Surrogate (AI/ML/ROM) models for acceleration of coupled codes

Nikolaos I. Prasianakis · Laboratory for Waste Management · Paul Scherrer Institut (PSI)

Contains several HERMES-Task 4 partner results as mention in the slides

EURAD-2 Annual Meeting / HERMES–DITOCO / Dublin / 09 September 2026

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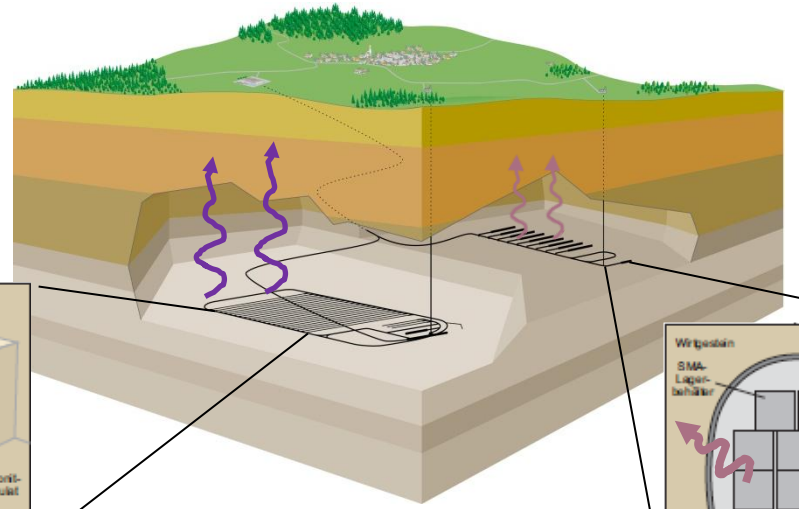
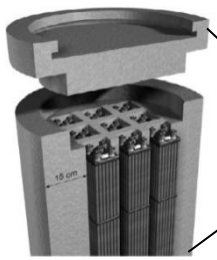
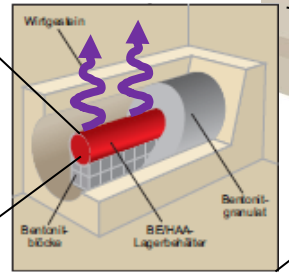
STRONGLY COUPLED PHENOMENA IN REPOSITORY SYSTEMS (THMC)

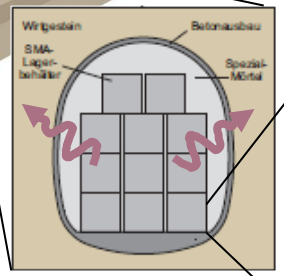
Thermal pulse
De-/re-saturation
Backfill degradation
Canister corrosion
Radionuclides release

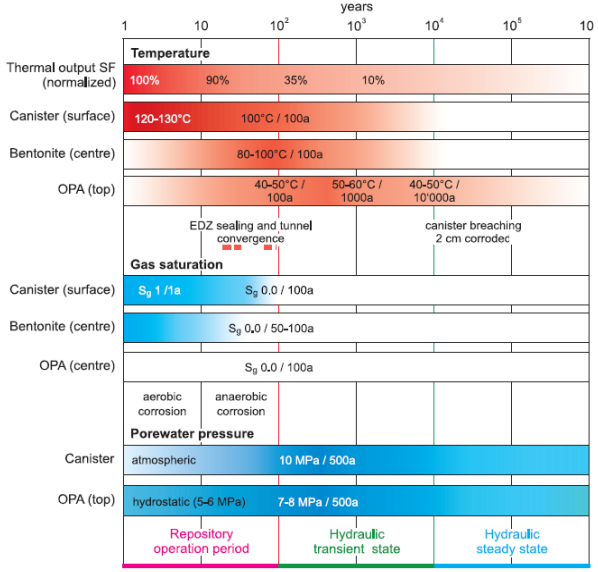


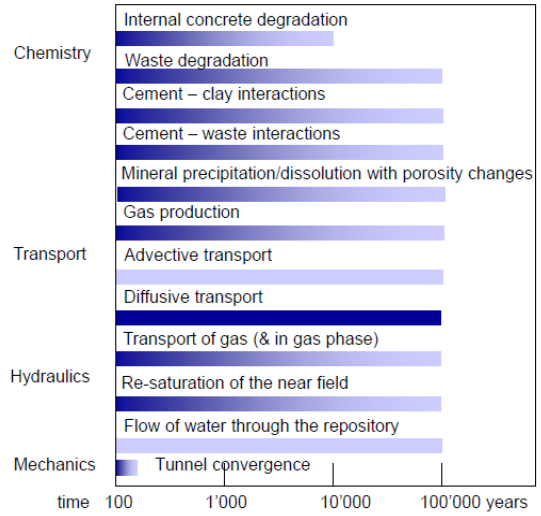
Waste degradation
Cement-clay interaction
Release of Gas & Radionuclides











HERMES TASK 4: ACCELERATING COMPUTATIONS

Task 4: Surrogate models of individual and coupled phenomena, Lead: PSI / TUL

15 European partners

Methods: Machine Learning and reduced order methods

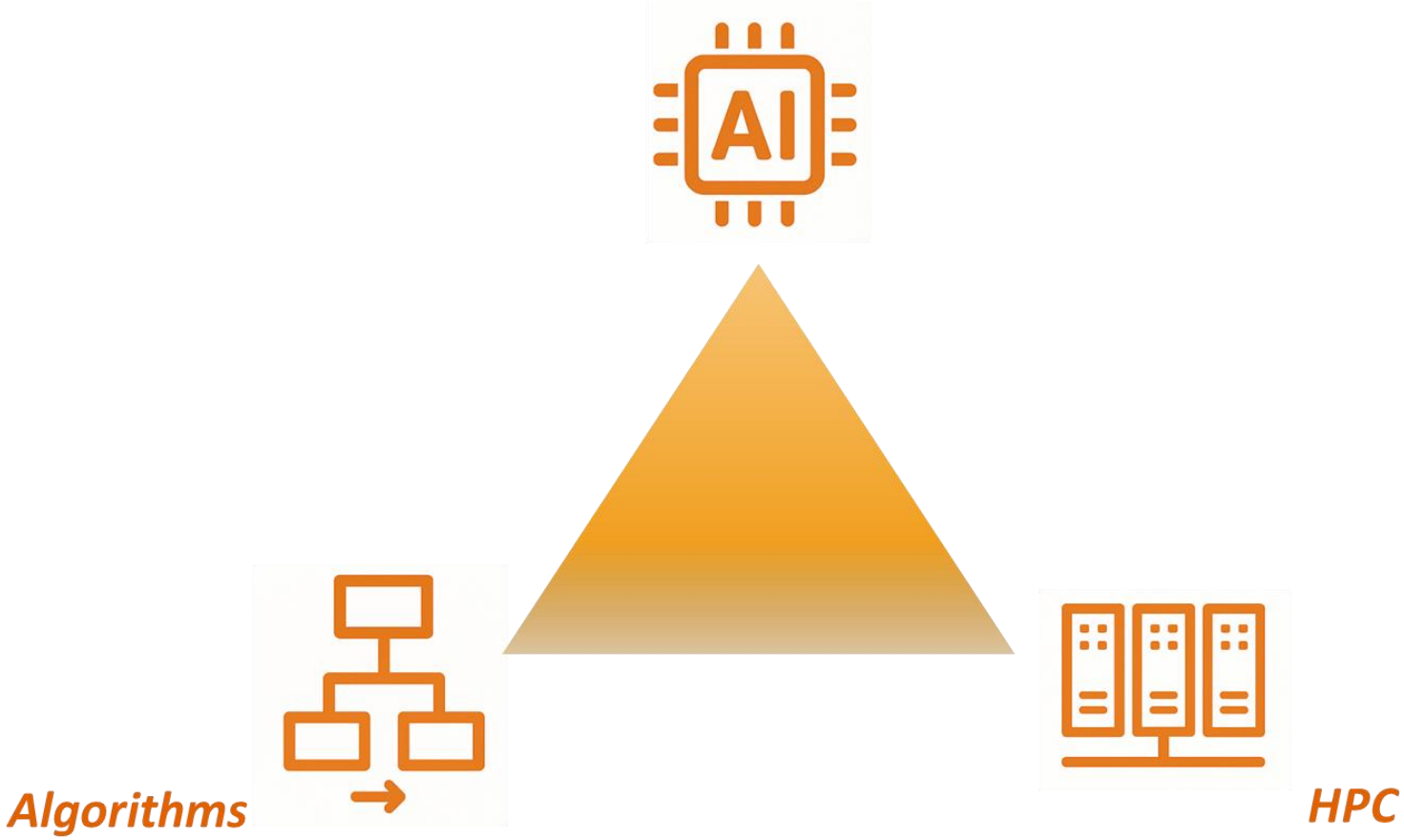
- Deep Learning Neural Networks
  (Forward, cascade forward, convolutional, recurrent, graph, liquid)
- Gaussian Processes
- Bayesian Regression
- Reduced order methods (ROM)
- Decision Trees (XGBOOST, DecTREE etc)
- Physics Informed Machine Learning (e.g. PINNS)
- ML based PDE modelling

Explore surrogates of subsystems, or of physical processes

Chemistry surrogates

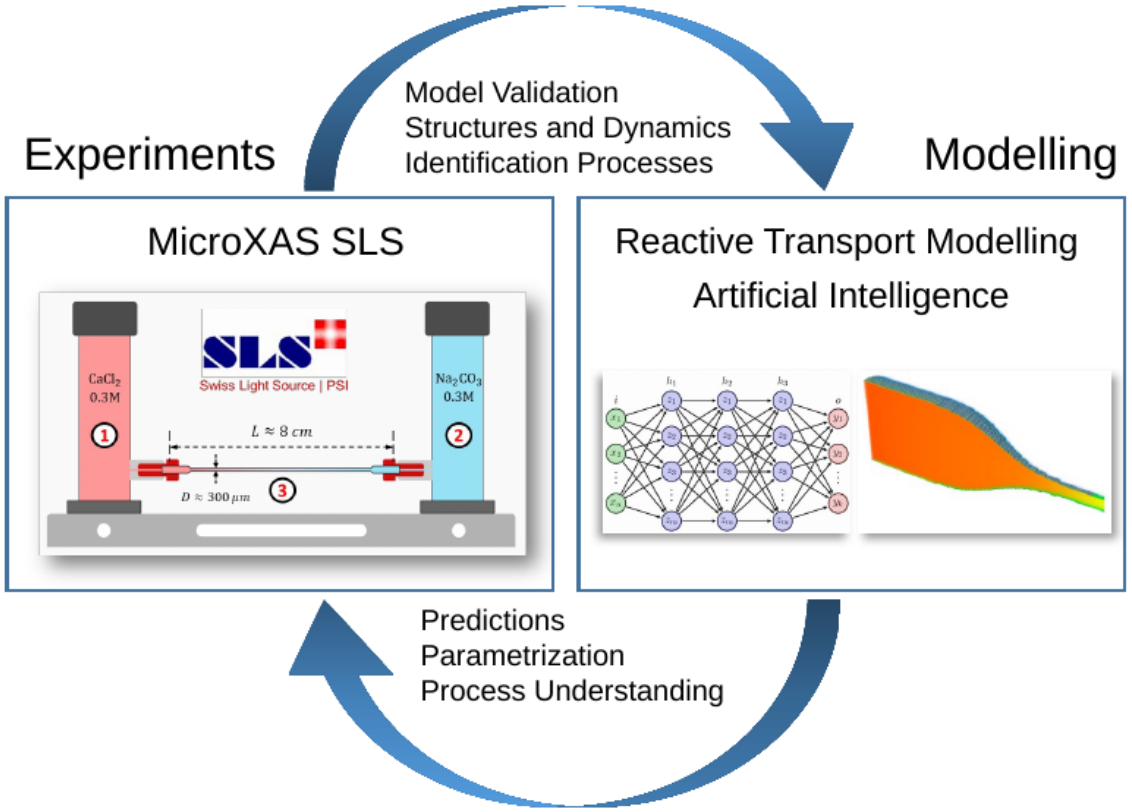
- Mechanics surrogates (including calculation of stresses from images)
- Hydraulics / Flow surrogates (including calculation of transport from images)
- Waste package level surrogates

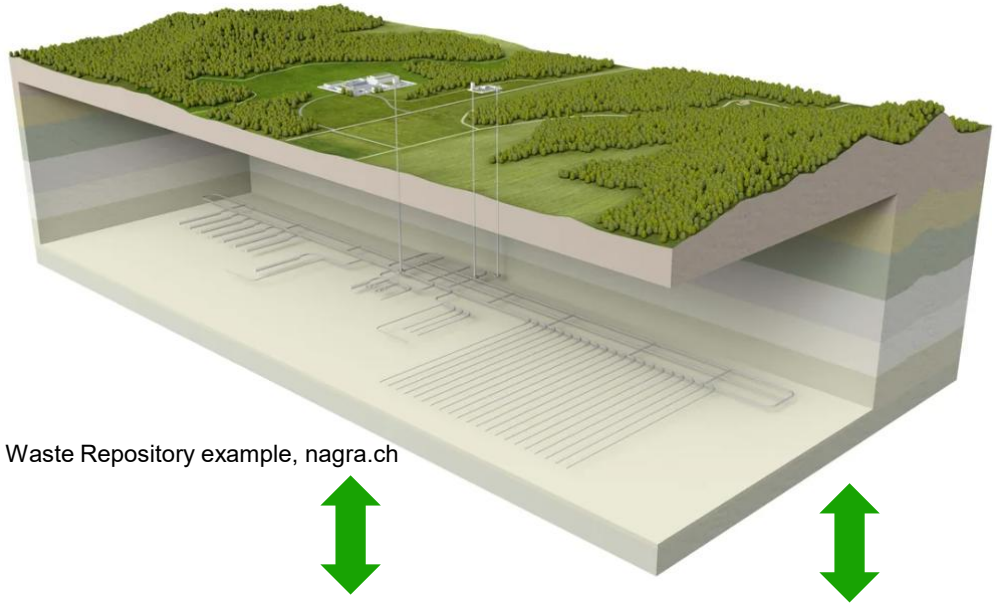
AI, SMART ALGORITHMS AND HPC PROVIDE PROVIDE THE NECESSARY ACCELERATION FOR REALISTIC SIMULATIONS IN REASONABLE TIME



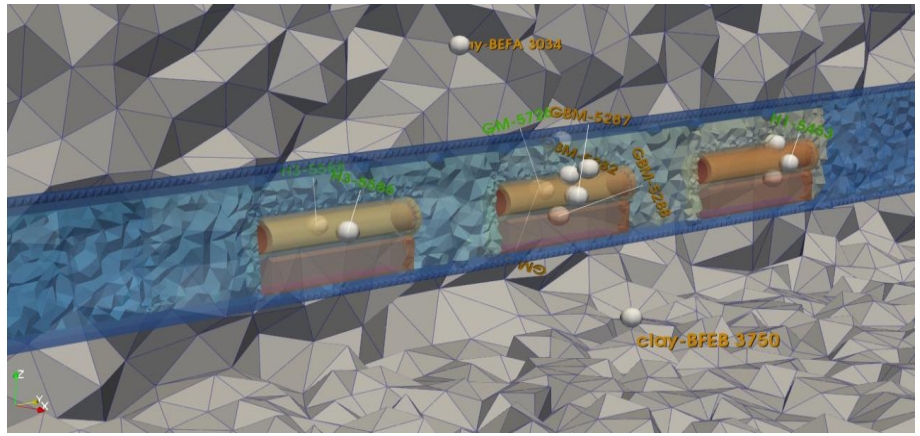
Target: make mechanistic simulations fast enough to interact/support the design of experiments.

MOTIVATION AND WHAT IS A DIGITAL TWIN IN THE HERMES CONTEXT





Waste Repository example, nagra.ch



(GEO)CHEMISTRY IS THE FIRST BOTTLENECK TO BE LIFTED

Accelerating chemistry in the field of combustion, reactive flows (1996 -)

Christo, F. C. et al."Artificial neural network implementation of chemistry with PDF simulation of H2/CO2 flames." Combustion and Flame 106, no. 4 **(1996)**: 406-427.

Accelerating geochemistry and geochemical reactive transport calculations (2016 -)

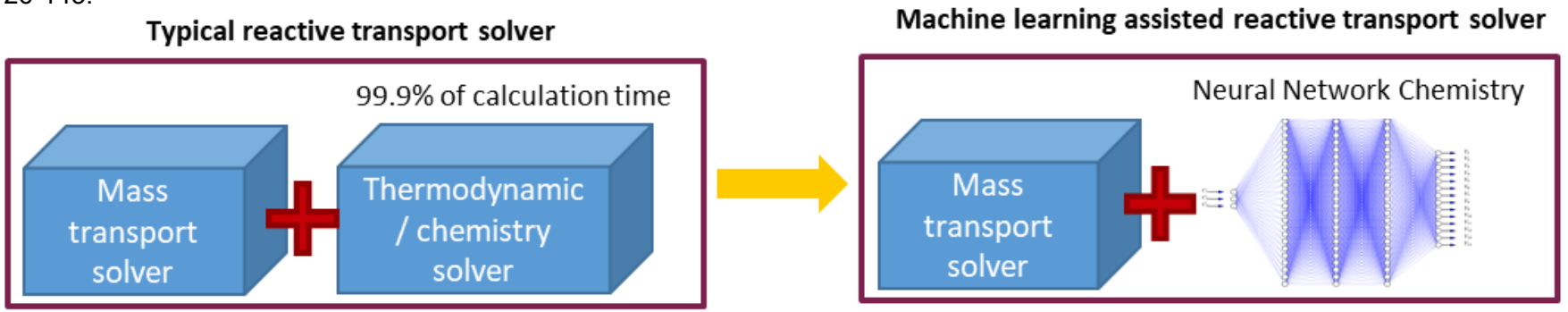
Jatnieks, J., De Lucia, M., Dransch, D. and Sips, M., (**2016)**. Data-driven surrogate model approach for improving the performance of reactive transport simulations. Energy Procedia, 97, pp.447-453.

Leal, A., Kyas S., Kulik D., Saar, M. arXiv:1708.04825 (**2017**)*, Transport in Porous Media* (**2020**).

Guerillot, D. R., and J. Bruyelle, 3rd EAGE Integrated Reservoir Modelling 504 (**2016**).

Laloy, E., and Jacques, D., *Computational Geosciences* 23, no. 5 (**2019**): 1193-1215.

Prasianakis, N.I., Haller, R., Mahrous, M., Poonoosamy, J., Pfingsten, W. and Churakov, S.V., (**2020**). *Geochimica et Cosmochimica Acta, 291*, pp.126-143.



GEOCHEMISTRY AND MACHINE LEARNING BENCHMARK EURAD-DONUT

Variable heading	Description	Unit	Min	Max
SiO2	Amount of SiO_2	mole	0.3	0.6
CaO	Amount of CaO_2	mole	0.9	1.4
H2O	Mass of water	kg	0.05	0.15
Al2O3	Amount of Al_2O_3	mole	0.03	0.07
K2O	Amount of K_2O	mole	0.006	0.012
SO3	Amount of SO_3	mole	0.02	0.05

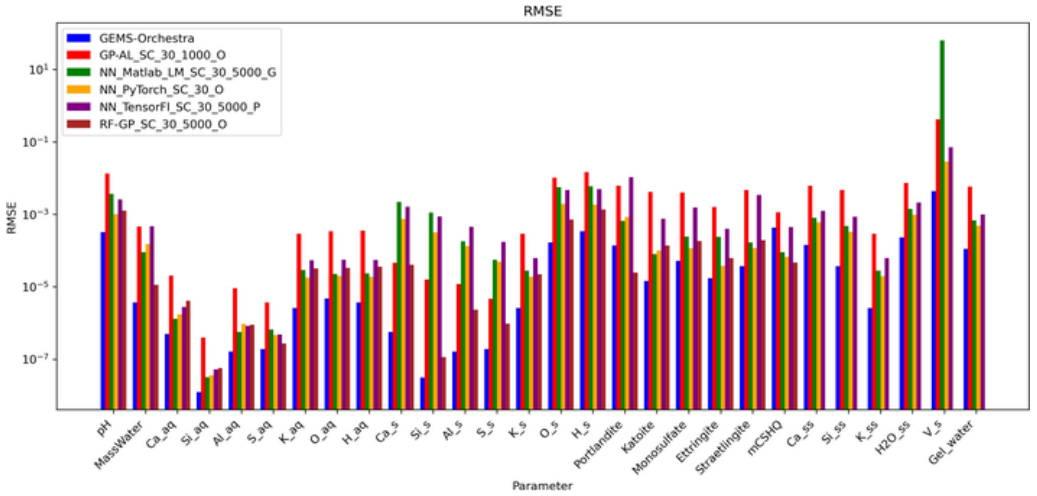
Machine Learning model

Data Management
FAIR principles

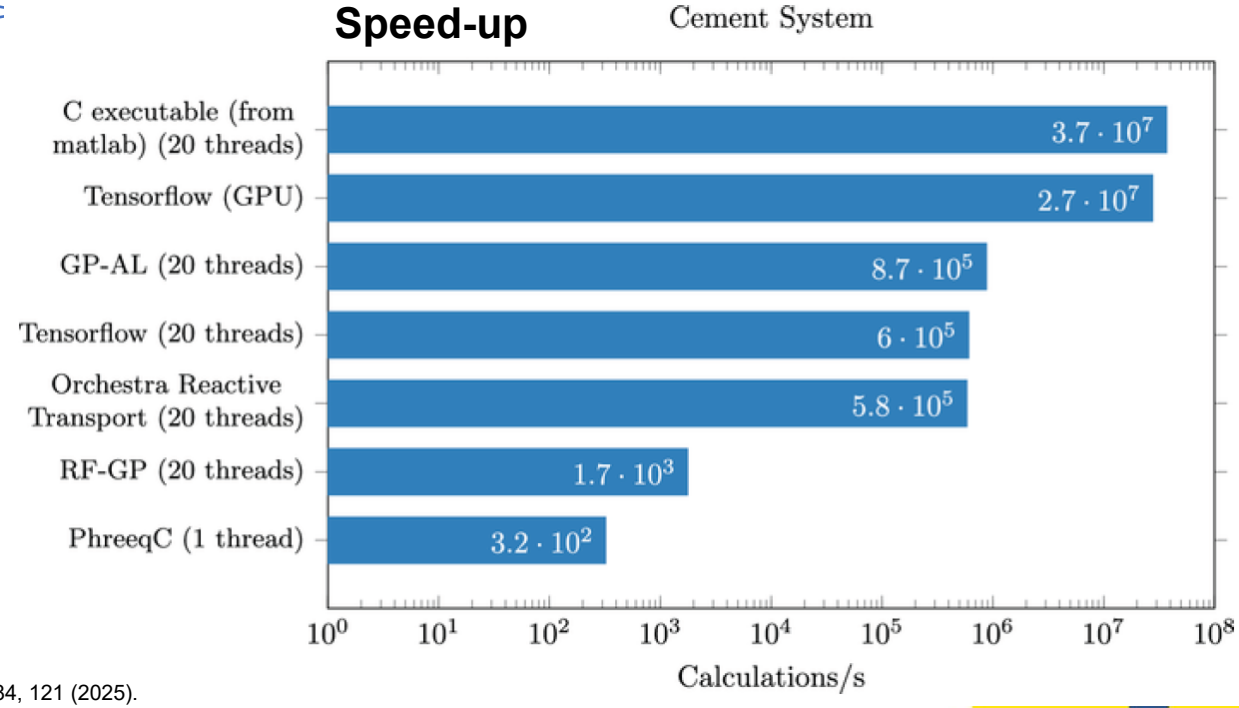
zenodo

Variable heading	Description
CaO	Amount of CaO
SiO2	Amount of SiO2
Al2O3	Amount of Al2O3
SO3	Amount of SO3
K2O	Amount of K2O
H2O	Mass of water
pH	pH
MassWater	Mass of water after reaction
Ca_aq	Amount of Ca in solution
Si_aq	Amount of Si in solution
Portlandite	Amount of portlandite
AmorfSi	Amount of amorf SiO2
Gibbsite	Amount of gibbsite
Katoite	Amount of katoite
Monosulfphate	Amount of monosulfoaluminate (monosulfate)
Ggypsum	Amount of gypsum
Eettringite	Amount of ettringite
Straetlingite	Amount of straetlingite
Chabazite	Amount of chabazite
.....	.....

Metrics of accuracy



Speed-up



Prasianakis et al., Environmental Earth Sciences 84, 121 (2025).

Geochemical calculations can be accelerated
How about reactive transport calculations?

➡ **GEOML-RT Benchmark within HERMES**

GEOML-RT SYSTEMS WHICH ARE EXPLORED

1

Cox - Cement degradation (D. Jacques, H. Meeussen). This benchmark focus on the cement degradation mechanisms, while clay is set as boundary condition

Mineral	Amount (mol/dm³)
Portlandite	0.5653
Amor-Si	0
Ca	0.04
CSHQ_JendD	0.166
CSHQ_JenH	0.110
CSHQ_TobD	0.125
CSHQ_TobH	5.47E-3

Figure 1: Cement evolution due to the geogemical contrast between cement and clay. System setup and cement composition details are shown.

2

Uranium Sorption on Clay (H. Meeussen, M. De Lucia). This benchmark focus on uranium transport including sorption. Advection and dispersion mechanisms are considered

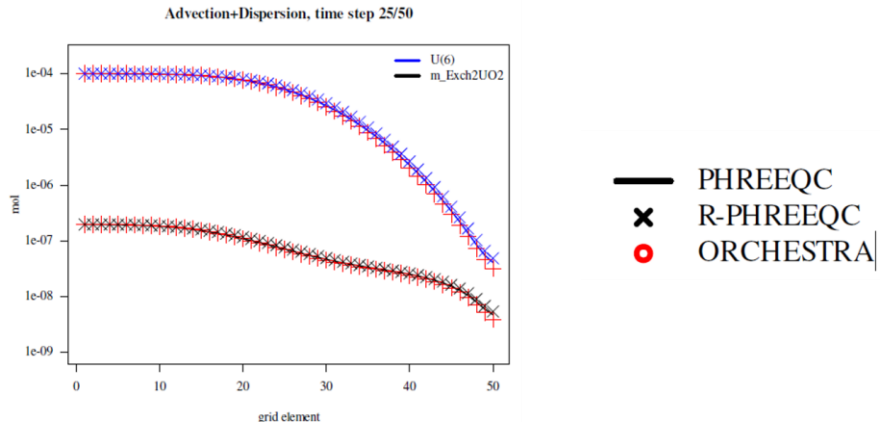
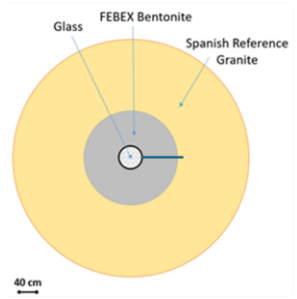


Figure 2: First results showing the profiles of U(6) and m_Exch2UO2 in an advection-dispersion-sorption setup.

3

Corrosion (J. Samper). This benchmark models the Iron corrosion and interaction with saturated bentonite.



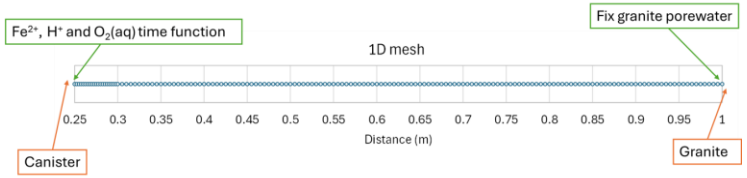
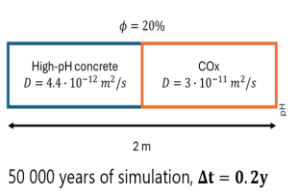
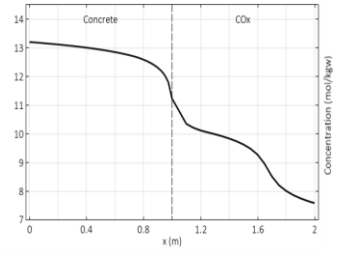


Figure 3: Setup where the cannister, bentonite and granite are modelled.

4

Cement-clay and processes at the interfaces (A. Idiart). This benchmark studies the interaction and alterations within both cement and clay materials





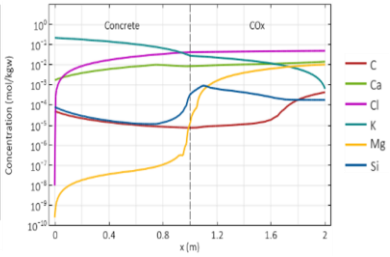
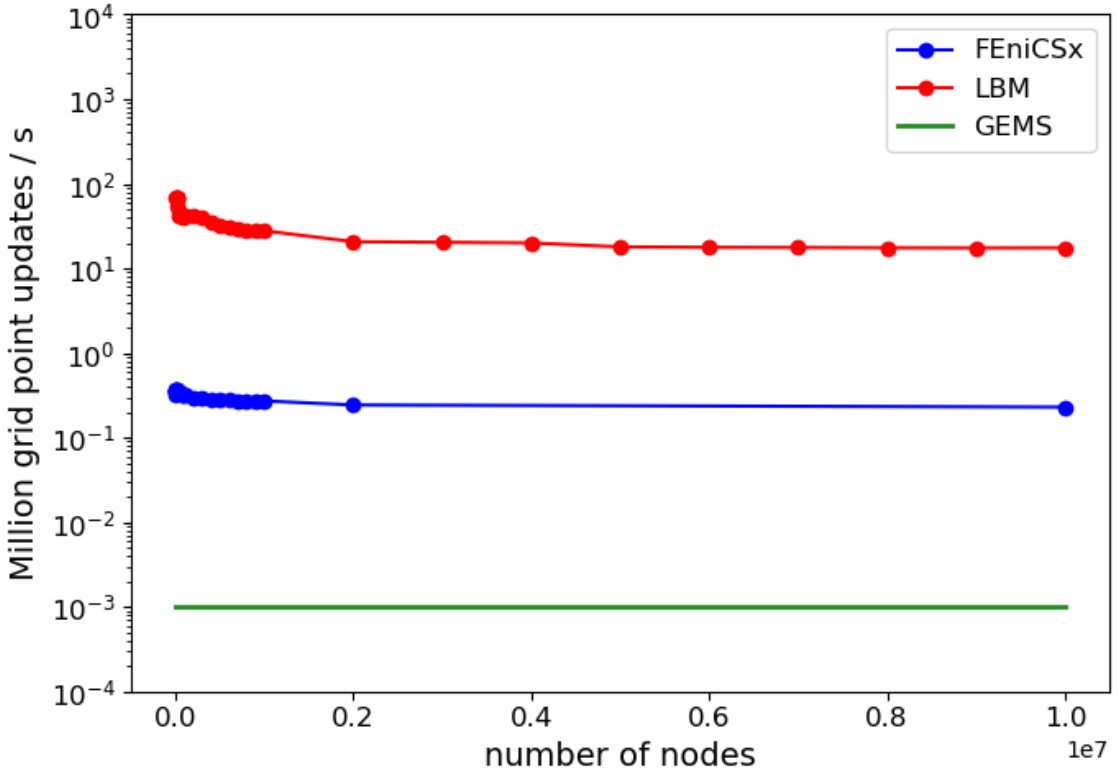


Figure 4:(left) System setup where cement and clay are modelled, (middle) porewater pH obtained with the reactive transport simulation after 50 kyears, (right) aqueous concentrations (mol/kgw) of porewater, obtained at 50 ky.

MASS TRANSPORT SOVLER EFFICIENCY – 1D_DIFFUSIVE_00_TRACER

Simulation time comparison for 100 years with increasing number of nodes, all simulations are performed in python using a single CPU core

#nodes	LBM time	LBM Million grid point updates /s	FEniCSx time	FEniCSx Million grid point updates /s
81	0.004	2.24	0.05	0.15
100	0.004	2.78	0.06	0.18
1 000	0.004	22.92	0.31	0.36
5 000	0.008	62.26	1.39	0.36
10 000	0.015	68.06	2.79	0.36
50 000	0.120	41.60	14.80	0.34
100 000	0.244	41.00	31.19	0.32
500 000	1.573	31.78	178.19	0.28
1 000 000	3.599	27.78	368.75	0.27
2 000 000	9.676	20.670	822.91	0.24
10 000 000	57.120	17.51	4357.539	0.23



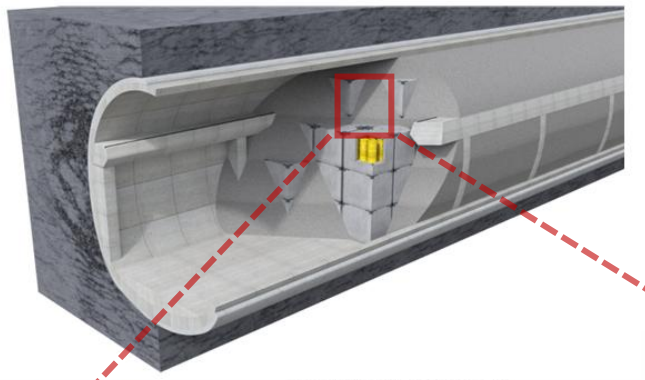
- LBM ~ 20 million grid point updates /s
- ORCHESTRA-RT ** ~ 10 million grid point updates /s ** 12 cores
- COREv5.2 ~ 0.8 million grid point updates /s
- FEniCSx ~ 0.25 million grid point updates/s
- GEMS ~ 0.001 million calculations/s

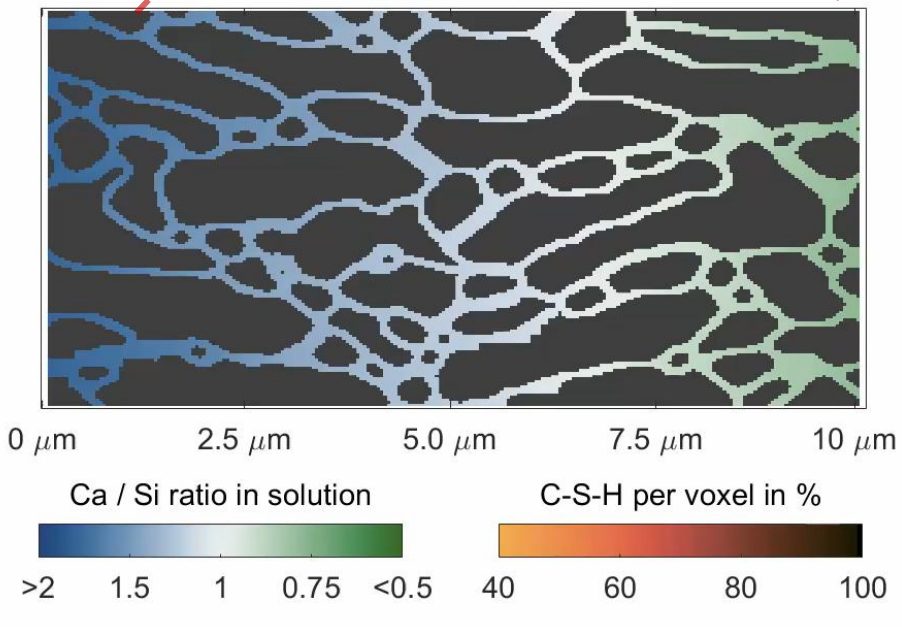
Mass transport + chemistry surrogate + adaptive timestep

PORE-SCALE INTERFACES: LATTICE BOLTZMANN METHOD

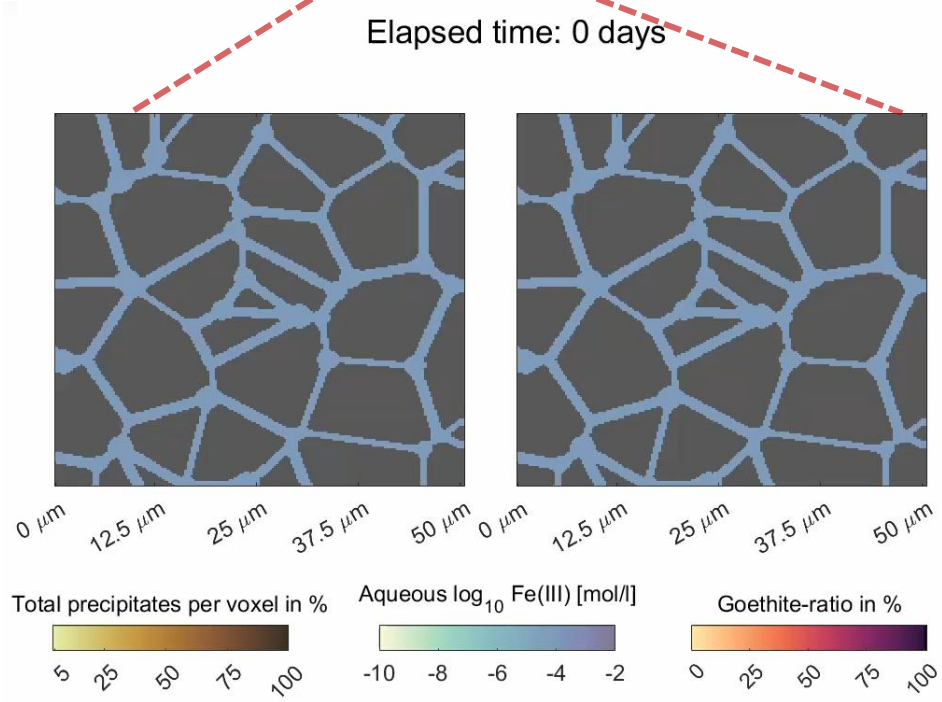
Cement - Clay

Nagra, (2022). NTB 21-02.



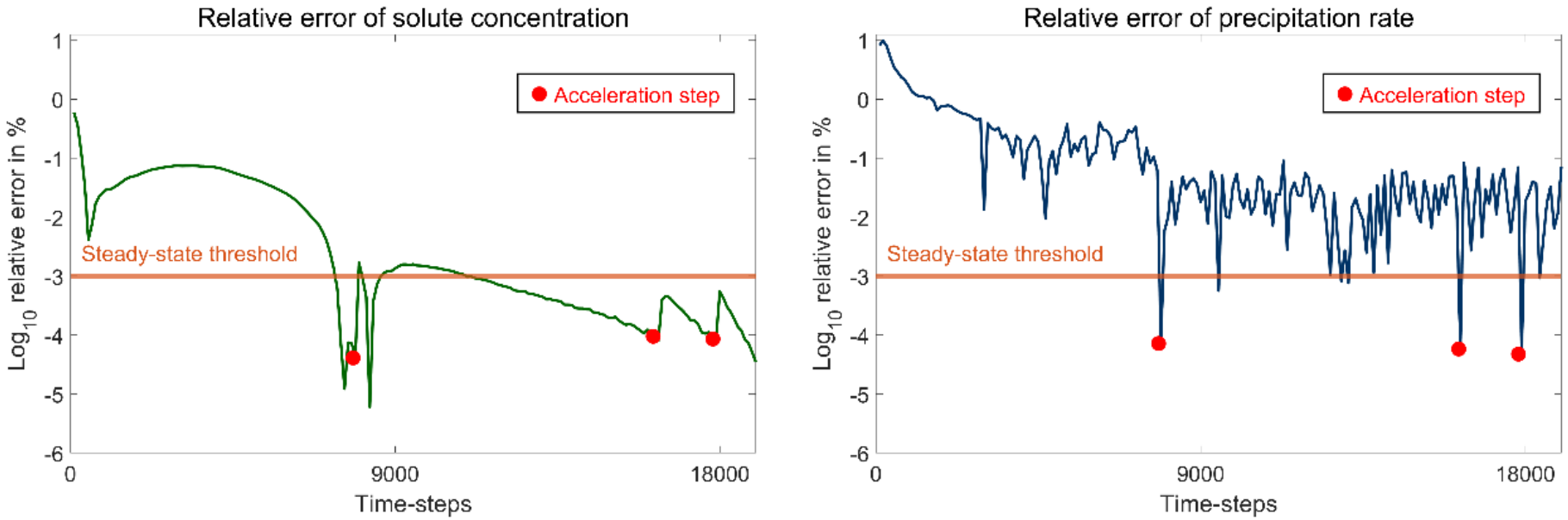


Cement - Steel



Baur, M. P., Churakov, S. V., & Prasianakis, N. I. (2026). Adaptive Time-Stepping and Machine Learning Approach for Pore-Scale Reactive Transport Simulations: MP Baur et al. *Transport in Porous Media*, *153*(3), 37.

ADAPTIVE TIME-STEPPING FOR MULTISCALE PROCESSES (IN TIME)



When all relevant thresholds are crossed a quasi-stationary state is reached and the simulation can advance at a larger timestep until change of the pore-space

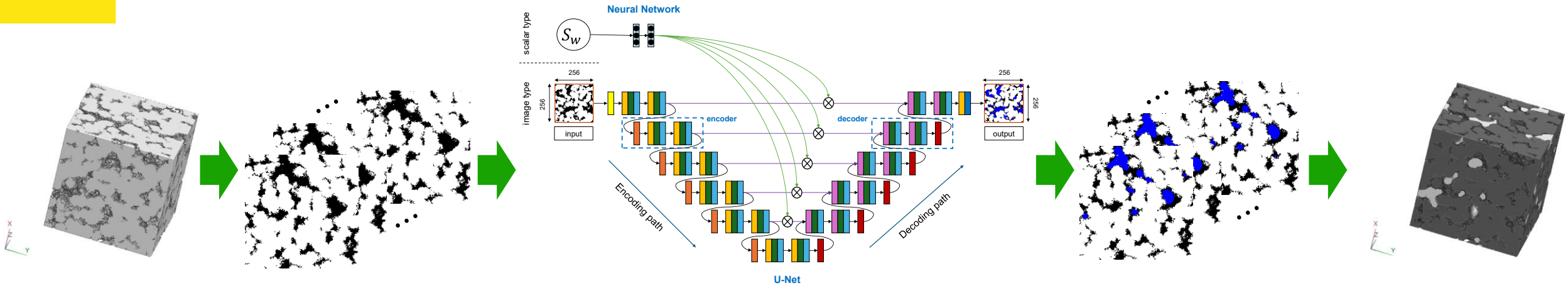
Combined with surrogate model: acceleration of up to **7 orders of magnitude**

Baur, Churakov & Prasianakis, Transport in Porous Media 153, 37 (2026) · ongoing HERMES work

Accelerating the estimation of rock transport properties at partially saturated conditions

eurad

ACCELERATING THE ESTIMATION OF EFFECTIVE ROCK PROPERTIES UNDER PARTIALLY SATURATED CONDITIONS

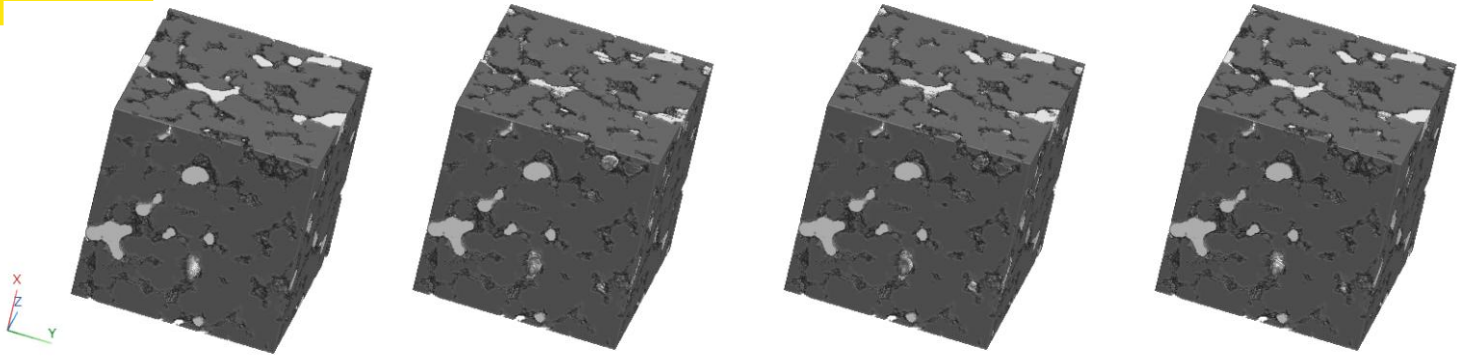


3-D saturated | 2-D saturated | Saturation-conditioned U-Net | 2-D partially saturated | 3-D partially saturated

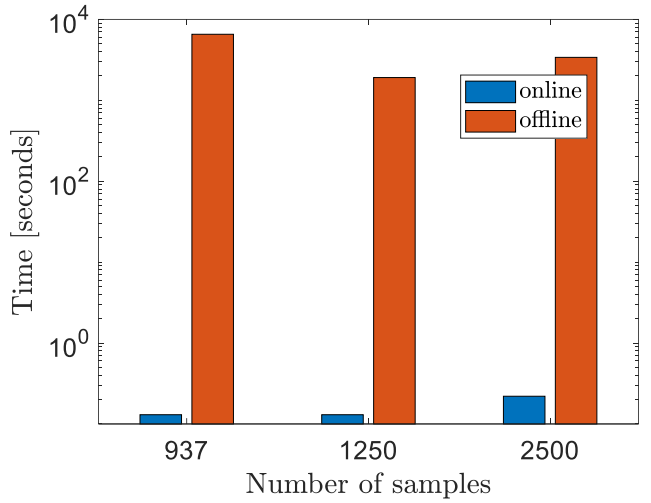
- The saturation-conditioned U-Net is trained to accelerate physics-based simulation based on Shan-Chen Lattice-Boltzmann
- It is to map 3D full-saturated images to 3D partially-saturated images with a given water saturation
- The model works on 2D basis to keep the architecture “small”, therefore, reducing the need of a large number of samples
- The basic idea is to condition U-Net skip connections using a shallow Neural Network model

Published: Santoso, R., Yang, Y., & Poonoosamy, J. (2026). Accelerating the Estimation of Effective Rock Properties Under Partially Saturated Conditions Through Saturation-Conditioned U-Net-Based Initialization. *JGR: Machine Learning and Computation*, 3 (4), e2026JH001287.

INFERRING THE WATER DISTRIBUTION



Reference	937 samples	1250 samples	2500 samples
S_w= 0.77	S_w = 0.82	S_w= 0.79	S_w= 0.77



- Using 2500 samples, we can predict accurately the gas phase distribution with $S_w = 0.77$ and ensure similar phase connectivity as the reference case
- A forward run requires 24 core-hours using 1 GPU in HPC Infrastructure
- The training requires 1 GPU for around 3 hours in HPC Infrastructure
- After training, the saturation-conditioned U-Net can deliver prediction (online) in 39 seconds using 1 CPU in a laptop

Published: Santoso, R., Yang, Y., & Poonoosamy, J. (2026). Accelerating the Estimation of Effective Rock Properties Under Partially Saturated Conditions Through Saturation-Conditioned U-Net-Based Initialization. *JGR: Machine Learning and Computation*, 3 (4), e2026JH001287.

Reduced Order Modelling (ROM)

TED experiment THM simulations

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- **Governing equations** (saturated medium with linear elasticity and cross anisotropy)

Thermal (T): $\boldsymbol{\lambda} \cdot \nabla^2 \mathrm{T} - \rho c \cdot \dot{\mathrm{T}} = \mathrm{Q}$

Hydraulical (p): $\frac{\boldsymbol{K}}{\mu_f(\mathrm{T})} \nabla \cdot (\nabla \mathrm{p}) - [3\mathrm{n} \cdot \alpha_f(\mathrm{T}) + 3(\alpha - \mathrm{n}) \cdot \alpha_s]\dot{\mathrm{T}} + \frac{1}{\mathrm{M}}\dot{\mathrm{p}} + \alpha \nabla \cdot \dot{\mathbf{u}} = 0$

Mechanical (u): $\nabla \cdot (\mathrm{D} : \nabla \mathbf{u}) - \alpha \nabla \mathrm{p} - \Theta \cdot \nabla \mathrm{T} = 0$

- **Full Order Model (FOM) discretization**

$$\begin{bmatrix} K_{TT} & 0 & 0 \\ 0 & K_{PP} & 0 \\ K_{UT} & K_{UP} & K_{UU} \end{bmatrix} \begin{Bmatrix} T \\ P \\ \mathbf{U} \end{Bmatrix} + \begin{bmatrix} C_{TT} & 0 & 0 \\ C_{PT} & C_{PP} & C_{PU} \\ 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} \dot{T} \\ \dot{p} \\ \dot{\mathbf{U}} \end{Bmatrix} = \begin{Bmatrix} F_T \\ F_p \\ F_{\mathbf{u}} \end{Bmatrix}$$

- **2 among 9 sub matrices are nonlinear due to:**

$\mu_f(\mathrm{T})$: viscosity of pore water

$\alpha_f(\mathrm{T})$: thermal expansion coefficient of pore water

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- **Governing equations** (saturated medium with linear elasticity and cross anisotropy)

Thermal (T): $\boldsymbol{\lambda} \cdot \nabla^2 \mathrm{T} - \rho c \cdot \dot{\mathrm{T}} = \mathrm{Q}$

Hydraulical (p): $\frac{\boldsymbol{K}}{\boldsymbol{\mu_f(T)}} \nabla \cdot (\nabla \mathrm{p}) - [3\mathrm{n} \cdot \boldsymbol{\alpha_f}(\mathbf{T}) + 3(\alpha - \mathrm{n}) \cdot \alpha_s]\dot{\mathrm{T}} + \frac{1}{\mathrm{M}}\dot{\mathrm{p}} + \alpha \nabla \cdot \dot{\mathbf{u}} = 0$

Mechanical (u): $\nabla \cdot (\mathrm{D} : \nabla \mathbf{u}) - \alpha \nabla \mathrm{p} - \Theta \cdot \nabla \mathrm{T} = 0$

- **Constitute a matrix of n snapshot solutions using n sets of parameter values $\boldsymbol{\mu}^*_{1-n}$ from 3D FOM:**

$$\mathbf{A} = \{\mathrm{THM}(\mathrm{t}_{1\sim \mathrm{N_t}}, \boldsymbol{\mu}^*_1), \mathrm{THM}(\mathrm{t}_{1\sim \mathrm{N_t}}, \boldsymbol{\mu}^*_2), \dots, \mathrm{THM}(\mathrm{t}_{1\sim \mathrm{N_t}}, \boldsymbol{\mu}^*_\mathrm{n})\}_{(5\times M)\times(n\times Nt)}$$

- **Derive reduced basis $\boldsymbol{\phi} = \{\phi_1, \phi_2, \dots, \phi_r\}$ based on POD as follows:**

$$\mathbf{R} = \mathbf{A}^{\boldsymbol{T}} \cdot \mathbf{A} \implies \mathbf{R}\boldsymbol{\varphi}_j = \boldsymbol{\sigma}_j \boldsymbol{\varphi}_j \implies \boldsymbol{\phi}_j = \frac{1}{\sqrt{\boldsymbol{\sigma}_j}} \mathbf{A}\boldsymbol{\varphi}_j$$

- **Governing equations in reduced basis:**

$$\begin{bmatrix} \mathbb{K}_{\mathrm{TT}} & 0 & 0 \\ \mathbb{K}_{\mathrm{UT}} & \mathbb{K}_{\mathrm{UU}} & \mathbb{K}_{\mathrm{UP}} \\ 0 & 0 & \mathbb{K}_{\mathrm{PP}} \end{bmatrix} \begin{Bmatrix} \mathbb{T} \\ \mathbb{U} \\ \mathbb{p} \end{Bmatrix} + \begin{bmatrix} \mathbb{D}_{\mathrm{TT}} & 0 & 0 \\ 0 & 0 & 0 \\ \mathbb{D}_{\mathrm{PT}} & \mathbb{D}_{\mathrm{PU}} & \mathbb{D}_{\mathrm{PP}} \end{bmatrix} \begin{Bmatrix} \dot{\mathbb{T}} \\ \dot{\mathbb{U}} \\ \dot{\mathbb{p}} \end{Bmatrix} = \begin{Bmatrix} \mathbb{F}_{\mathrm{T}} \\ \mathbb{F}_{\mathbf{u}} \\ \mathbb{F}_{\mathrm{p}} \end{Bmatrix},$$

where $\mathbb{K}_{\mathrm{UT}} = \mathbb{W}^{\mathrm{T}}\mathrm{K}_{\mathrm{UT}}\mathbb{Z}$, $\mathbb{D}_{\mathrm{PU}} = \mathbb{Q}^{\mathrm{T}}\mathrm{D}_{\mathrm{PT}}\mathbb{W}$, $\mathbb{F}_{\mathrm{U}} = \mathbb{W}^{\mathrm{T}}\mathrm{F}_{\mathrm{U}}$, …;

$\mathbb{U} = \mathbb{W}^{\mathrm{T}}\mathrm{U}$, …;

$\mathbb{Z}$, $\mathbb{Q}$, $\mathbb{W}$ are respectively reduced basis for T, p, and **U**

- **Project $[\mathbb{T}, \mathbb{U}, \mathbb{P}]$ from reduced basis back to original FOM space $[\mathrm{T}, \mathbf{U}, \mathrm{P}]$:**

$$\mathrm{T} = \mathbb{Z}\mathbb{T};\ \mathbf{U} = \mathbb{W}\mathbb{U};\ \mathrm{P} = \mathbb{Q}\mathbb{P}$$

A REDUCED ORDER FOR THE TED THM EXPERIMENT:

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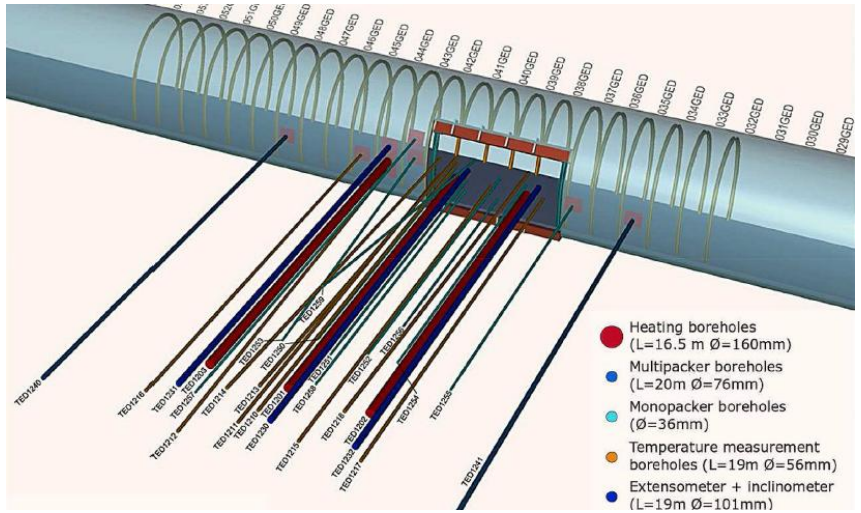
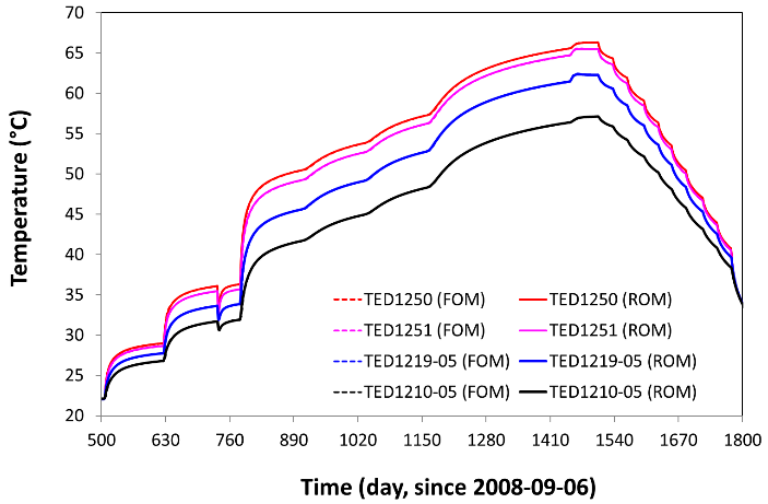
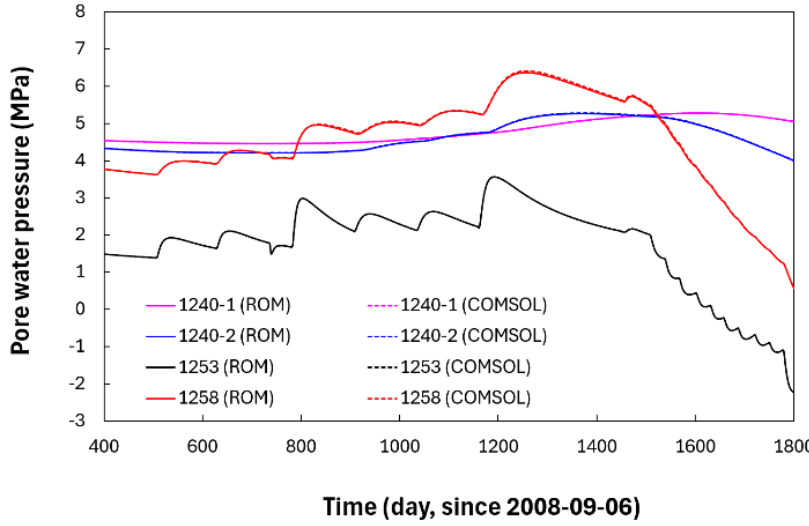
- was developed in MATLAB with livelink to COMSOL which significantly reduced the time to generate the necessary snapshot Full Order Model (FOM) solutions
- was applied to 3D coupled THM modelling of an in-situ TED heating test performed in France with excellent agreement with FOM by COMSOL
- **Achieved already a 12–16× speed-up in the calculation**





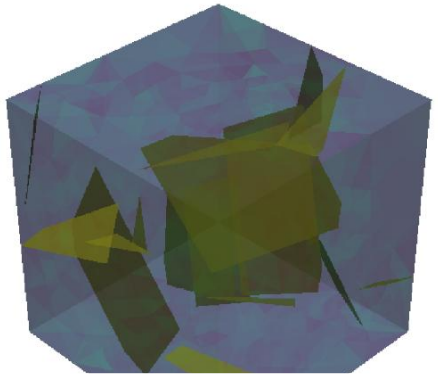


Groundwater flow through fractured rock units (Multi-level monte Carlo)

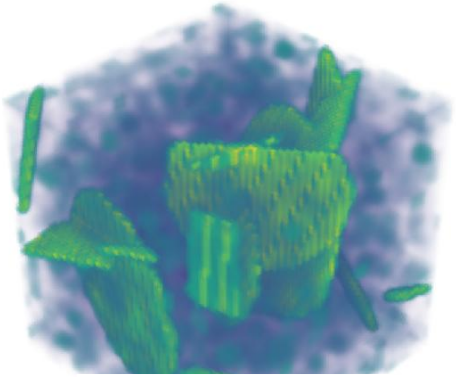
TECHNICAL UNIVERSITY OF LIBEREC

MULTI-LEVEL MONTE CARLO WITH A CNN UPSCALING SURROGATE TO ADDRESS UNCERTAINTY

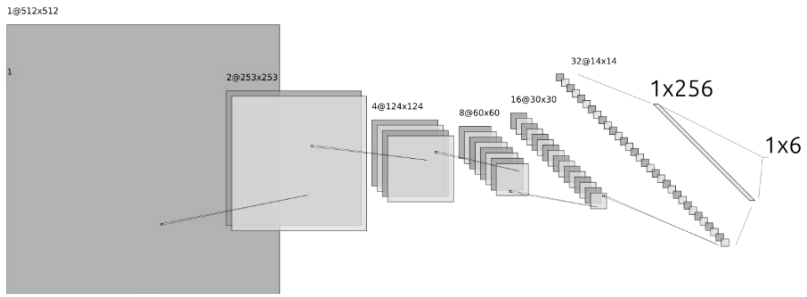
Špetlík, Březina 2026
Convolutional surrogate for 3D discrete fracture–matrix tensor upscaling



tensor field + fractures



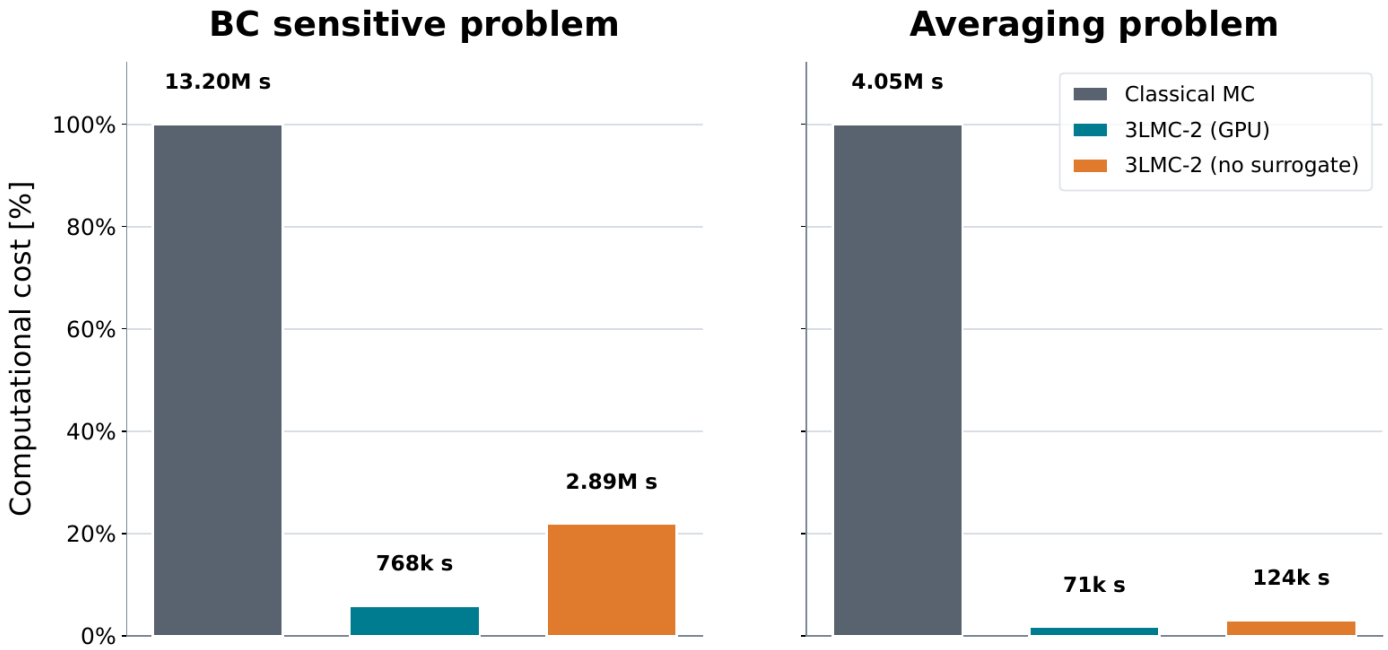
voxelized to 64x64x64



convolutional neural network

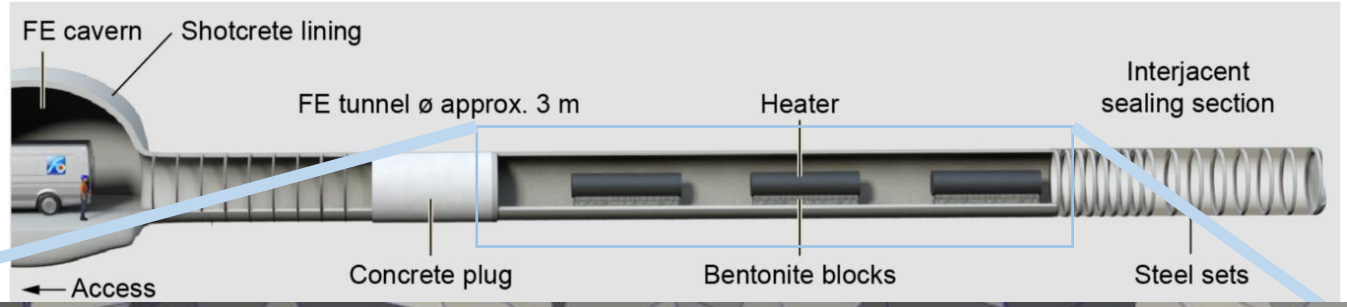
- MLMC efficiency demonstrated on two Darcy flow problems
- surrogate more helpful on challenging problems
- best results for 3 level MLMC, efficiency sensitive to level mesh step

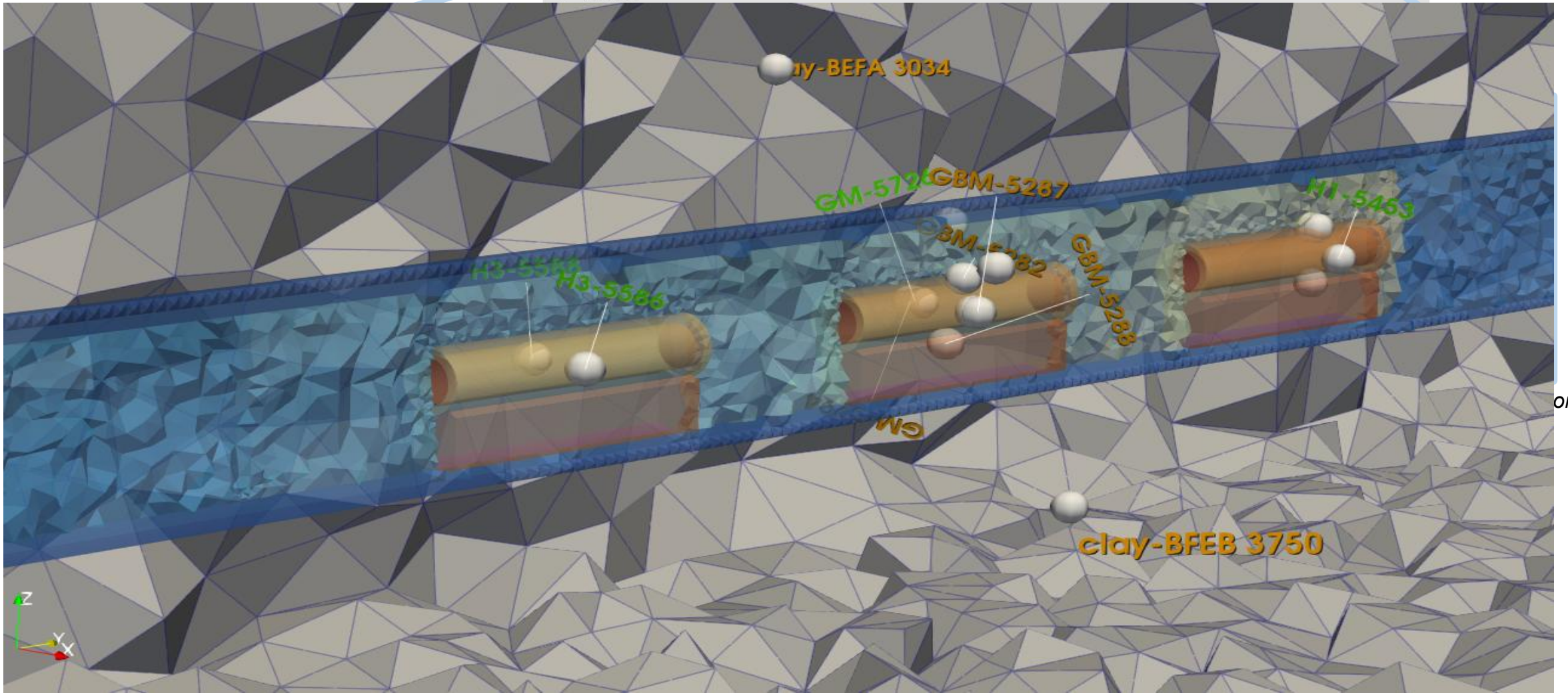
50x speed up



Coupled modelling of the Mont Terri FE Experiment

MONT TERRI
FE IN-SITU EXPERIMENT





ory

INTEGRATING SENSOR DATA, PHYSICS AND MACHINE LEARNING

Sparse sensor data

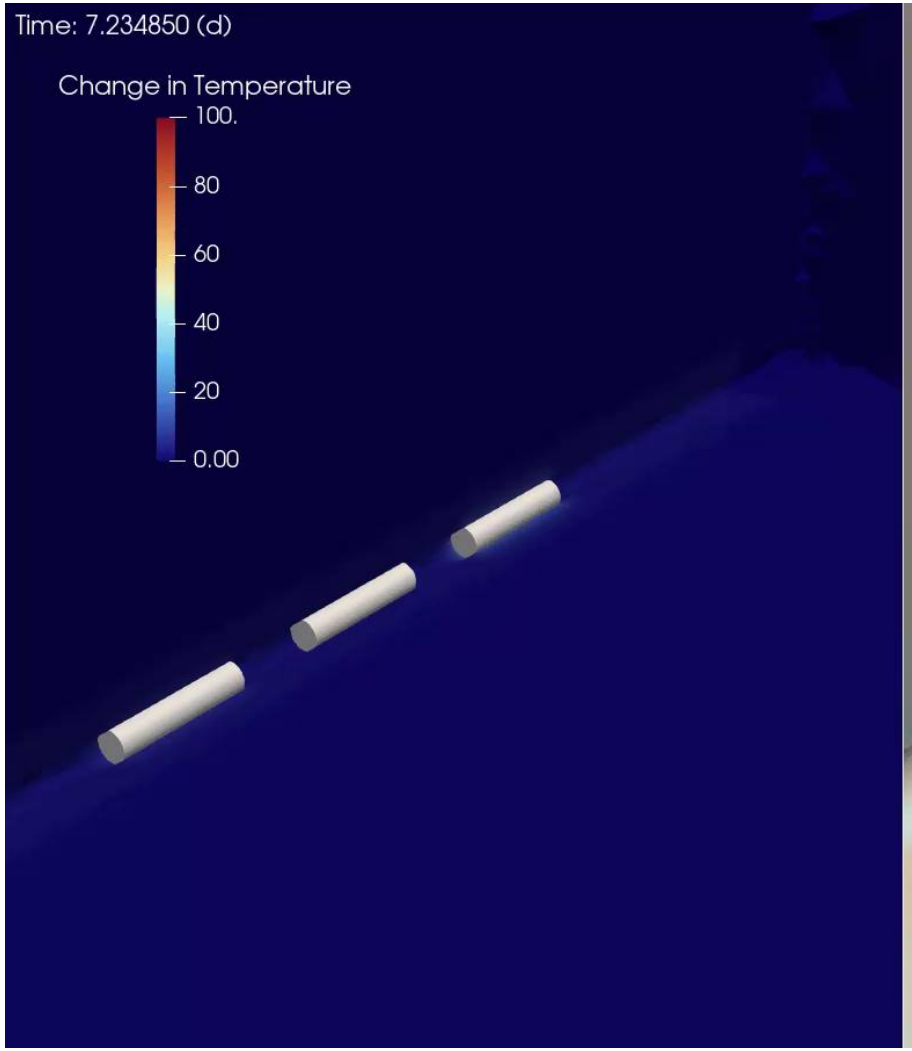
temperature
humidity / saturation
displacement

3D physics

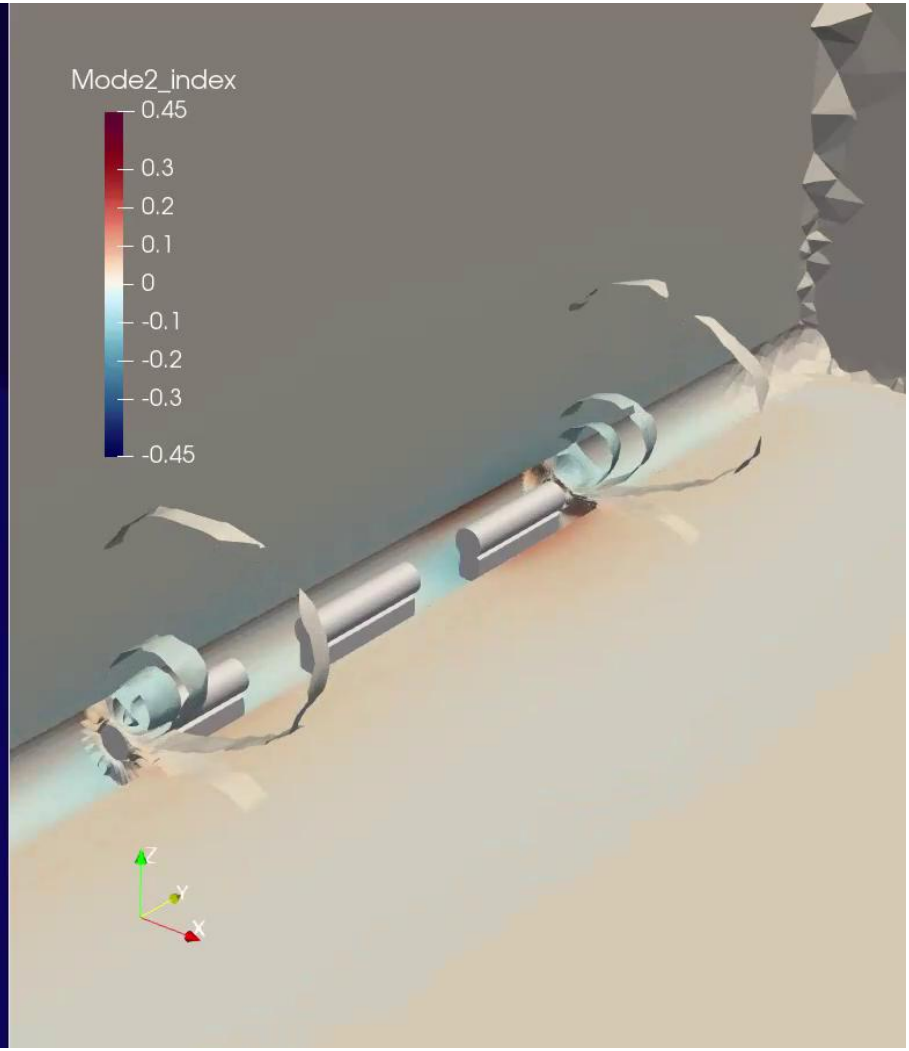
realistic geometry, material properties and boundary conditions, Temperature, Stresses

ML assist

Reconstruct humidity field from sparse sensor data



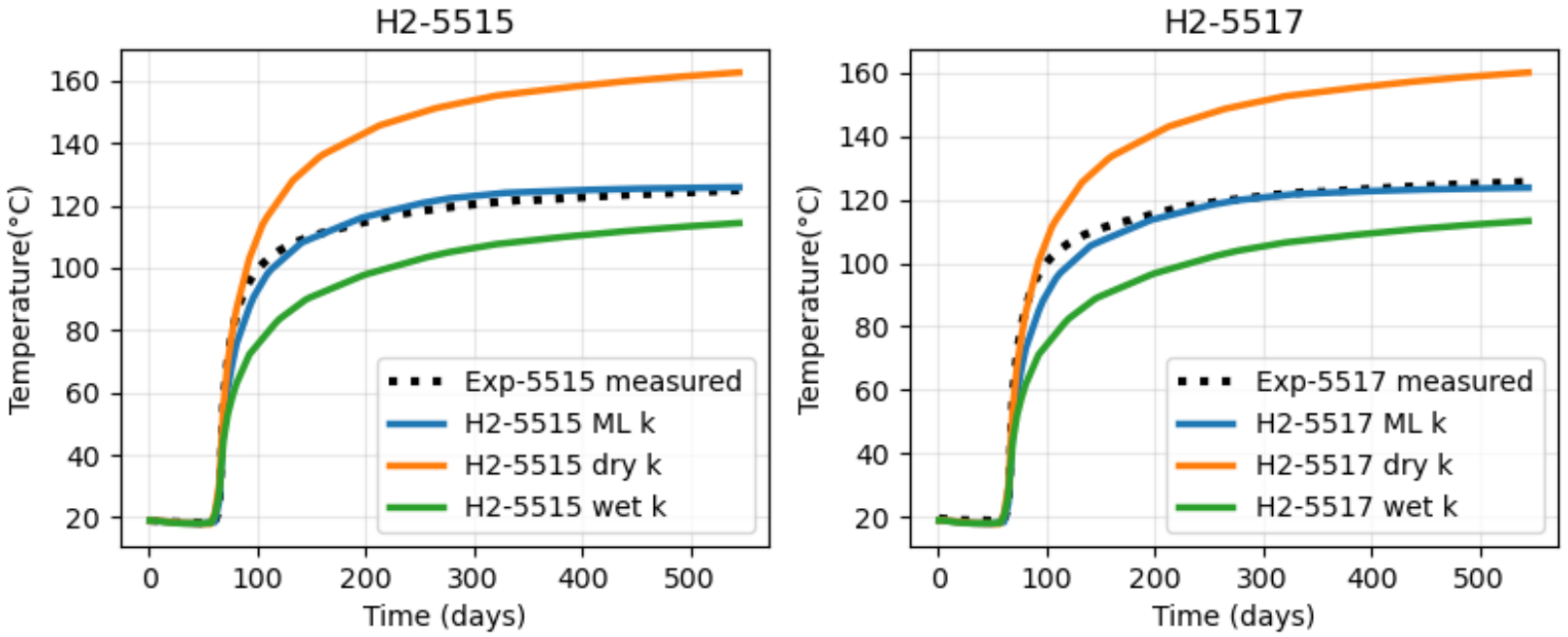
Temperature



Stresses

Urpi et al, (HERMES), Hu et al., International Journal of Heat and Mass Transfer 213 (2023);

TOWARDS A FIELD-SCALE DIGITAL TWIN: SENSOR DATA + 3D PHYSICS + ML



- Simulation is much faster than the monitored experiment and can be updated by daily sensor data
- Identify erroneous sensors or experimental discrepancies with designed set-up
- Visualization of the experiment
- **Combining monitoring data with coupled models supports interpretation of the experiment and provides a basis for testing predictive capabilities relevant to repository design and assessment.**

SUMMARY

Complementary methods accelerate coupled simulations: machine-learning surrogates, reduced-order models and adaptive algorithms address different computational bottlenecks.

Fast and validated coubled codes enable broader analysis: multiscale studies, inverse modelling and design optimisation can be explored more efficiently across coupled processes and repository scenarios, supporting the development of a **digital twins.**

Explainability, accuracy and benchmarking remain essential: establishing when accelerated models are reliable, and how their performance compares with established approaches is central for their adoption in future coupled workflows

Questions / discussion