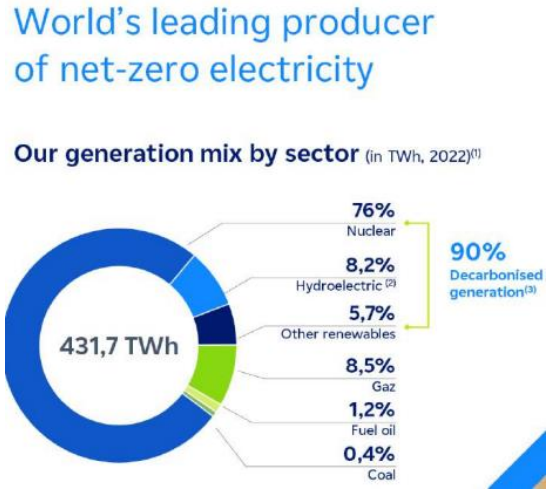
Feedback on the Use of MUMPS in EDF Codes

MUMPS User Days 2023

O.Boiteau (EDF R&D – Paris-Saclay Lab)

EDF at a Glance: an Environmentally-Conscious Multinational Electric Utility



40.3M

Customers worldwide(1)

171,490

Employees throughout the world

Our *raison d'être* is to build a net zero energy future with electricity and innovative solutions and services, to help save the planet and drive wellbeing and economic development.

Wherever our Group operates, we want to invent a new energy model to address the climate crisis: lower-carbon, more efficient, less of an impact on the environment and on people.

€ 649M

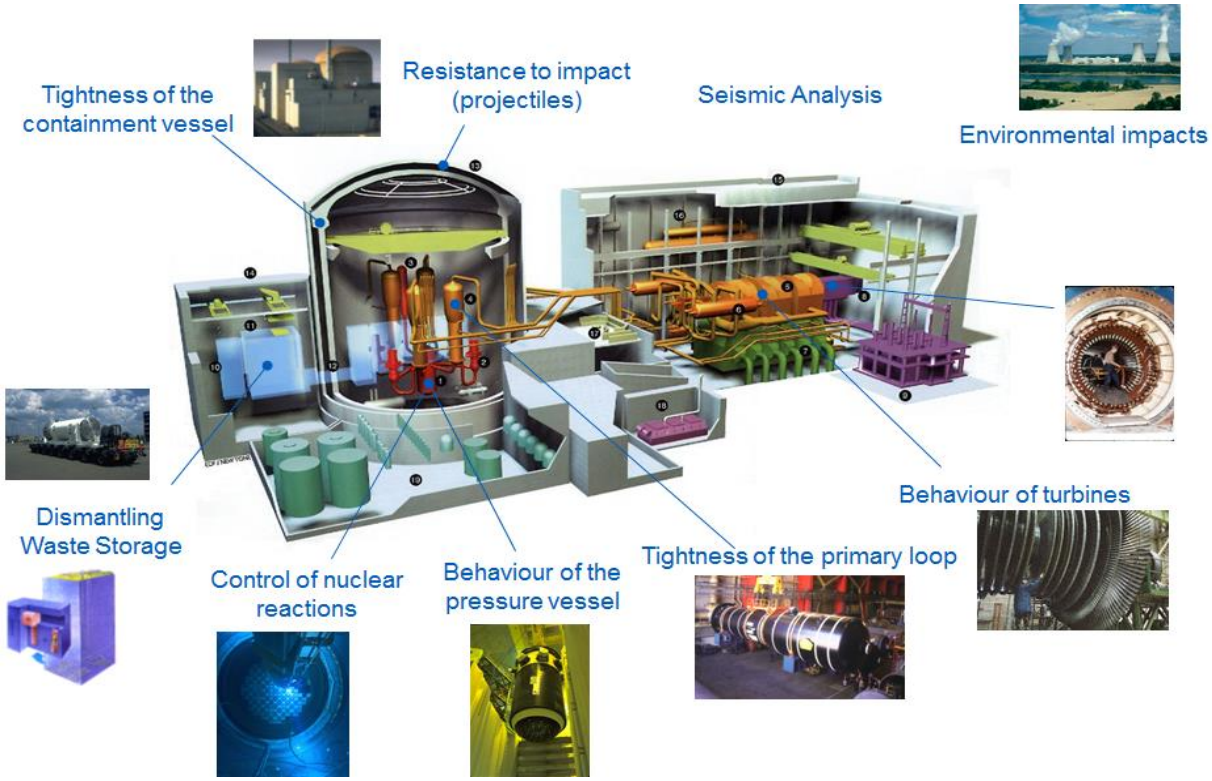
Research and development budget

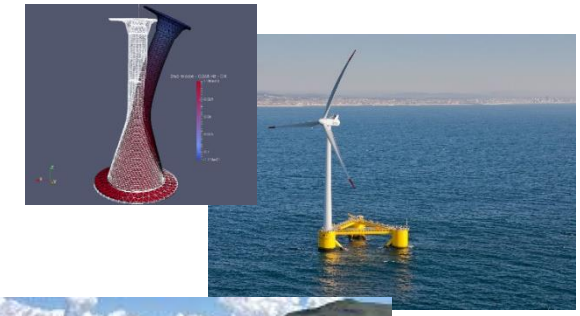
€ 143.5Bn

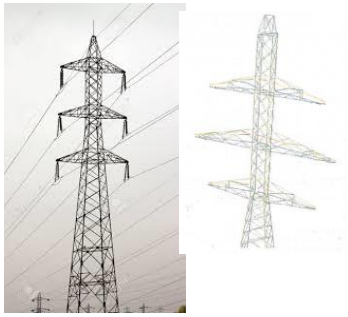
Sales

Numerical Simulation at EDF for What ?

- **In-house technical backing:** strong Engineering and R&D divisions
- **Physical testing/simulation** are key tools; often **in-house open source codes**







- Guarantee safety
- Improve performances/costs
- Maintain assets
- Face unexpected events
- Ageing issues

Great Benefit of the High Performance Computing (‘HPC’)

DataCenter NOE
Val de Rueil (France)

TOP 500 97ième

cluster
GAIA -2018
1200 nodes of **36** cores
RAM >192Go
3Pflops

TOP 500 67ième

cluster
CRONOS - 2021
2000 nodes of **48** cores
RAM >192/768Go
7Pflops

- ✓ Less simplifying assumptions,
- ✓ More information,
- ✓ More calculation scenarios,
- ✓ Take into account incertainties.

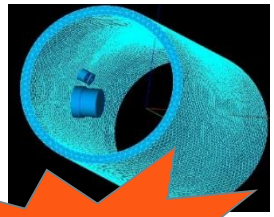
- Relevance of simulations,
- Studies more precise, closer to reality,
- Our codes > tools to support Engineering Division in adressing real-life industrial problems.

Computational Softwares used by Engineers, Experts and Researchers

- **All-purpose tools**
  - ✓ **Studies**: user-friendly, highly versatile…
  - ✓ **Researches:** continuous integration of new models/methods, prototyping…
  - ✓ **Quality Management:** robust/reliable, tested/qualified (V&V)…

Often in-house open-source codes,

not « black-box » closed sources ones



Electromagnetics, NDT code

CRESCENDO

code_Carmel

Material's structure research code

- **Research codes/Prototypes**

code_aster

Thermomechanical code

telemac

Free-Surface Flow solver

code.saturne

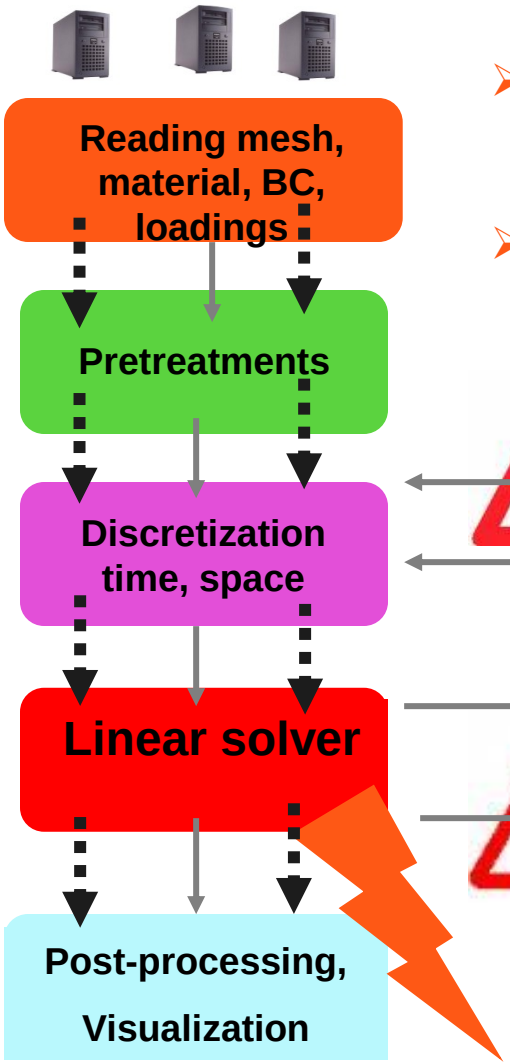
CFD

But also,

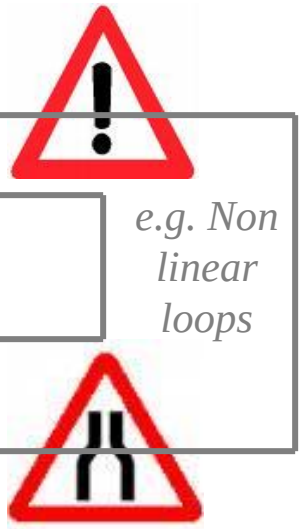
Neutronics for nuclear

Production management, trading…

A Common Requirement: HPC Linear Algebra Tools



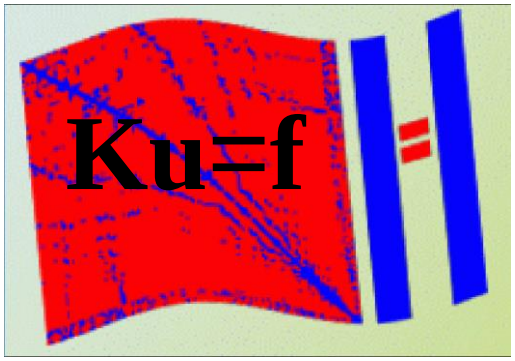
- Sparse linear solver: historically the first step that was improved. We selected the best algorithms, parallelized…
- **Performance AND robustness**, user-friendliness, versatility issues, numerical skills…



e.g. Non linear loops

e.g. Time loop

Bottleneck in CPU time and RAM peak



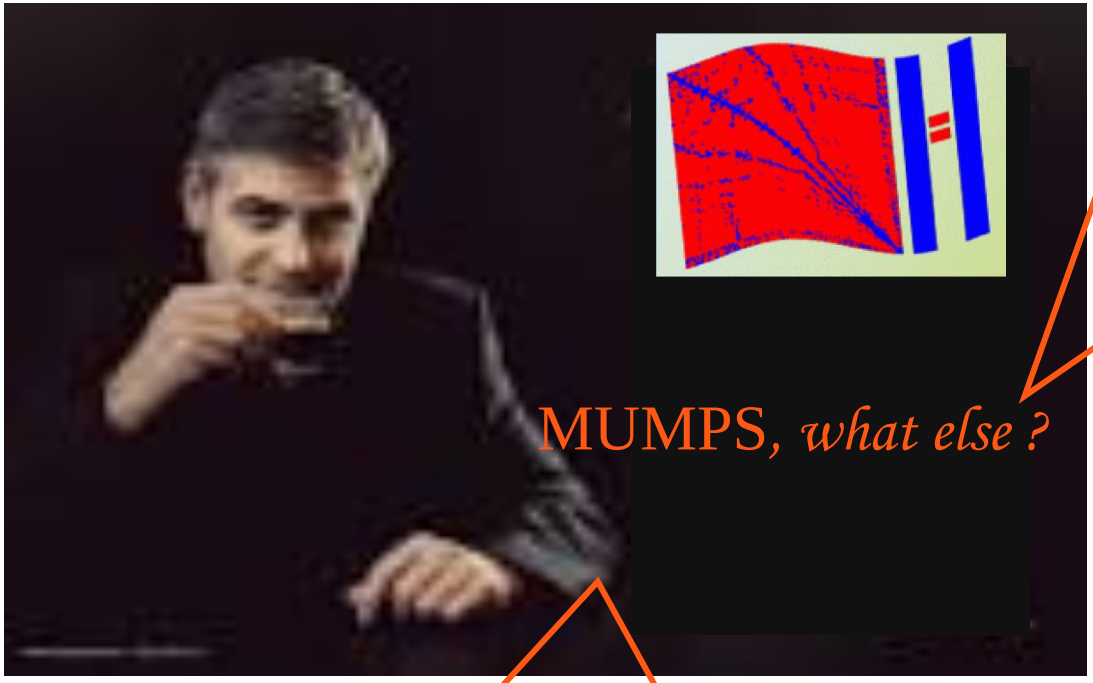
Components may be crucial for feasibility of a study

Our Codes' Best Friend : MUMPS package

CERFACS INP Inria ens de lyon université de BORDEAUX

Mumps Technologies

Solution of sparse systems of linear equations



18-year fruitful and win-win partnership

EDF>MUMPS: ***(EDF Project P_QUASI)***

- Functional/numerical feedback,
- Bug report/industrial validation in our QA in-house codes.
- Support for (e.g. PhD M.Gerest) developments/researchs

MUMPS>EDF:

- Numerical expertise, software patches…
- Tips and tricks.

Best-in-class tool according to the criteria:

Robustness x Performance x Versatility x User-friendliness

ALTAIR AIRBUS Ansys INES

EDF esi get it right® HEXAGON MICHELIN

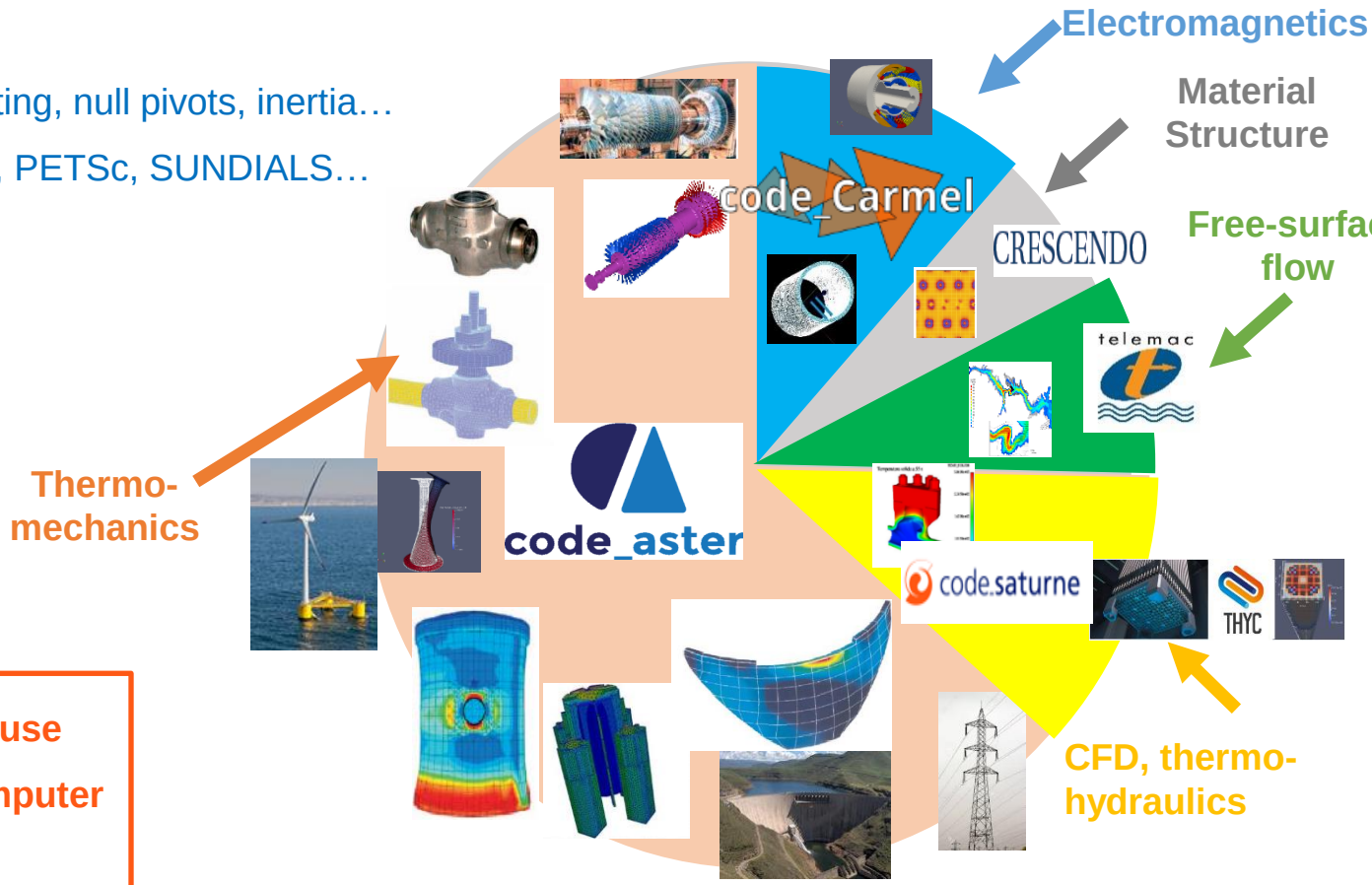
SAFRAN SIEMENS TotalEnergies

EDF

Uses of MUMPS in EDF Codes

- Real indefinite poorly conditioned matrix, sometimes singular: **1000 dof <Size <500 million dof ！**
- **Crucial steps:** analysis/factorization (direct solver), solve (preconditioner/eigenvalue/ODE)
- **Performance:** MPI/OpenMP (CPU), BLR, mixed precision…

- **Numerical skills:** pivoting, null pivots, inertia…
- Coupled with ARPACK, PETSc, SUNDIALS…



Intensive industrial use

Multicore desktop computer and cluster

Significant Impact on Studies

- **FEASIBILITY: make them possible !**
  - ✓ Too slow: acceptable computation time,
  - ✓ Too much RAM consumption: mutualize RAM of cluster nodes.

- **ACCELERATOR: make them easier, secure their computation steps**
  - ✓ Speed-up X10, X100 compared to previous options: sequential native-solvers (often not questionned for decades)…
  - ✓ Computation times: **hours/days** instead of **days/weeks**.

- **CLOSER TO REAL-LIFE: improve quality**
  - ✓ Finer mesh, more precise loading/BC…
  - ✓ More elaborate: parametric study, sensitivity study, parameter estimation, data assimilation…

- **INNOVATIVE APPROACHES: try new kind of analysis**

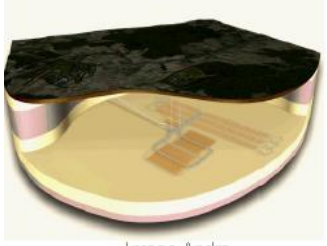
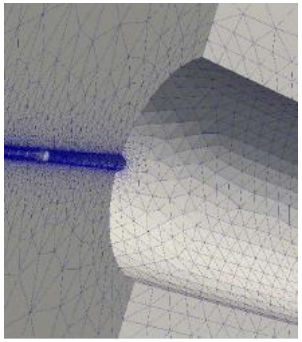


Image Andra

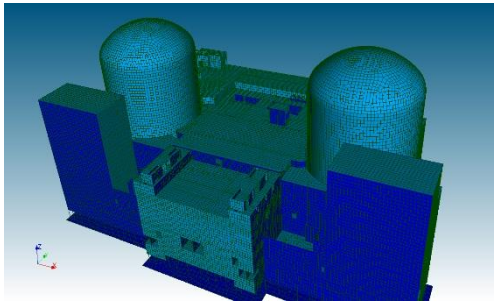
EURAD project:

Porous media

#dof=5,2M



4 nodes
30 min/t (2018-EOLE)
9 min/t (2022-GAIA)
PETSc + MUMPS preconditioner



Seismic analysis
Post Fukushima analysis
Huge eigenmode computation

#dof=1,5M
#eigenmode=3481

code_aster

FEASIBILITY

Dismantling
Waste
Storage

Seismic Analysis

Integrity
Graphite Cores

Without

FAILURE

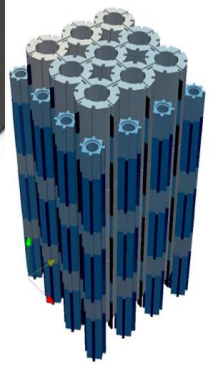
Moisture
Separator-Reheater

40 nodes EOLE: 40MPI x 28 OpenMP
Computation time < **30min**
Spectrum slicing + ARPACK + MUMPS
direct solver

Maintenance of nuclear power plant
Constrainted computation time < 2 weeks

#dof=7,7M à 20M

2 nodes Aster5: 8 MPI x 6 OpenMP
Computation time = **3 days**
MUMPS direct solver



EDF Energy CBNA model:

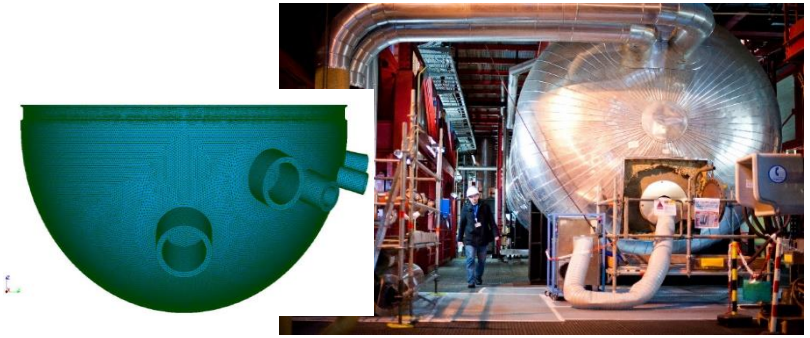
#time steps=100

#contact=250,000 !!!

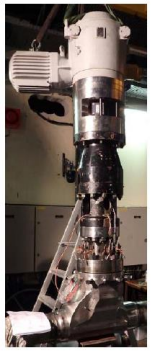
#dof=3,6M

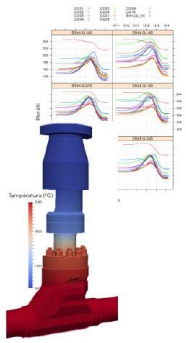
2 nodes EOLE: 16 MPI x 3 OpenMP
Computation time = **4 days**
MUMPS direct solver

EDF



STUDY ACCELERATOR





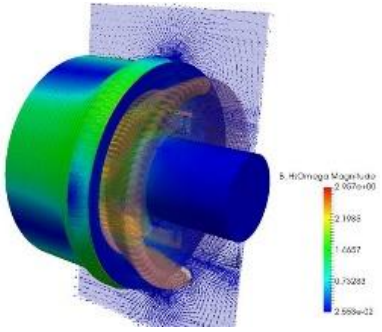
code_aster

Industrial valves/actuators

Thermal-shock, plasticity contact, links beetween mesh parts: **numerically difficult**

#dof=2M

2 nodes Aster5: 8 MPI x 6 OpenMP
days instead of **weeks**
MUMPS direct solver



code_Carmel

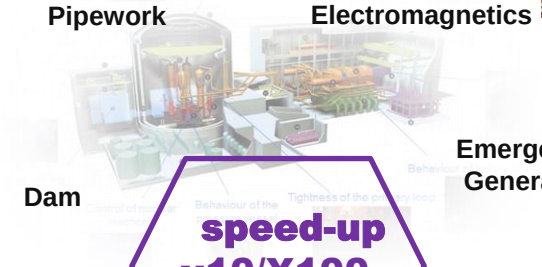
Generator/ alternator/ transformer issues

#dof=several millions

8 nodes EOLE: 24 MPI x 4 OpenMP
One week instead of months
MUMPS direct solver

Pipework

Electromagnetics



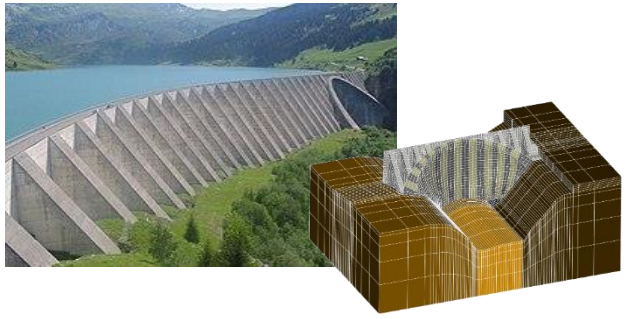
Dam

Emergency Generator

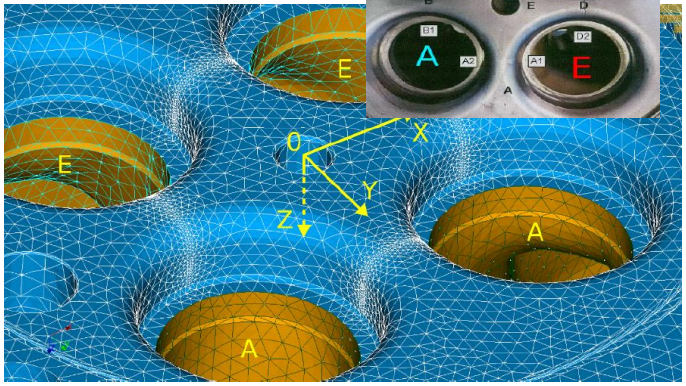
speed-up x10/X100...

code_aster

Seismic re-assessment
Non linear, FE mixing
#dof = 0,5M
#dt = thousands



4 nodes Aster5: 48 MPI x 1 OpenMP
3 days instead of **one month**
MUMPS direct solver



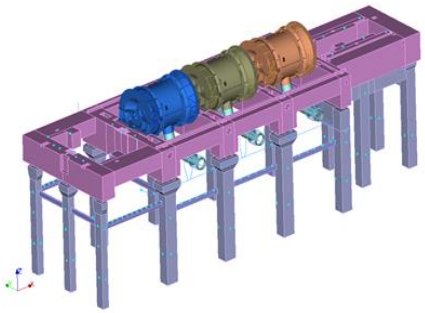
Cylinder heads of diesel engine
Cracking study for French Nuclear Regulatory Authorities

#dof=2,5M

EDF

1 nodes EOLE
Less than a day instead of **weeks**
MUMPS direct solver or preconditioner of FGMRES (PETSc)

code_aster



4 nodes EOLE
3.5min instead of **2h22min**
Spectrum slicing+ ARPACK+MUMPS direct solver

9 nodes

2,5 days (2018-EOLE)

8 hours (2022-GAIA)

MUMPS direct solver

Turbine of nuclear plant
Eigenmode computation
Need of more precise simulation: 3D instead of 1D
Computation time constraint (because of parameter fitting): ~ minute !

#dof=2,4M in 3D instead of 0,1M in 1D

INNOVATIVE APPROACHES

Turbogenerator

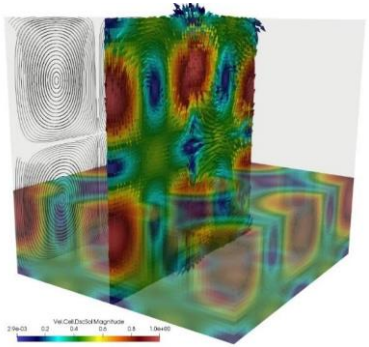
Tightness of the containment vessel

CFD/primary loop

Innovation

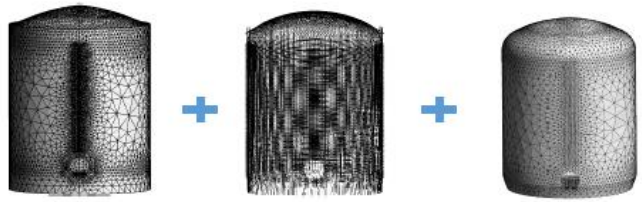
!!! #dof= 495 M !!!
Our record size for MUMPS
Preconditioner of MINRES (BLR+single)

MUMPS works and
could be competitive vs multigrid approach



FE mixing: concrete and pre-tension cables
numerically difficult

#dof=2,6M



3D stationary Stokes problem: Taylor-Green-vortices
Compatible Discrete Operator (CDO) schemes
Velocity linear systems inside Uzawa or Golub-Kahan algorithms

Conclusions and Perspectives (1/2)

- **MUMPS, a 'best-in-class' linear sparse solver:**
  - ✓ Very effective and constantly being improved, without deteriorating its basis**: robustness, versatility….**
  - ✓ Concentrate of innovations,
  - ✓ Industrial product that is now a reference.

- **Heavy use of MUMPS in EDF's *in-house* codes**

MUMPS/HPC: tools for research and engineering

- ✓ *Standard study*: very useful (time-accelerator),
- ✓ *Large study*: mandatory (feasibility, closer to real life),
- ✓ *Innovative study*: make it happen.

- **But also links « in-house code » - « linear algebra package » needs steady adjustments.**

Often, questioning about external libraries induces improvment in the caller code.

→ Progressive HPC rewriting of old legacy codes

Conclusions and Perspectives (2/2)

- **Work in progress in MUMPS:**
  - ✓BLR,
  - ✓Mixed precision (BLR, IR…),
  - ✓GPU,
  - ✓Ordering (SCOTCH),
  - ✓Algebraic iterative linear solver….

- **18-year fruitful and win-win partnership EDF-MUMPS,**
  - Thanks to the utmost professionalism/expertise of the MUMPS team
  - And its kindness/availability/perenity

MAKE

DIRECT SOLVER

GREAT AGAIN!

Thank you !