ALLIANCES : SIMULATION PLATFORM FOR RADIOACTIVE WASTE DISPOSAL

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ABSTRACT

CEA, ANDRA and EDF are jointly developing the software platform Alliances whose aim is to produce a tool for the simulation of nuclear waste storage and disposal. This type of simulations deals with highly coupled thermo-hydro-mechanical-chemical and radioactive (T-H-M-C-R) processes. Alliances aim is not to develop a new scientific calculation code but to accumulate within the same simulation environment the already acquired knowledge and to gradually integrate new knowledge. The release 1 of Alliances was distributed to users in December 2003. The next releases of Alliances (2.x) include more physical phenomena like reactive transport in unsaturated flow, thermal and mechanical models and their coupling with hydraulics and alteration of waste package coupled with the environment. Beyond, his first application domain for high level nuclear waste disposal, Alliances can be used for a large range of computations in the field of porous media simulation.

1. INTRODUCTION

The safety assessment of nuclear waste disposals needs to predict coupled thermo-hydro-mechanical-chemical and radioactive (T-H-M-C-R) processes, involving phenomena such as heat generation and transport (due to radioactive decay of nuclear waste), infiltration of groundwater (hydrological processes), swelling pressure of buffer material due to saturation (mechanical processes) and chemical evolution of buffer material and porewater (chemical processes). It appeared as necessary to develop and assess numerical tools that model these physical mechanisms.

Therefore, the French Atomic Energy Commission (CEA), and the French Agency for Radioactive Waste Management (ANDRA) have been jointly developing since 2001 the software platform Alliances. The French Electric company (EDF) joined the project in 2003. The aim of the project is to obtain a numerical platform enabling the simulation of all phenomena governing storage and disposal safety with the following characteristics: (i) Efficient coupling of different numerical codes; (ii) Simulation of multi-physical and multi-scale phenomena; (iii) Uncertainties analysis related to data and models; (iv) Studies management and traceability.

More precisely, the physical models currently implemented are: flow in unsaturated and saturated porous media, radionuclide transport in unsaturated/saturated media,

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chemistry/Transport coupling in saturated media with feedback of porosity changes on transport properties, thermo-hydraulic and mechanical coupled processes (THM), thermo-aerolics, alteration of waste packages and their interaction with its environment.

The next releases of Alliances will include more physical phenomena: mainly reactive transport in multiphase flows to take into account gas migration.

These models lead to a large set of non-linear differential equations that can be solved on 3D meshing by using finite element like methods. Main numerical components currently integrated in Alliances use a scalar architecture. Current works are done on massively parallels architecture which will available in the next release of Alliances.

Alliances goal is not to develop a new scientific tool but to accumulate within the same simulation environment the already acquired knowledge and to gradually integrate new ones. Therefore, it is based on the following three fundamental choices:

- Seamless integration of legacy codes as software components ;
- Allow efficient coupling between components by sharing a common data model for mesh and field;
- Sharing Salome (www.salome-platform.org) open source components for pre and post processing.

Special attention is paid to the qualification and validation program. It proceeds by tests with a gradual complexity: first comparing calculations to analytical solutions, then defining benchmark exercises between codes implemented in the platform and external ones. The tests validate the different aspects of the application validity domain of the modules. For each test, several options are tested: selected codes, size of the grid, methods of discretization (Finite Volume, Mixed Hybrids Finite elements...), linear solver. The tests are included in a non regression test suite.

ANDRA safety studies were done with the platform during 2004-2005. Several computations were also carried out at CEA mainly on reactive transport simulations.

Alliances is currently available on PC/Linux computer system and on the CEA supercomputer facilities CCRT.

Specific accommodation could be established for a free utilisation of Alliances for research applications (contact the corresponding author)

This paper is organized as follows. Section 2 is devoted to the software architecture and coupling methodology. The Alliances capabilities are described in section 3. Some applications are presented in section 4. Finally we give a conclusion and prospects for further work.

2. SOFTWARE ARCHITECTURE

2.1 A Multi-Level architecture

In order to correspond to the software strategy a multi-level architecture has been chosen (see figure 1).

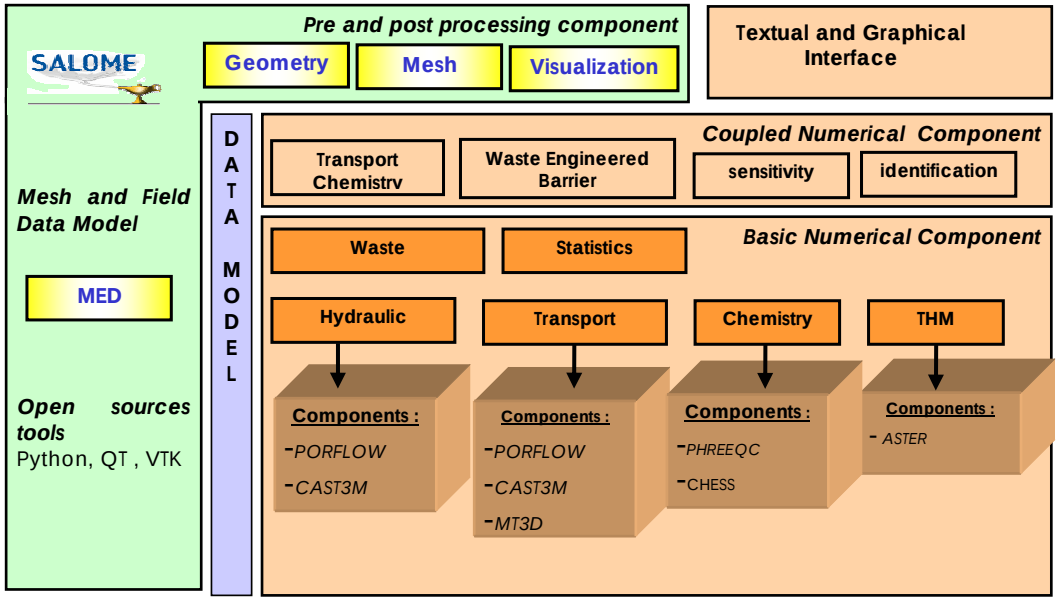

FIGURE 1. Alliances multi-level architecture.

The **basic numerical components** come from the integration of legacy external codes. Each component corresponds to a specific application (Hydraulic, transport, thermo-hydro-mechanic, etc.). This application can result from coupled processes but the coupling is in this case internal to the integrated code. A component satisfies a given programming interface but may have several implementations (i.e. link to different codes), this property is widely used, for example a transport calculation can be performed with Cast3m or Traces, the choice between one or the other implementation is only specified by a limited set of parameters. These components can be used by a stand-alone way or via coupled numerical components.

The coupled numerical components correspond to multi-physics applications which are implemented via coupling algorithms between the basic numerical components (see part 3)

The **common data model** supports the communication way between the different components. This data model contains all the characteristic values (geometrical, physical, and numerical) used for the modelling and the simulation. The data model joins the physical properties to the geometrical characteristics. This data model is based for the mesh and field part on the MED format (see next section).

A specific **mesh and field data model** is used. It is based on **MED structure,** a format developed by CEA and EDF in the context of the Salome project. Both file and memory

formats are available. File format uses HDF5 (Hierarchical Data Format) technologies allowing efficient, compact and portable data storage. Different tools for basic fields manipulation have been developed (addition, norm computation, ...). Each integrated code can exchange with this format via specific drivers.

The use of Salome platform gives access to the **pre and post processing tools**: geometry and meshing generator, visualization.

The **user interface** is based on a textual mode using Python scripting and a graphical mode using QT and VTK instructions.

2.2 Coupling methodology

In Alliances, for some applications, as THM, the integrated codes already implement the coupling algorithms. But for other applications, as chemistry/transport or waste package / environment, the coupling should be done at the platform level.

For this reason a key objective of Alliances is to give the capability for coupling algorithms development between existing codes.

The choice of Python was done as central language rather than PVM or MPI.

First of all, it provides an access via an high level language to the components programming interface, though allowing scientist an easy prototyping of coupling algorithm even if they are not expert in low level programming as C++.

Moreover, in order to optimize cpu cost, the data exchange needs to be made through memory. For this reason codes are integrated in the platform as dynamic libraries, Python being well adapted to this type of wrapping. More precisely each code appears in Alliances as a Python classes with specific methods for initialisation, computation, data exchange. The codes are themselves written in different languages (C, C++, Fortran , Fortran 90). There exist several tools to help in Python wrapping. In Alliances we mainly use swig for C and C++ codes and F2PY for Fortran ones.

As previously mentioned several codes can be used for the same physical application. For example, in the chemistry/transport coupling two codes are used for the chemistry part due to model complementarities in the codes.

The algorithms are written at a global level independently from involved codes specificities in order to facilitate the evolution of platform (integration of new codes, coupling algorithms optimisation). Each code share the same Application Programming Interface (API).

Thanks to the efficient coupling implementation, different algorithms leading to explicit or implicit coupling can be performed. The only limitation being the ability of a component to provide necessary information (derivatives for example). The usual way is to use for light coupling sequential iterative strategy mainly base on an operator splitting approach. For stronger coupling, specific work needs to be done in order to develop adapted algorithms [*Bouillard et al*., 2005].

3. ALLIANCES MAIN CAPABILITIES AND CORRESPONDING INTEGRATED COMPONENTS

3.1 General Capabilities

Alliances take into account 2D and 3D unstructured meshes.
For each application the users have the possibility to use different code with the same input and output format (data model, mesh, field)

3.2 Hydraulic and mass transport

The flow simulation takes into account saturated media in transient and steady state and unsaturated media with constant gas pressure (Richards model)
The mass transport model deals with an arbitrary number of species and includes convection-diffusion transport, radioactive chains, radioactive decay, dissolution/precipitation process and chemical retention modelled through a delay factor (Kd, Langmuir, Frendlich).

3.3 Chemistry/Transport coupling

The reactive transport model describes the spatial and temporal evolution of a set of chemical species that are, on one hand, submitted to transport phenomena and, on the other hand, submitted to chemical reactions. Transport phenomena are convection, diffusion and dispersion in porous media. Chemical reactions may be in equilibrium or under kinetics, in liquid (acid-base redox reactions), solid (precipitation/dissolution) or sorbed (cation exchanges) phases. The influence of an heat field evolution on the chemistry is also taking into account (including thermal transport computation).

The corresponding physical model is made of a set of partial derivative equations describing species transport in liquid phase, and a set of non linear algebro-differential equations corresponding to the chemical reactions that model species interactions.

The implementation already done in Alliances uses a sequential iterative algorithm [*Yeh and Tripathi, 1989*]. Specific works are under development in order to implement more implicit coupling schemes as Quasi-Newton's methods and Non Linear Conjugate Gradient Methods [*Bouillard et al.*, 2005].

3.4 Thermo hydraulic and mechanical thermo hydraulic coupling

The thermo hydraulic module is used for the simulation of two phase flows in porous media, taking into account thermal loading and coupling. The thermal propagation equation represents thermal diffusion and also advection mechanisms due to transport of energy by the liquids. Two fluids are simulated, a gas mixture and a liquid. Partial vaporization of the liquid is modelled as well as dissolving of the gas into the liquid. Fick diffusion can occurs in the gas mixture. In the two phases flows module, the deformation of solid phase is represented in a very coarse way, by a linear relation between porosity variations and liquid pressure.

The Thermo Hydro mechanical module uses a widely more sophisticated representation of the solid phase. Conversely, hydraulic simulation is more simple: only one liquid phase can be present. The total mechanical stress tensor is the sum of the effective stress tensor-related to deformation of the skeleton- and an isotropic contribution related to liquid pressure with the Biot coefficient. The same coefficient links porosity evolution and liquid pressure variations. These relations induce a strong coupling between hydraulic equations and

mechanical ones. The mechanical behaviour is a plastic rock model based on Hoek and Brown criterion. A softening mechanism is implemented, including dilatancy effects. The plastic equivalent deformation is regarded as a measurement of the damage of the material. Consequently the hydraulic permeability can increase drastically when plastic deformation expands. This relation induces also a strong coupling between hydraulic and mechanical phenomena. The coupling between temperature and solid deformations is very classical and needs the use of two thermal expansion coefficients (one for the liquid, one for the skeleton).

3.5 Sensibility Analysis

Alliances sensibility analysis tool allows to lead an uncertainty analysis (determine and study the variation of the output parameter, considering the variation of all the uncertain input parameters) or a sensitivity analysis (determine the importance of the variation of the input parameters on the variation of the output parameters) with a probabilistic approach.

A study decomposes into three steps: define the sampling, execute the application for each set of date and analyze the results for the uncertainty and sensitivity point of view.

The sampling module assigns a probability distribution function to each uncertain parameter. This function can be continuous or discreet. The Sampling can be generated by a Simple Random Sample or the Latin Hypercube Sampling method.

The uncertainty analysis is made by calculating classical statistical indicators from the results: moments (mean, standard deviation), quantiles (median, quartiles, and extreme quantiles), curves (Cumulative Function Distribution, Complementary Cumulative Function Distribution, Boxplots …).

The sensitivity analysis is carried out by comparing correlation coefficients between the studied result and each uncertain input parameter. These coefficients can be classic (Pearson, Spearman) partial (PCC/ PRCC) or regression coefficients (SRC/ SRRC).

3.6 Packages models coupled with the environment

Different models are available for the description of bitumen, glass or generic container degradation. These models consist of a set of non linear differential equations that are coupled with hydraulic and mass transport models.

3.7 List of integrated codes

- Hydraulics and Transport:
  - Cast3M (CEA, France) with Mixed Hybrid Finite Elements and Finite Volumes [*Bernard-Michel et al. 2004*]
  - Porflow (ACRI, USA) with Finite Volumes
  - Traces (IMFS, France) with Mixed Hybrid Finite Elements
  - MT3D (USGS, USA) with Finite Volumes [*Zheng and Wang, 1998*]
- Geochemestry:
  - Chess (ENSMP/CIG, France) [*van der Lee and de Windt, 2002*]
  - Phreeqc (USGS, USA) [*Parkhurst and Appelo, 1999]*
- Thermo-aerolics: Trio-U (CEA, France)
- Thermo-Hydro-Mechanics: Aster (EDF, France) with Finite Elements
- Sensibility analysis:
  - Kalif (CEA, France) for data sampling
  - Pastis (ANDRA, France) for statistic analysis.

4. APPLICATIONS EXAMPLES

4.1 Andra Safety computation

The Law of 30 December 1991 confers to Andra the mission of assessing the feasibility of a repository of high-level and long-lived (HLLL) waste in a deep geological formation. In this context, Andra has recently produced a report, the "dossier 2005 argile", on which the feasibility has been studied.

Alliances platform has been used in the establishment of the Dossier 2005, to carry out deterministic safety calculations, especially in order to quantify radiological impact, from the waste to the human being, through the multi-system barrier. In figure 2, two types of results are presented.

A probabilistic study has also been carried out, taking into account the simultaneous variation spectrum of the various parameters. The study has considered twenty probabilistic input data and for each one, the specific probability distribution function was established. In order to have the most coherent set of input data, constraints and correlations have also been used and managed by Alliances.

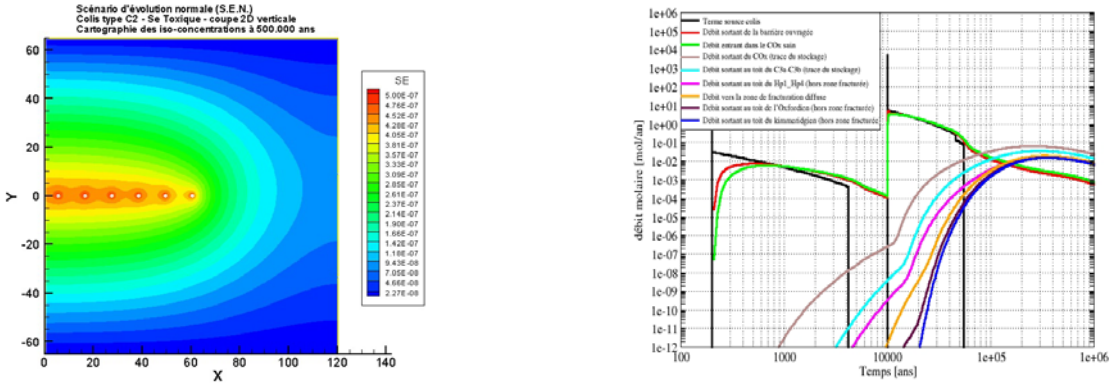

FIGURE 2. Plume of concentration (mol/m3)of toxic Selenium at 500.000 yr in the near field (left), Molar flux (mol/yr) of I129 through the repository and the geological barrier (right)

4.2 Uranium migration in a soil with various redox conditions

Measurements performed in a polluted site show that [U] varies in time, increasing in winter and decreasing in summer according to Eh variations. The numerical platform Alliances has been used to model and simulate the site [*Montarnal et al., 2006*]. In the simulation, water in equilibrium atmospheric PO2 infiltrates a subsurface aquifer and leaches a zone enriched in UO2(s). Several simulations have been performed with an increasing complexity for the soil geochemistry, including N and S aqueous redox chemistry. Modelling shows the dissolution of UO2(s) and the subsequent uranium migration. When SO42- and S2O32- are taken into account, the UO2(s) solubility increases due to the formation of SxOy-U aqueous complex. Numerical results (see figure 3) are in qualitative agreement with experimental measurements and show the interest of the use of such a coupled reactive transport code.

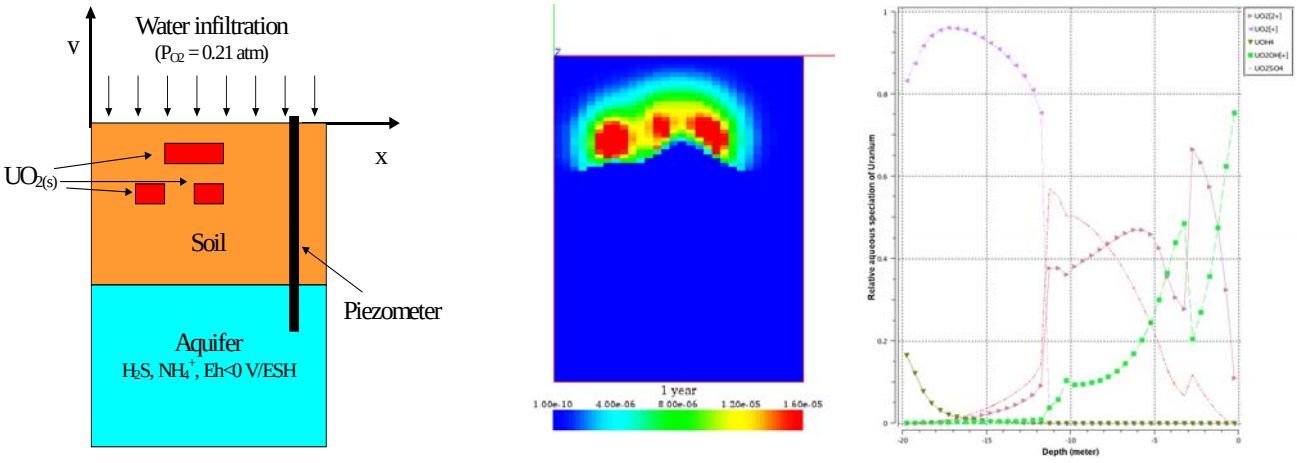

FIGURE 3. Uranium migration : Schematic representation of the studied polluted site (left), Total concentration of uranium (mol/l) calculated at 1 year (midle), Vertical profiles of relative aqueous speciation of uranium, at x=7.5 m and t=2 years (right)

5. CONCLUSIONS AND PROSPECTS

The software platform Alliances is currently available for various multi-physics simulations in porous media such hydraulic, reactive transport, thermo-hydro-mechanics, etc…Its specific software architecture give an easy access to different numeric codes for the same application. Coupling algorithms can be implemented with a modular approach allowing flexible developments. ANDRA safety studies were done with this version of the platform during 2004-2005. Several computations were also carried out at CEA mainly on reactive transport simulations.

Next releases of Alliances will increases the physical capabilities mainly to take into account gas migration via a full multiphase approach. An evolution of the software architecture will also be done in order to be able to deal with massively parallel computers.

Beyond, his first application domain for high level nuclear waste disposal, Alliances can be used for a large range of computations in the field of ground water simulation.

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