

Topical Session 3: Digital transformation (HERMES & DITOCO)



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

AGENDA

Digital transformation

Introduction – DITOCO , HERMES (Réka Szőke, Sergey Churakov)

DITOCO

Green Paper – Arto Laikari

White Paper – Pablo Cayon

HERMES

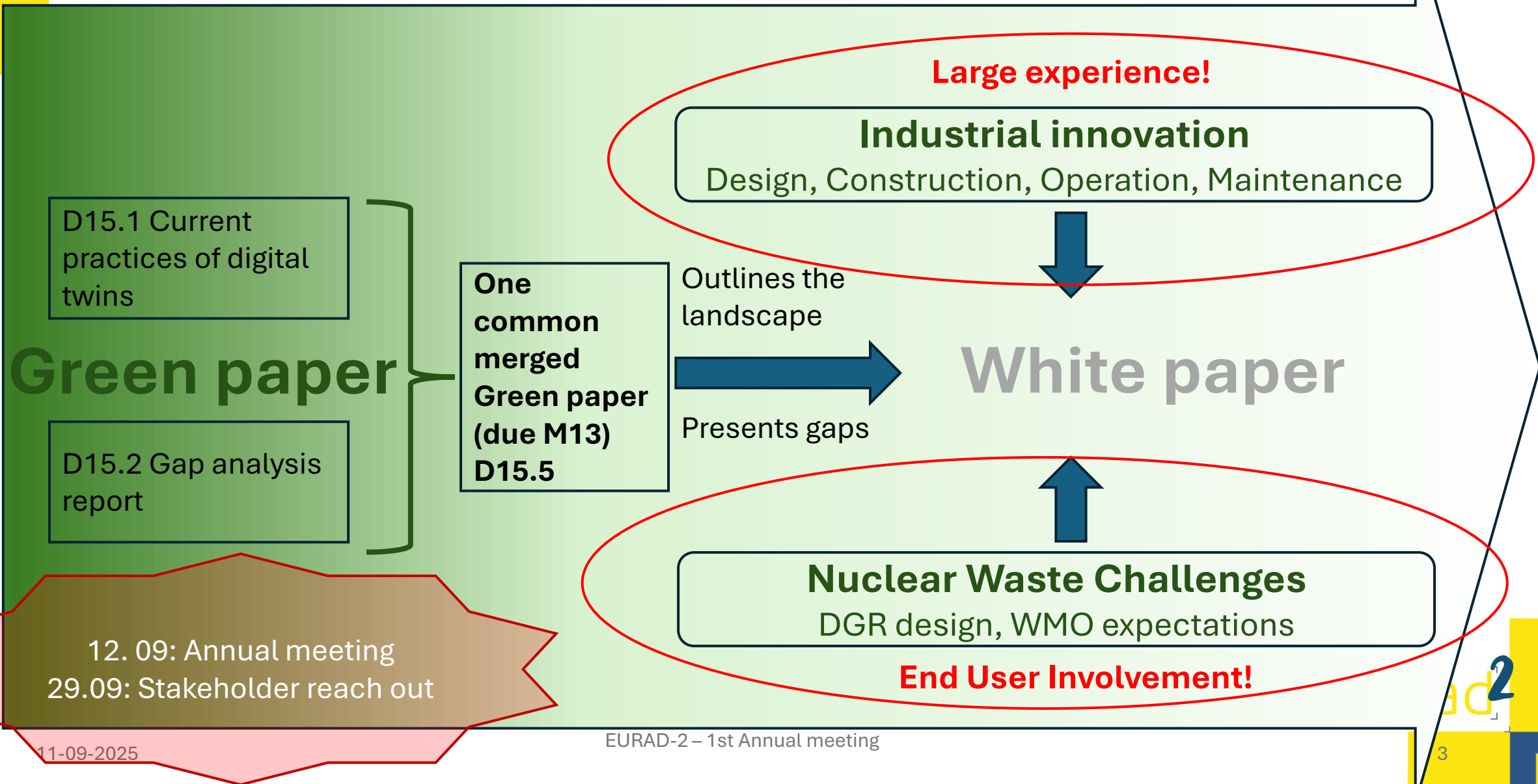
HERMES-Model/Data-HUB development –
Olaf Kolditz

**Application of AI in reactive transport
modelling** – Nikolaos Prasianakis

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

Q & A

eurad²



NAGRA'S INTEGRATED DIGITAL ENVIRONMENT

Dynamic Repository Modelling (DRM)

Design → Construction → Optimization

Integrated Geo-Model (IGM)

Common Project Environment (CPE)

Building Information Modelling (BIM)

Information & Data Centre (IDC)

Digital Twin

feeds into

Digital Safety Case

HERMES - MODELHUB

WebLayer

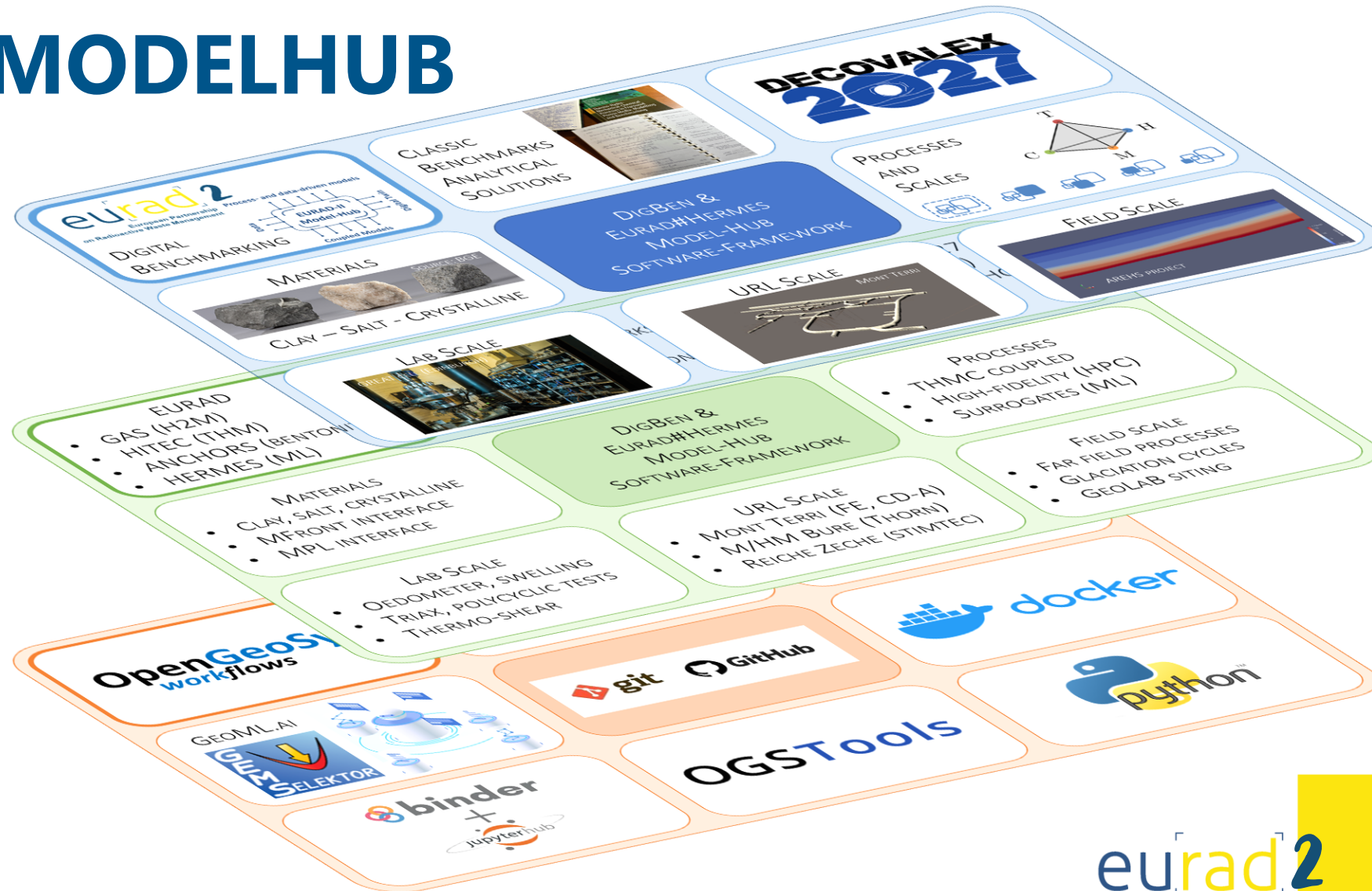
structured user-web-interface
organized by thematic areas:
materials, processes, scales >
projects

InfoLayer

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

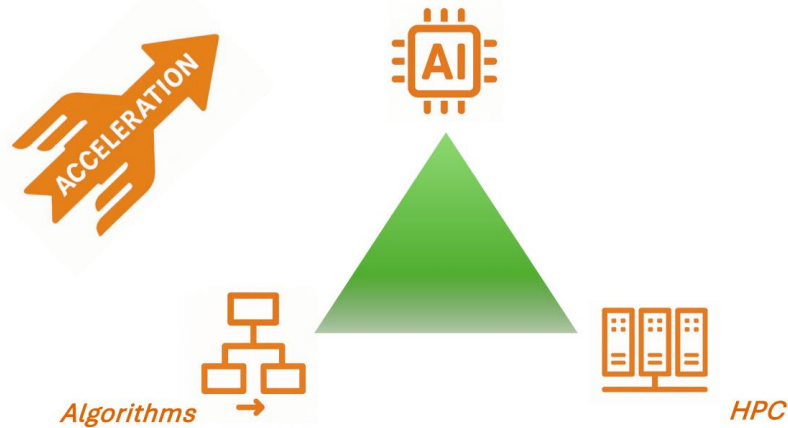
JupyterLab

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



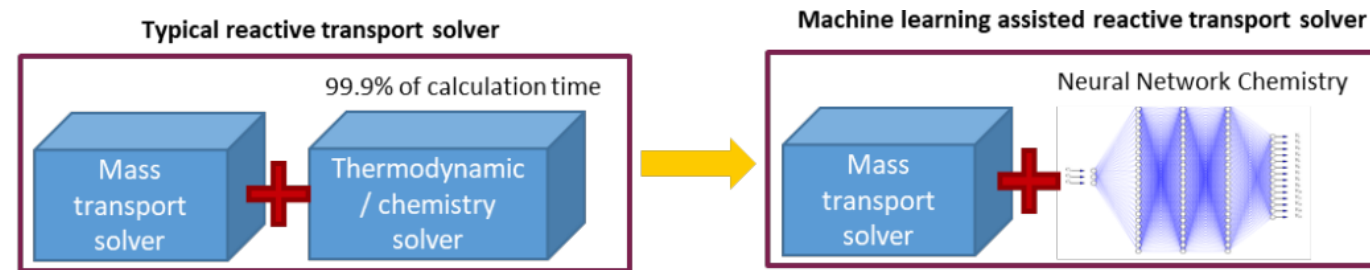
HERMES – USE OF AI/ML IN REACTIVE TRANSPORT

- Using AI in the computation system that greatly increase the speed of the simulations.



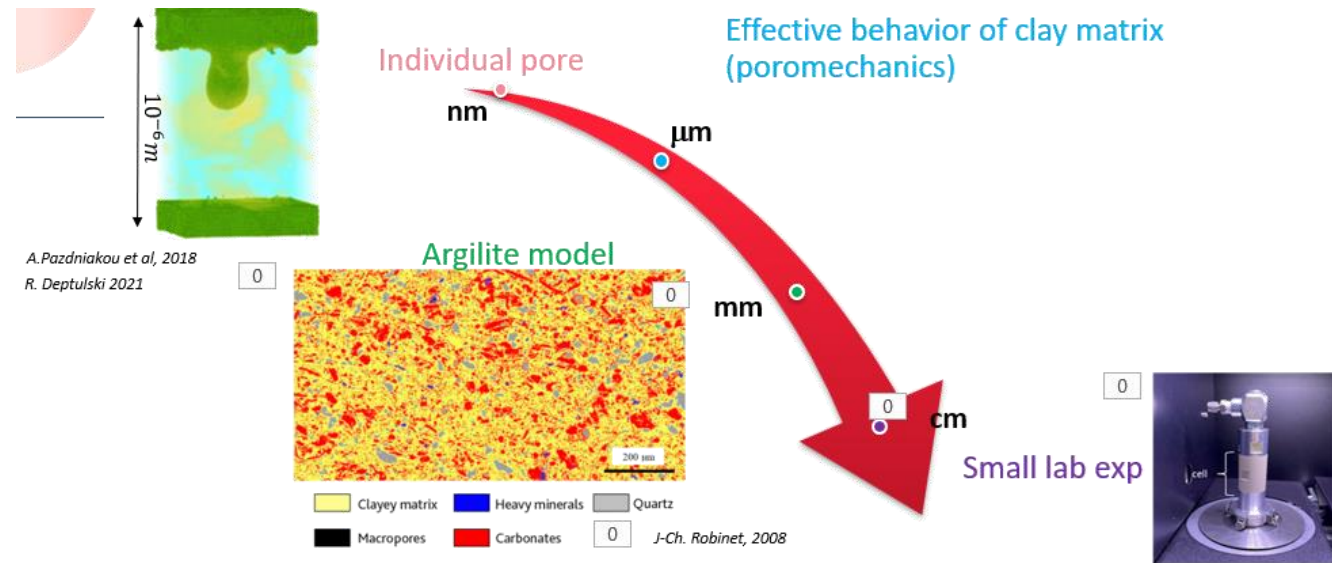
- In addition to increasing the speed of simulations, the accuracy of the physical model behind the calculations cannot be compromised.

- Surrogate models are simplified models that approximate complex, high-fidelity systems or simulations
- By learning the input-output behavior from a limited set of data, surrogate models provide faster, less costly results
- Surrogate models provide a significant acceleration to the THMC simulation codes



ML TECHNIQUES IN GAS TRANSPORT

- Example of the application of ML techniques in a gas transport calculation problem: changing the scale of the simulation between pore-scale and reservoir-scale simulations to laboratory scale
- The use of physics-based neural networks (PINNs) is planned in the calculation of scale-up routes.
- These are physics-based machine learning methods that seamlessly integrate physical knowledge with data.





TAKE-AWAY MESSAGES

- A lot of experience is gathered in the field of Digital Twins in the industry
- To have an effective co-operation an effective dialog with the End-Users is important
- Dynamic Repository Modelling: approach to follow the lifecycle of a DGR
- AI / ML are the important and effective tools
- It is important to focus on the accuracy of the physical models as well as the improvement of the speed of the simulations