SUPPORTING IMPLEMENTATION AND OPTIMISATION OF NUCLEAR WASTE DISPOSAL BY DEVELOPING AND IMPROVING NUMERICAL METHODS AND TOOLS FOR MODELLING COUPLED PROCESSES

eurad
European Joint Programme on Radioactive Waste Management

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CONTEXT

Understanding of multi-physical Thermo-Hydro-Mechanical-Chemical coupled processes (THMC) occurring in radioactive waste disposal is a major and permanent issue to support optimization of design and safety case abstraction. Numerical simulations are necessary to make predictive multi-physical analyses for time periods and space scales larger than experiments can cover. These numerical simulations require integrating, in a consistent framework, an increasing scientific knowledge acquired for each of the individual components of a system for radioactive waste disposal. This implies to consider couplings of different and non-linear processes from a wide range of materials with different properties as a function of time and space in ever-larger systems. The development of cutting-edge and efficient numerical methods is thus necessary, in the scope of having useful, powerful and relevant numerical tools for assessments. It is also necessary to manage the uncertainties associated to the input data feeding the models and the representation of the processes, to assess the range of variability of the results and to identify the main parameters and processes driving the behavior of the systems of interest. Managing uncertainties in these complex systems require the improvement and the development of innovative, appropriate and efficient numerical methods.

WP MAIN OBJECTIVES

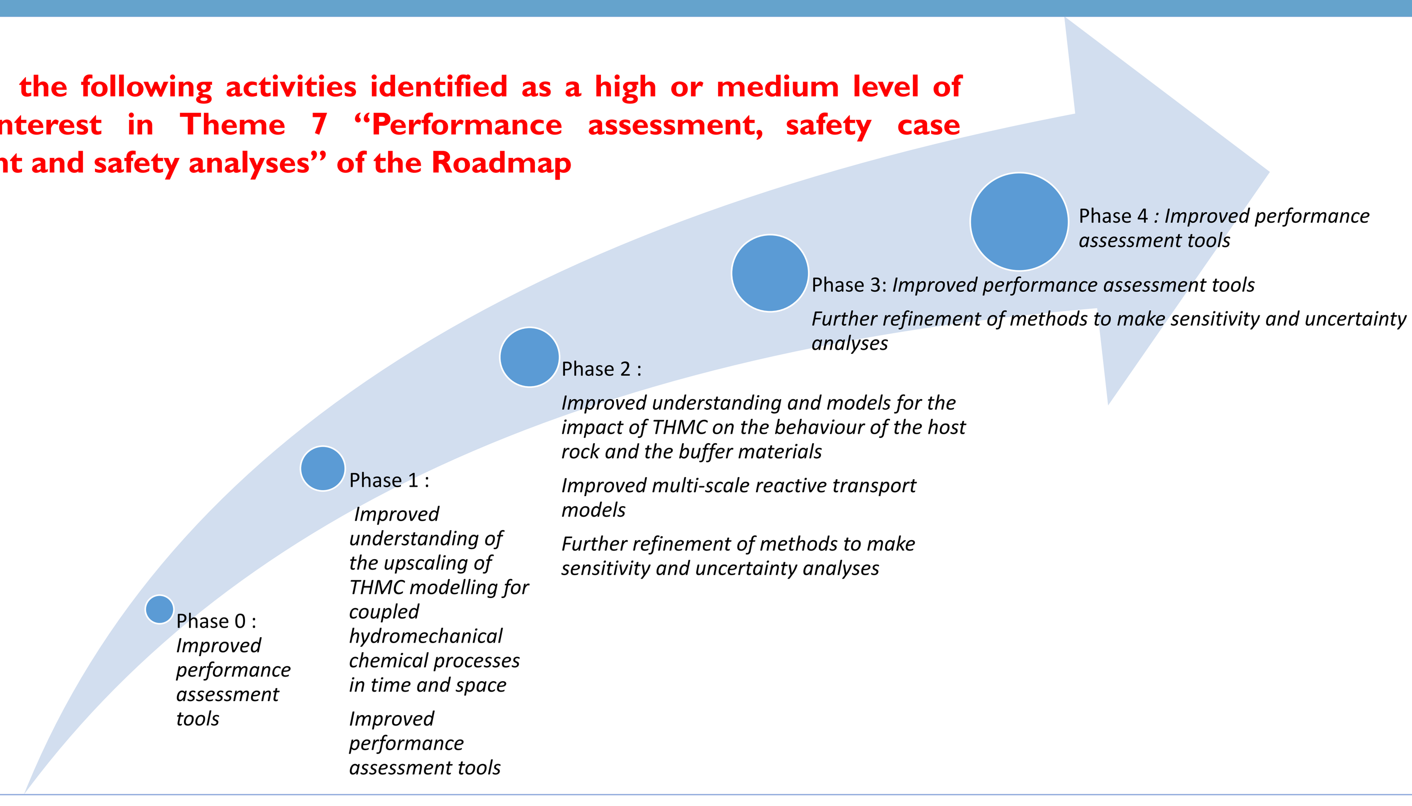
- Development of relevant, performant & cutting-edge **numerical methods that can easily be** implemented in existing or new tools, in order to carry out high-performance computing to study of **highly coupled processes** in large systems (reactive transport, 2-phase flow & THM modelling in porous and fractured media);
- Development of numerical **scale transition schemes** for coupled processes (meso to macro scale, or pore to Darcy scale) supporting the study of specific multi-scale couplings e.g. chemo-mechanics;
- Development of **innovating numerical methods** to carry out uncertainty and sensitivity analyses;
- **Benchmark exercises**, on representative test cases, to test the efficiency of developed methods (robustness, accuracy, time computational) on relevant tools.

WP MAIN IMPACTS

- **Improvement of multi-physical understanding of radioactive waste disposal**
- **Supporting design and abstraction for safety case**
- Bring together at European level diverse scientific communities to reinforce innovation through cross-fertilization
- Skills developments for young researchers through thesis or postdoc funding
- Interaction with civil society through strategic studies (e.g. UMAN)
- High scientific-technical impact (via open peer-publications, benchmark exercises, etc...)

LINK WITH SRA

Addressing the following activities identified as a high or medium level of common interest in Theme 7 "Performance assessment, safety case development and safety analyses" of the Roadmap



REFERENCE

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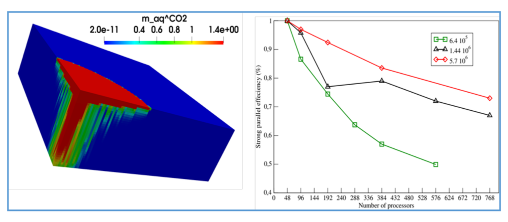
- Steefel, C.I., Yabusaki, S.B., Mayer, K.U., 2015. Reactive transport benchmarks for subsurface environmental simulation. Computational Geosciences 19, 439
- Bildstein O., Claret, F. , Lagneau V. 2021. Guest editorial to the special issue: subsurface environmental simulation benchmarks. Computational Geosciences 25, 1281-1283
- Sochala, P., Chiaberge, C., Claret, F. , Tournassat C., 2022 Uncertainty propagation in pore water chemical composition calculation using surrogate models. Sci Rep 12, 15077

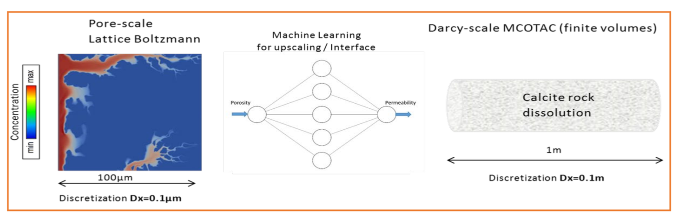
For more information

DONUT AT A GLANCE

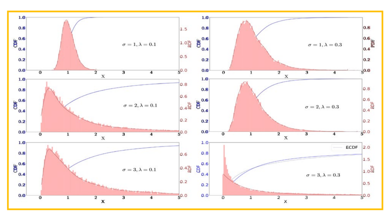
Task 1 Management (Leader F. Claret & G. Pepin)



Task 2 Numerical methods for high performance computing of coupled processes (Leader C. Cances)



Task 3 Scale transition schemes for coupled processes (Leader O. Kolditz & N. Prasianakis)

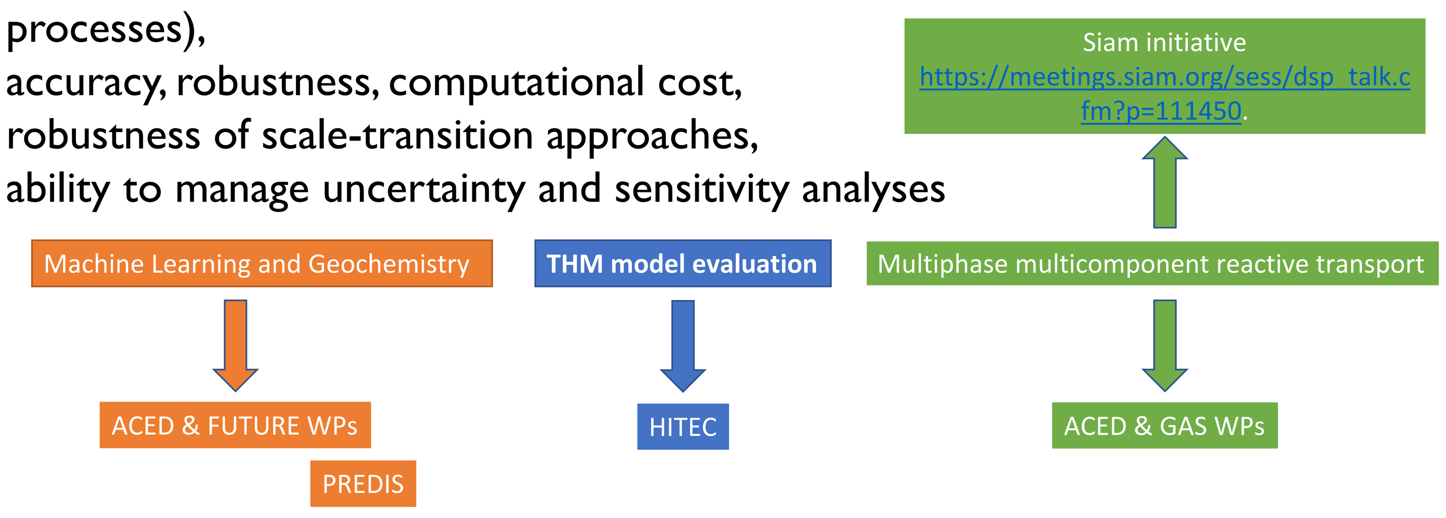


Task 4 Tools and methods to quantify/derive uncertainties induce by coupled processes (Leader A. Baksay)

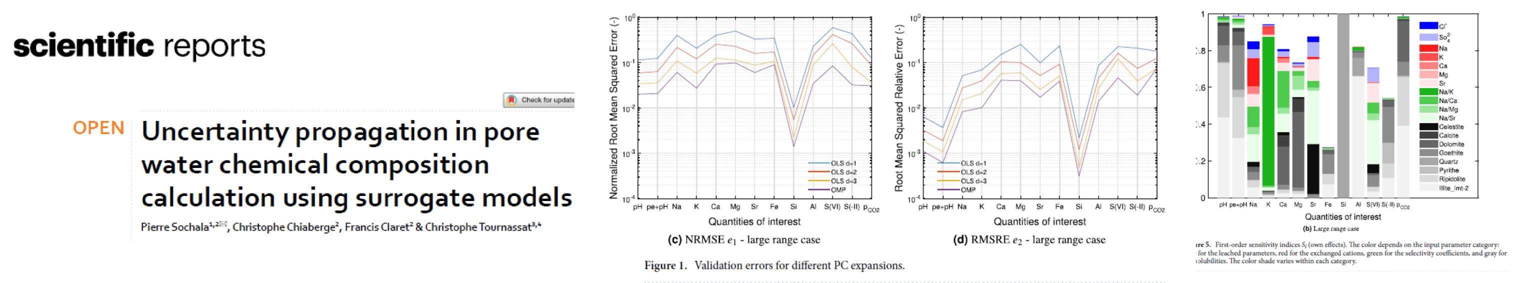
Task 5 Benchmarks of methods and tools for coupled processes (Leader D. Lukin) :

In addition to the specific work that will be conducted by each partners, a specific outcome of DONUT is the definition of benchmarks that will be use both inside DONUT and outside to foster interactions. While international benchmarks initiative are existing (Steefel et al., 2015; Birkholzer et al., 2019; Bildstein et al., 2021), the goal here is to define benchmarks of methods and tools to quantify efficiency and added-value in terms of :

- increase of knowledge (e.g. better physical representation, integration of couple processes),
- accuracy, robustness, computational cost,
- robustness of scale-transition approaches,
- ability to manage uncertainty and sensitivity analyses



ON THE USE OF SURROGATE MODELS



PERSPECTIVES : DIGITAL TWINS

Seen as potential opportunity:

- Contribution to decision-making process at operational phase
- A federative and interoperable tool to give information for the operational & long-term phases, and supporting project development (design, safety)
- Unified, accessible, readable environment of phenomenological evolution (space/time) : integration of "Coupled" multi-physical numerical simulations and Integration / treatment of measured data
- Combined with VR, communication tool

For our repository case, long term R&D effort effort and following fields : data treatment and data mining, model calibration, model reduction, multi-physical couplings, interoperability between tools, etc

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