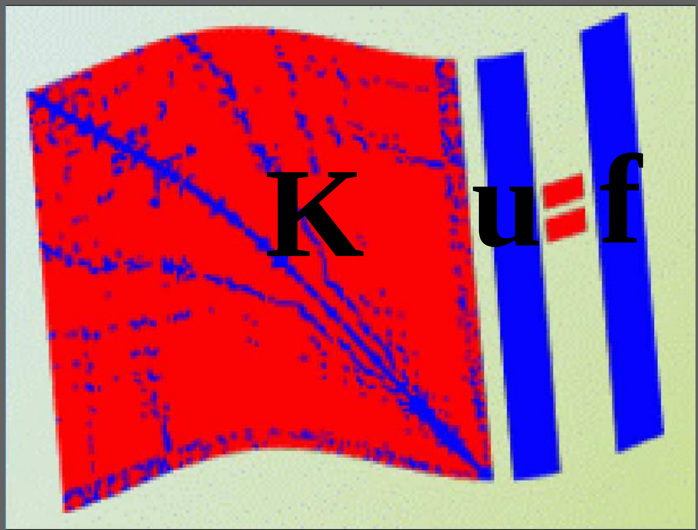


Thermomechanical and hydraulic industrial simulations using MUMPS at EDF

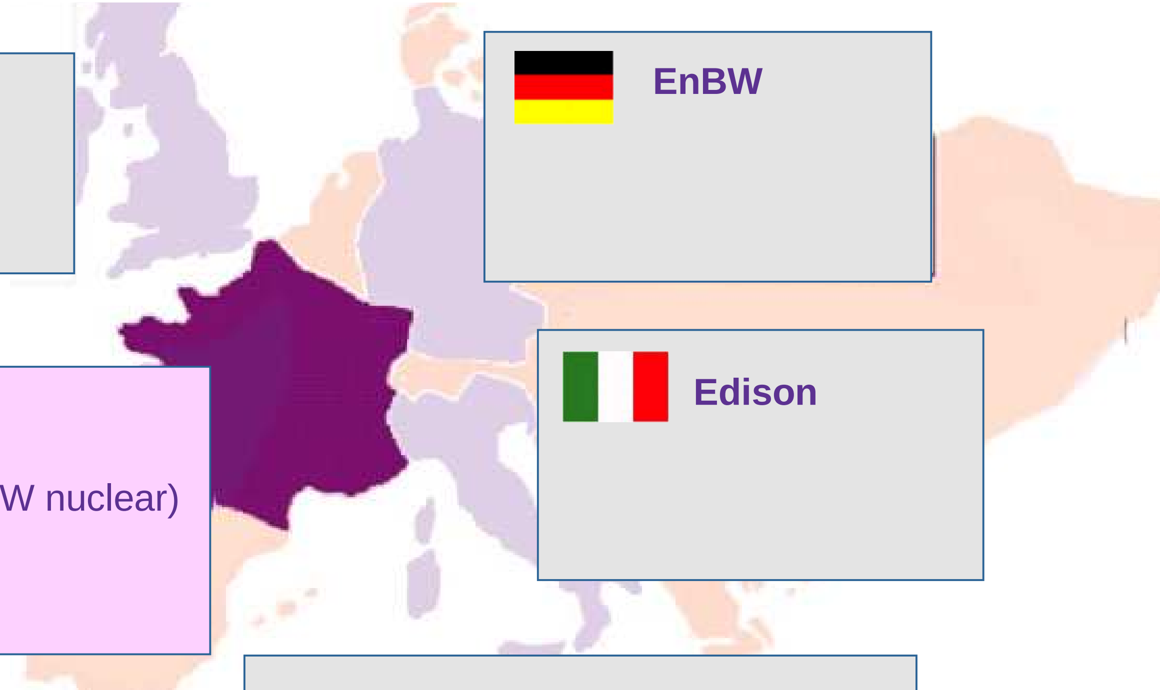
MUMPS User group meeting

15 april 2010

O.Boiteau, C.Denis, F.Zaoui

MUltifrontal Massively Parallel sparse direct Solver

1a. EDF Group: a European Electricity Utility with strong R&D involvment



EDF Energy

EnBW

EDF

Capacity: 101 GW (63 GW nuclear)
Customers: 28 Million
Networks: 1 340 000 km
Gas: 3 Gm^3

Edison

Sales: €64.3 billion
Global customer base: 38,1 million
Employees worldwide: 161,000
Installed capacity: 128.2 GW
R&D: €1 million/day

1b. Operation, Maintenance & Optimization of complex systems at EDF

Software Quality Plan
(requirements of the Nuclear
Structures Safety Authority)

Permanent objectives

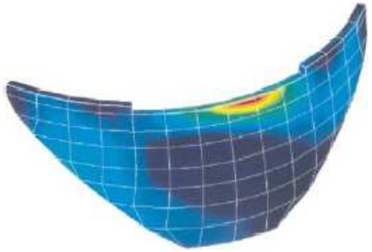
- guarantee safety,
- improve performances/costs,
- maintain assets.

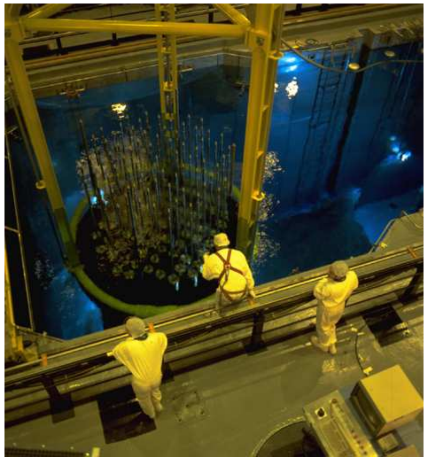
Changing operating conditions

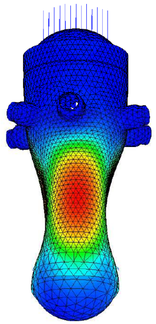
- face unexpected events, ageing issues, maintenance,
- improve performance through new technologies, new operating modes and system-wide optimization,
- adapt to evolving set of rules (safety, environment, regulatory).

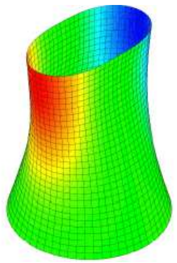
In-house technical backing

- expertise: strong Engineering and R&D Divisions,
- physical testing and simulation are key tools from the outset.





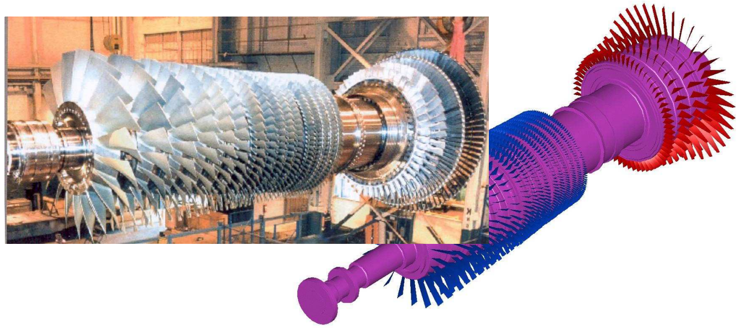


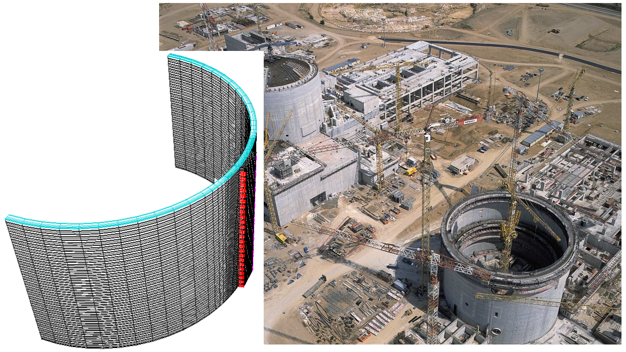


1c. Workflow of EDF physical simulation codes

eDF R&D

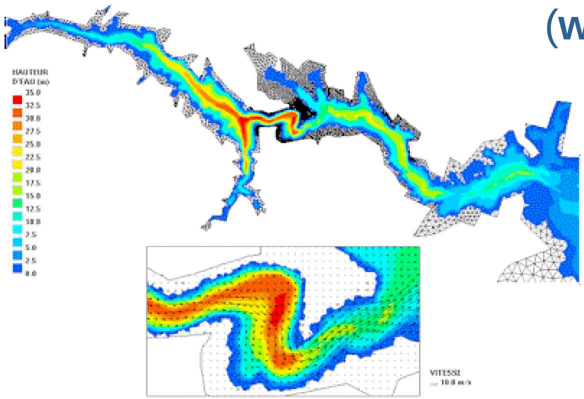
1d. Use of MUMPS in two EDF physical simulation codes



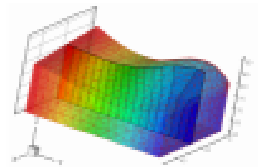


Code_Aster: A finite element code for analysis of structures and thermomechanics studies and researchs (**www.code-aster.org**).

TELEMAC system: a group of numerical modeling softwares for free surface water, sedimentology, waves, water quality, underground flows (**www.telemacsystem.com**) …



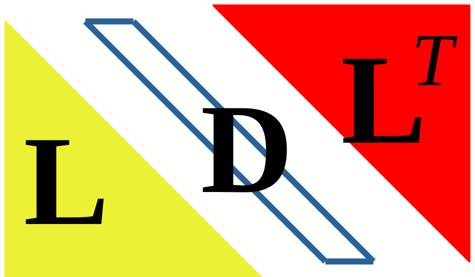
telemac



EDF R&D

2a. The bootleneck is the linear system step

- Direct methods versus iterative ones



$$Lw = f$$

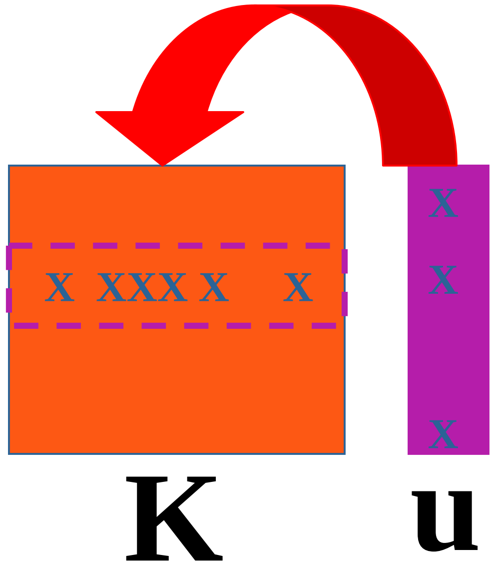
$$Dv = w$$

$$L^{T}u = v$$

$$Ku = f$$

Aster keyword METHODE

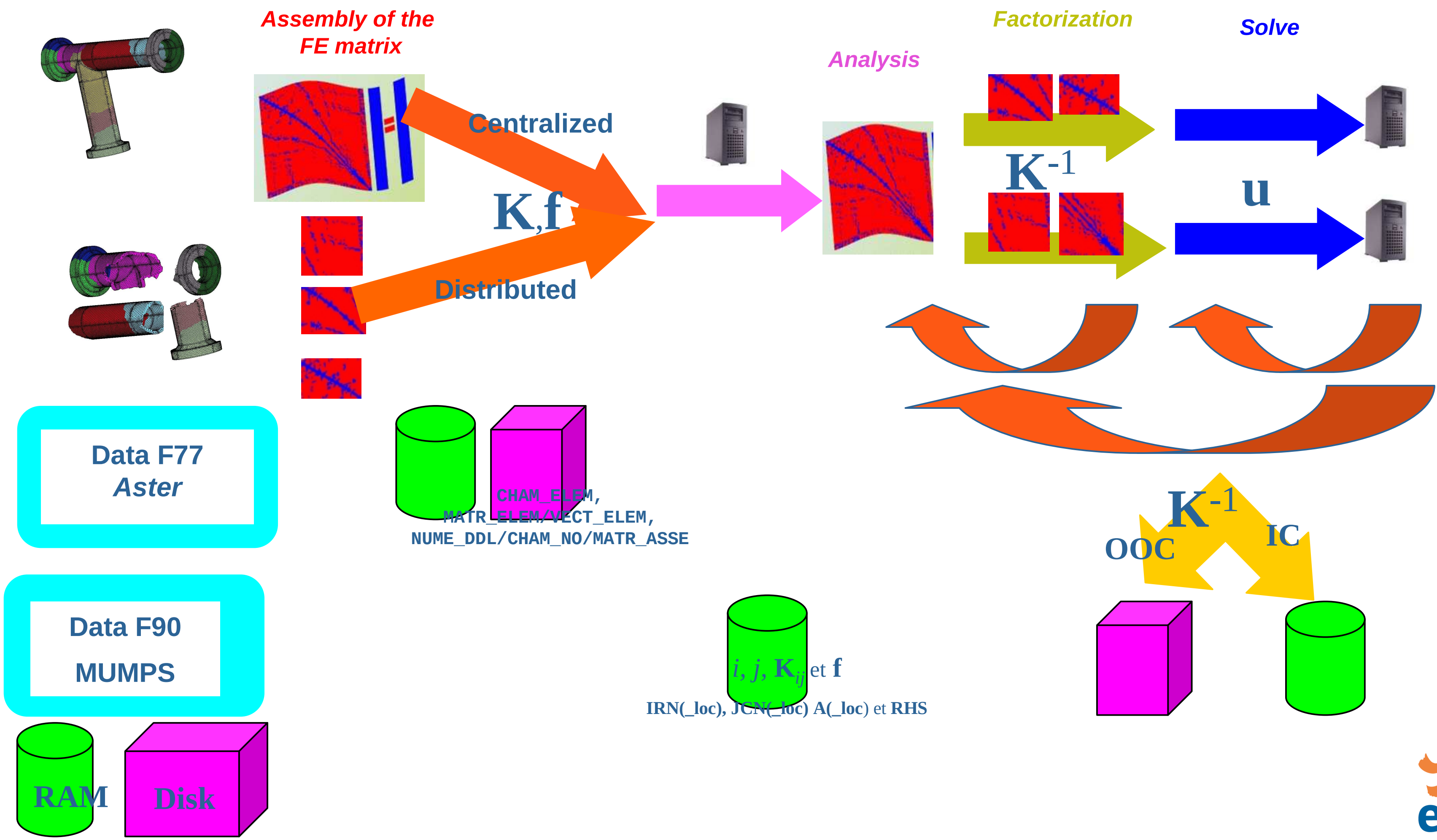
LDLT	GCPC
MUMPS	PETSC
MULT_FRONT	FETI



2b. *Code_Aster* & MUMPS (1/3)
A story of sparse linear system !

Flexibility/Efficiency,
Distributed parallelism,
Out-of-core capabilty

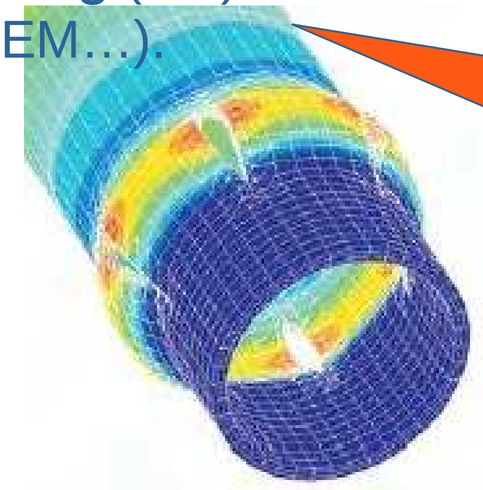
- (Usually) General real symmetric < 5 millions dof;



2b. *Code_Aster* & MUMPS (2/3)
A story of sparse linear system !

- (Often) **Bad conditionning** (10^8) and indefinite matrix (mixte FE, Lagrange multipliers, X-FEM…).

__X-FEM on a pipe__: enriching the sane mesh with special FE to simulate multi-cracking.



Numerical robustness, Pivoting/scaling strategies, Error analysis and iterative refinement.

- Detection of **singular matrice** (lacks/excess of boundary conditions, eigenvalue problem, null space analysis…).

Zero-pivot detection option

- (Sometimes) Unsymmetric, SDP, complex arithmetic, reuse of the analysis phase for several solves.

Full range of possibilities

2b. *Code_Aster* & MUMPS (3/3)
A story of sparse linear system !

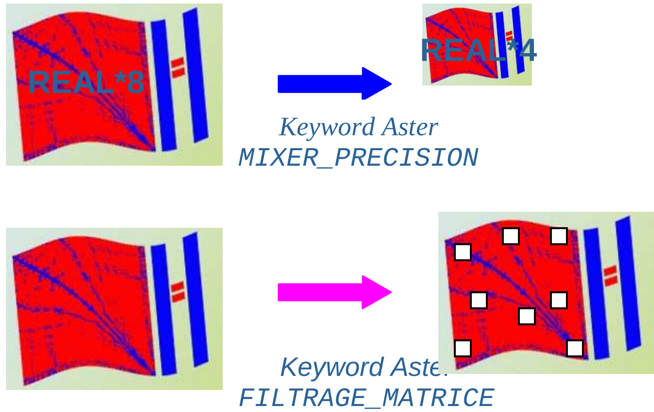
Matrix, RHS *Aster*

Matrix, RHS MUMPS

Solver Tool-kit

➢Mixte-precision strategies:

- Direct solver in non linear analysis with Newton-like algorithm,
- Krylov solver (linear or not): coarse/cheap/ robust preconditioner.



Non-linear analysis of a device holder :

N=0.2M, NNZ=6.5M, Facto=103 M, cond=2.10^{6}

Direct solver: RAM/CPU improvments 50% / 10%

Krylov preconditionner: 50% / 78%

➢Various kinds of linear systems:

- One-shot resolution,
- (Often) **Multiples right-hand sides** (Newton with periodic reactualization of the tangent matrix…),
- (Sometimes) Concurrent resolutions (Schur complement-like solves in contact-friction problems…).

Flexibility

EDF R&D

2c. Feedbacks of the software integration/use

- More than 100 *Aster* test-cases (seq. and //) using MUMPS, dozens of MUMPS parameters available to the Aster'User.

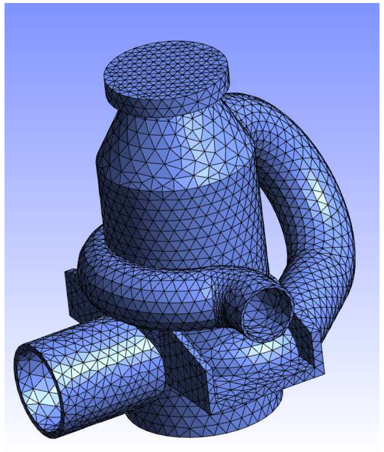
- **Steady software workings in the Aster/MUMPS'** links: bug tracking, optimization, upgrade, user training…

Often questioning/debugging about exterior librairies induce improvment in the caller code (data workflow…)

Year	2006	2007	2008	**2009**
# Works about *Code_Aster*/MUMPS	28	36	56	**103**

- Daily use throught *Code_Aster* at EDF R&D/Engineering

2d. Some results (1/3)



N=0.8 M

nnz=4,5 M / K^{fact}=372M

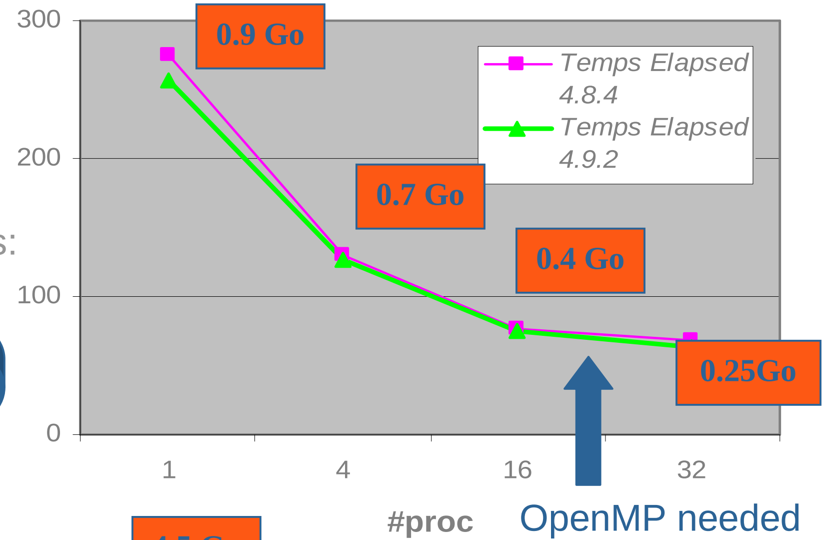
(77%) **Th. speed-up** 4/16/32 procs:

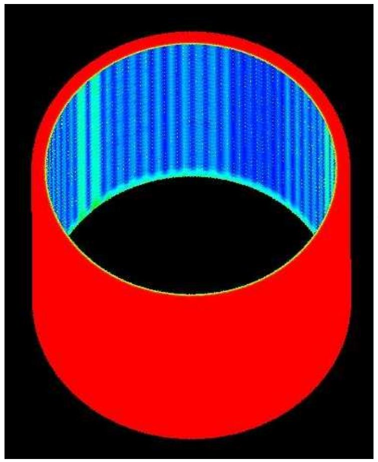
2.4/ 3.6/ 3.9

Real speed-up 4/16/32 procs:

2.1/2.0 3.6/3.6 3.9/3.9

Good Speed-ups





N=0.8 M

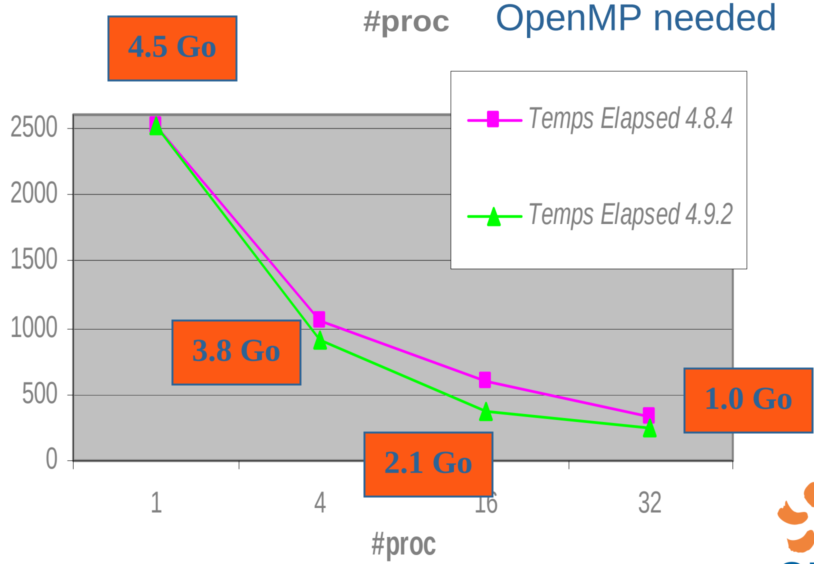
nnz=71 M / K^{fact}=1900M

(95%) **Th. speed-up** 4/16/32 procs:

3.5/ 9.1/ 12.5

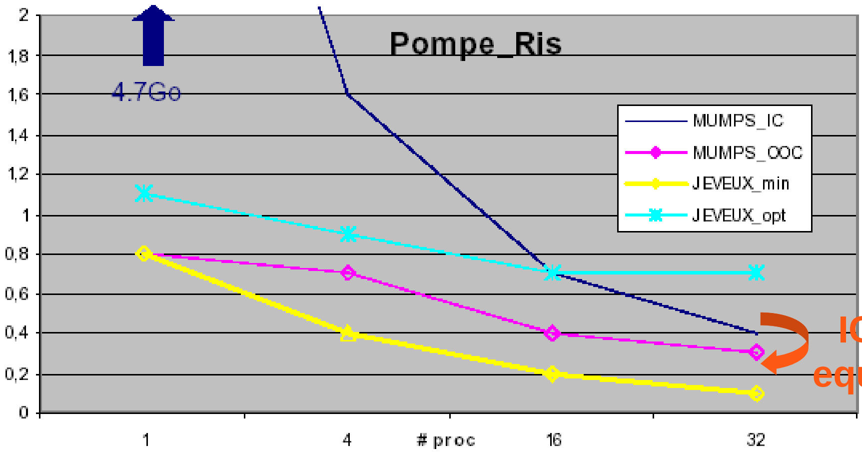
Real speed-up 4.8.4/4.9. 2:

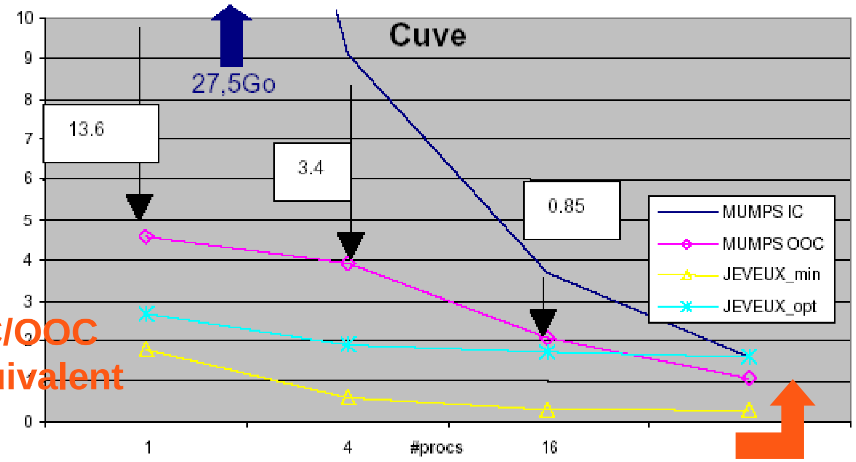
2.4/2.7 4.3/ 6.7   7.7/10.3



2d. Some results (2/3)

- **RAM memory consumption**

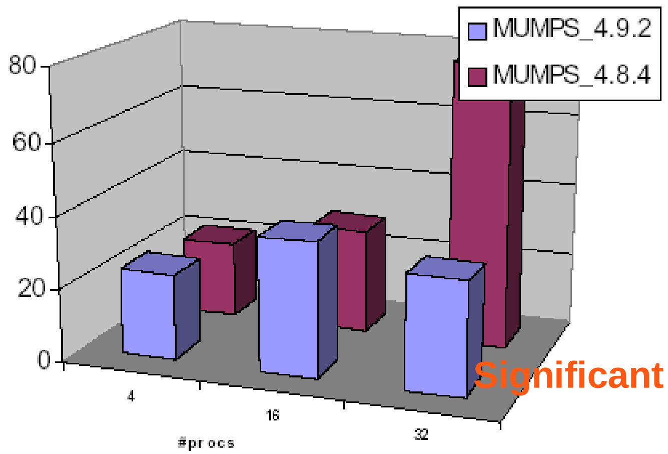


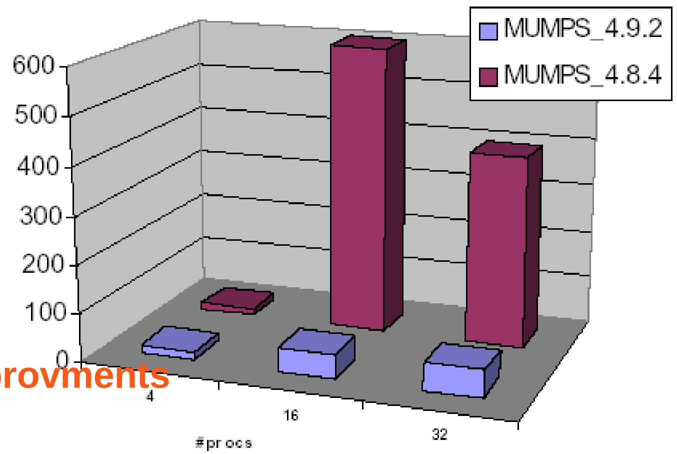


x4 on MUMPS OOC

x6 on Aster memory

- **Unbalance RAM** memory consumption between cores





Significant improvments

2e. Conclusions regarding *Code_Aster*/MUMPS

- **Daily use** throught *Code_Aster* at EDF R&D/Engineering ('best-in-class' tool)

Much more important than performances,
we particulary appreciate the MUMPS
Software Quality and the reactivity/friendliness of its team.

- **Partnership** throught the ANR SOSLTICE

Agence Nationale de la Recherche ANR
www.agence-nationale-recherche.fr

- Wish for future MUMPS functionalities/Letter to Santa Claus
    - Hybrid parallelism (MPI/Threads),
    - OOC capability (analyse step, integer, automatic),
    - Reuse of the factorized Matrix between two runs (restart mode),
    - Parallele Incomplete factorization…

- Test and benchmark of others strategies/librairies: DD, multigrid, PastiX, HIPS/MaPhys…

3. TELEMAC : an Integrated Modelling System

Free Surface Hydrodynamics

TELEMAC2D – TELEMAC3D

Sedimentology

SISYPHE – TELEMAC3D

Water Quality

(coupled) TELEMAC

Waves

ARTEMIS – TOMAWAC

Groundwater Flows

ESTEL2D – ESTEL3D

Smoothed Particle Hydrodynamics

SPARTACUS

3. First tests of MUMPS in TELEMAC (context)

Telemac has a common library of parallel iterative solvers developped at EDF + 1 direct sequential solver (YSMP) recently included

7 // iterative solvers :

- **developped and maintained at EDF**
- **very good performances in most cases**
- **but fail to converge with ARTEMIS !**

MUMPS in comparison ?

➡ **YSMP :**

- **works with ARTEMIS**
- **limitation on the problem size**
- **robustness not so good**
- **no parallelism**

MUMPS in replacement ?

3. First tests of MUMPS in TELEMAC (description)

SEQUENTIAL TESTS (PC Linux Workstation) :

- **ARTEMIS** (MUMPS vs YSMP) : *Mild Slope equation (FEM)*
- **TELEMAC2D** (MUMPS vs Iterative solvers) : *Shallow Water (2D FEM)*

PARALLEL TESTS (HP supercomputer) :

- **ARTEMIS** (MUMPS)
- **TELEMAC3D** (MUMPS vs Iterative solvers) : *Navier-Stokes (3D FEM)*

3.a Sequential Test : ARTEMIS

MUMPS in L.D.L^t mode with 2 systems to solve, 3-6 iterations

MUMPS is about 50% faster than YSMP (N ~ 100.000)

There is no more problem of robustness

→ **As expected, MUMPS easily outperforms YSMP**

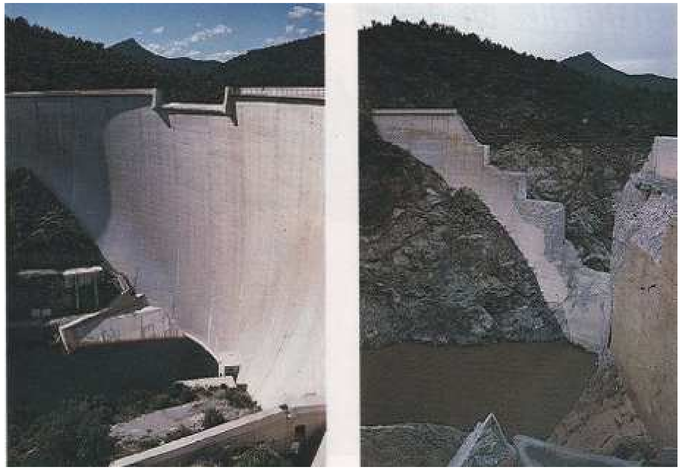
Example :
N = 338.930
NNZ(upper) = 2.532.299

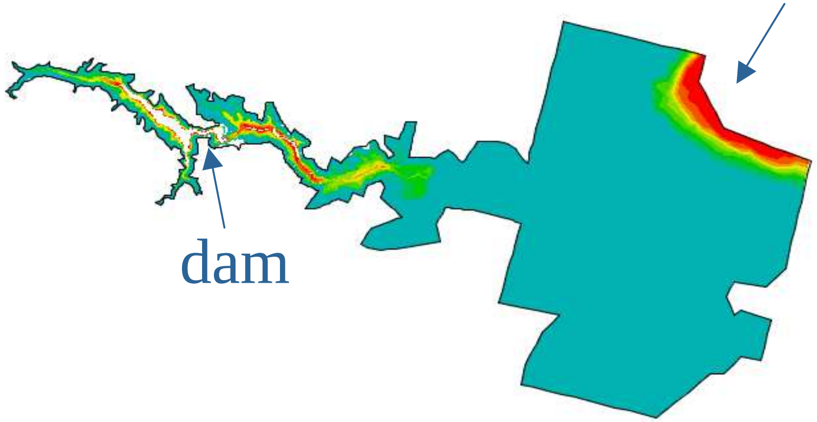
Ordering	NNZ(L+U-I)
Pord	26M
Scotch	27M
Metis	27M
Amf	29M
Amd	31M
Qamd	31M

$T_{MUMPS} = 9s$

3.b Sequential Test : TELEMAC2D

Simulation of a dam break : Malpasset (1959)





Simulation of 1000 s with DT = 1 s

(L.D.L^T and systematic analysis for MUMPS) N = 153.253 NNZ = 1M

Global computation times (for the same precision on results ;-)

Iterative : 19'33''

YSMP : 47'02''

MUMPS : 60'44''

Improvement :

No systematic analysis **or** suppress zeros?

/2 ?

3.c Parallel Test : ARTEMIS

Case Flamanville

(12 = 6x2 sparse linear systems to be solved with N= 169 465)

Experiments performed on HP supercomputer

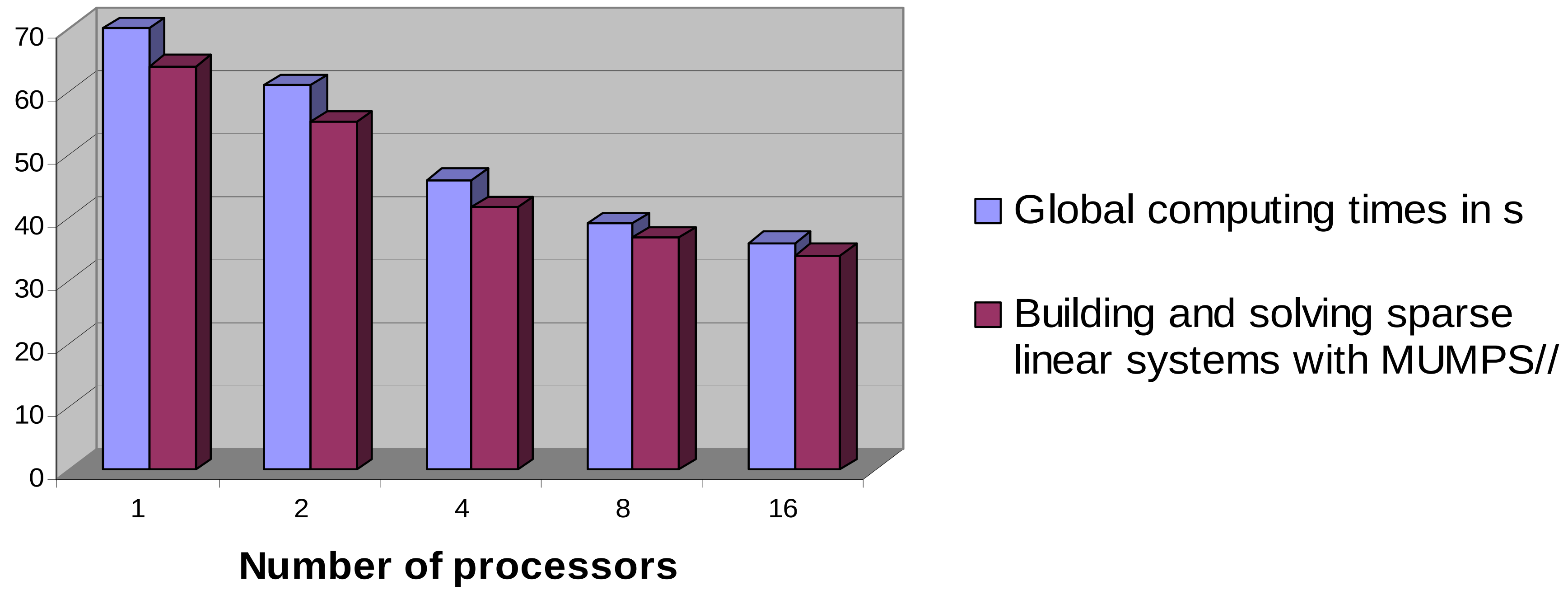
MUMPS used in distributed mode (icntl(18)=3) double precision

METIS (sequential) used as reordering method

Remember : iterative methods do not converge !

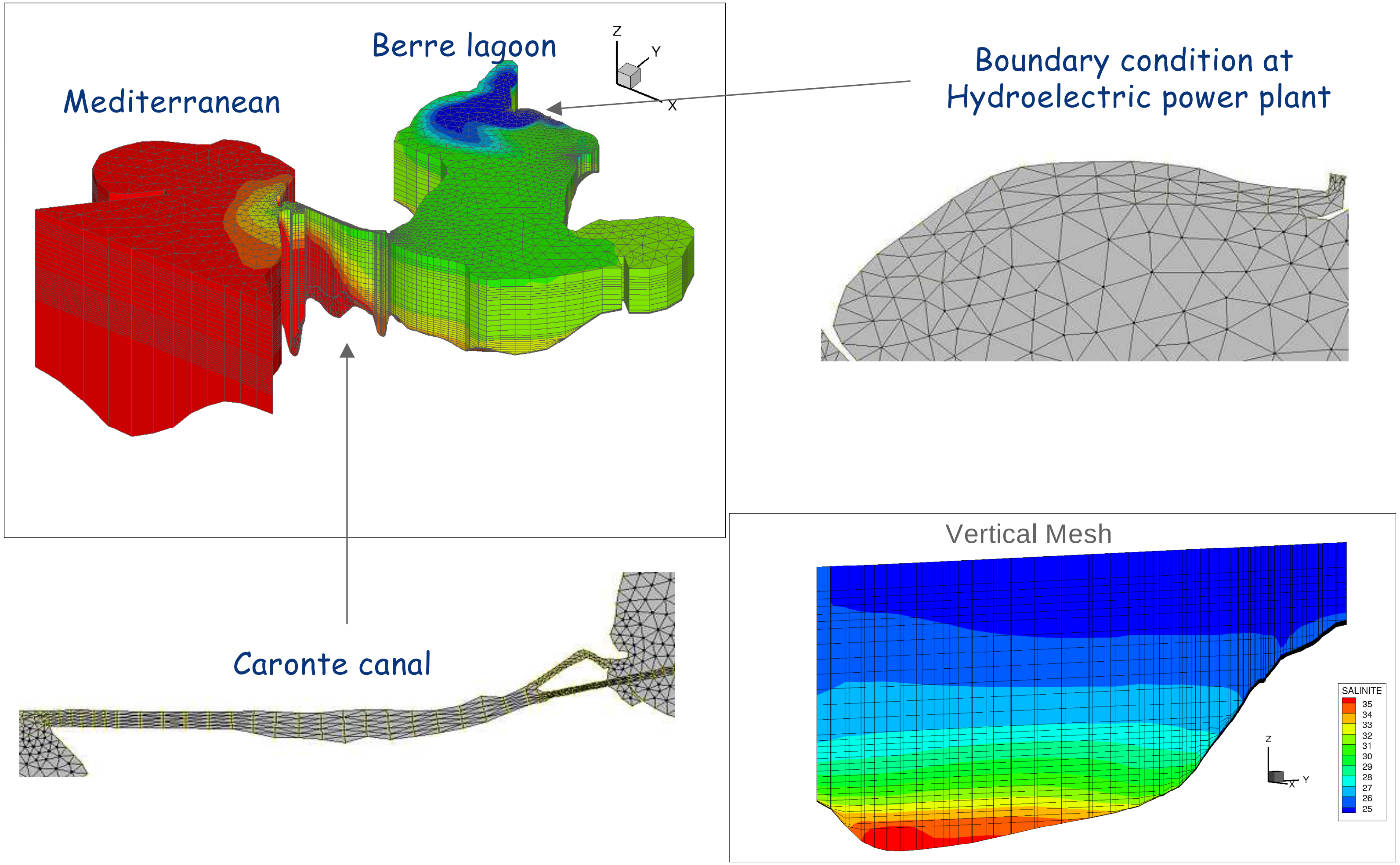
3.c Parallel Test : ARTEMIS

ARTEMIS// using MUMPS// (C. Denis)



MUMPS can now be used to deal with larger ARTEMIS problems !

Evolution of the salinity in the Berre Lagoon (South of France)



3.d Parallel Test : TELEMAC3D

One time step, 4 sparse linear systems need to be solved

- sparse linear system **S1**, N=4 098 700, Number of entries in factors ~1,7 10^9
- sparse linear system **S2**, N= 204 935, Number of entries in factors ~8,5 10^6
- sparse linear system S3, N= 4 098 700, Number of entries in factors ~1,7 10^9
- sparse linear system S4, N=4 098 700, Number of entries in factors ~1,7 10^9

MUMPS// used in distributed mode (icntl(18)=3)

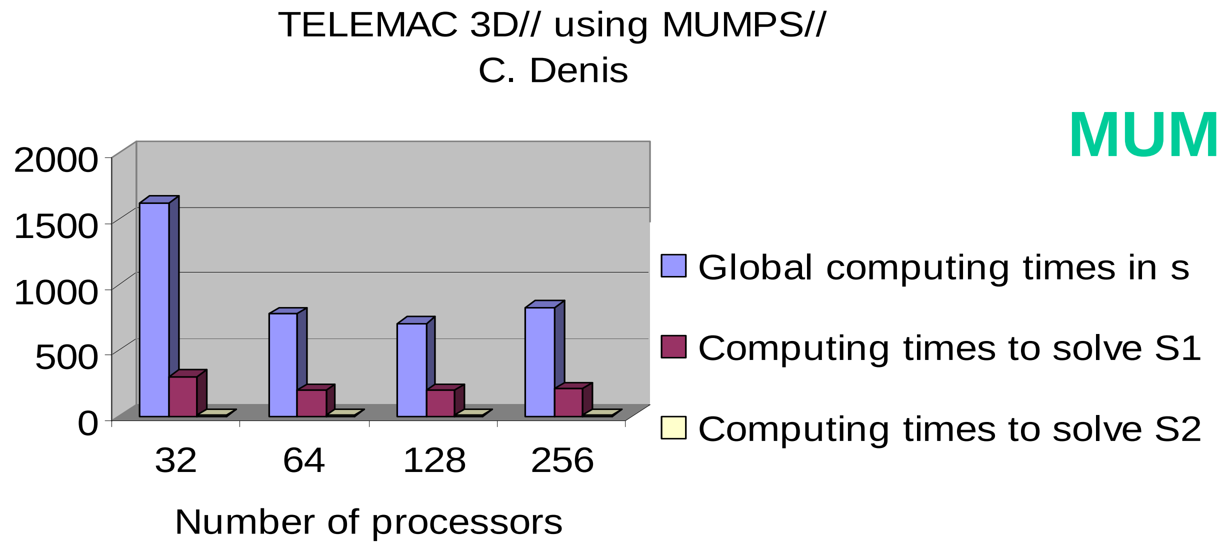
Scotch (sequential) used as reordering method

Experiments are performed on a HP Cluster on 32, 64 and 128 processors

Comparison are made with the iterative methods //

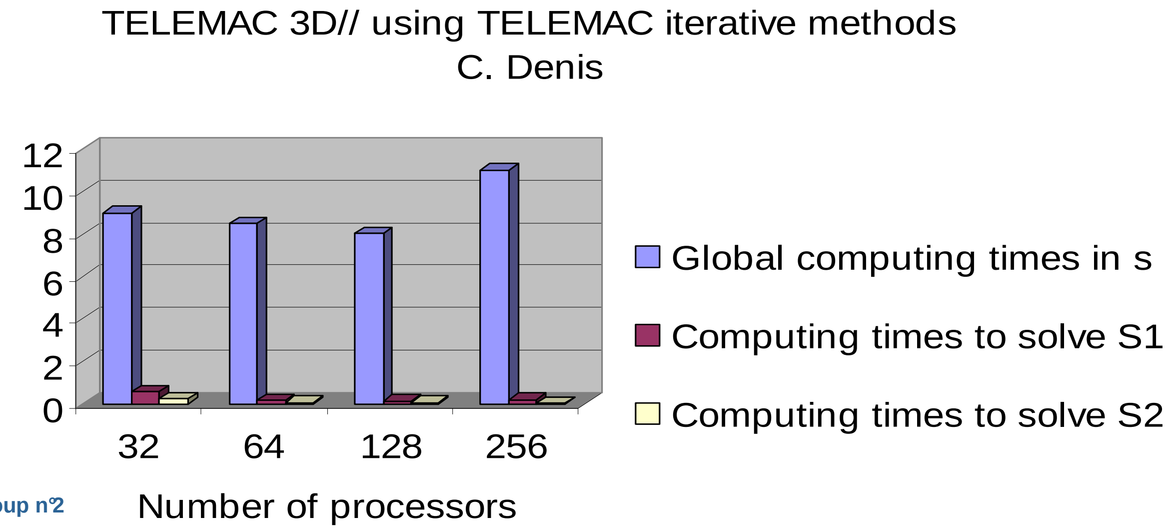
Iterative methods for this problem require few iterations to converge

3.d Parallel Test : TELEMAC3D



MUMPS

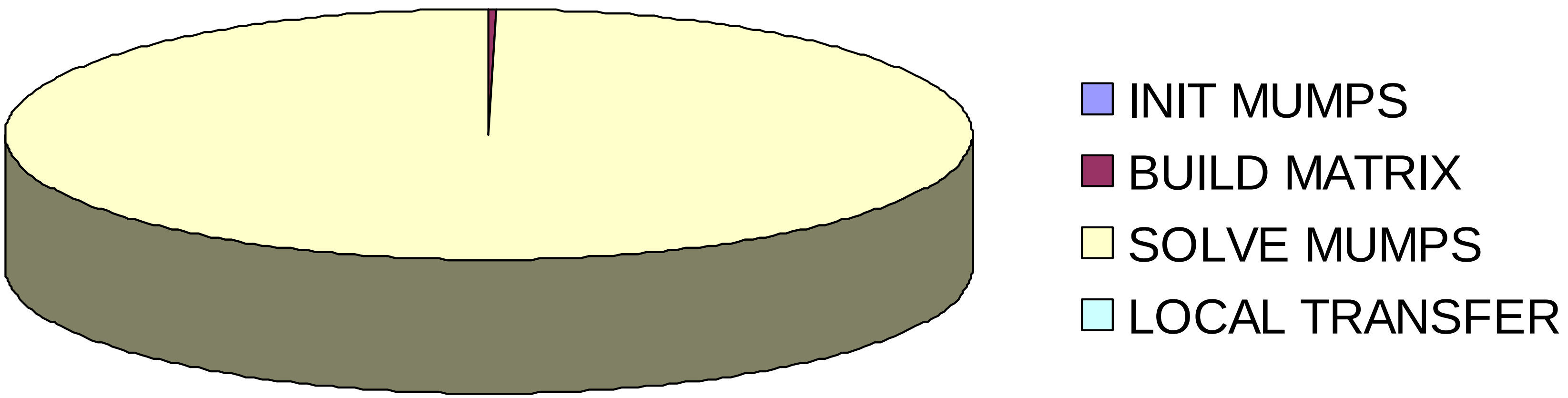
Ite. Method



3.d Parallel Test : TELEMAC3D

The solve phase is dominated by MUMPS algorithm

Computing times to solve S1 with 256 procs
(C. Denis)



3.d Parallel Test : TELEMAC3D

Precision on results are identical…

The numerical scheme has to be conservative in terms of water mass

Loss of (water) mass	32	64	128	256
with MUMPS	-0.2698488E-05	0.1625352E-06	-0.1430511E-05	0.1625688E-06
with iterative methods	-0.2698488E-05	0.1625352E-06	-0.1430511E-05	0.1625688E-06

3. Conclusions regarding TELEMAC/MUMPS

MUMPS and iterative methods are both useful depending of the sparse linear system to solve

Very useful when the sparse linear system to be solved is not well conditioned (ARTEMIS)

Not surprisingly, the conjugate gradient method gives best performances than MUMPS// when it needs a few number of iterations to converge for a well-posed problem (TELEMAC3D)

Future works :

- To improve the performance of ARTEMIS//
  - Optimisation of the matrix building by using MUMPS with complex numbers
  - solve in sequential the local sparse linear system with MUMPS and solve the interface problem
  - Implementation of MaPhys or HIPS in the TELEMAC system