INRIA's Large-Scale Initiative "C2S@Exa" Computer and Computational Sciences at Exascale

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General objective and contributions

✓ Establishment of a continuum of skills in the applied mathematics and computer science fields for a multidisciplinary approach to the development of numerical simulation tools that will take full benefits of the processing capabilities of emerging high performance massively parallel architectures

✓ Activities and contributions are organized along a three-level structure from **generic building-blocks** to **large-scale applications**

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Project structure and activities (1/3)
Level 1 – Towards generic and scalable algorithms

✓**Computer science topics**

Upstream from the core topics which are centered on *the development of high performance numerical schemes and algorithms*

✓**Algorithmic aspects**

*E*mphasis on the development of generic numerical libraries and solvers in order to benefit from all the parallelism levels with the main goal of optimal scaling on very large numbers of computing entities

✓**Robustness, accuracy and scalability issues of numerical schemes**

Generic design issues of high performance numerical schemes for systems of partial differential equations

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Project structure and activities (1/3)
Level 1 – Towards generic and scalable algorithms

- **Topics that will be addressed (among others):**
  - resource management and scheduling strategies,
  - runtime systems,
  - component-based programming model,
  - high level parallel programming model,
  - energy effective fault tolerant protocols for HPC applications,
  - performance execution models for fault-tolerant applications,
  - techniques and tools for static and dynamic processing of numerical data sets,
  - resilience for sparse linear algebra.

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Project structure and activities (2/3)
Level 2 – Towards robust, accurate and highly scalable numerical schemes for complex physical problems

✓ Study of the systems of PDEs that model the scientific and engineering use cases considered in the project

✓ Topics of interest include discretization in space of underlying systems of PDEs (high order approximation, adaptivity, etc.), solution algorithms base on continuous models (domain decomposition algorithms, physics base preconditioners, etc.) and numerical methods adapted to multi-scale and multi-physics problems

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Project structure and activities (2/3)

Level 2 – Towards robust, accurate and highly scalable numerical schemes for complex physical problems

- ✓ **Topics that will be addressed (among others):**
  - ✓ core numerical linear algebra kernels,
  - ✓ sparse direct solvers,
  - ✓ preconditioned iterative solvers,
  - ✓ continuous solvers (i.e. defined at the PDE level),
  - ✓ numerical schemes for transport, diffusion, convection-diffusion, waves and N-body models.

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Project structure and activities (3/3)
Level 3 – Towards exascale computing for the simulation of frontier problems

✓ Large-scale simulations using high performance numerical computing methodologies resulting from the activities undertaken in the bottom and intermediate levels

✓ With the involvement of external partners from research laboratories or industrial groups that will help in defining and dimensioning a number of frontier problems

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Project partnership

- ✓ **Level 1: core project-teams**
  - ✓ Computer scientists
  - ✓ Algorithmists
  - ✓ Numerical mathematicians
- ✓ **Level 2: associated project-teams**
  - ✓ Numerical mathematicians of the core project-teams and from researchers of associated INRIA project-teams that are experts of the underlying PDE models
- ✓ **Level 3: external partners**
  - ✓ Researchers and engineers from third-parties organizations, laboratories or industries

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Core project-teams: numerical mathematicians

BACCHUS [INRIA Bordeaux – Sud-Ouest]

Parallel tools for numerical algorithms and resolution of essentially hyperbolic problems

CALVI [INRIA Nancy – Grand-Est]

Scientific computing and visualization

HIEPACS [INRIA Bordeaux – Sud-Ouest]

High-end parallel algorithms for challenging numerical simulations

NACHOS [INRIA Sophia Antipolis – Méditerranée

Numerical modeling and high performance computing for evolution problems in complex domains and heterogeneous media

SAGE [INRIA Rennes – Bretagne Atlantique]

Simulations and algorithms on Grids for environment

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Core project-teams: computer scientists

AVALON [INRIA Grenoble – Rhône-Alpes]
Large algorithms and software architectures for service oriented platforms

GRAND-LARGE [INRIA Saclay – Ile-de-France]
Global parallel and distributed computing

MOAIS [INRIA Grenoble – Rhône-Alpes]
Programming and scheduling design for applications in interactive simulation

ROMA [INRIA Grenoble – Rhône-Alpes]
Resource Optimization: Models, Algorithms, and scheduling

RUNTIME [INRIA Bordeaux – Sud-Ouest]
Efficient runtime systems for parallel architectures

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Software development activities

- ✓ Numerical linear algebra
  - ✓ GPREMS, HIPS, MAGMA/PLASMA, MAPHYS, MUMPS, PASTIX
- ✓ PDE solvers
  - ✓ FLUIDBOX, GYSELA, MPFRAC, MAXW-DGTD, SISMO-DGTD, etc.
- ✓ Programming models/languages, runtime systems
  - ✓ DHICO, FORESTGOMP, HWLOC, KAAPI, STARPU, PACO++, etc.
- ✓ Others tools
  - ✓ EPSN, NUM3SIS, PAMPA, SCOTCH, etc.

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Scientific and technical challenges

- ✓ **Nuclear energy production**
  - ✓ Nuclear fusion
    - ✓ CEA Cadarache
- ✓ **Environmental applications**
  - ✓ Earthquake dynamics
    - ✓ BRGM [Public institution in earth science applications for the management of surface and subsurface resources and risks]
  - ✓ Groundwater flow and reactive transport
    - ✓ ANDRA [National Radioactive Waste Management Agency]

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- Numerical linear algebra
  - MUMPS [ROMA]
  - PaStiX/HIPS [BACCHUS]
  - MaPhys [HIEPACS]
- PDE solvers
  - RealFluids [BACCHUS]
  - ScalFMM [HIEPACS]
- Other tools and environment
  - PAMPA [BACCHUS]

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- PDE solvers
  - H2OLab [SAGE]
  - Selalib [CALVI]
- Other tools and environment
  - NUM3SIS [NACHOS/OPALE]
- HPC tools and environment
  - StarPU and Hwloc [RUNTIME]
  - IER [GRAND-LARGE]
  - TakTuk and Kaapi [MOAIS]

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Scientific and technical challenges: ANDRA use case

In the field of phenomenological description and performance/safety assessment, ANDRA has to perform many numerical simulations, in particular to quantify flow and solute transfer in saturated or unsaturated porous media, from the waste package to the human being, and through the repository and geological environment

Simulations have to take into account many physical processes, applied to different components (from the waste packages to the geological media) and material (clay, concrete, iron, glass, etc.) on very large time (up to one million years) and scale (from centimeter to tens of kilometers

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Scientific and technical challenges: ANDRA use case

Two levels of simulations are carried out

- ✓ Complex physicochemical processes, involving strong couplings (such as chemical-transport, 2 phase-flow with radionuclide transfer, thermo-hydro-mechanics problems) but solved on small systems with grids up to many thousands of elements
- ✓ Simplified physicochemical processes (leak coupling) consisting of modifying in space and time hydraulic and solute transfer parameters, but solved on big systems with grids of many millions of elements. Global system is split into embedded compartments whose scales are bigger and bigger

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Scientific and technical challenges: ANDRA use case

Ex : deep geological repository

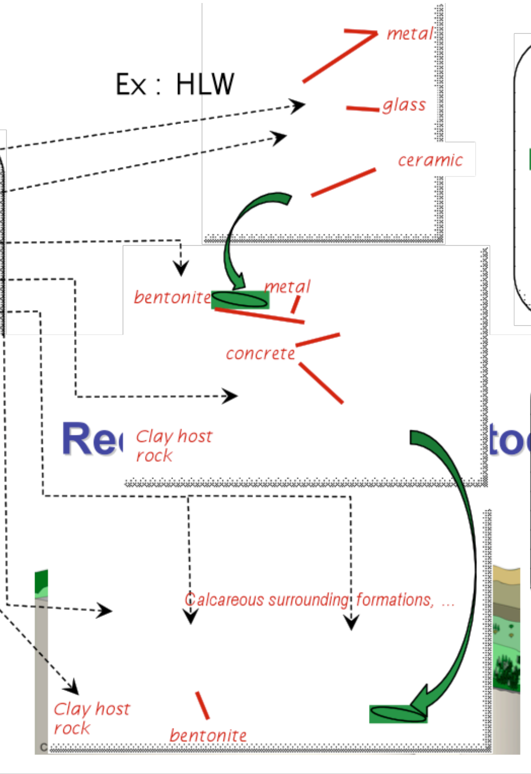
Multi components

- Waste
- Waste package
- Galleries
- Disposal cell
- Access (shaft…)
- Modules and zones
- Geological medium

Multi materials

- Glass
- Ceramic
- Metal
- Concrete
- Clay based (bentonite)
- Clay host formation
- calcareous, …

Ex : HLW



Multi processes

Thermal (T), Hydraulical-Gas (H), Mechanical (M), Chemical (C), Radiological (R) Solute Transfer in porous media (Tr).

with or without couplings (strong to low)

Multi spatial scale

- *centimetric to metric :*	waste
- *metric to decametric*	disposal cell
- *hectometric to kilometric*	disposal
- *pluri-kilometric*	geological medium

→ Management > 7 orders of magnitude

Multi temporal scale

Up to 1 million years

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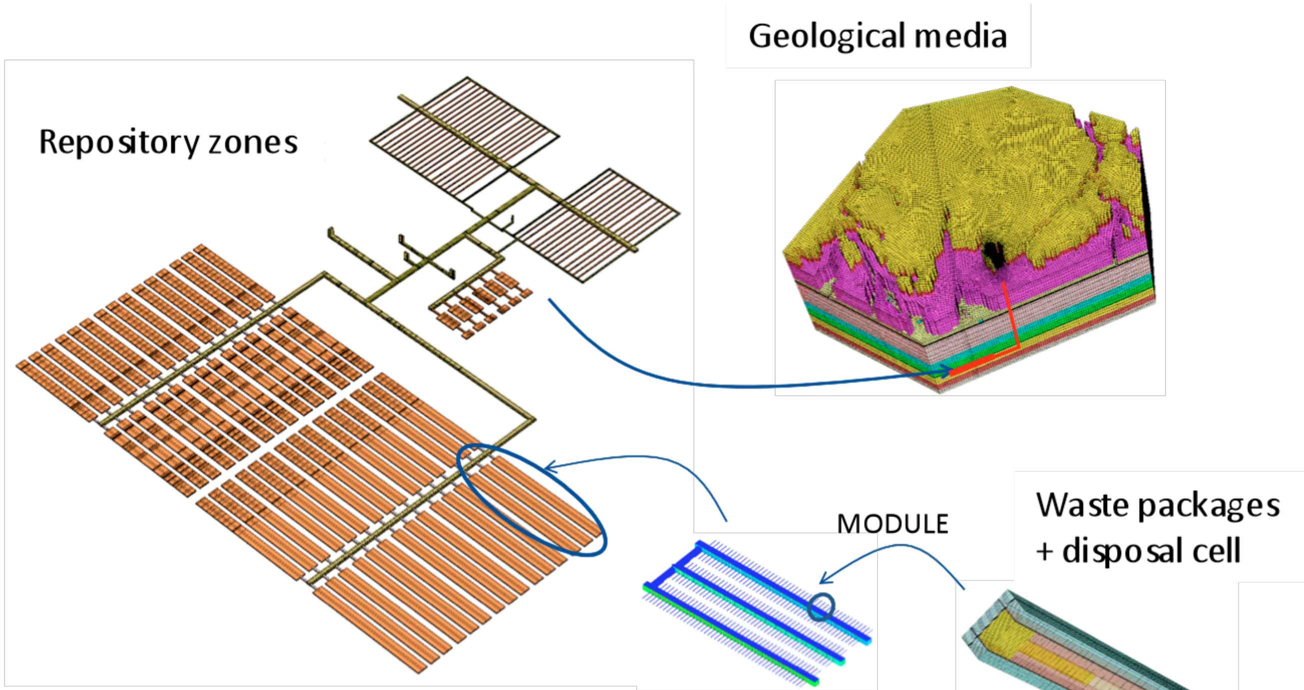
Scientific and technical challenges: ANDRA use case



Radioactive wave management scenario
based on simplified physicochemical processes

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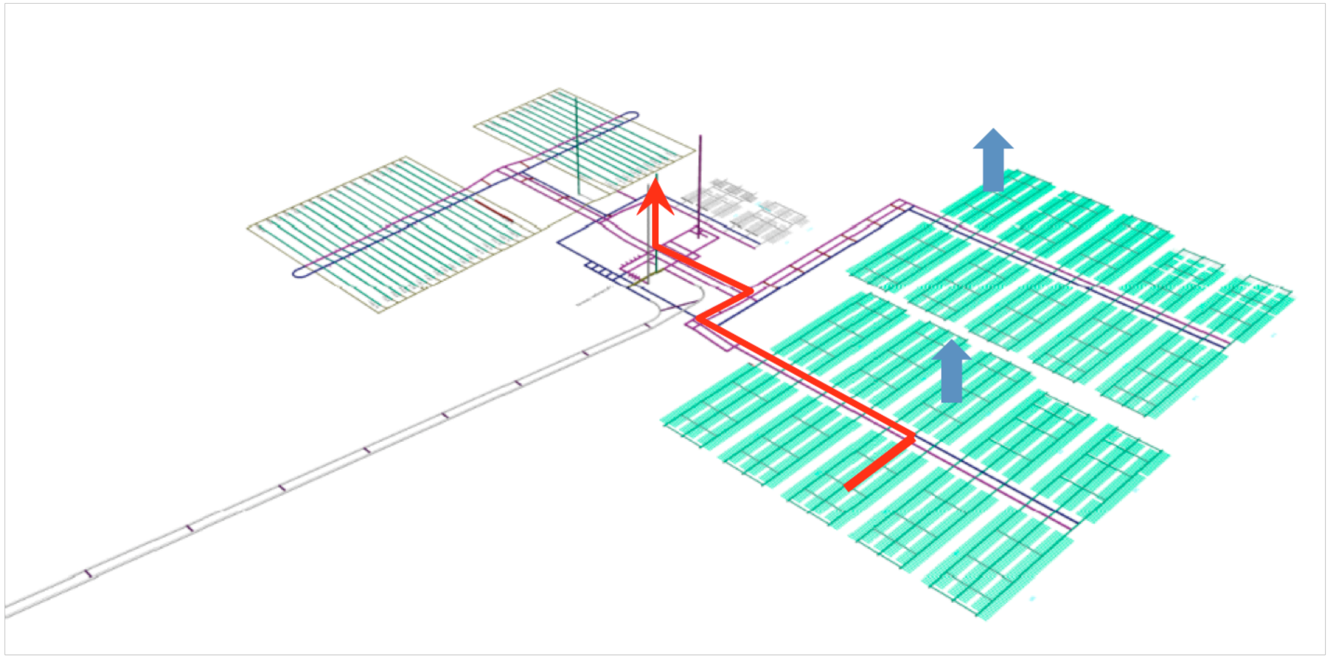
Scientific and technical challenges: ANDRA use case



Computational setting of geological repository structures and its environment

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Scientific and technical challenges: BRGM use case

Earthquake dynamics. Modeling seismic wave propagation in large sedimentary basins with extremely high velocity contrasts over tiny superficial layers is one of the most challenging problems in computational seismology. Seismic risk assessment begins with the description of the earthquake source. This is why obtaining correctly the source image is crucial. The particularity of the earthquake source includes a discontinuous process (faulting) controlled by fracture mechanics, and this makes it difficult to simulate numerically. These physical processes are three dimensional and large scale computing resources are mandatory to investigate the impact of strong motion seismic events

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Scientific and technical challenges: BRGM use case

CO2 sequestration. In the context of greenhouse gas emission into the atmosphere, CO2 capture and storage into geological formation has been considered recently as one of the mitigation option. Mathematical models and numerical simulators are essential tools in addressing problems and questions that arise in the context of CO2 storage in the deep subsurface. They are necessary for the clarification of safety, feasibility and economic issues and rely on complex three-dimensional modeling of coupled phenomena

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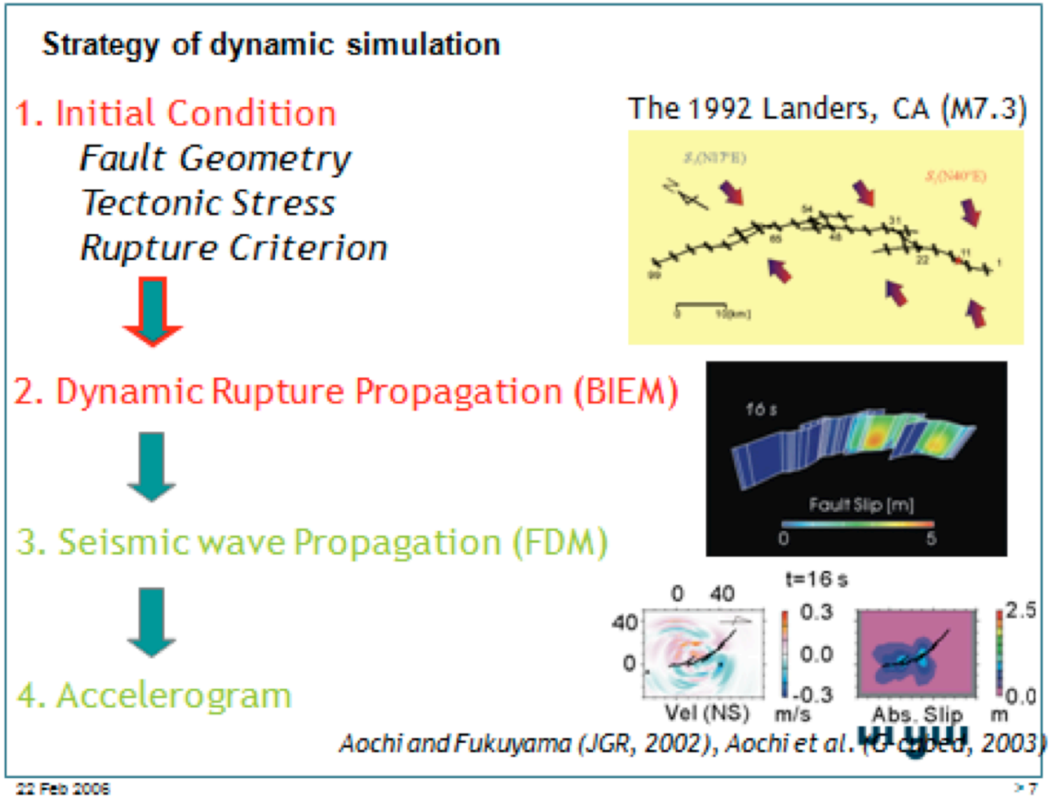
Scientific and technical challenges: BRGM use case

Earthquake modeling with the different physical processes and the numerical methods associated.
Example of the Landers, California earthquake (M7.3) in 1992



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Scientific and technical challenges: BRGM use case

Capture and storage of Carbon Dioxide from CO2CRC, Australia, 2010