eurad
European Joint Programme on Radioactive Waste Management

HERMES

DITOCO2030

# TOPICAL SESSION 3 - DIGITAL TRANSFORMATION

## DITOCO2030 and HERMES

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# HERMES & DITOCO2030: 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.

***WP-HERMES is RD&D project aiming 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****.*

***WP-DITOCO2030 is a StSt project aiming to lay-out the path on how to close the R&D gap*** *between the currently fragmented digital twins (DT) of individual disciplines, common data environments and decision-making platforms* ***to better understand*** *the* ***opportunities & limitations of DT*** *in* ***their deployment*** *in* ***whole life cycle of waste management.***

# HIGH FIDELITY SIMULATIONS

*High-fidelity simulations* refer to **accurate and detailed model-based representations of real-world** systems, processes, or phenomena involving advanced computational models, precise data inputs, sophisticated computational algorithms and use of advanced High-Performance-Computing (HPC).

**Detailed System representation:**

- High resolution spatial representation of the system with its components and material properties
- Description of coupled physical phenomena, complex material behavior and system interactions
- Close match of real-world observations (monitoring data)

**Computational Challenges**

- High computational demands
- Handling of complex equations and large (in time & in space)  datasets

## SURROGATE MODELS

*Surrogate models* are simplified **mathematical approximations** of more complex, computationally expensive models. Surrogate models are designed based on the high-fidelity reference data developed with the aim to **reduced computational costs** while **providing required accuracy**.

**Key Features of Surrogate Models:**

- *Efficiency*: Much lower computational costs compared to the reference high-fidelity models.
- *Accuracy*: Provide key outputs parameters within acceptable error margins.
- *Flexibility* and *application* range: Use generic approach for various types of engineering problems. Interpolate data from the original complex model or real-world experiments.

**Key application domains:**

- *Optimization*: Multi-factor optimization of model parameters and system design.
- *Uncertainty Quantification*: Assessing variability of the input-outputs relationships.
- *Sensitivity Analysis*: Identification of most impactful system parameters.
- *Real-Time Decision Making*: Providing quick approximations in dynamic or interactive environments.

# What is a Digital Twin?

## What is the Digital Twin for Eurad-2?

A key challenge lies in aligning & integrating the diverse objectives of Digital Twin technologies (ranging from digital engineering to long-term safety) across multiple disciplines, including geology, performance assessment, systems optimization, realization, and infrastructure.

**Achieving a coherent & functional integration across these areas remains a significant difficulty.**

*Have repositories been constructed? | Nagra*

# VISION OF DITOCO2023

- **to agree on what is needed** from the individual disciplines in a DT,
- **at what point in time**
- **to what level of detail**, in order to use the DT for effective decision-making during the planning, construction, operation and maintenance of radioactive waste management facilities, and for interactions with stakeholders.

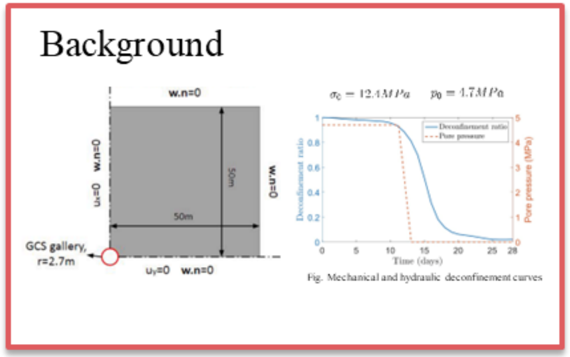
The study will **identify** the major challenges to tackle and set key performance indicators to identify the **expertise & capacity that is needed** to address the RD&D challenges.

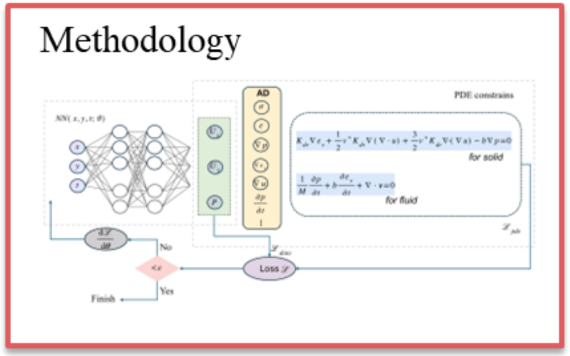
The added value lies in the evidence-based ***i)*** identification & management of risks, ***ii)*** performance assessment of safety margins, ***iii)*** optimization of design configurations, ***iv)*** calculation of costs to completion, ***v)*** engagement improvement with stakeholders.

# SURROGATE MODES EXAMPLES

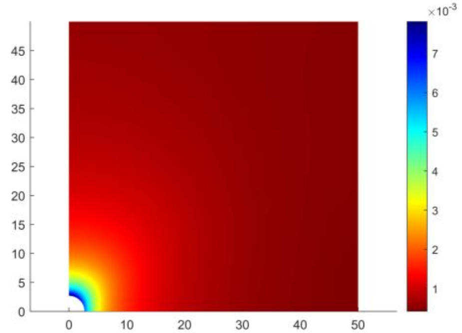
**Surrogate models or proxy models provide a significant acceleration to the THMC simulation codes.**
**How: Apply, benchmark and implement scientific machine learning methods**

Numerical study of Hydromechanical response using Physics-Informed Neural Networks (PINN) Method

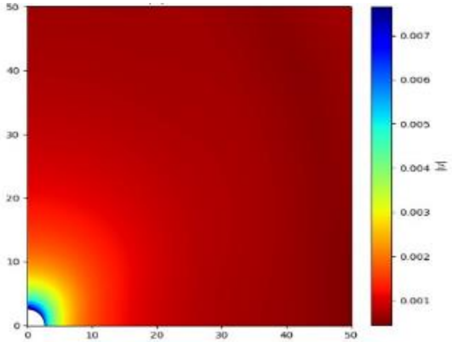



FEM



PINN

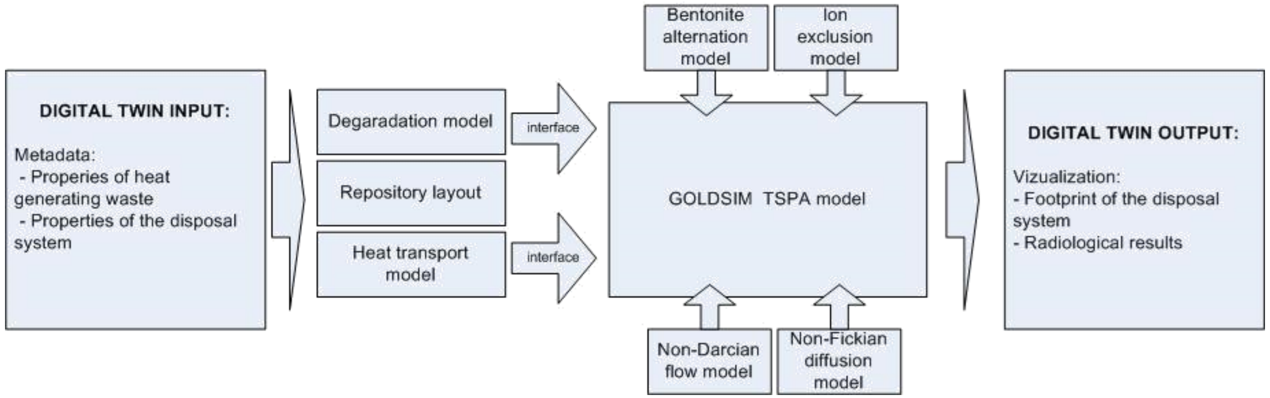


Displacement distribution (FEM Vs PINN)

LaMCUBE
Laboratoire de mécanique, multiphysique, multiéchelle

# TAILORED MODELS FOR FIELD SCALE MOCK-UPS

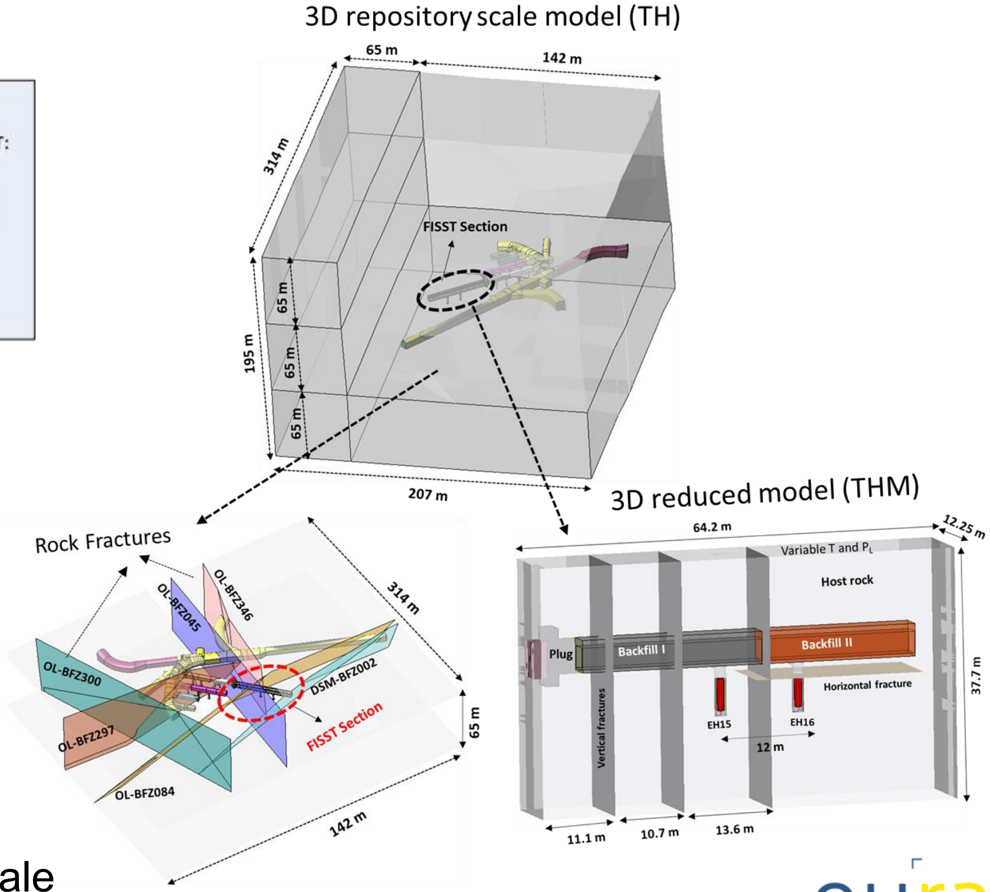
- **FISST (Full scale In-Situ System Test) backfilled tunnel with two deposition holes, each one containing a canister embedded in expansive clay in ONKALO, Olkiluoto (Finland)**




(I) calibration of THM material models

(II) performing 3D TH simulations with the “in situ” test real geometry (Digital Twin);

(III) predictive THM calculations in 3D at a reduced (simplified) scale



# MODEL-HUB: DATA AND MODEL INTEGRATION

**WebLayer**

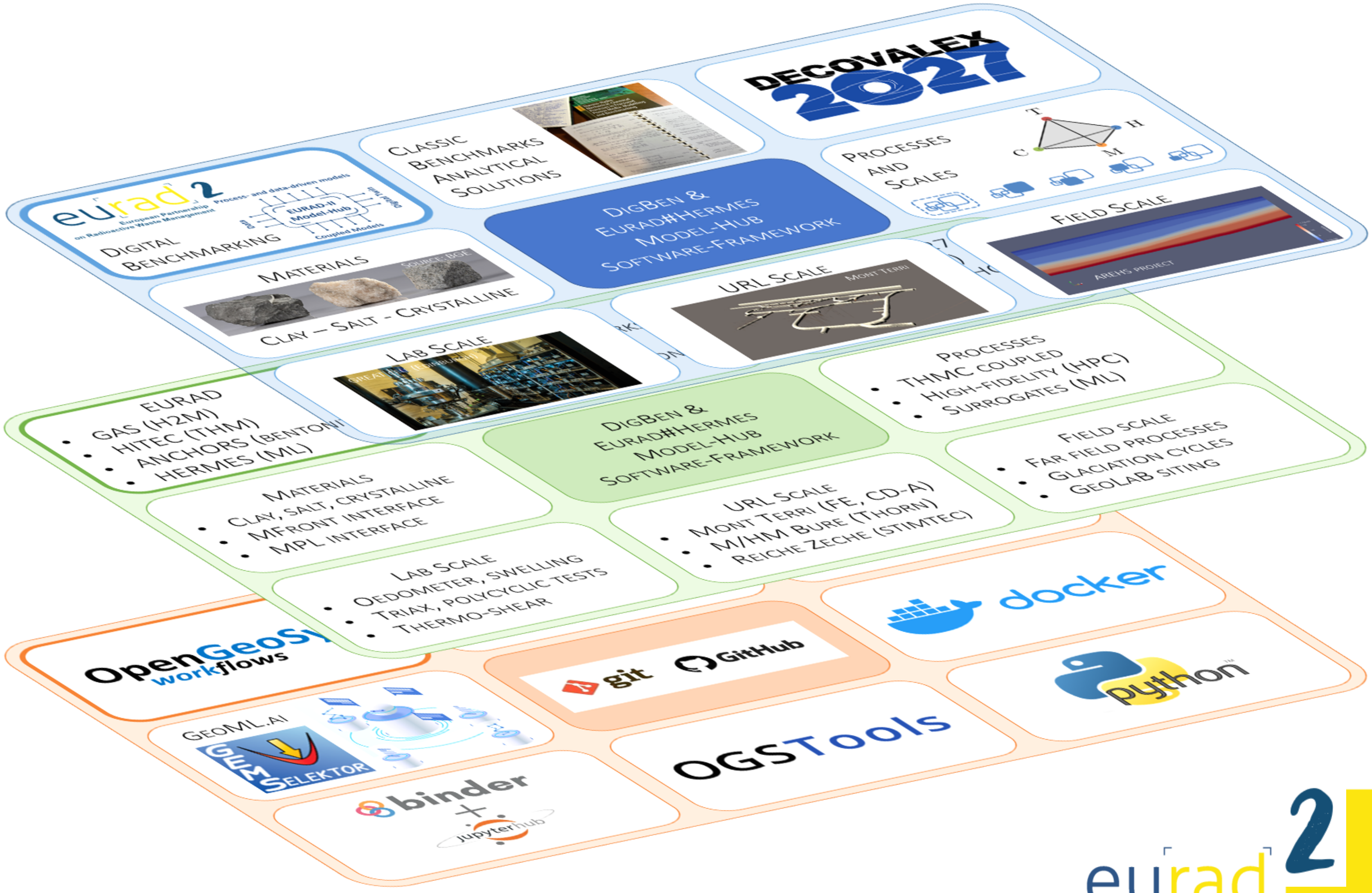
structured user-web-interface organized by thematic areas: materials, processes, scales > projects

**InfoLayer**

specific information about thematic areas including literature links > list of current benchmarks and examples (extending)

**JupyterLab**

interactive Jupyter Notebooks of benchmarks and examples < coding area for interactive work



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## AIM OF THE DIGITAL TRANFORMATION DISCUSSION

- Status update on development, use and application of high-fidelity models coupled models
- RD&D challenges and knowledge gaps
- Define the meaning of DT in nuclear waste management community
- Prospective on design and use DT in nuclear waste disposal (e.g., use cases, pilot studies, …)
- Innovative approaches for integration of knowledge from simulation of coupled processes into digital twins

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# DIGITAL TRANFORMATION SESSION AGENDA

10’ Réka Szőke & Sergey Churakov Introduction and scope

**20’ Arto Laikari Insights from DITOCO green paper**

**20’ Pablo Cayón Insights from DITOCO white paper**

**20’ Olaf Kolditz HERMES-Model/Data-HUB development**

**20’ Nikolaos Prasianakis Application of AI in reactive transport modelling**

**20’ Magdalena Dymitrowska Macroscopic and pore-scale modelling of gas transport**

**10’ Réka Szőke & Sergey Churakov Concluding remarks**

Reporter: Attila Baksay (TS-Enercom)

Observer: Alex Papafotiou (Nagra);

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