Development and improvement Of NUmerical methods and Tools for modelling coupled processes (DONUT)

F. CLARET/BRGM, Berlin, 3-4 December 2018

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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 Expected 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...)

DONUT Participants

Organisations
✓ **Andra**, France (WMO) ▪ BRGM, France
✓ **CEA**, France (RE) ▪ EDF, France
✓ **CNRS**, France (RE) ▪ ULille, France ▪ Unice, France
✓ **COVRA,** Netherlands (WMO)
✓ **ENRESA**, Spain (WMO) ▪ UDC, Spain
✓ **FZJ**, Germany (RE) ▪ HZDR, Germany ▪ UFZ, Germany
✓ **GRS**, Germany (TSO)
✓ **IRSN**, France (TSO)
✓ **LEI,** Lithuania (RE)

Organisations
✓ **MTA EK**, Hungary (RE) ▪ SORC, Hungary
✓ **NRG**, Netherlands (TSO)
✓ **PSI,** Switzerland (RE)
✓ **SCK-CEN**, Belgium (RE)
✓ **SURAO**, Czech Republic (WMO) ▪ CTU, Czech Republic ▪ CU, Czech Republic ▪ IGN, Czech Republic ▪ TUL, Czech Republic ▪ UJV, Czech Republic
✓ **TS Enercon,** Hungary (TSO)
✓ **TUS,** Bulgaria (RE)
✓ **UHELSINKI**, Finland (RE) ▪ TUT, Finland

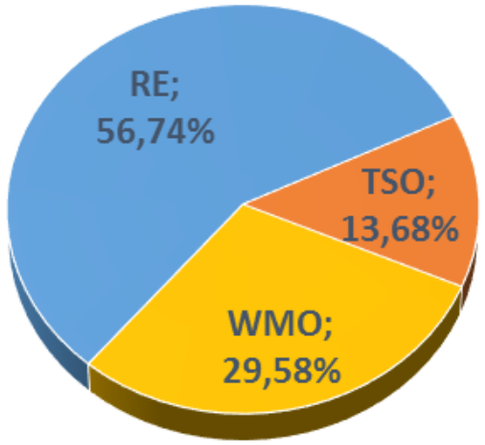
WP – Task Breakdown and WP Board

- Contact details for the WP leader/how to contact the WP if interested in being connected/associated f.claret@brgm.fr

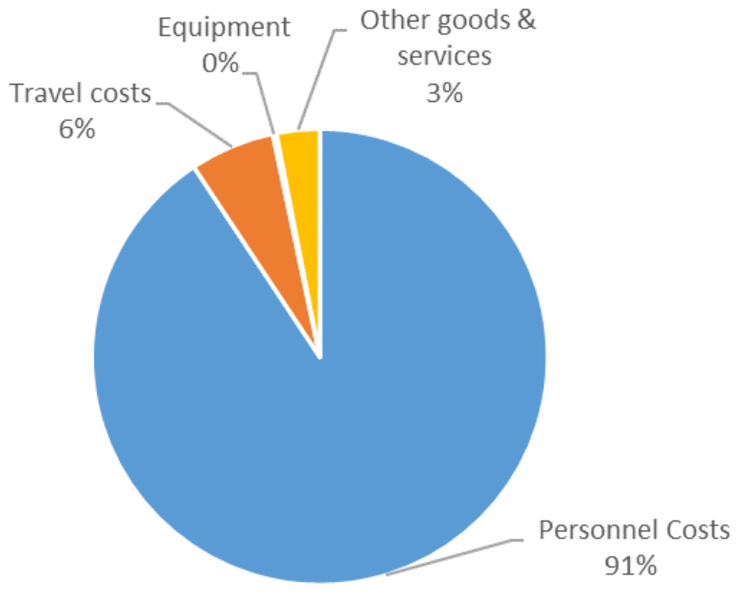
- **Task1 – Coordination**
  - **Leader:** Francis Claret (BRGM)
- **Task 2 - Numerical methods for high performance computing of coupled processes**
  - Leader: Clement Cances (INRIA/Lille University)
- **Task 3 - Scale transition schemes for coupled processes**
  - Leaders: Olaf Kolditz (UFZ), Nikolaos Prasianakis (PSI)
- **Task 4 - Tools and methods to quantify/derive uncertainties induced by coupled processes**
  - Leader: Attila Baksay (TS ENERCON LTD)
- **Task 5 - Benchmarks of methods and tools for coupled processes**
  - Leader: Dimitry Lukin (SURAO)

WP – Planned resources

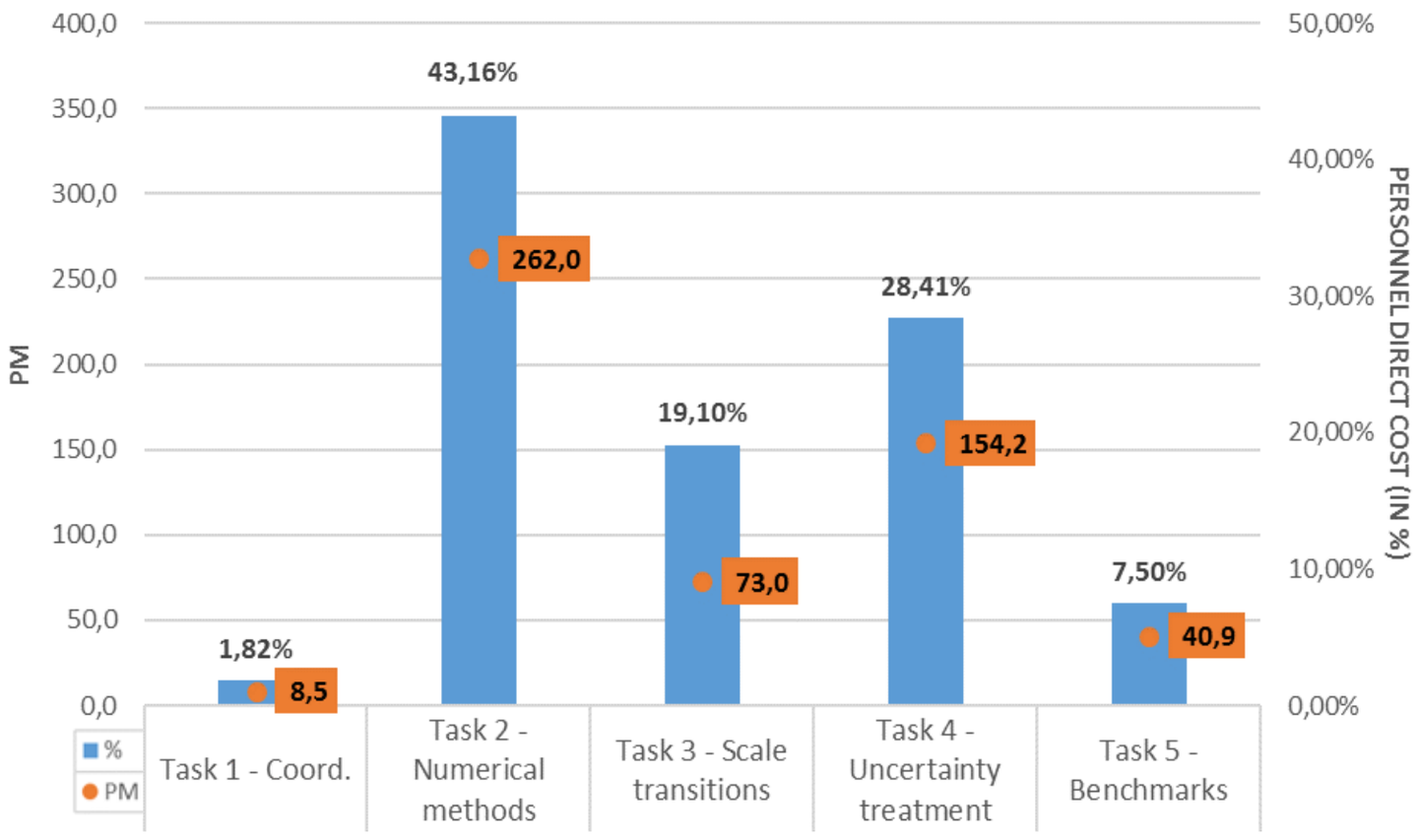
DONUT WP:
Distribution of EC Contribution between categories of Actors



DONUT WP - Budget distribution between categories of direct costs



DONUT WP:
Personnel costs breakdown per task (in % and in PM) - Total PM: 538,6



DONUT Task 2 - Numerical methods for high performance computing of coupled processes

Goals:

- To design and implement efficient numerical algorithms taking advantage of the latest research achievements for solving complex coupled problems. In particular, the following axes play a central role in this task:
  - **numerical algorithms for parallel computing (e.g., linear solvers, domain decomposition,...)**
  - **efficient multiscale numerical methods for coupled problems**
  - **grid adaptivity and adaptive stopping criteria based on a posteriori error estimates**
- The methods and tools that are developed will be made available within the other tasks of the WP to benchmark their efficiency and to the whole community (others WP and beyond) thanks to scientific publications, versatile codes development associated to a thorough documentation.

DONUT Task 2 - Numerical methods for high performance computing of coupled processes

- **Deliverables**:
  - D2.1 (m18): Intermediate report describing numerical method improvement and their transferability in numerical tools. Amongst other, it will describe how the developments can be linked and implemented in existing tools used by partners and it will document input/output interface [Task leader]. All partners involved in this task will contribute to this report.
  - D2.2 (m24): Report describing the benchmarks to be carried out during the project (common for all tasks) [BRGM]. It is worth noticing that prior to benchmarks definition a workshop will be organized with other WP to set up and defined relevant benchmarks.
  - D2.3 (m46): Updated report describing numerical method improvement and their transferability in numerical tools as well as benchmarks realization [Task leader]. All partners including in this task will contribute to this report.

DONUT Task 3 - Scale transition schemes for coupled processes

- Main **objectives** of this task are to:
  - Provide numerical methods to **bridge spatial scales**
  - Provide tools that enable the consideration of **chemo-mechanical** process couplings
- **Deliverables**:
  - D3.1 (m18): Intermediate report describing improvement and implementation of scale transition methods improvement and their application for multiscale simulations. [Task leaders]. All partners involved in this task will contribute to this report.
  - D3.2 (m24): Report describing the benchmarks to be carried out during the project (common for all tasks) [BRGM]
  - D3.3 (m46): Final report describing upscaling scheme and benchmark realisation [Task leaders]. All partners involved in this task will contribute to this report.

DONUT Task 4 - Tools and methods to quantify/derive uncertainties induced by coupled processes

- Main **objectives** of this task are to
  - Developments of innovating numerical methods to treat uncertainty and sensitivity analysis on complex coupled representative cases (big system, many media and input data) **with strong non-linearities**: global/local sensitivity analysis with specific tools (surrogate/metamodels such Chaos polynomia, neural network, adjoin state methods, …)
  - Developments of mathematical representations of uncertain parameters applied for coupled processes (correlations, …)
- **Deliverables**:
  - D4.1 (m18): Intermediate report describing numerical developments realized to treat uncertainty. [Task leader]. All partners including in this task will contribute to this report.
  - D4.2 (m24): Report describing the benchmarks (with a focus on surrogate models) to be carried out during the project (common for all tasks) [BRGM].
  - D3.3 (m46): Final report describing numerical developments realized to treat uncertainty. [Task leader]. All partners including in this task will contribute to this report.

DONUT Task 5 - Benchmarks of methods and tools for coupled processes

- This task will focus on:
  - Development of **suitable benchmarks**, mainly derived from THGas, THM, and reactive transport test-cases at large time and space scales (porous/fractured and free media),
  - **Implementation** of numerical methods developed at task 2, 3 and 4 in existing tools used by each involved partner,
    - benchmarks of methods and tools to quantify efficiency and added-value in terms of :
    - increase of knowledge (better physical representation, more integrated systems, …)
    - accuracy, robustness, computational cost,
    - robustness of scale-transition approaches
    - Ability to manage uncertainty and sensitivity analyses
- **Deliverables**:
  - D 5.1 (m18): The description of key points needed to be evaluated in numerical methods for coupled processes (SURAO, ENRESA, COVRA, ANDRA, GRS)
  - D5.2 (m24): Report describing the benchmarks to be carried out during the project (common for all tasks) [BRGM].
  - D5.2 (m46): Final report describing benchmark realizations and (i) influence of the development carried out in other tasks on the quantification of improvement (ii) comparison, when possible, of tools on which numerical methods have been implemented [Task leader]. All partners involved in this task will contribute to this report.

Key challenges & objectives for Year 1

- In addition to detailed work description that can be found in the submitted document, the first year the work carried out in the WP will be:
  - Organizing and holding the WP kickoff meeting
  - Establishing the communication within the WP
  - Ensuring that the partners follow the agreed work plan and taking mitigation actions if necessary
  - Organizing the T+1 years annual meeting
  - Make the partners contributing to State of the Art report (due month 6)