PAMSIM Project: Massive parallelism in numerical simulations for mechanics

Forum TERATEC
June 29, 2016

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EDF R&D

Outline

- Needs for numerical simulation at EDF
- About **`code_aster`** as a solver in Salome-Meca platform
- Highlights on some applications
- PAMSIM : towards a massive parallel version of **`code_aster`**
- Conclusion and call for contributions

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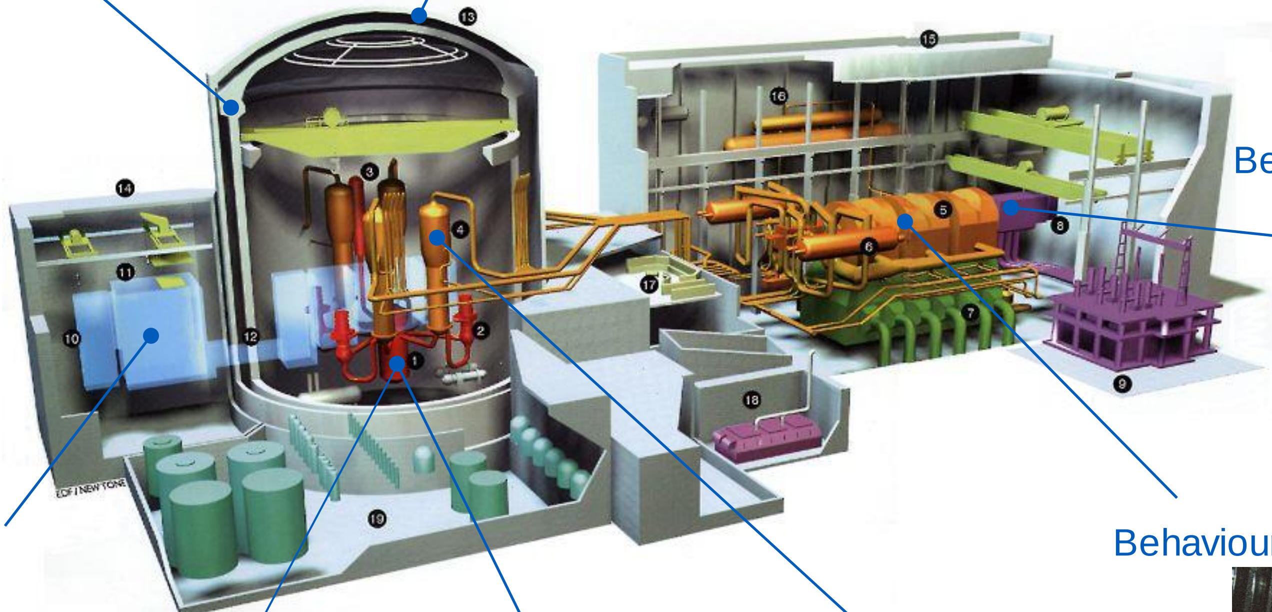
Needs for numerical simulations

Tightness of the containment vessel

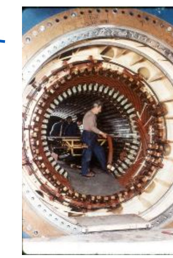
Resistance to impact (projectiles)

Seismic Analysis

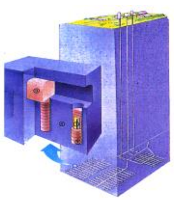
Environmental impacts



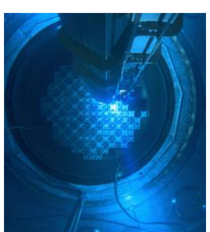
Behaviour of generators



Dismantling Waste Storage



Control of nuclear reactions



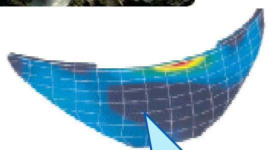
Behaviour of the pressure vessel

Tightness of the primary loop

Behaviour of turbines

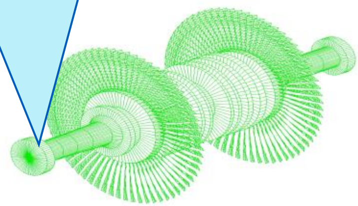
EDF

50 years of structural mechanics simulation …



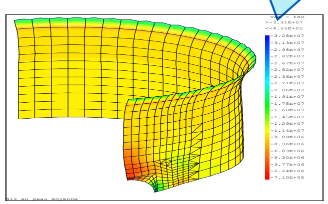
1960-70: First dam linear FE simulation (EDF apps then ASKA)

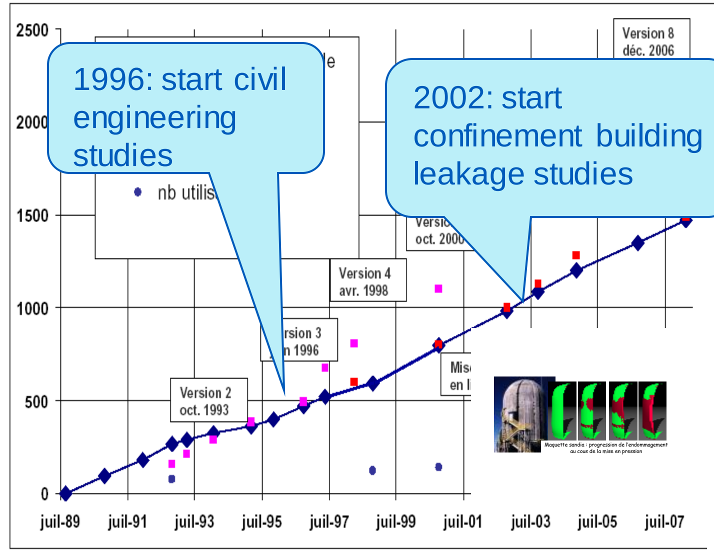
Pylon Optimization (OPSTAR)



1970-80: design studies, on type of FE, linear, specific limit conditions

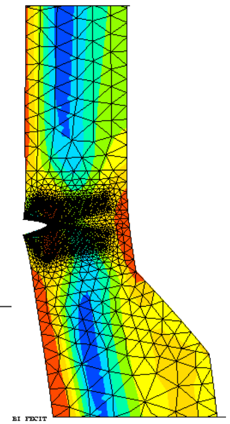
1980: 3D non linear breaking simulation: vessel damage surface detection



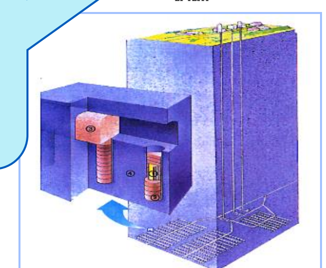


1996: start civil engineering studies

2002: start confinement building leakage studies



Now: Civil engineering, Steel thermal fatigue, Damage, lifetime, Earthquake resistance, Coupled Thermal – hydraulic – mechanical, Material ….



60 | 70 | 80 | 90 | 2000 | 2010 | 2020

1989: birth of Code_Aster

2001: Code_Aster is open source

2011: Salome-Meca 2011.2 is the qualified software

EDF

… unified for 27 years through code_aster development

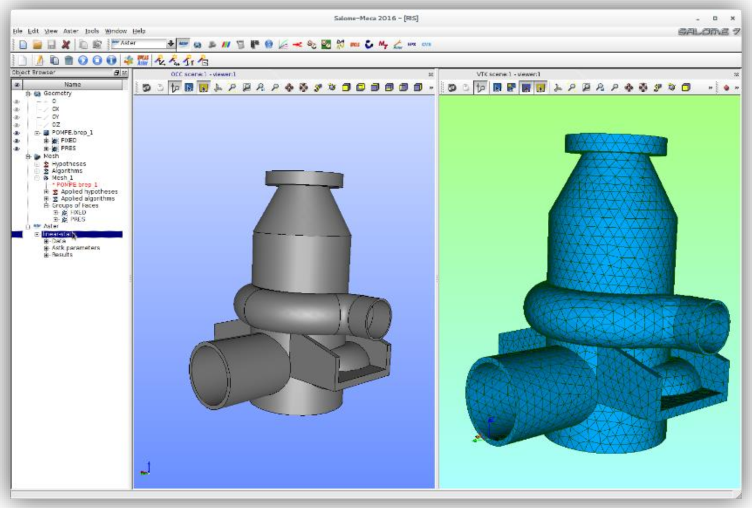
- An all-purpose FEA software for structural mechanics :

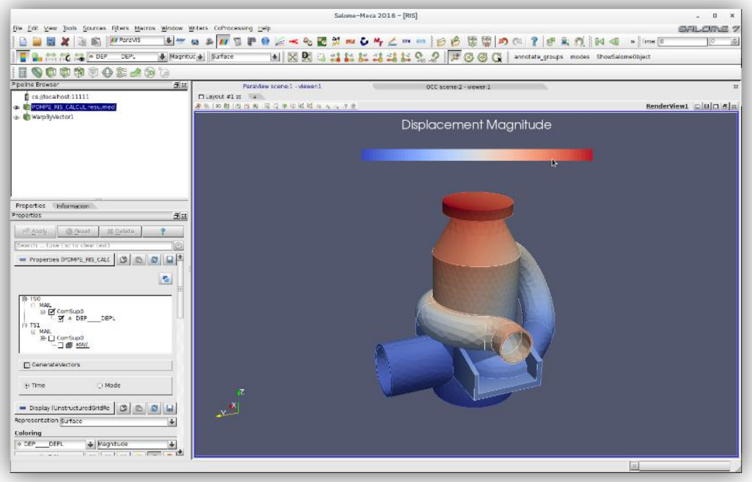
code_aster

- Plugged in a user-friendly interoperable environment :

Salome-Meca

www.code-aster.org





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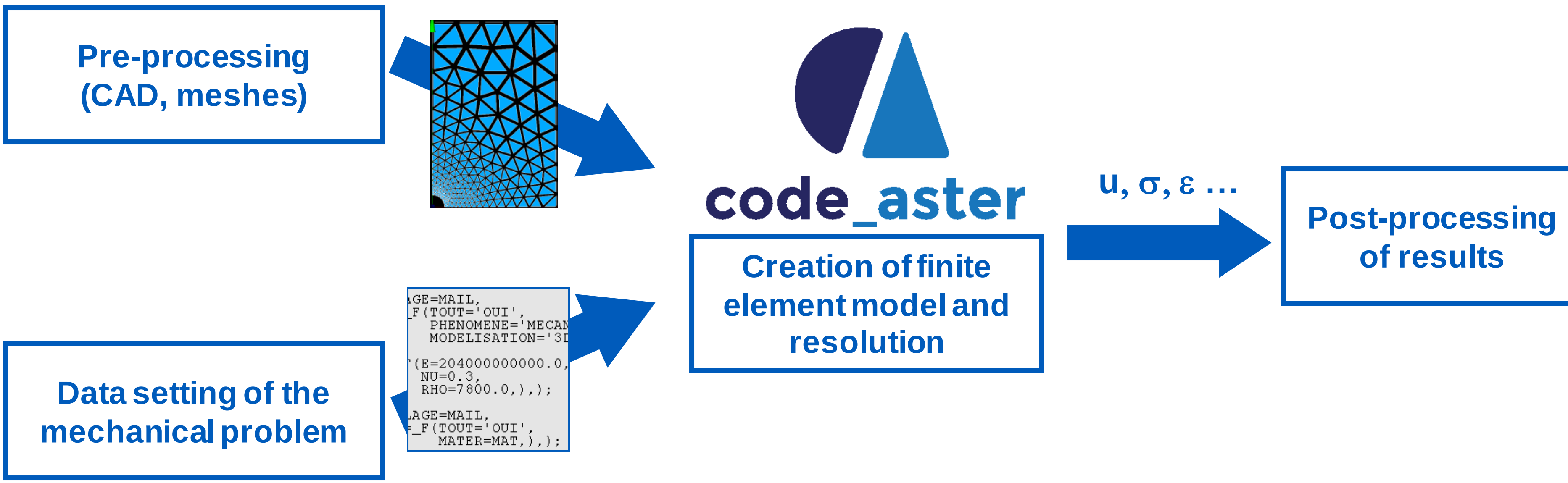
General presentation of *Code_Aster*

Code_Aster is a « stand-alone » thermo-mechanical solver

- No integrated GUI to create geometries and meshes
- No colourful post-processing
- With study data prepared in a text file



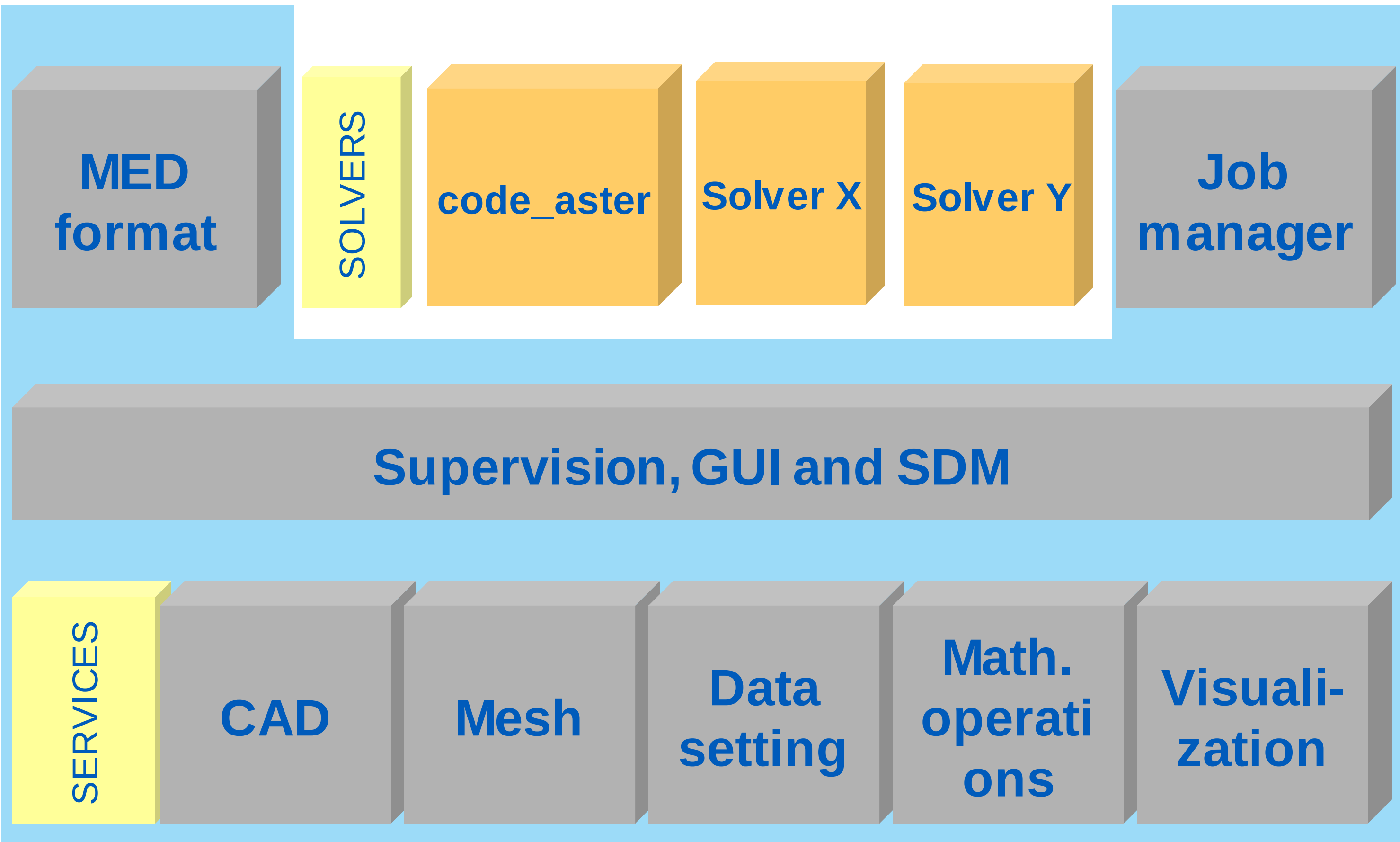
- Input: mesh and data setting
- Output: physical fields (displacement, strain, stress, temperature …)

General presentation of *Code_Aster*

- An all-purpose code for themo-mechanical study of structures
  - With a wide variety of models
    - More than 400 finite elements: 3D, 2D, shells, beams, pipes …
    - More than 100 constitutive laws
    - A wide range of solvers: mechanical statics and dynamics, vibrations, modal and harmonic analysis, thermo-hydro-mechanical coupled problems, thermics, metallurgy, acoustics …
  - A computational software used by engineers, experts and researchers
    - Studies: a need of a robust, reliable, tested and qualified industrial simulation code at EDF
    - Researches: continuous integration of new models in the development versions

Presentation of SALOME platform

- **SALOME is a generic framework for pre- and post-processing**



Salome_Meca platform for simulation in mechanics

SALOME generic platform

- CAD
- Meshing
- Supervision and study data management
- Post-processing, mathematical operations

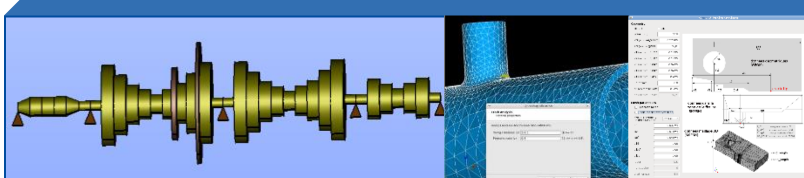
code_aster

epx europlexus software

Edyos

Mechanical solvers

- code_aster : implicit mechanics
- Europlexus : explicit dynamics
- Edyos : bearings modelling



Skill modules

- Rotating machinery, fracture mechanics, penstock modelling
- …

EDF

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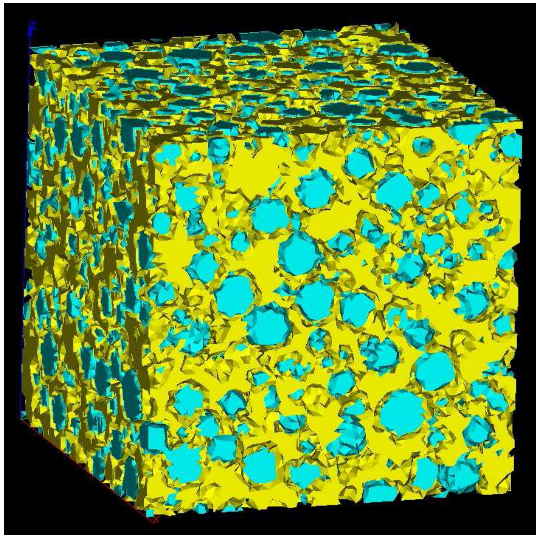
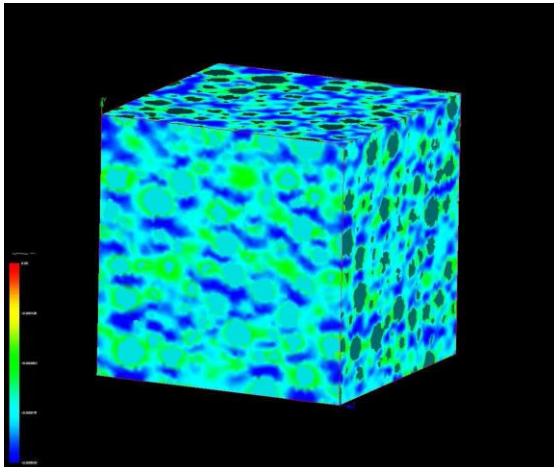
Concrete behavior: numerical identification of effective properties

- Issue
  - mastery of concrete structures subjected to aging associated with environment terms
- Goal
  - Numerical identification of effective properties of such concretes
- Study
  - a virtual experiment using computations with Code_Aster, with homogeneous schemes, in order to find the elastic and viscous properties of concrete to estimate the creep behaviour
- Results
  - Computed modulus: 33.0 GPa / measured modulus 33.7 GPa



3D concrete : 1116541 elements and 2024 inclusions



Deformation: visualization of compression bands

Identification and validation of micro-mechanical laws for austenitic steels

- Issue
  - the study of the behavior and lifetime of reactor components for nuclear power plants at polycrystals scale
- Goal
  - develop a method to compare the kinematic fields measured in polycrystals during tests performed by scanning electronic microscope (SEM) and those from the simulation of these tests.
- Study
  - simulation with code_aster of the tensile tests, with the boundary conditions nodal displacements measured over time on the edges of the field
- Results
  - Quite good agreement between simulation and measurements after updating procedure of parameters

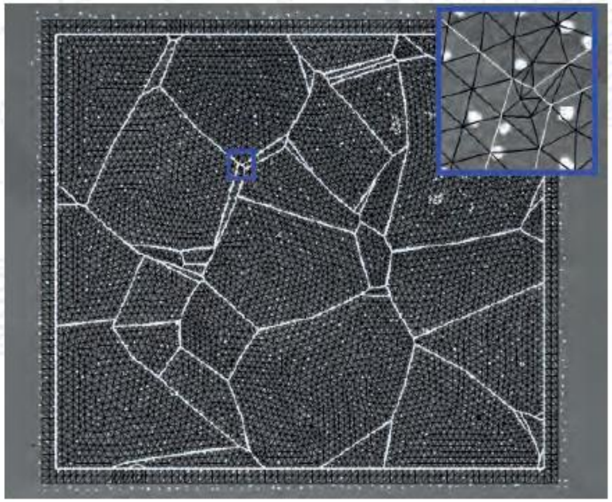
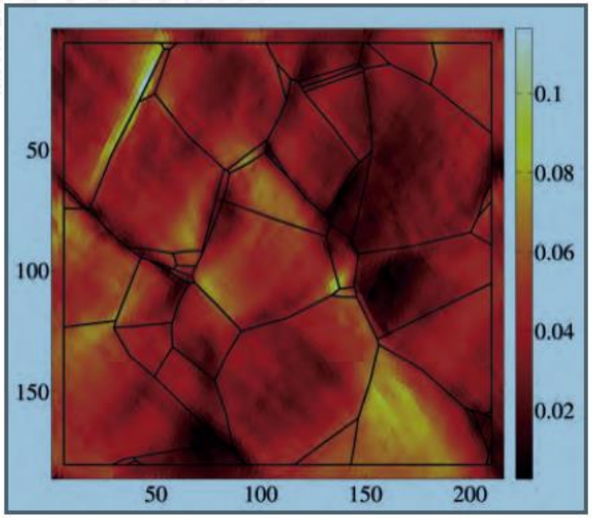


Figure 1:

(a) Maillage non-structuré de la microstructure expérimentale superposé à l'image MEB de la région d'intérêt. La barre d'échelle fait 100 µm.



(b) Champ de déformation longitudinal mesuré pour une déformation macroscopique de 5%. Les axes sont exprimés en micromètres.

Modeling the intergranular cracks by corrosion under contraints for stainless steel

Issue

- initiation and propagation of intergranular corrosion under constraint that affects nickel based alloys and austenitic stainless steels exposed to primary water of REP

Goal

- develop a method to compare the kinematic fields measured in polycrystals during tests performed by scanning electronic microscope (SEM) and those from the simulation of these tests.

Study

- simulation of the IGSCC with Code_Aster on a polycrystalline aggregate to quantify the coupling material-chemistry-mechanics mechanisms supposed to be involved in the initiation and propagation of cracks

Results

- The simulation reproduces, on small aggregates, experimentally observed phenomena: connection and coalescence of cracks, pH effects, effect of irradiation

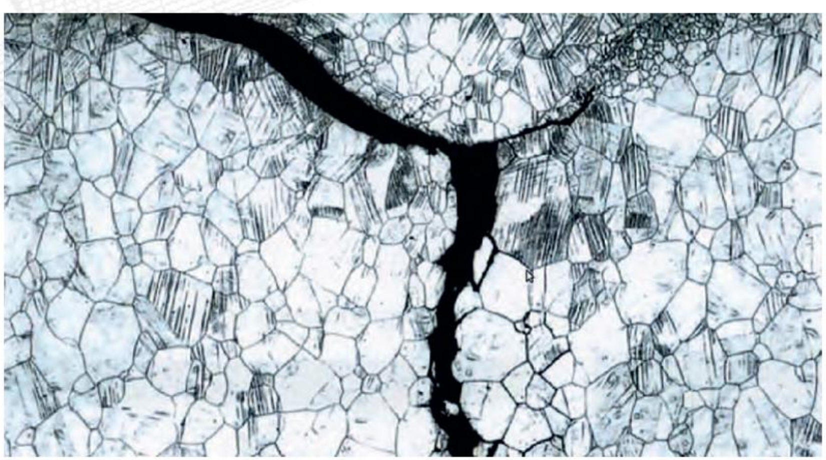


Figure 1: Fissure inter-granulaire due à l'IGSCC.

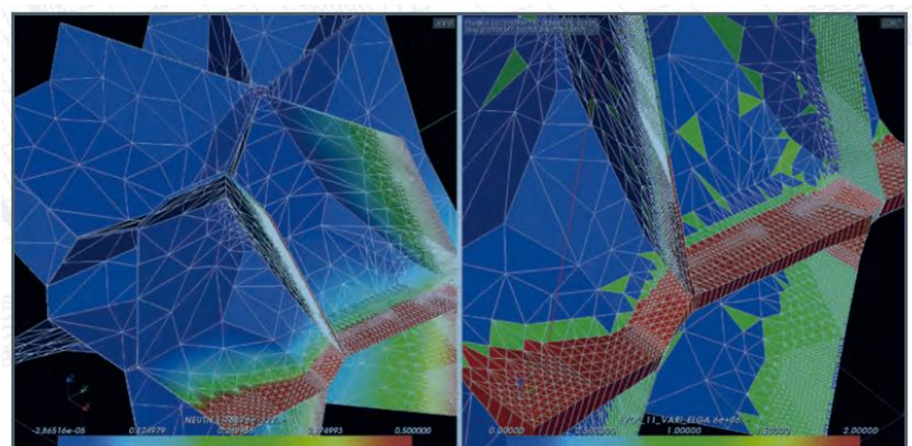


Figure 2: Joints de grains oxydés (en rouge, à gauche) et rompus (en rouge, à droite).

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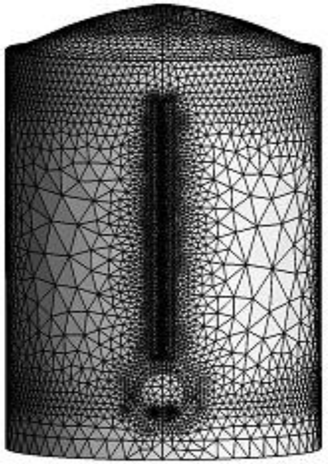
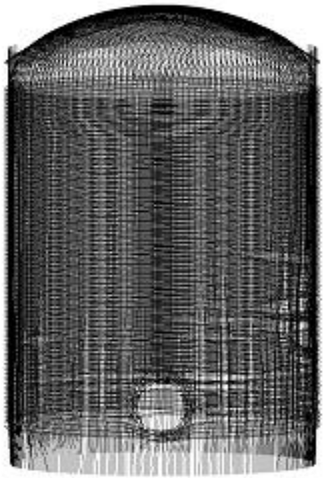
Specific features of mechanical models

- Small size compared to other physical domains being poorly conditioned
  - Using finite elements of different types (3D, shells, beams)
  - Using linear relationships between degrees of freedom imposed by the Lagrange multipliers
  - Using specific behavior laws that change the nature of being resolved equations (loss of ellipticity)
- Most frequently require the resolution of a linear system
- Typical example: reactor building model
  - Mixing 3D, shells and beams
  - Many Lagrange multipliers (about 30% of DDL)
  - Current solvers are not suitable



Concrete



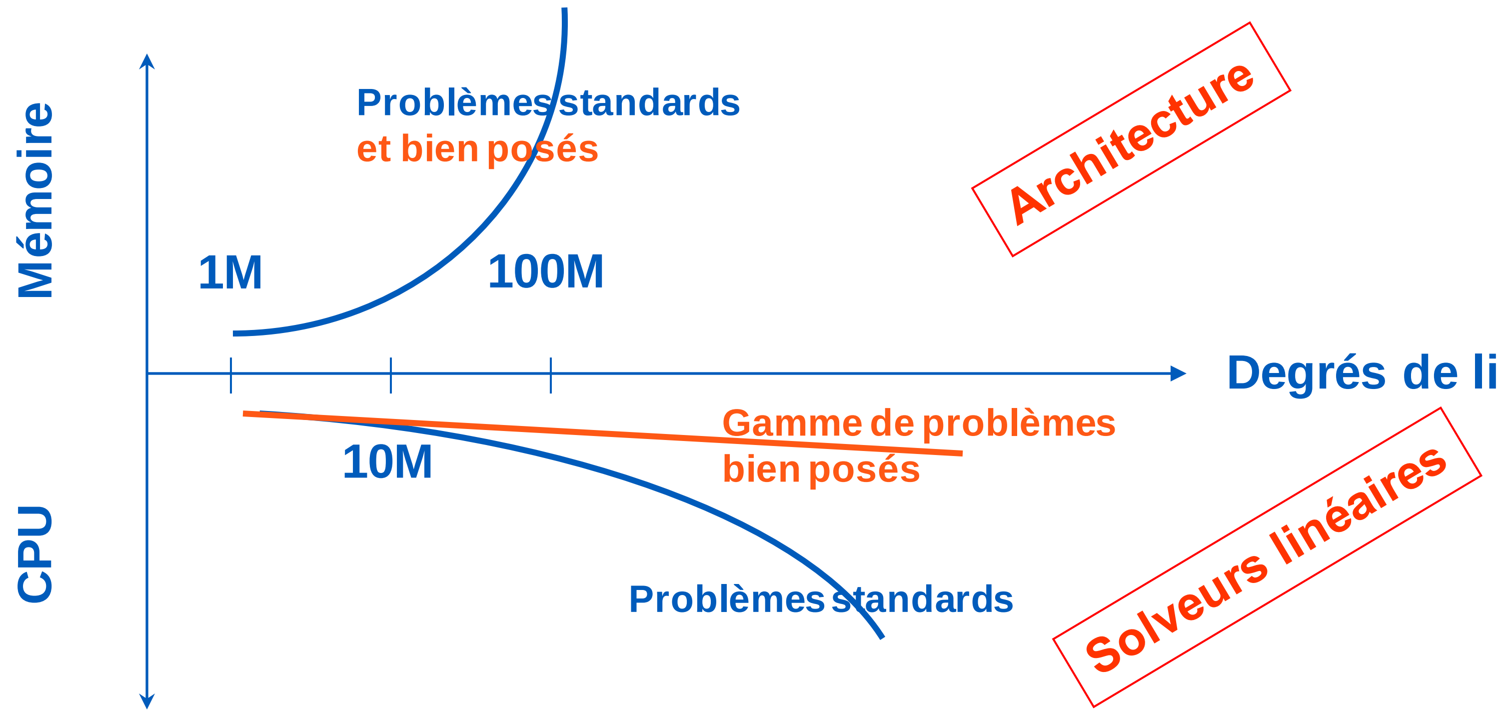
Pretension cables

Identified priorities

- Objectives
  - 1: Reliability
    - Essential for the intended applications
  - 2: Robustness
    - Imposed by the population of users, who are mechanical engineers
  - 3: Performance
    - Important to ensure a return time consistent with the time of the industrial user and allow to move a scale in size models so as to refine the description of the physical and earn margins
- Development actions
  - Distribution of data structures
  - Using algebraic scalable linear solvers
    - Multigrids
    - Hybridization of direct and iterative methods

State of the art of HPC in structural mechanics

- Significant return time but less critical than the memory consumption
  - Better memory distribution allows moreover to win on both fronts



- EDF supercomputers: more and more cores, less and less memory by core
  - Risk of non-suitability of the code available architectures

Situation of Code_Aster before starting PAMSIM

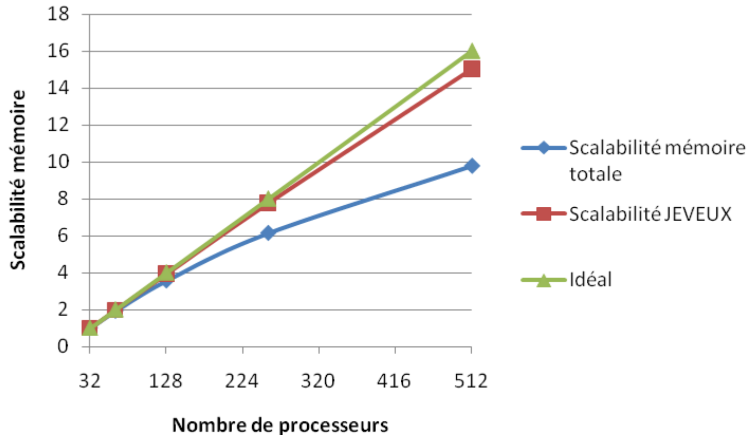
- Two assessments were performed in 2008 and 2012 on the parallel features
  - Parallel performance has improved since 2008 as evidenced by six industrial studies
  - Code_Aster is now a parallelized computation code but do not effectively takes advantage of massevely parallel machines (typically, the efficiency collapses beyond 100 processors)
  - The assessment is shared by a study conducted in 2012 by SGI on industrial codes

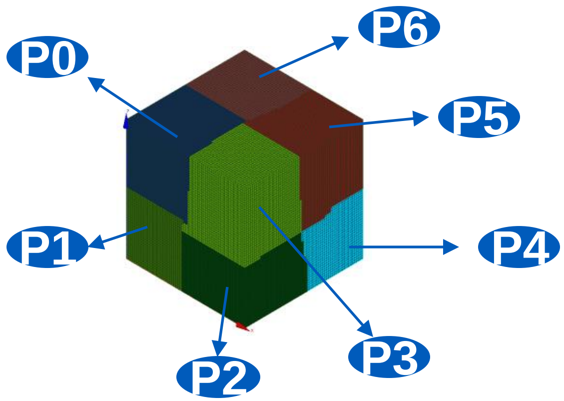
Workload	Applications	Scaling: # threads
CFD	Fluent, StarCCM+, CFX, OpenFOAM, Powerflow	2048
Comp. Electromagnetic	FEKO, FMSLIB, HMSS	256
Reservoir	Eclipse,Intersect, VIP, Nexus	512
Seismic	ProMAX, EPOS, Geocluster	1-1024
Structural Mechanics (Implicit)	ABAQUS, ANSYS Nastran,	1-32
Structural Mechanics (Explicit)	LS-Dyna, Pam-Crash, Radioss	512

Source : SGI (2012)

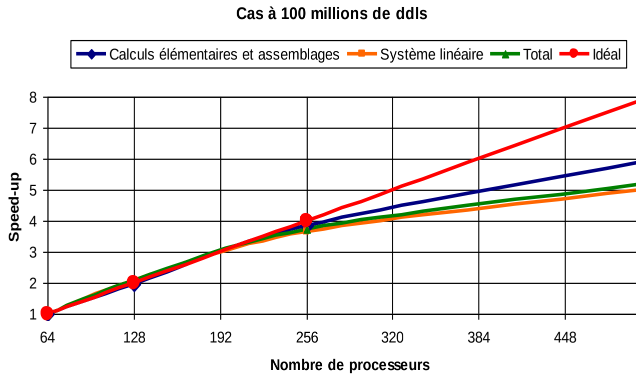
Conclusions of a feasibility study

- A significant increase in parallel performance in structural mechanics is possible
  - Division of domains for memory distribution and parallelism of elementary computations





  - Parallel linear solver for the distribution of CPU cost (best performance obtained with multi-grid solvers)



Launching of the PAMSIM project

- Submitted to the call « *Calcul Intensif et Simulation Numérique N°2* » launched in 2015 by BPI France in the framework of PIA

- Objective
  - develop and make available to economic actors a massively parallel version, robust and validated, of the EDF reference code for simulation in mechanics, Code_Aster.

- A consortium of 7 partners :
  - EDF R&D
  - NECS, ALNEOS, PHIMECA
  - LMT Cachan
  - CERFACS, IFPEN

- From 2016 to 2018

- A total estimate cost of 2,89 M€

And during the construction of the project ...

BENCH MARK

April 2015 issue . . .

NAFEMS Benchmark Challenge

Survey of Computing Platforms for Engineering Simulation

NAFEMS World Congress

Flammability Risks Through Dispersion Modelling

Concrete Material Modelling

THE INTERNATIONAL MAGAZINE FOR ENGINEERING DESIGNERS & ANALYSTS FROM **NAFEMS**

Results for implicit FEM

- Maximum number of ddl
  - < 100k : ~ 12 %
  - 100k - 10M : ~ 54 %
  - 10M - 100M : ~ 20 %
  - 100M - 1B : ~ 14 %
  - > 1B : 0 %

  PAMSIM objective (10M - 100M and 100M - 1B)

- Number of used cores
  - 1 - 8 : ~ 34 %
  - 9 - 64 : ~ 31 %
  - 65 - 1024 : ~ 29 %
  - 1024 : ~ 6 %

  PAMSIM objective (65 - 1024 and 1024)

And during the construction of the project ...

- Barrier to uptake according to the survey :

1) Purchase cost of the hardware and maintenance

2) Prohibitive licence cost of the HPC software

- Code_Aster is a free open source software

3) Poor performance of the software

- Objective of PAMSIM : up to 1024 cores for industrial studies

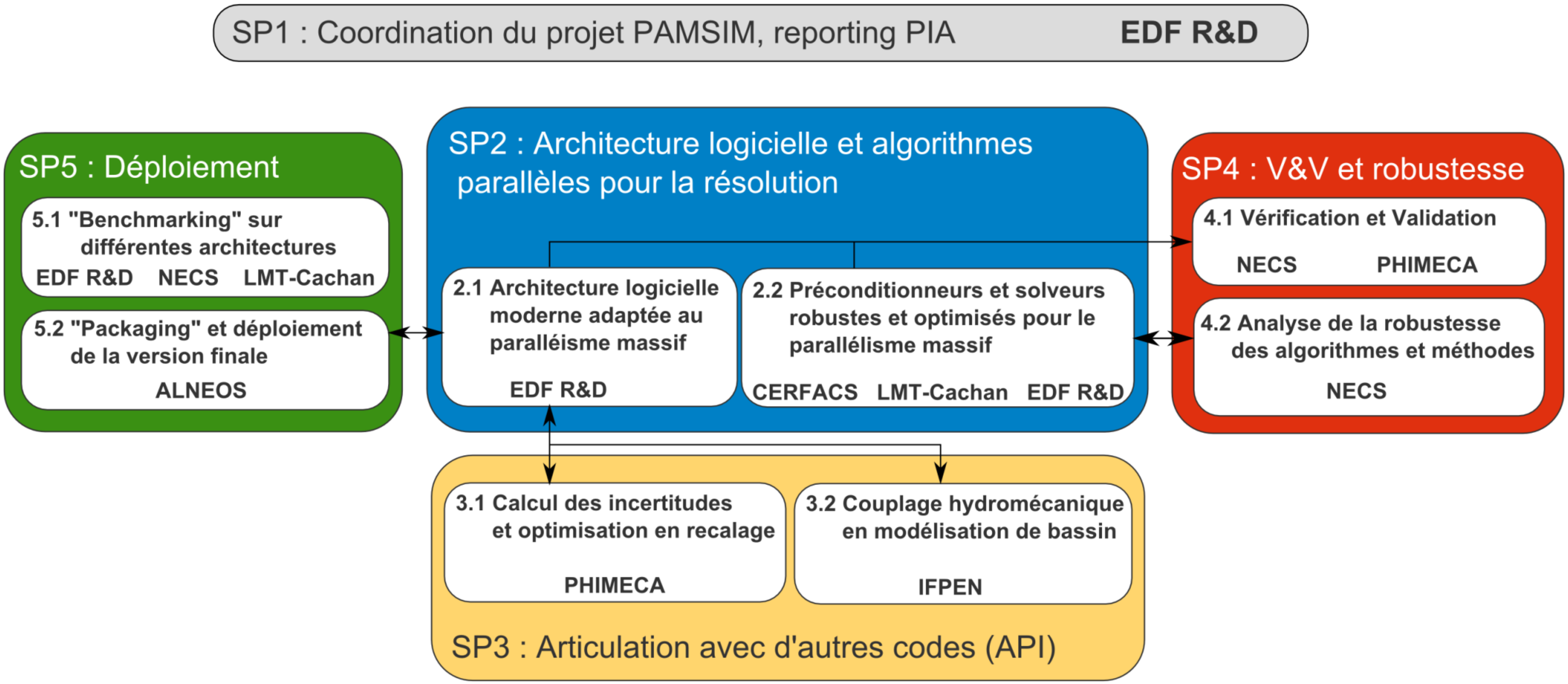
4) Difficulty in managing increasing volume of simulation date

- another PIA project launched by EDF R&D : AVIDO

5) Difficulty in automating workflow between different software

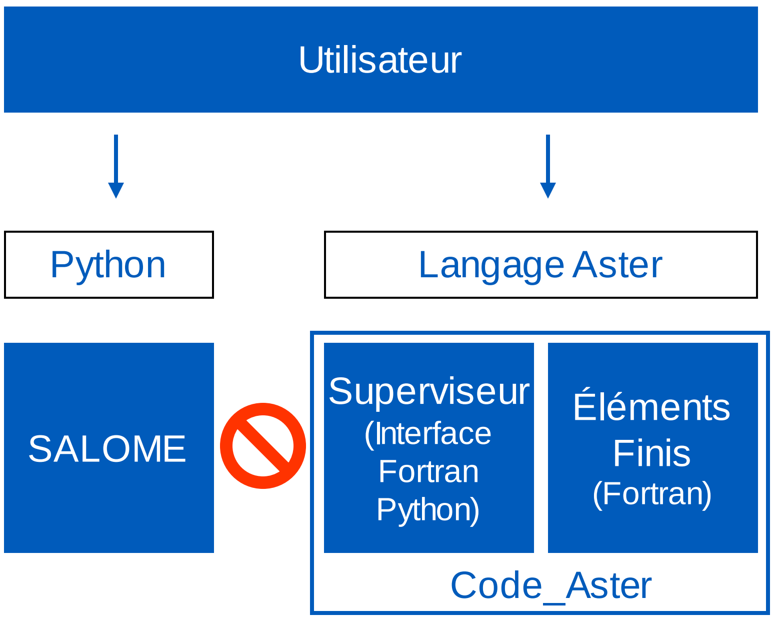
- Coupling possibility of code_aster with other codes foreseen by PAMSIM

PAMSIM Project organisation

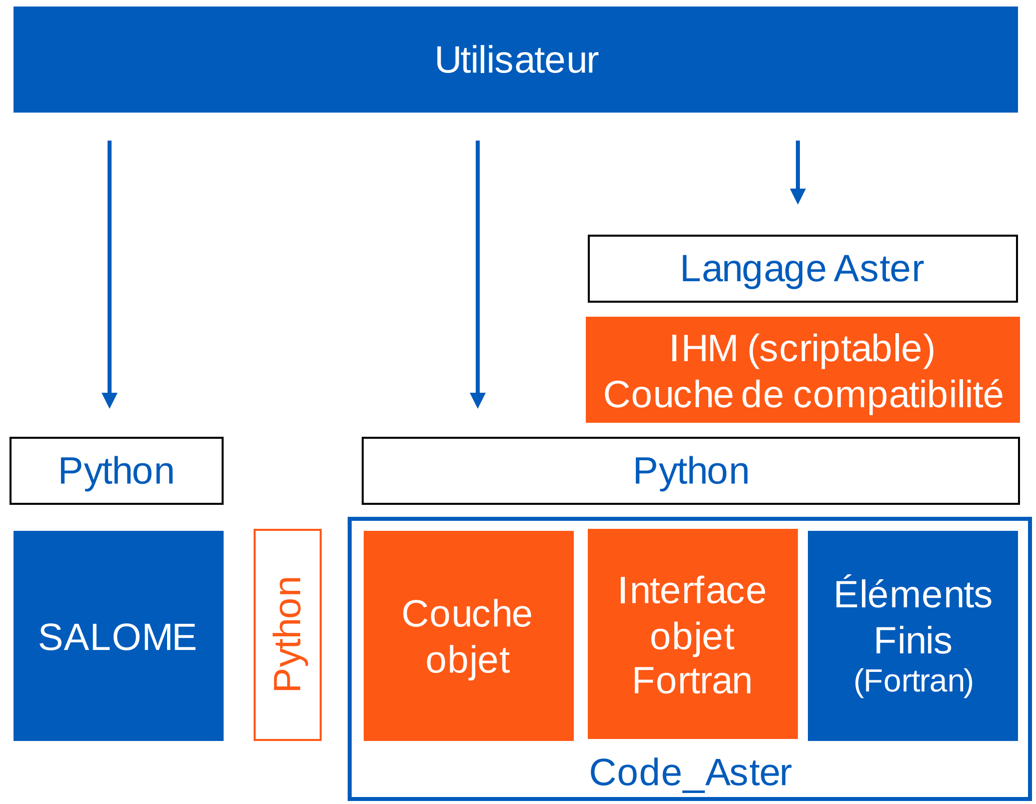


Transition to a modern architecture

Now



Proposed



From a moderate to a massive parallelism

- Current parallel features

Direct solver MUMPS with shared memory parallelism

Good scalability up to 32 processors

Excellent robusteness

Iterative solvers (PETSc library)

Punctual distribution of memory

Lack of robustness without an appropriate booster

- Future parallel features

Total distribution of memory over the calculation domain

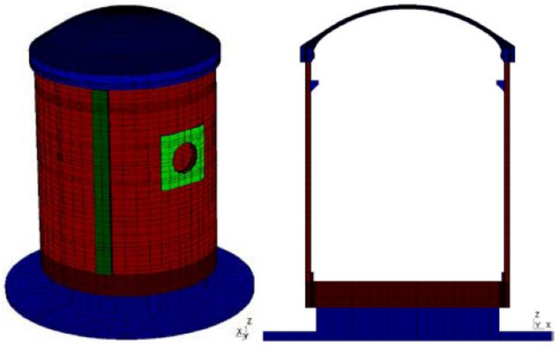
Scalability goal of up to 1024 proc

Satisfying the 3 objectifs:

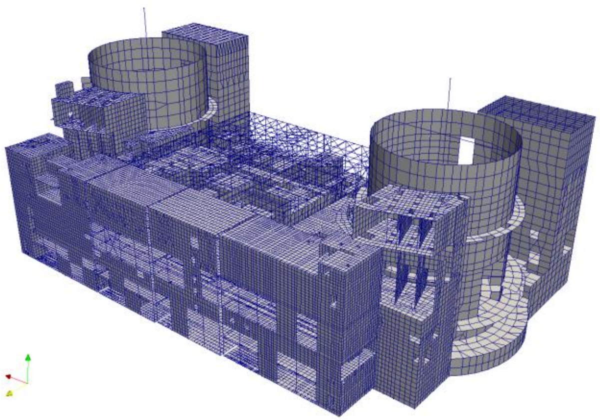
- reliability
- robusteness
- performance (lower CPU time and memory per proc)

Target EDF applications

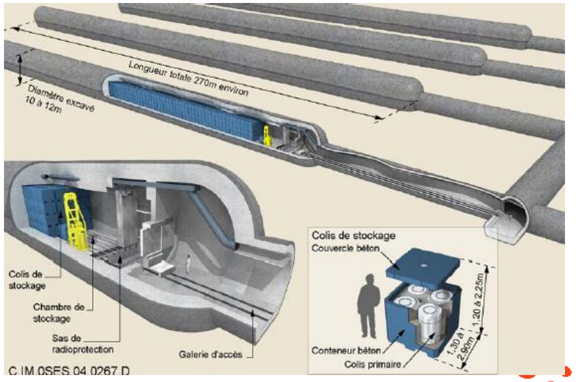
- Civil Engineering (VERCORS model)
  - 2015: simulation of damage to a containment portion (smaller than the experimental tests)
  - 2019 (preparation of the final test on the model): simulation of damage on the entire containment, several million degrees of freedom needed for each modelized crack



- Earthquake
  - 2015: simulation of damage to a single building under earthquake
  - 2020: several buildings with realistic SSI



- Nuclear residual storage
  - 2015: 3D simulation of excavation with consideration of material nonlinearities
  - 2019: 3D simulation of excavation of two perpendicular galleries (crossover) with structural details and nonlinearities



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Conclusions

- EDF launched in 2016, with six other partners, the development of a massively parallel version of Code_Aster in the PIA project PAMSIM

- The architecture of the code, its solvers and boosters will evolve to allow the launch of the calculations up to 1024 proc with optimized memory usage

- The future massively parallel Open Source version of Code_Aster will be available on HPC facilities (GENCI, HPCSpot, …)

Call for contributions

- If you would like to contribute to the verification and validation of future massively parallel version of Code_Aster, with an application on the simulation of materials, your help will be appreciated by the consortium PAMSIM !

- Contacts
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  - Hassan BERRO, Hassan.berro@edf.fr


Merci