APPLICATION OF AI IN REACTIVE TRANSPORT MODELLING

Topical Session 3 – Digital transformation: DITOCO2030 and HERMES

Nikolaos I. Prasianakis, PSI Switzerland

Presentation includes results of HERMES Task 4

Co-funded by the European Union under Grant Agreement n° 101166718

HERMES TASK 4

• Surrogate models (of individual and coupled phenomena)

Task Partners: [SCK CEN] [SURAO] [TUL] [IGN] [TU BAF] [MUL] [FZJ] [PSI] [GFZ] [UNIPR] [UDC] [Amphos 21] [KIT] [CNRS] [ANDRA]

- **Task leading: N. Prasianakis (PSI, Switzerland)/ J. Brezina (TUL, Czech Rep.)**
- **Aim:**
  Create surrogate models of individual processes and of several coupled processes. Surrogate models or proxy models provide a significant acceleration to the simulation codes. The topics which will be addressed are relevant to Chemistry, Gas-Mass-Heat transport and Mechanics (THMC). In the core of this task is the application, benchmarking and implementation of machine learning methods and codes which go beyond the state of the art.

Task 4.1: Acceleration of computations for individual processes and phenomena
Task 4.2: Surrogate models for coupled processes and multiphysics

TASK 4: SURROGATE MODELS

- 15 Participants from 10 countries across Europe.

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

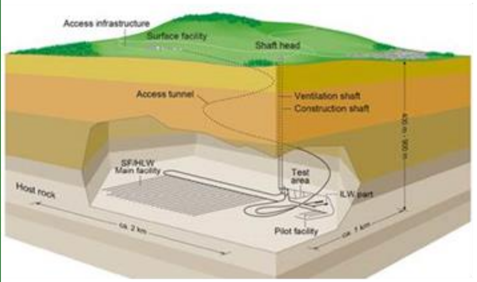
Chemistry surrogates
Mechanics surrogates (including calculation of stresses from images)
Hydraulics / Flow surrogates (including calculation of transport from images)
Waste package level surrogates

NEED FOR RT, MULTISCALE MULTIPHYSICS AND DIGITAL TWINS

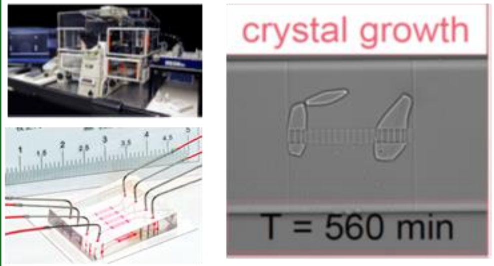
Digital Twin is a modelling based tool of increased realism. For geochemical applications, it should cover several spatial and temporal scales, as well as all major underlying mechanisms.

Digital Twin

Real physical process



Field scale, nuclear waste repository



Laboratory experiment, microfluidics

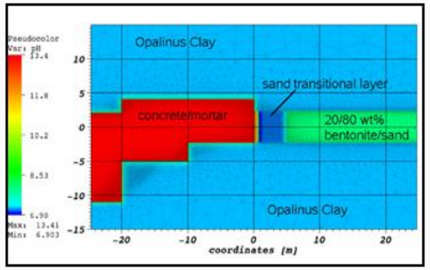
Design optimization

Predictive capability

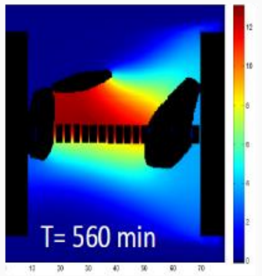
Process Understanding

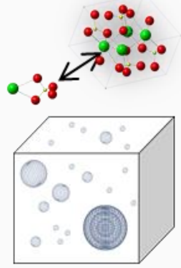
Numerical Diagnostics

Physics based models



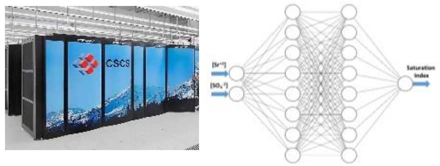
Field scale, numerical simulation



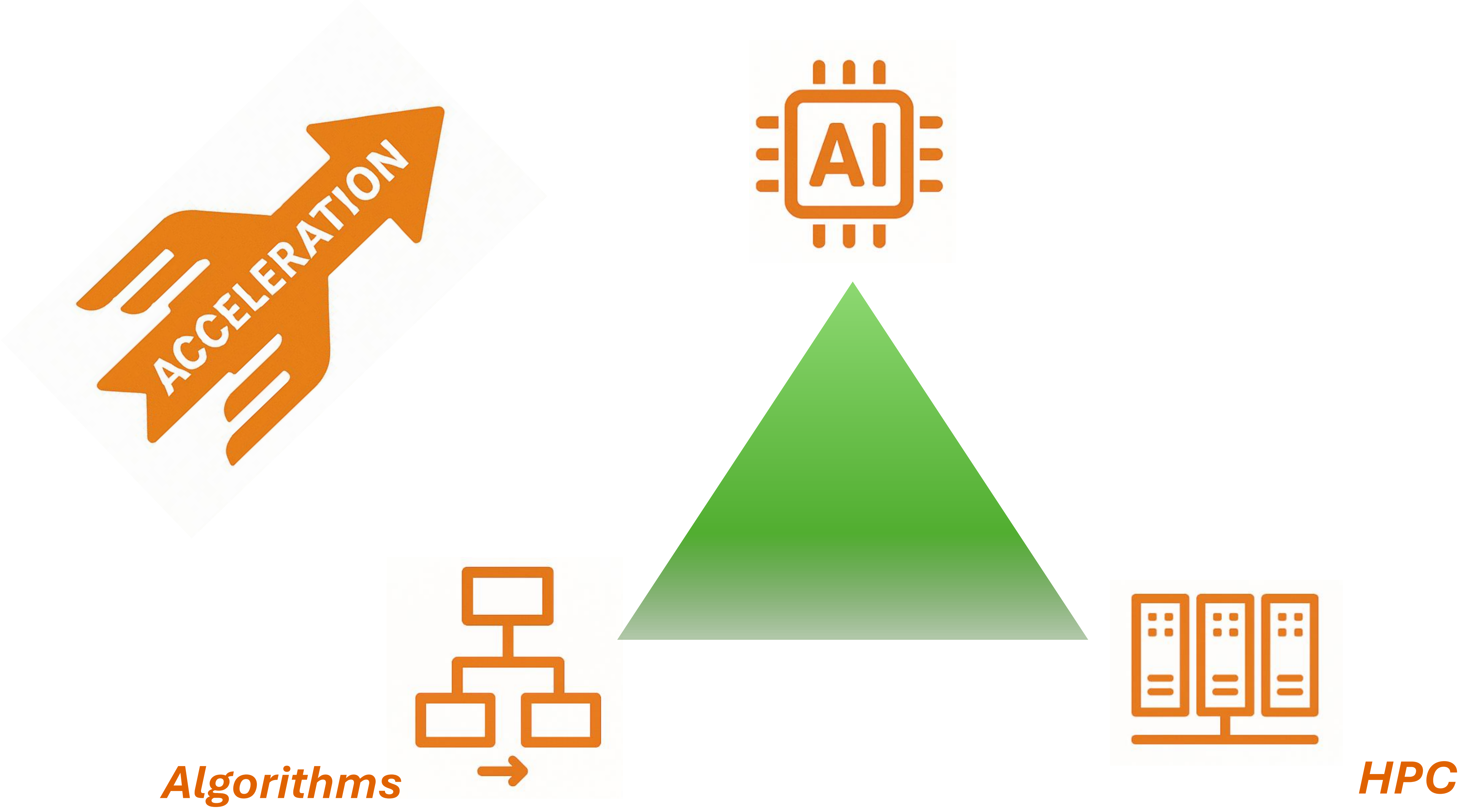


Cross-scale microfluidic precipitation simulation

- High fidelity simulations
- Multiscale description
- Multiphysics description
- Ultrafast computations Sensitivity analysis
- Machine learning
- Augmented reality of experiment
- Real-time experiment companion

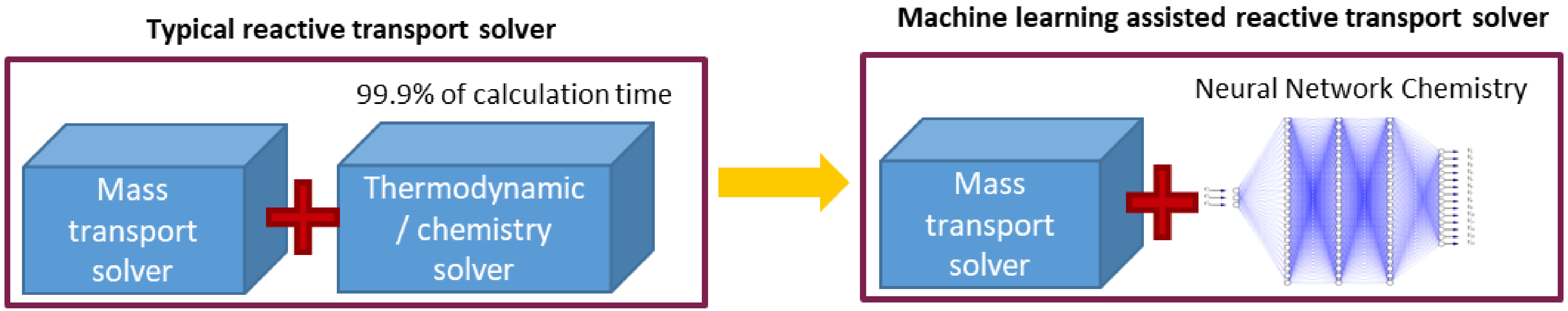


MULTISCALE MULTIPHYSICS, OPTIMIZATION AND DIGITAL TWINS

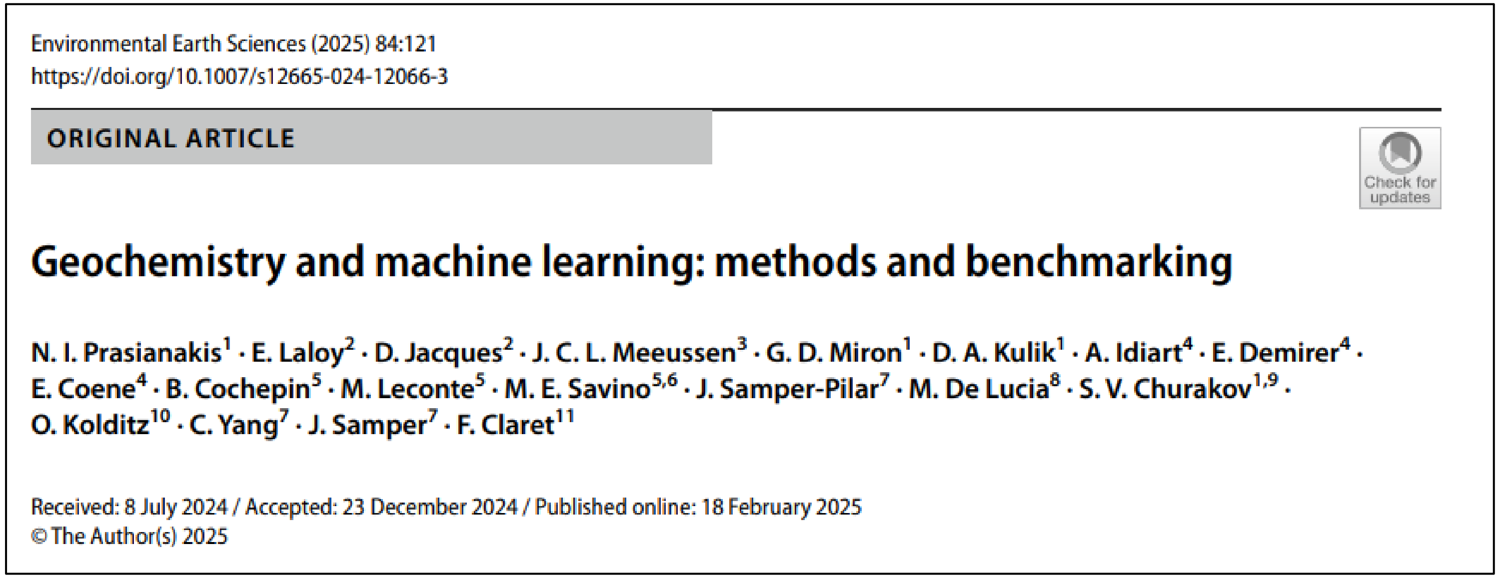


MACHINE LEARNING FOR ACCELERATING CODES: CHEMICAL REACTIONS

- In reactive transport simulation a transport and a chemical solver are usually coupled.
- The thermodynamic/chemical calculations consume > 99.9% of the total simulation time.
- Chemistry based machine learning for acceleration of the geochemistry has been showcased in several works.



EURAD-DONUT


Environmental Earth Sciences (2025) 84:121
https://doi.org/10.1007/s12665-024-12066-3

ORIGINAL ARTICLE

Check for updates

Geochemistry and machine learning: methods and benchmarking

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Data Management
FAIR principles

Switch

zenodo

GEOCHEMISTRY AND MACHINE LEARNING BENCHMARK WITHIN EURAD

HERMES

eurad European Joint Programme on Radioactive Waste Management

NRG

UNIVERSITE D'ORLEANS

PAUL SCHERRER INSTITUT PSI

SCK•CEN

brgm

cea

université PARIS-SACLAY

AgroParisTech Talents d'une planète soutenable

ANDRA

AMPHOS 21 SCIENTIFIC AND STRATEGIC ENVIRONMENTAL CONSULTING

UFZ HELMHOLTZ Zentrum für Umweltforschung

GFZ Helmholtz-Zentrum POTSDAM

UNIVERSIDADE DA CORUÑA

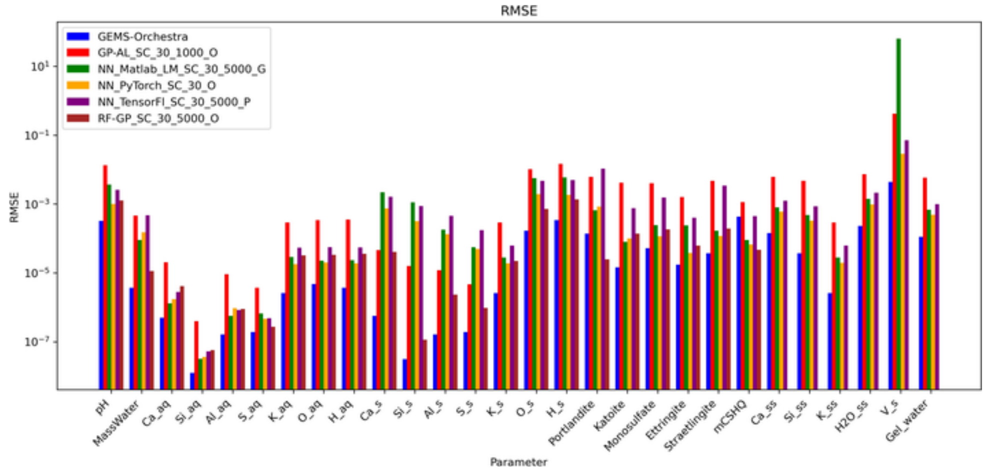
enresa

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

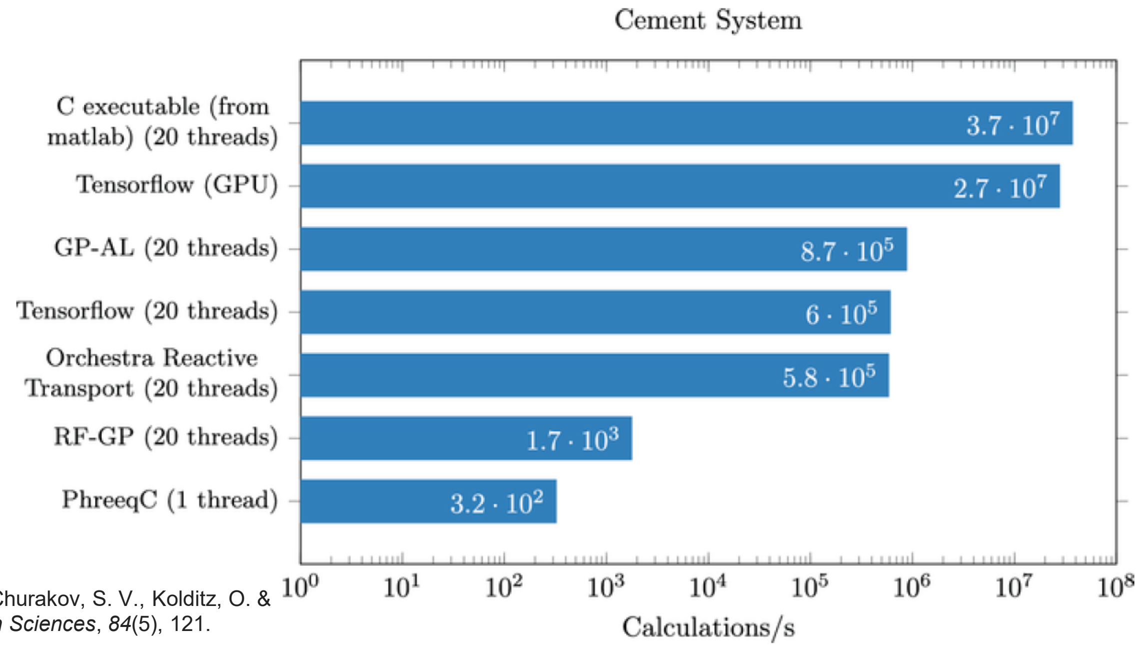
Machine Learning model

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

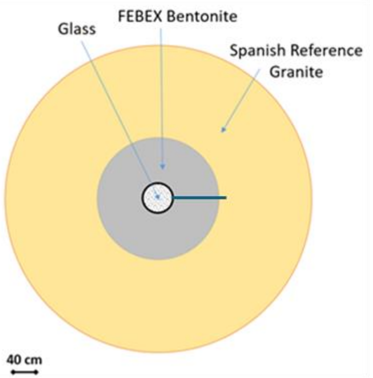


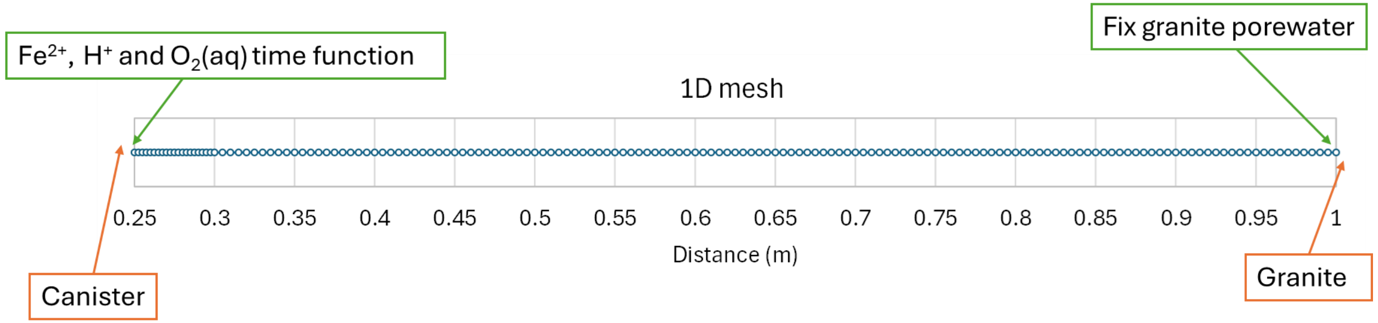
Prasianakis, N. I., Laloy, E., Jacques, D., Meeussen, J. C. L., Miron, G. D., Kulik, D. A., De Lucia, M., ...Churakov, S. V., Kolditz, O. & Claret, F. (2025). Geochemistry and machine learning: methods and benchmarking. *Environmental Earth Sciences*, *84*(5), 121.

GEOML-RT : REACTIVE TRANSPORT BENCHMARK

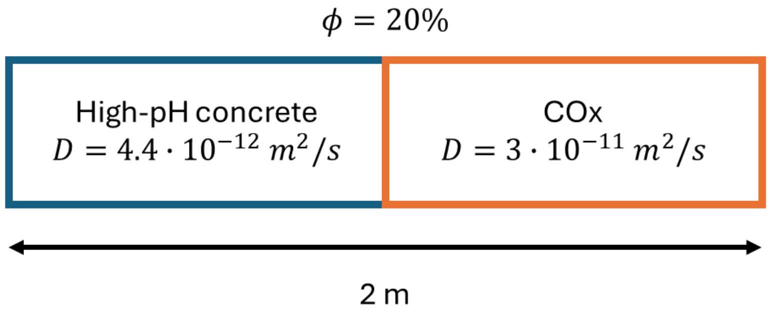
Several participants across EURAD-2 benchmarking reactive transport codes with ML-accelerated geochemistry

- Uranium sorption and transport (GFZ)
- Cement degradation (SCK – PSI)
- Iron corrosion benchmark (UDC, J. Samper et al.)

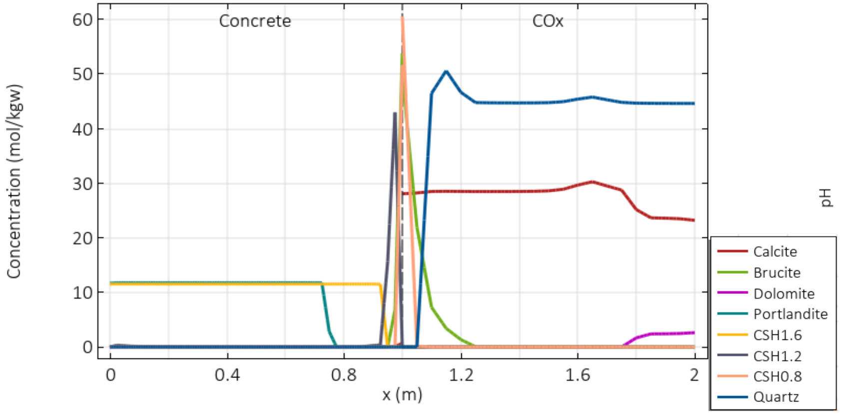


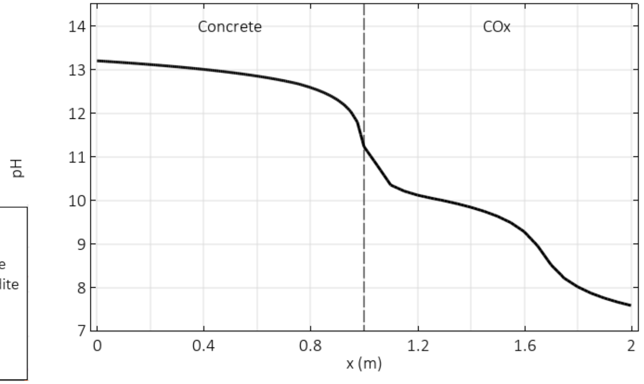


- Processes at the interfaces: Cement-Clay (Amphos, A. Idiart et al.)



50 000 years of simulation, $\mathbf{\Delta t = 0.2y}$





REACTIVE TRANSPORT CORROSION MODEL

- **Following steps for model complexity:**
  - More minerals under equilibrium
  - More aqueous complexation
  - Cation exchange

Minerals	LogK
Calcite + H^+ ⇔ Ca^{2+} + HCO_3^-	1.850
Magnetite + $6H^+$ ⇔ $3Fe^{2+}$ + $0.5O_2$ (aq) + $3H_2O$	-6.560
Goethite + $2H^+$ ⇔ Fe^{2+} + $1.5H_2O$ + $0.25O_2$ (aq)	-8.090
Quartz ⇔ H_4SiO_4	-3.7400

Cation exchange	$K_{Na\text{-}cation}$
Na^+ + X-K ⇔ K^+ + X-Na	0.138
Na^+ + 0.5 X_2-Ca ⇔ 0.5 Ca^{2+} + X-Na	0.2924
Na^+ + 0.5 X_2-Mg ⇔ 0.5 Mg^{2+} + X-Na	0.2881
Na^+ + 0.5 X_2-Fe ⇔ 0.5 Fe^{2+} + X-Na	0.5

Aqueous complexes	Log K
$CaCO_3$(aq) + H^+ ⇔ Ca^{2+} + HCO_3^-	7.1100
$CaHCO_3^+$ ⇔ Ca^{2+} + HCO_3^-	-1.100
$CaOH^+$ + H^+ ⇔ Ca^{2+} + H_2O	12.78
CO_2(aq) + H_2O ⇔ H^+ + HCO_3^-	-6.350
CO_3^{2-} + H^+ ⇔ HCO_3^-	10.33
KOH(aq) + H^+ ⇔ K^+ + H_2O	14.460
$MgCO_3$(aq) ⇔ Mg^{2+} + CO_3^{2-}	-2.980
$MgHCO_3^+$ ⇔ Mg^{2+} + HCO_3^-	-1.040
$MgOH^+$ + H^+ ⇔ Mg^{2+} + H_2O	11.680
$NaHCO_3$(aq) ⇔ Na^+ + HCO_3^-	0.250
$NaCO_3^-$ ⇔ Na^+ + CO_3^{2-}	-1.270
NaOH(aq) + H^+ ⇔ Na^+ + H_2O	14.750
OH^- + H^+ ⇔ H_2O	14.000
Fe^{3+} + $0.5H_2O$ ⇔ H^+ + $0.25O_2$ + Fe^{2+}	-8.485
$FeHCO_3^+$ ⇔ Fe^{2+}+ HCO_3^-	-1.440
$FeCO_3$ (aq) ⇔ Fe^{2+}+ CO_3^{2-}	4.640
$FeCl^+$ ⇔ Fe^{2+}+ Cl^-	-0.140
$FeCl^{2+}$ + $0.5H_2O$ ⇔ Fe^{2+} + Cl^- + H^+ + $0.25O_2$(aq)	-9.885
$FeOH^+$+ H^+ ⇔ Fe^{2+}+ H_2O	9.500
$FeOH^{2+}$ ⇔ Fe^{2+}+ $0.5H_2O$ + $0.25O_2$(aq)	-6.295
$Fe(OH)_2$(aq) + $2H^+$ ⇔ Fe^{2+}+ $2H_2O$	20.60
$Fe(OH)_3$(aq) + $2H^+$ ⇔ Fe^{2+} + $2.5H_2O$ + $0.25O_2$(aq)	4.075
$Fe(OH)_4^-$ + $3H^+$ ⇔ Fe^{2+} + $3.5H_2O$ + $0.25O_2$(aq)	13.115
$Fe(OH)_2^+$ + H^+ ⇔ Fe^{2+} + $1.5H_2O$ + $0.25O_2$(aq)	-2.815
$Fe_2(OH)_2^{4+}$ + $2H^+$ ⇔ $2Fe^{2+}$ + H_2O + $0.5O_2$(aq)	-14.020
H_2(aq) + $0.5O_2$ ⇔ H_2O	46.07

J. Samper, A. Mon

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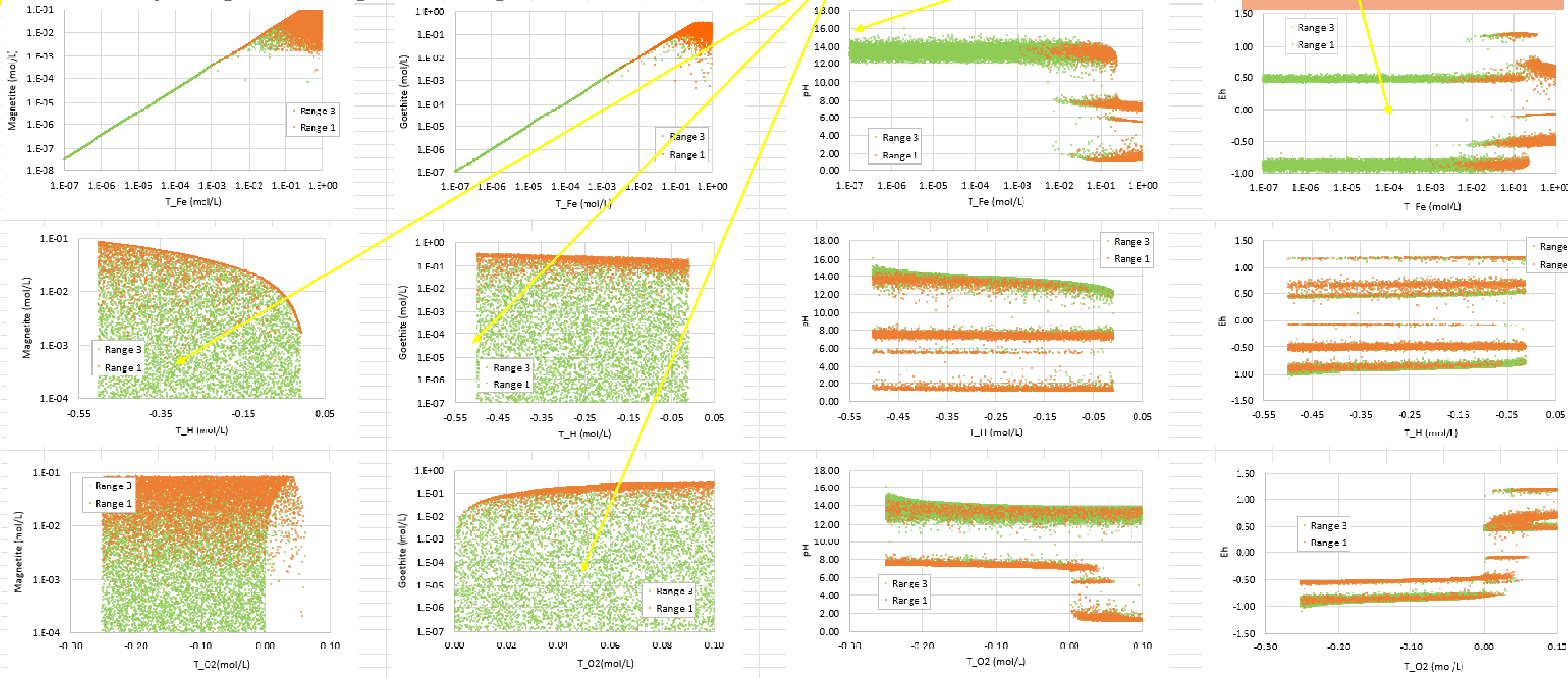
REACTIVE TRANSPORT CORROSION MODEL

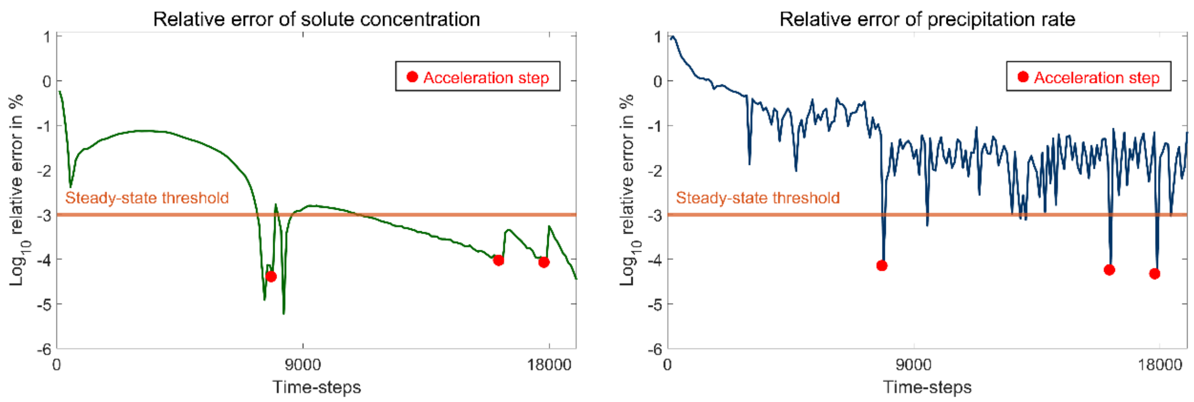
- Exploring a new range of training data

Small goethite and magnetite precipitation is better represented

- Small Fe concentrations are better represented
- pH and Eh gaps remain

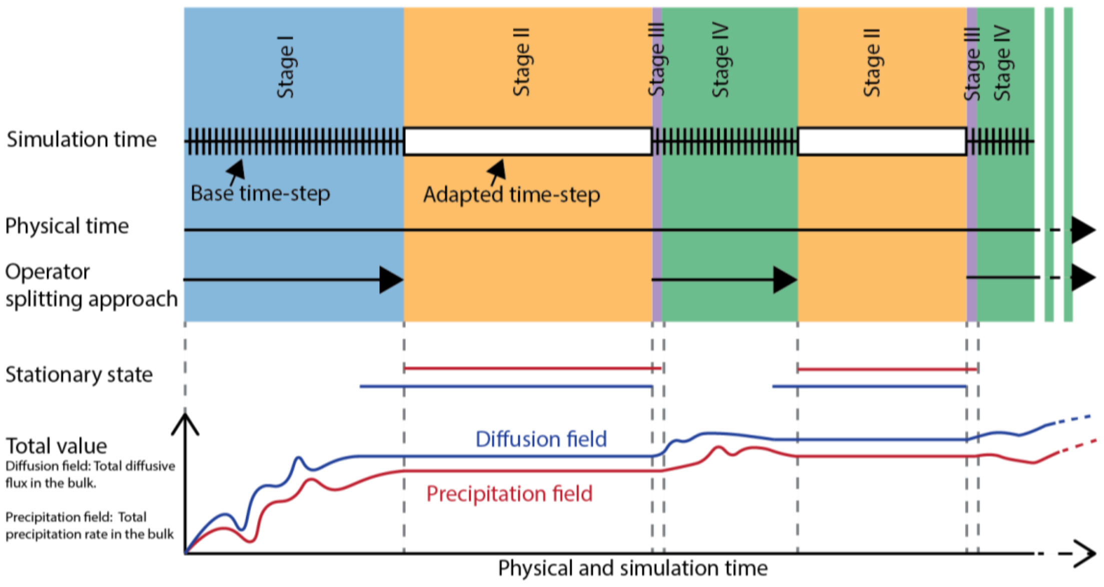


ACCELERATION OF LB ALGORITHM FOR PORE LEVEL SIMULATIONS

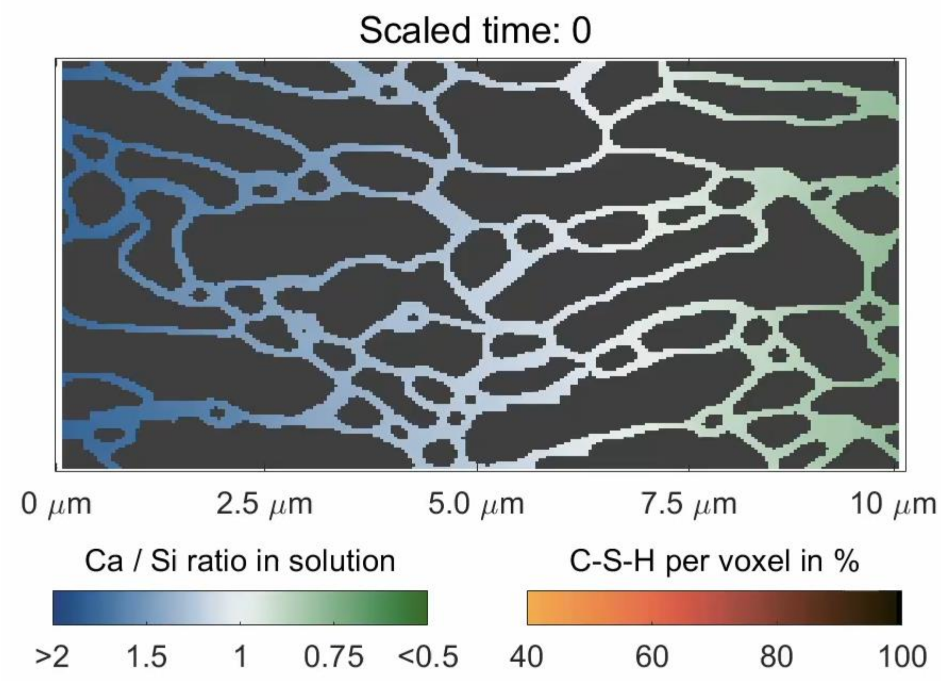


- Cement – clay interface (CSH precipitation in Clays)

- Adaptive time step speed-up 3-4 orders of magnitude
- **Combined ML-chemistry + adaptive timestep Speed-up of 6 orders of magnitude.**



Stage I:	Initial transient state
Stage II:	Temporary occurence of quasi steady state (TOSS)
Stage III:	Disturbance of TOSS
Stage IV:	Rearranging transient state



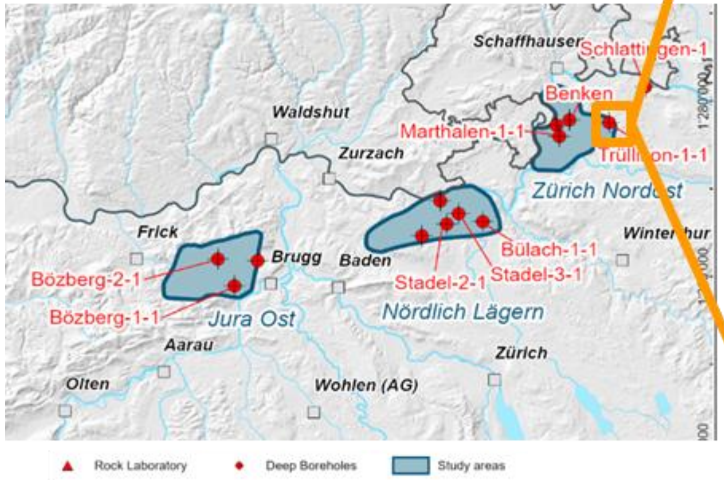
M. Baur, S. V. Churakov, N.I. Prasianakis (submitted); Synergy with SNF PRINCE project

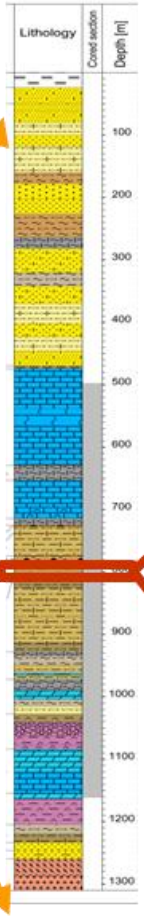
AI FOR THE ACCELERATION OF THE MODELLING WORKFLOW: LITHOLOGY CLASSIFICATION AND MINERAL CONTENT REGRESSION

HERMES

PSI nagra

9 boreholes
~ 6 km extracted drill cores
+ photos (continuous data)
+ laboratory data (at selected points)





Computer Vision based Core Processing

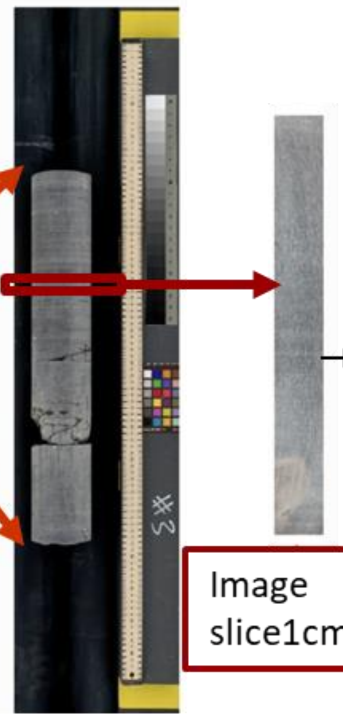
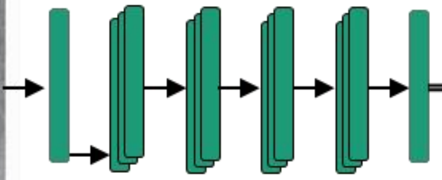


Image slice1cm

AI Classification & Regression Model



Lithological Classification 96.7% Accuracy

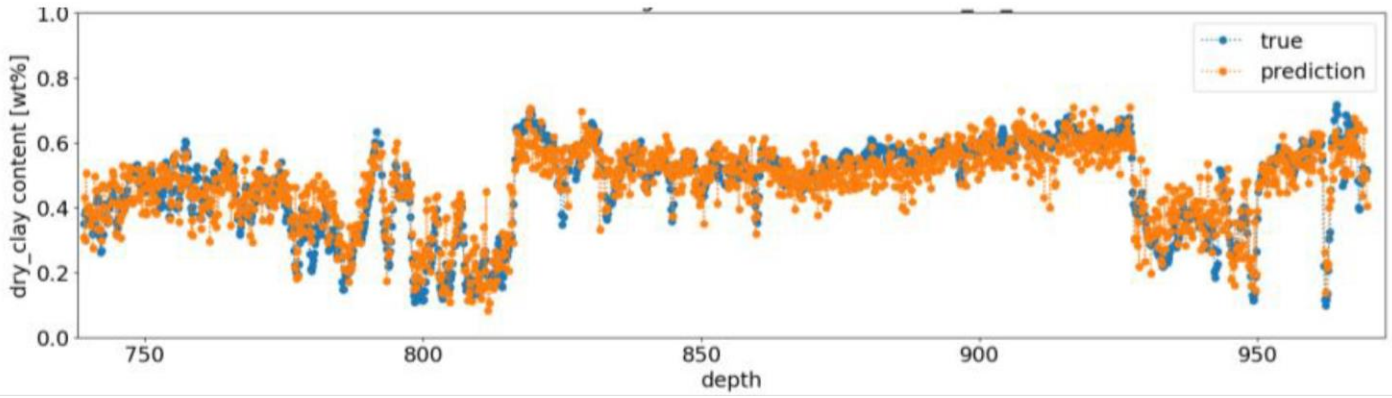
Mineralogical Prediction
Clay
Carbonate
Silicate

Similar accuracy as MultiMin

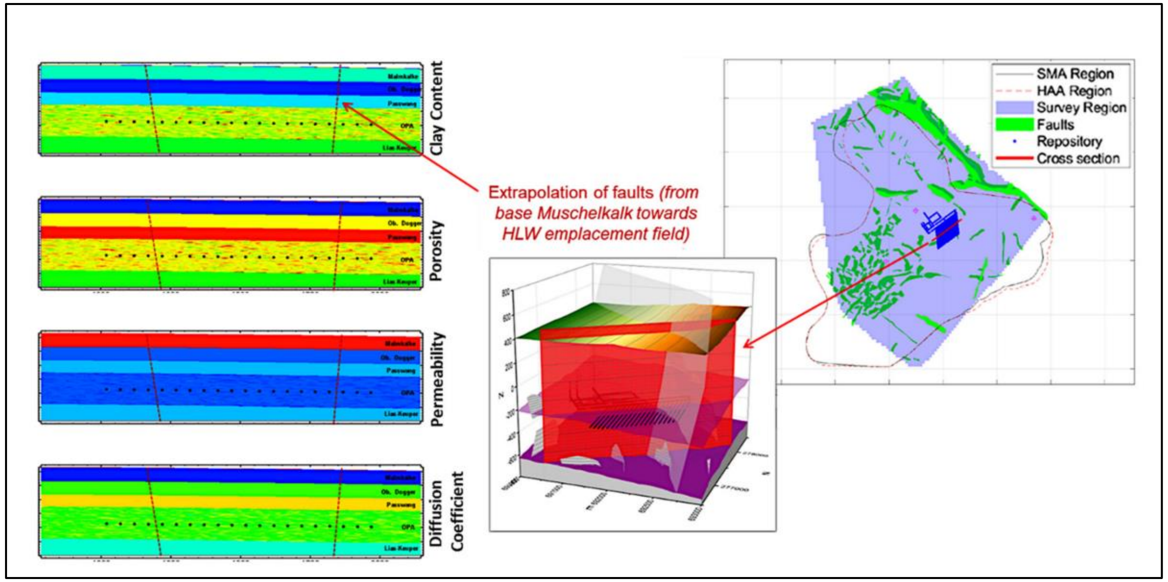
Boiger R., Churakov S.V., Ballester Llagaria I., Kosakowski G., Wüst R., Prasianakis N.I. (2024) Direct mineral content prediction from drill core images via transfer learning. Swiss Journal of Geosciences, 117(1), 1-26. https://doi.org/10.1186/s00015-024-00458-3

DRILL BOREHOLE -> AI ANALYSIS -> GEOLOGICAL MODEL

High resolution model result
14% relative error to XRD
➔ Same level of accuracy with
state of the art statistical models



Can assist the **high resolution** rapid construction of geological model



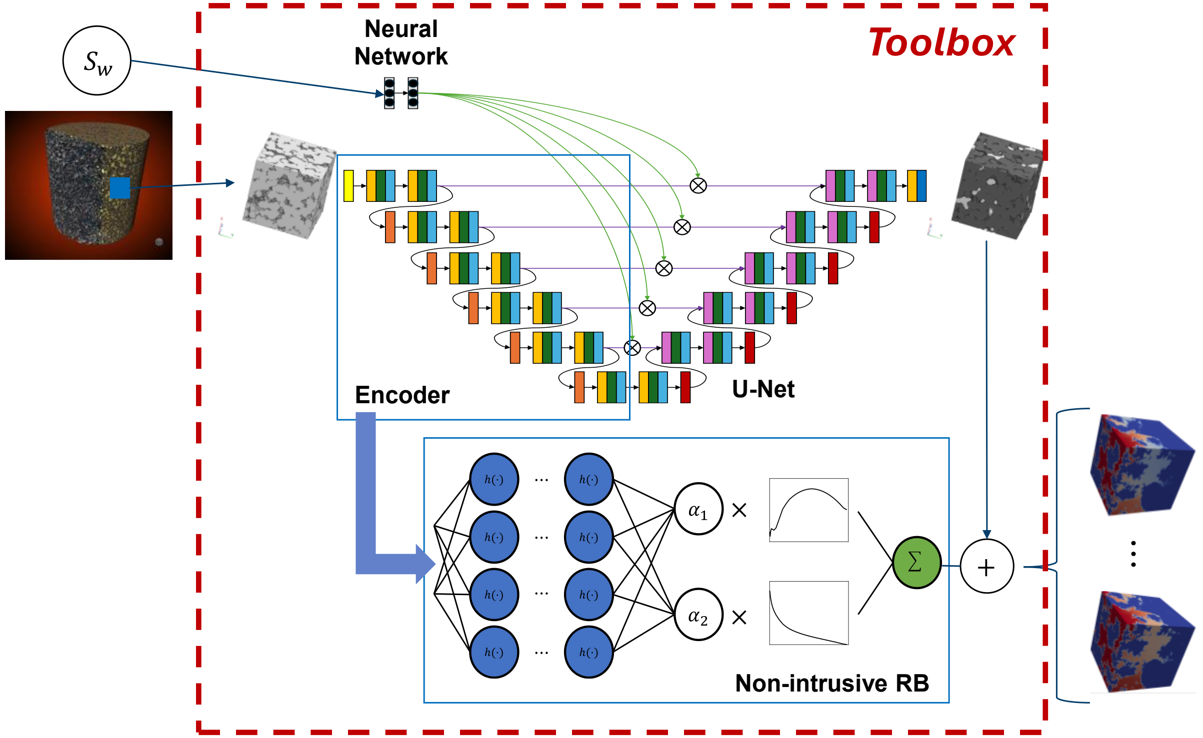
Q: How to map a few borehole data to the reservoir scale domain ?

Example image of geological model from: Papafotiou et al. , *Energies* **2022**, *15*, 6121. https://doi.org/10.3390/en15176121

DEVELOPMENT OF PROCESS-BASED ML TOOLBOX FOR ASSISTING 3D EXPERIMENTS IN PARTIALLY SATURATED CLAY

1. **Aims:**
   - Developing a process-based machine learning toolbox/framework to assist real-time 3D experiments and understanding reactive flow
2. **Modeling approach:**
   - **Saturation-conditioned U-Net** for mapping gas phase distribution and dimensionality reduction
   - **Non-intrusive reduced basis method** for mapping to states, such as concentration
3. **Numerical methods:**
   - Lattice Boltzmann method for generating partially saturated condition and states
4. **Vision:**
   - Enabling imaging fast & and identification of events e.g. mineralization at gas/liquid interfaces or gas bubble nucleation

   - Enabling efficient calibration of nucleation and geochemical parameters, as well as deriving effective properties, for radionuclides transport in partially saturated clay



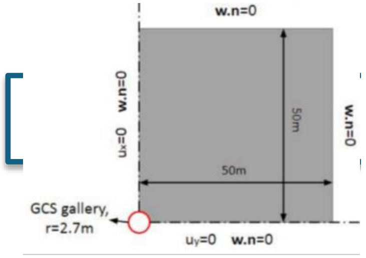
Santoso et al. (in prep) & codes will be made publicly available

J. Poonoosamy
R. Santoso
Y. Yang



NUMERICAL STUDY OF HYDROMECHANICAL RESPONSE USING PHYSICS-INFORMED NEURAL NETWORKS (PINN)

Background



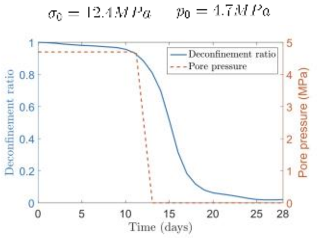
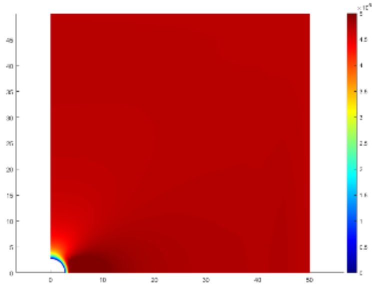
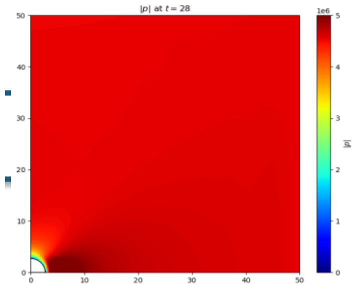


Fig. Mechanical and hydraulic deconfinement curves

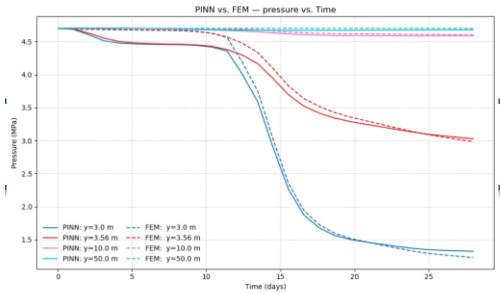
Result: Pressure distribution



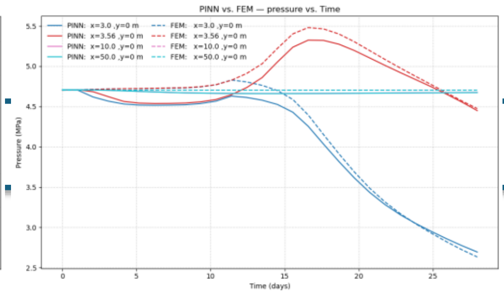
FEM



PINN

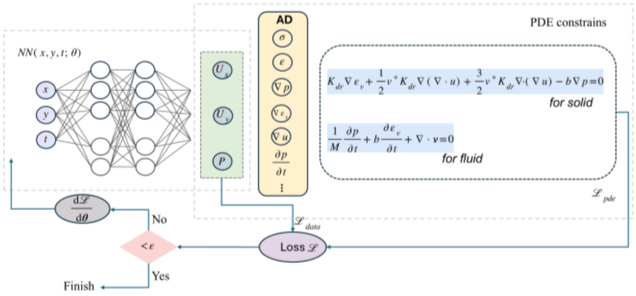


Points on y-axis

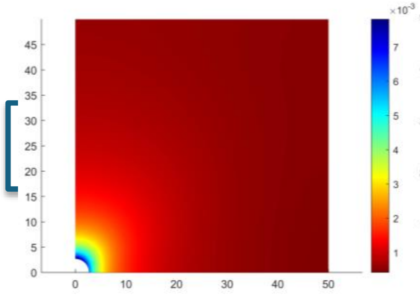


Points on x-axis

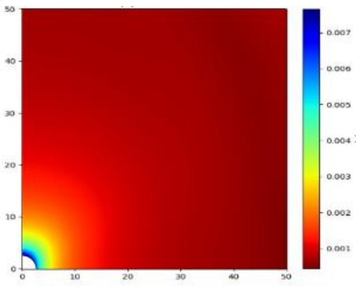
Methodology



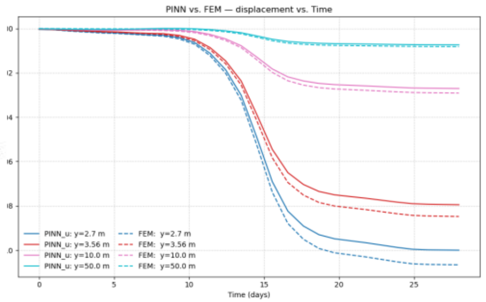
Result: Displacement distribution



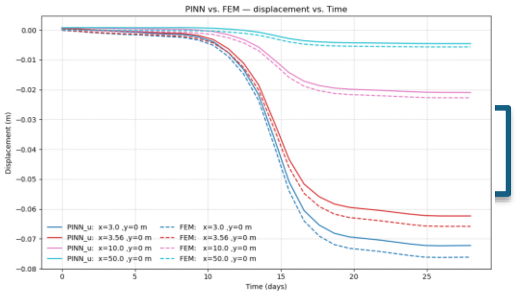
FEM



PINN



Points on y-axis



Points on x-axis

Laboratoire de mécanique, multiphysique, multiéchelle

Rong-Fei LIU, Jian-Fu SHAO

AI/ML DEVELOPED IS FULLY BASED ON PHYSICS AND THERMODYNAMICS

- Training Data: solid Thermodynamic data or high fidelity physical simulations
- Model architecture and weights is available
- Possibility to run statistical tests to understand model dynamics
- Measures of accuracy / comparison to experiments
- AI applied in domain of expertise
- Understand the limitations

Validated and reliable

Results justified
By physics and thermodynamics

SUMMARY

- Advancements in **AI/ML supported reactive transport** are on-going within EURAD 2
  => Mostly at the level of **individual systems** and **simple process coupling.**

- **Integration of codes and unifying workflows** will be needed to increase the complexity and realism of the simulations -> **Digital Twin**

- AI/ML can support the modelling and accelerate calculations
  => suitable for **sensitivity**, **optimization** and **inverse modelling** studies

- Advancement of **coupled algorithms** is still needed to provide the fundament for AI/ML

HERMES

THANK YOU

European Partnership
on Radioactive Waste Management