analysis/porodict.html</a>
Dualfoil.py	Dualfoil.py is a flexible application programming interface that allows for hierarchical control over the dualfoil legacy code (Newman model) and visualization modules.	<a href="https://github.com/iSchomer/Dualfoil_Storage_Device">https://github.com/iSchomer/Dualfoil_Storage_Device</a>
<b>Hydrocarbon reservoirs</b>		
VideoGPT	A conceptually simple architecture for scaling likelihood-based generative modeling to natural videos	<a href="https://wilson1yan.github.io/videogpt/index.html">https://wilson1yan.github.io/videogpt/index.html</a>
MultiscaleDRPNet	An effective way to fuse multiscale digital rock images for better characterization of heterogeneous porous media	<a href="https://github.com/theanswer003/MultiscaleDRPNet">https://github.com/theanswer003/MultiscaleDRPNet</a>
EDSR modeling	A GitHub repository for deep-learning image enhancement, pore-network, and continuum modeling from X-Ray Micro-CT images	<a href="https://github.com/scijsj/EDSRmodelling">https://github.com/scijsj/EDSRmodelling</a>
The Multiphysics Object-Oriented Simulation Environment (MOOSE)	It is a finite-element, multiphysics framework that provides a high-level interface to some of the most sophisticated nonlinear solver technology	<a href="https://github.com/idaholab/moose">https://github.com/idaholab/moose</a>
Finch	Finch is a MOOSE-based application for modeling advective flows in heterogeneous porous media using the finite volume method	<a href="https://github.com/cpgr/finch">https://github.com/cpgr/finch</a>
TensorFlow	It has a comprehensive, flexible ecosystem of tools, libraries, and community resources that lets researchers push the state-of-the-art in ML and developers easily build and deploy ML-powered applications	<a href="https://github.com/tensorflow/tensorflow">https://github.com/tensorflow/tensorflow</a>
Keras: Deep Learning for humans	Keras is a deep learning API written in Python, running on top of the ML platform TensorFlow. It was developed with a focus on enabling fast experimentation	<a href="https://github.com/keras-team/keras">https://github.com/keras-team/keras</a>
The developed MLP-SSD and MLP-PSO codes	To examine the effectiveness of hybrid methods in predicting the permeability of the rock	<a href="https://github.com/mmehrad1986/Hybrid-MLP">https://github.com/mmehrad1986/Hybrid-MLP</a>
Brittleness prediction using machine learning	This repo contains Jupyter notebooks to estimate brittleness using elastic and	<a href="https://github.com/tobio/Brittleness-">https://github.com/tobio/Brittleness-</a>

		mineralogical properties and to predict brittleness using ML	Prediction-using-Machine-Learning
ML Surrogate Data Optimization	Binary	Build a surrogate model for NPV forecasting taking binary well placement data as input	<a href="https://github.com/joao bertini/MLSurrogateBinaryDataOptimization">https://github.com/joao bertini/MLSurrogateBinaryDataOptimization</a>
OPM data		Contains all relevant datasets and simulation results that are required to test the OPM simulators thoroughly	<a href="https://github.com/OPM/opm-data">https://github.com/OPM/opm-data</a>
<b>Carbon capture and sequestration</b>			
ARC-MOF		A diverse database of MOFs with DFT-derived partial atomic charges and descriptors for ML	<a href="https://zenodo.org/records/7600474">https://zenodo.org/records/7600474</a>
CoRE MOF 2014		A database of nearly 2,900 MOF structures with ddec partial atomic charges	<a href="https://zenodo.org/records/3986573">https://zenodo.org/records/3986573</a>
CoRE MOF 2019		An update to the CoRE MOD database with over 14k porous, 3D MOF structures	<a href="https://zenodo.org/records/3370144">https://zenodo.org/records/3370144</a>
CoRE-COF		Solvent-free and disorder-free structure files of nearly all the experimental COFs published in the literature	<a href="https://github.com/core-cof/CoRE-COF-Database">https://github.com/core-cof/CoRE-COF-Database</a>
IZA		This database offers structural information on all of the zeolite framework types that have been approved by the structure commission of the International Zeolite Association (IZA-SC)	<a href="http://www.iza-structure.org/databases/">http://www.iza-structure.org/databases/</a>
CURATED-COF		Clean, uniform, and refined with automatic tracking from the experimental database (curated) COFs from the literature	<a href="https://www.materialscloud.org/discover/curated-cofs#mcloudHeader">https://www.materialscloud.org/discover/curated-cofs#mcloudHeader</a>
Quantum MOF (QMOF)		A public dataset of quantum-chemical properties for more than 20k MOFs and coordination polymers derived from high-throughput periodic DFT simulations	<a href="https://figshare.com/articles/dataset/QMOF_Database/13147324">https://figshare.com/articles/dataset/QMOF_Database/13147324</a>
Polymer Gas Separation Membranes		An open-source database for experimentally measured and reported polymer gas permeabilities	<a href="https://research.csiro.au/virtualsecreening/membrane-database-polymer-gas-separation-membranes/">https://research.csiro.au/virtualsecreening/membrane-database-polymer-gas-separation-membranes/</a>
<b>Groundwater</b>			
Water Database 6.1	Resources	Image reconstruction, Image resolution, Data Classification, Data regression, Image segmentation	<a href="http://wrdb.com/">http://wrdb.com/</a>
R For Water Resources, Data Science		Multivariate linear regression, Partial differential equations, Non-linear system of equations, Matrix operation, Graph theory	<a href="https://www.github.com/r4wrds">https://www.github.com/r4wrds</a>
WE geophysics/water, water-resources		Artificial neural networks, Deep and convolutional neural networks, Generative adversarial neural networks, Ensemble learning, SVM, SOM, Gaussian process	<a href="https://github.com/WEgeophysics/watex">https://github.com/WEgeophysics/watex</a> <a href="https://github.com/topics/water-resources">https://github.com/topics/water-resources</a>

DeePore, Porous materials	Morphological properties, Hydrodynamic characterization, Mechanical properties, Thermal properties, Electrical properties	<a href="https://github.com/ArashRabbani/DeePore">https://github.com/ArashRabbani/DeePore</a> , <a href="https://github.com/topics/porous-materials">https://github.com/topics/porous-materials</a>
SWE_FVM, gmsfem-fem-fvm	Finite difference method (FDM), Finite volume method (FVM), Finite element method (FEM), Lattice Boltzmann method (LBM), Volume of fluid method (VOF)	<a href="https://github.com/NikitaMatkevich/SWE_FVM">https://github.com/NikitaMatkevich/SWE_FVM</a> , <a href="https://github.com/vmasaha/gmsfem-fem-fvm">https://github.com/vmasaha/gmsfem-fem-fvm</a> ,