HERMES:

High fidElity numeRical siMulations of strongly coupled processes for rEpository syStems

Churakov S.V., Baksay A., Brezina J., Dieudonné A.-C., Garcia E., Kolditz O., Laloy E., Prasianakis N.I. Samper J. *On behalf of WP-Consortium*

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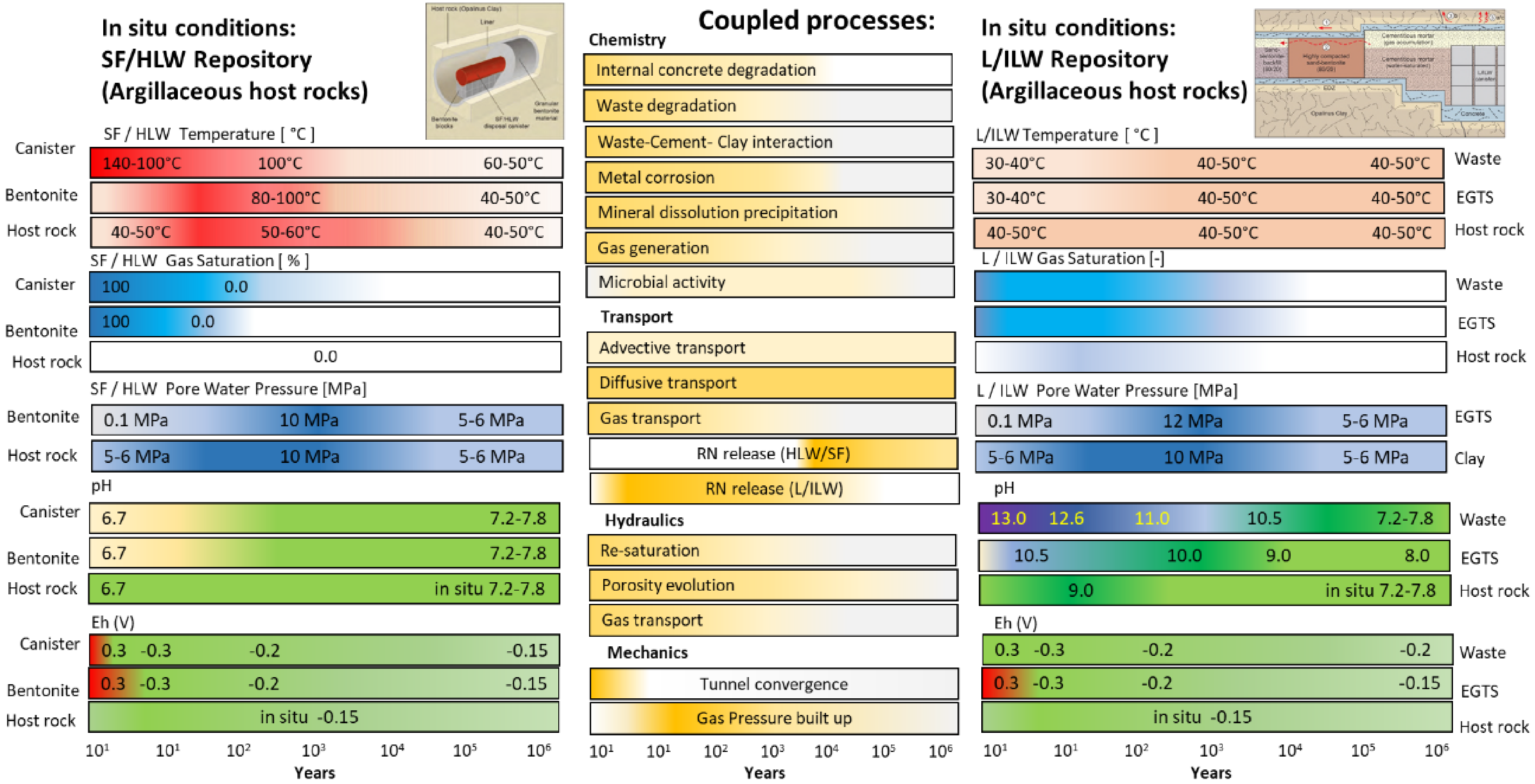
COUPLED PROCESSES IN REPOSITORY SYSTEMS



Churakov SV, Claret F, Idiart A, Jacques D, Govaerts J, Kolditz O, Prasianakis NI, Samper J (2024) *Position paper on high fidelity simulations for coupled processes, multi-physics and chemistry in geological disposal of nuclear waste*. Environmental Earth Sciences, 83, 521. doi:10.1007/s12665-024-11832-7

Kolditz O, Jacques D, Claret F, Bertrand J, Churakov SV, Debayle C, Diaconu D, Fuzik K, Garcia D, Graebling N, Grambow B, Holt E, Idiart A, Leira P, Montoya V, Niederleithinger E, Olin M, Pfingsten W, Prasianakis NI, Rink K, Samper J, Szöke I, Szöke R, Theodon L, Wendling J (2023) *Digitalisation for nuclear waste management: predisposal and disposal*. Environmental Earth Sciences, 82:42. doi:10.1007/s12665-022-10675-4

PROJECT BACKGROUND & AIMS

Despite the continuous growth of the computational resources, the **realism of the current models applied in the simulations of repository systems remains severely limited in terms of dimensions, time-space resolution and process couplings**. Major challenge remains to be efficiency of the process couplings in the available computer simulation tools.

Some orders of magnitude improvement in the computational efficiency can be obtained by replacing the physical based solvers or its components with high-fidelity surrogate models. Particularly promising are the surrogate models based on **machine learning** for specific aspects of **THMC coupled models**, **data exchange between models at different scales**, **reduction of big data** and extraction of constitutive relations from big **numerical, experimental and monitoring datasets**.

*This **WP aims at the development of high-fidelity numerical models for simulations of strongly coupled THMC processes** in repository nearfield, repository design optimisation and interpretation of mock-up experiments using a combination of physics-based models and accelerated computing assisted with machine learning and artificial intelligence.*

RELATION TO SRA DRIVERS

- ***Scientific Insight:*** *Family of high fidelity/high computation throughput coupled models for multiscale simulations of THMC processes in repository nearfield and host rocks offered via an open access EURAD model-hub*
- ***Scientific Insight:*** *Improved understanding of in situ repository evolution controlled by coupled phenomena*
- ***Innovation for Optimisation:*** *Surrogate models for inverse modelling and large-scale simulations for sophisticated optimisation of repository design with respect to THMC-FEPS (Features Events Processes)*
- ***Innovation for Optimisation:*** *Dedicated proxy (simplified) models for optimisation, PA/SA and repository design. Integration of the models into DT definition conducted in WP17. Adjustment of the modelling framework according to the output of WP17 on the DT formulations.*
- ***Knowledge Management:*** *Unified collaborative platform and protocols for surrogate model development. Open access database with experimental datasets (including numerical data) for model testing*

MAJOR TARGETS TO THE FIRST 2 PROJECT YEARS

Recent developments in the field of data sciences and computational efficiency of surrogate models on modern computer infrastructure opens the way for realisation of efficient coupled numerical models (Digital Twins) for real time numerical analysis of laboratory and field experiments, repository design, components optimisation and comprehensive safety analysis. Such numerical tools are essential for repository conceptualisation and the repository design optimisation in both advanced- and early-stage waste disposal programs

This project will play a central role in facilitating collaboration between WPs focused on experimental studies and application of the results to SA/PA

Major activities for the first project phase (2024-2026) comprise:

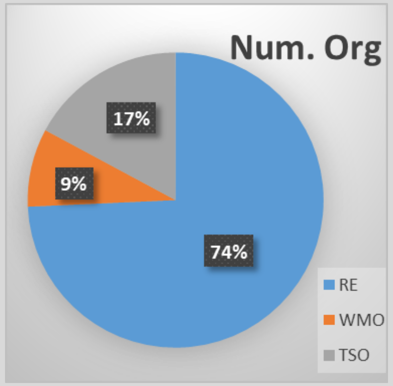
- Road map for model development and process coupling including definition of interfaces between models and codes
- Demonstration of an order of magnitude of speed up of surrogate model for specific processes versus conventional simulations
- Joint definition of interface for the process coupling according to the output of WP17 on the Digital Twins

PARTICIPATING ORGANISATIONS

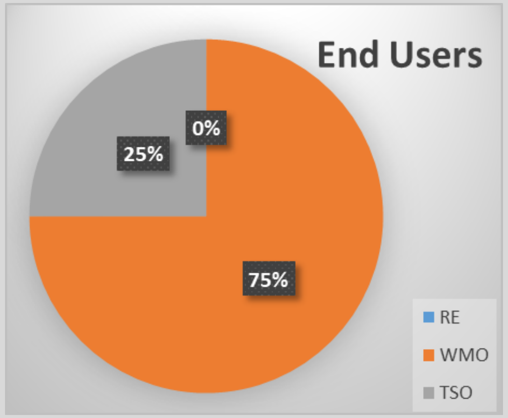
AGES	AMPHOS 21	Andra	BGR	CEA	CNRS	CNRS-LaMcube	ENRESA	EDF	GFZ
Golder WSP	GRS	IGN	Inria	IRSN	JUELICH	KIT-IMB/MPA	Mitta	MUL	NRG
NTW	SCK CEN	SURAO	TU Delft	TUL	TUS	UCLM	UDC	UFZ	UL-Geo Ressources
Univ. Lille	UNIPR	TS Enercon	TUBAF	x	x	x	x	Nagra	PSI
				x	x	x	x		

PARTICIPATING ORGANIZATIONS

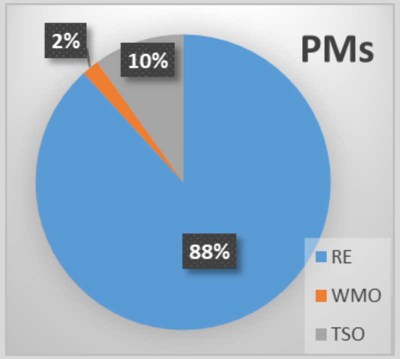
Participating organisations	Num
RE	26
WMO	3
TSO	6



Effort per colleges	PMs
RE	452
WMO	10
TSO	51



Number of End-Users	Num
RE	0
WMO	3
TSO	1



WP GOVERNANCE

Res.	Task title	Task leaders	
		Main Task leader	Co Leader
5%	**Task 1:** Management & coordination of the WP	*Sergey Churakov PSI, RE, CH* 	*Olaf Kolditz, UFZ, RE, DE* 
15%	**Task2:** Knowledge Management	*Laloy Eric, SCK CEN, RE, BE* 	*Enrique Garcia, Enresa, WMO, ES*
30%	**Task 3:** THMC-Process couplings and computational performance	*Olaf Kolditz, UFZ, RE, DE* 	*Anne-Catherine Dieudonné, TU Delft, RE, NL* 
25%	**Task 4:** Surrogate models of individual phenomena	*Nikolaos Prasianakis, PSI, RE, CH* 	*Jan Brezina, TUL, RE, CZ* 
25%	**Task 5:** Tailored models for SA/PA and field scale mock-ups	*Attila Baksay, TS Enercon, TSO, HU* 	*Javier Samper, UDC, RE, ES* 

PMO Contact: Vaidas Matuzas (JRC, the Netherlands) 

TASK 2 KM: COLLABORATIVE HUB FOR CODE DEVELOPMENT AND DATA MANAGEMENT

...

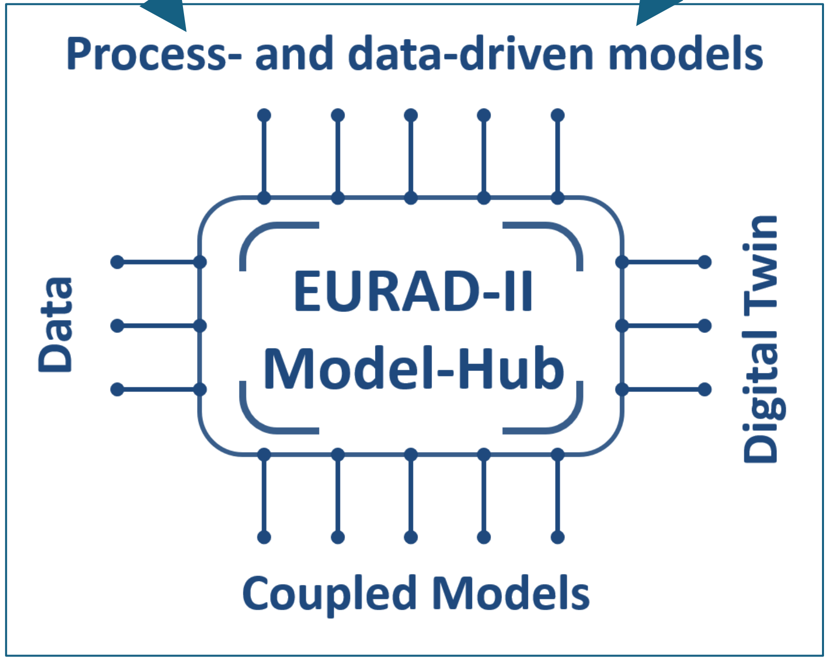
HERMES JupyterLab

GeoML.AI / GeoML.EU

...

binder
git
docker
jupyterhub

MODATS



DITOCO 2023

Demonstration examples:

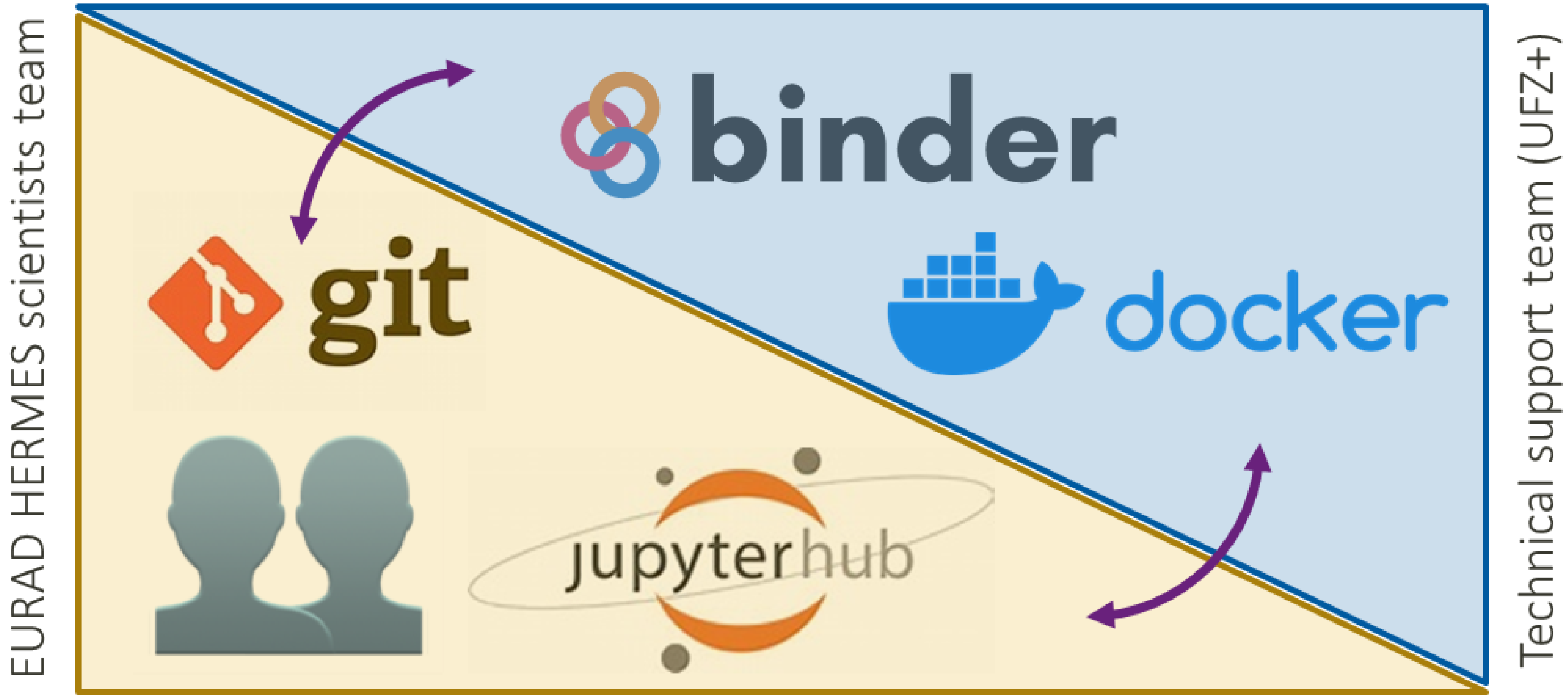
- Benchmarks
- URL experiments
- ...

- Code coupling via Python interfaces
- Process-Coupling and data-driven models
- ...

TASK 2 KM: COLLABORATIVE HUB FOR CODE DEVELOPMENT AND DATA MANAGEMENT

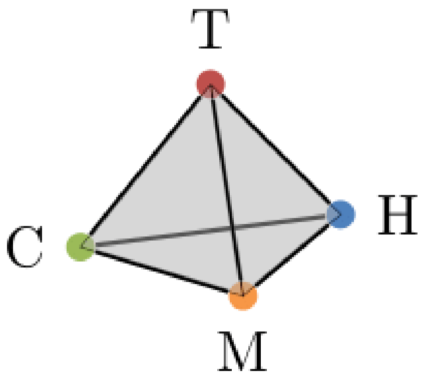
Technical concept: to be introduced and further tuned during HERMES Kick off Meeting

binder: providing the computational web-platform
docker: providing the software environment (Python et al.)



git: version-management for repos (scientists + hermes)
jupyterhub: working environment for scientists

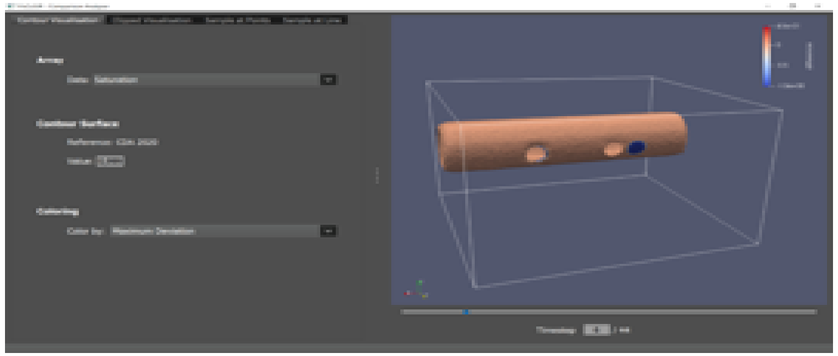
TASK 3: PROCESS COUPLING AND COMPUTATIONAL PERFORMANCE

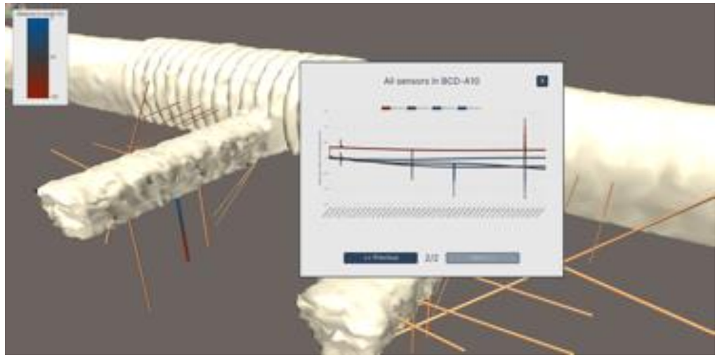


Benchmarking coupled processes and computational performance

- TH2M processes for different repository concepts (LILW, HLW) concerning all stages of gas transport during lifetime of repositories
- THMC processes related to canister-buffer interaction (chemo-mechanical), mechanical damage
- THC reactive transport models of interfaces related to canister corrosion, glass dissolution, corrosion of iron
- Proving thermodynamic consistency of coupled models

Benchmark contributions to the Model-Hub





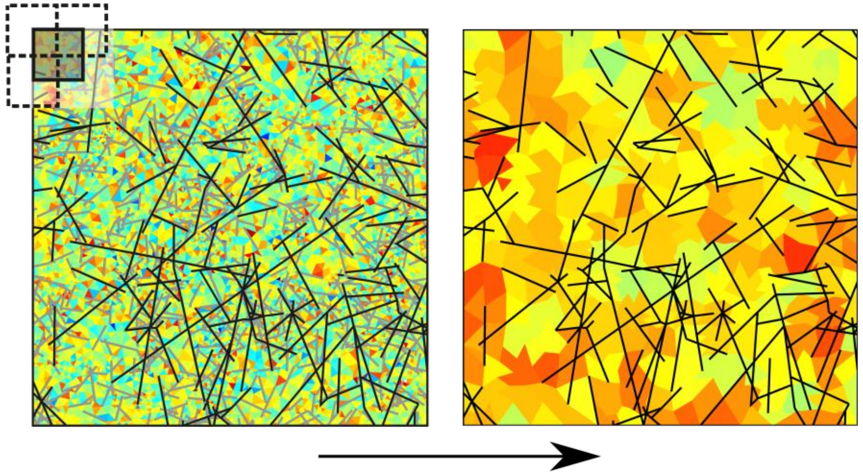
TASK 3: PROCESS COUPLING AND COMPUTATIONAL PERFORMANCE

Inverse modelling, sensitivity analysis and upscaling

- Lab and field experiments from URLs as data base
- Upscaling: statistical and analytical homogenisation, examples: derivation of effective properties from pore-scale modelling (TH2M processes), upscaling evolution of CM processes for cementitious materials, upscaling of transport models based on discrete fracture matrix
- Sensitivity analysis: multilevel Monte Carlo, local (adjoint state) and global sensitivity methods (VARS, Sobol, Kucherenko analyses)
- Inverse modelling: reduced-order models (ROM) or proxy-based approaches (design-of-experiment)

Data and model integration

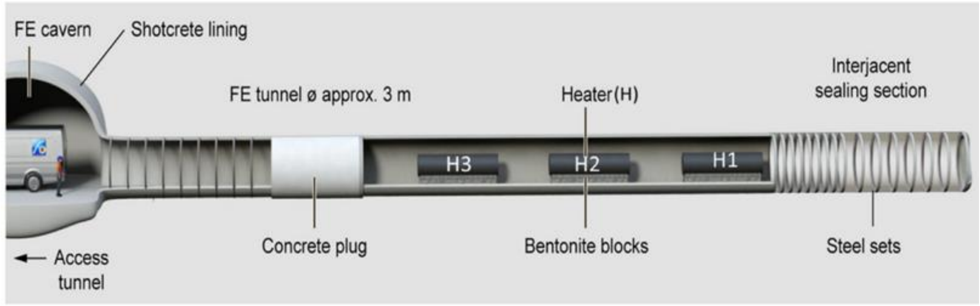
- MODATS legacy
- DITOCO2030 link
- SODOKU link



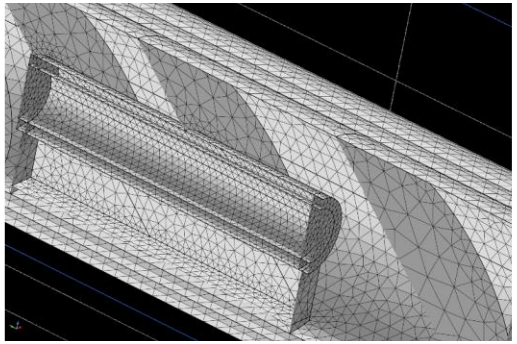
TASK 4: SURROGATE MODELS OF INDIVIDUAL PHENOMENA

Development of surrogate models of individual processes and of several coupled processes.
The topics to 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.

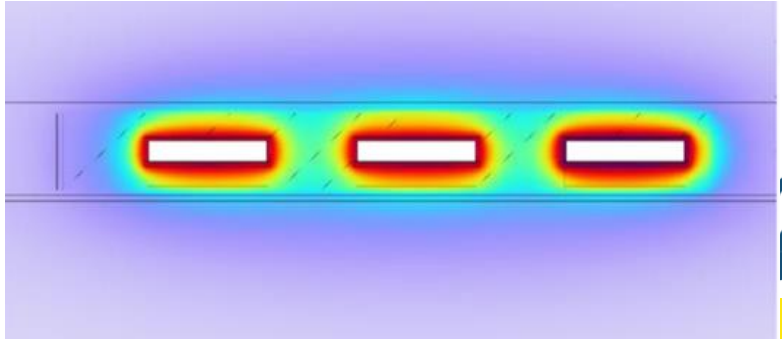
Task 4.1: Acceleration of computations for individual processes and phenomena
Task 4.2: Surrogate models for coupled processes and multiphysics



Example: Mont Terri Full Emplacement Experiment

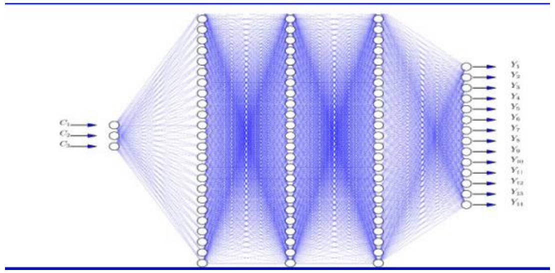


Discretization



Temperature Distribution

TASK 4.1: SURROGATE MODELS



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
- 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

N.I. Prasianakis, E. Laloy, D. Jacques, J.C.L. Meeussen, G.D. Miron, D. A. Kulik, A. Idiart, E. Demirer, E. Coene, B. Cochepin, M. Leconte, M. E. Savino, J. Samper II, M. De Lucia, S. V. Churakov, O. Kolditz, C. Yang, J. Samper, F. Claret (2024) Geochemistry and Machine Learning: review of methods and benchmarking Environmental Earth Sciences (in review)

TASK 4.2: SURROGATE MODELS FOR COUPLED PROCESSES AND MULTIPHYSICS

Target of this task will be the:

-main MC processes and the mutual interplay between mechanical properties and chemical aggressions.

-Application of reactive transport modelling to study the geochemical evolution of an interface under non-isothermal conditions, as well as coupled geochemical systems: cement/water, uranium sorption and steel/corrosion products/bentonite interactions.

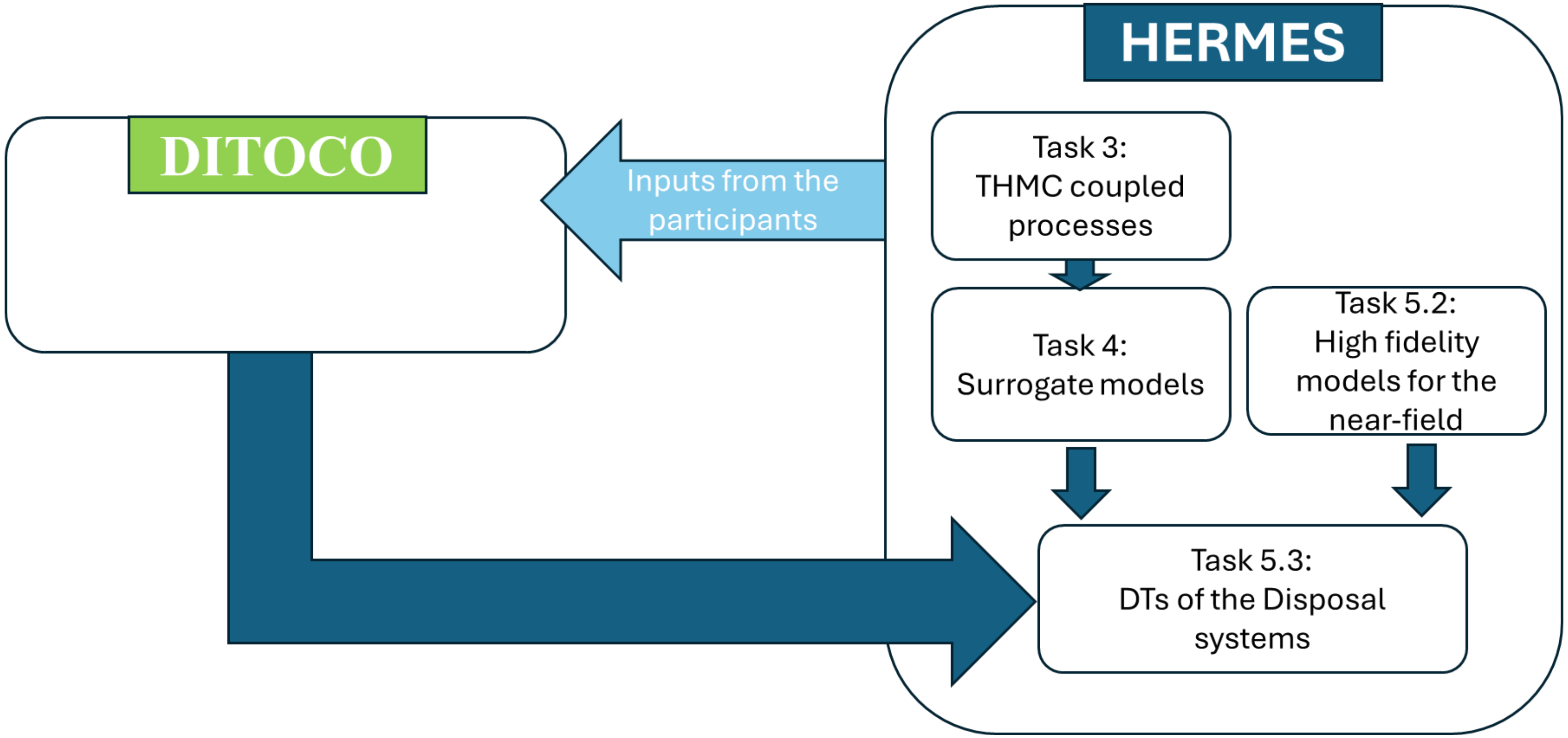
-Improvement and extension the ML techniques to be used as the geochemical solver in coupled reactive transport problems at the pore-scale and at continuum scale.

-High resolution 3D modelling of THMC processes with focus at the Mont-Terri FE-Experiment including spatial heterogeneities. Machine learning techniques including physics-informed ML, upscaling techniques, as well as analytical homogenization methods will be used. Application test-cases will be relevant to multi-physical couplings, linked with the radioactive waste disposal scale.

TASK 5 - TAILORED MODELS FOR SA/PA AND FIELD SCALE MOCK-UPS

The aim of the task is modelling of repository scale systems and simulations of field scale experiments.

The purpose is to use the approaches and results of the development carried out in other Tasks of HERMES to create modeling tools that are capable of used in safety case, in design and optimization of radioactive waste disposal systems.



SUBTASKS IN TASK 5

Subtask 5.1: Real time simulation of field-scale experiments

- Mont Terri
- FISST test in ONAKLO
- DECOVALEX

Subtask 5.2: High fidelity models for repository near field simulations and assessment of waste package integrity

- Long term geochemical evolutions on bentonite-granite, carbon steel-bentonite, vitrified waste-carbon steel interfaces
- Multiscale and multifidelity transport model for DT development
- Evolution of the environment in the near-field close to heat generating waste

Subtask 5.3: Dedicated models for optimization and repository design and integration of the models into Digital Twin concepts to be formalized in WP 17

- Consolidating the models created in the work package into tools capable of performing analyses that can be used in the design and optimization of the radioactive waste disposal system.
- The resulting models are digital twins of the disposal systems, the formalism of which is described in DITOCO

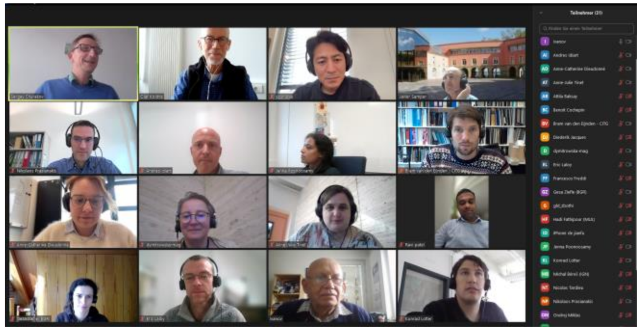
OPERATIONAL LINK BETWEEN EURAD I AND EURAD-II WPS

SUDOKU	Development of coupled models for surface disposal facility
DITOCO2030	Definition of interfaces between physical/surrogate models and digital twins.
RAMPEC	Data, models, and knowledge exchange for simulation of solutes and RN transport in cementitious systems and argillaceous rocks
LOPERA	Development of surrogate models for waste matrix evolution
DITUSC	Joint exchange meeting/workshop on best practices for treating thermodynamic data and requirements for thermodynamic databases
ANCHORS	Data and models exchange on the bentonite evolution on the repository near field. A joint workshop on THMC characterisation and modelling of bentonite behaviour.
DONUT, ACED, MODATS, and PREDIS	A proof of concept for the successful use of machine learning and surrogate modelling for the isolated coupling and repository components has been demonstrated, including benchmarking exercises, in the ongoing WPs in EURAD-I (e.g. DONUT, ACED, MODATS) and PREDIS.

CHALLENGES

- Adjustment of the project plan to the 2+2 Years format
- Personnel recruitment: PhD student hiring may not be feasible for some organisations due to 2*2 years funding constraints
- Alignment of model development and application with the progress of experimental WPs Eurad II
- Right balance between models generality and specific requirements in safety case applications
- Access to HPC infrastructure

STEPS TOWARDS SUCCESS:



- **Build up on developments and benchmarking exercises initiated in EURAD-I**
- **Existing collaborations in previous international projects (DECOVALEX, Mont Terri)**
- **Clusters building during project preparation phase**

COMMING SOON:

- Kick off meeting 4-5 November 2024, PSI, Switzerland

THANK YOU FOR YOUR ATTENTION !