The MUMPS library: news since last users'day

MUMPS team, Lyon-Grenoble, Toulouse, Bordeaux

MUMPS Users'Group Meeting
April 2010

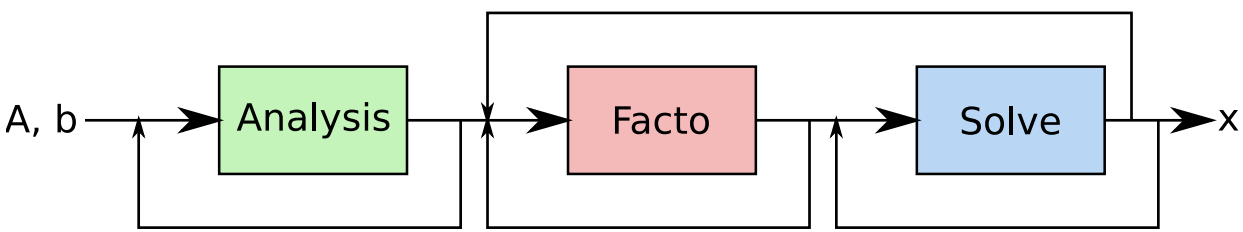
MUMPS

What is MUMPS

Initially funded by LTR (Long Term Research) European project PARASOL (1996-1999)

MUMPS (**MU**ltifrontal **M**assively **P**arallel sparse direct **S**olver) solves sparse systems of linear equations $Ax = b$ in three phases :

1. Analysis : matrix is preprocessed to improve its structural properties ($A'x' = b'$ with $A' = P_n P D_r A D_c Q P^t$)
2. Factorization : matrix is factorized as $A = LU$ or LDL^T
3. Solve : the solution x is computed by means of forward and backward substitutions



MUMPS (MUltifrontal Massively Parallel Solver)

http://graal.ens-lyon.fr/MUMPS and http://mumps.enseeiht.fr

Platform for research

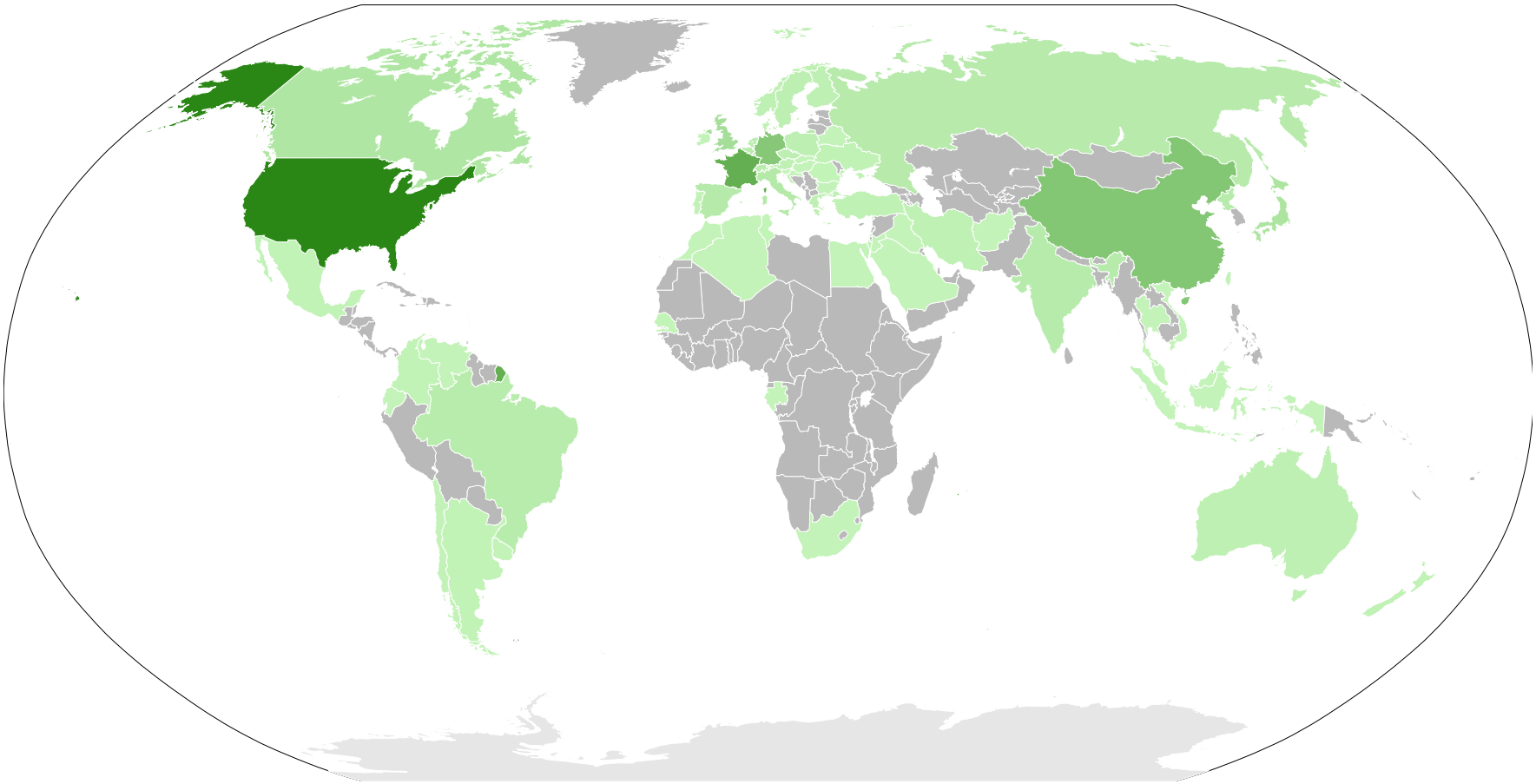
- Research projects
- PhD thesis
- Hybrid methods

Competitive software package used worldwide

- Co-developed by Lyon-Toulouse-Bordeaux
- Latest release : MUMPS 4.9.2, Nov. 2009, $\approx$ 250 000 lines of C and Fortran code
- 1000+ downloads per year from our website, half from industries : Boeing, EADS, EDF, Petroleum industries, Samtech, etc.
- Integrated within commercial and academic packages (Samcef from Samtech, FEMTown from Free Field Technologies, *Code_Aster* or Telemac from EDF, IPOPT, Petsc, Trilinos, ...).

User's distribution map

1000+ download requests per year



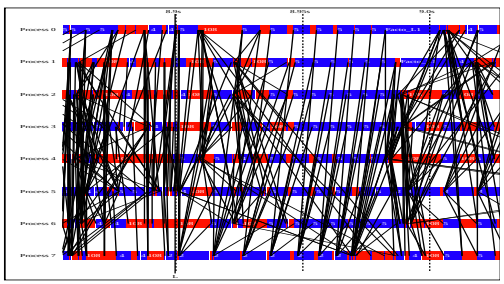
MUMPS vs other sparse direct solvers

Address wide classes of problems

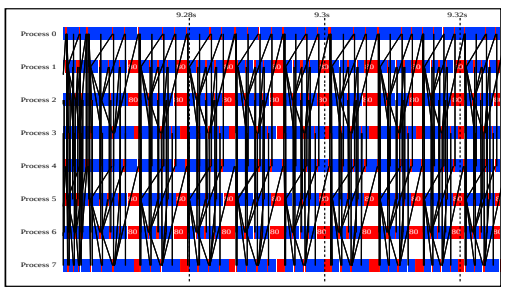
- Good numerical stability (dynamic pivoting, preprocessing)
- Wide range of numerical features

Management of parallelism

- Dynamic and asynchronism approach (more complex than static approaches)



MUMPS

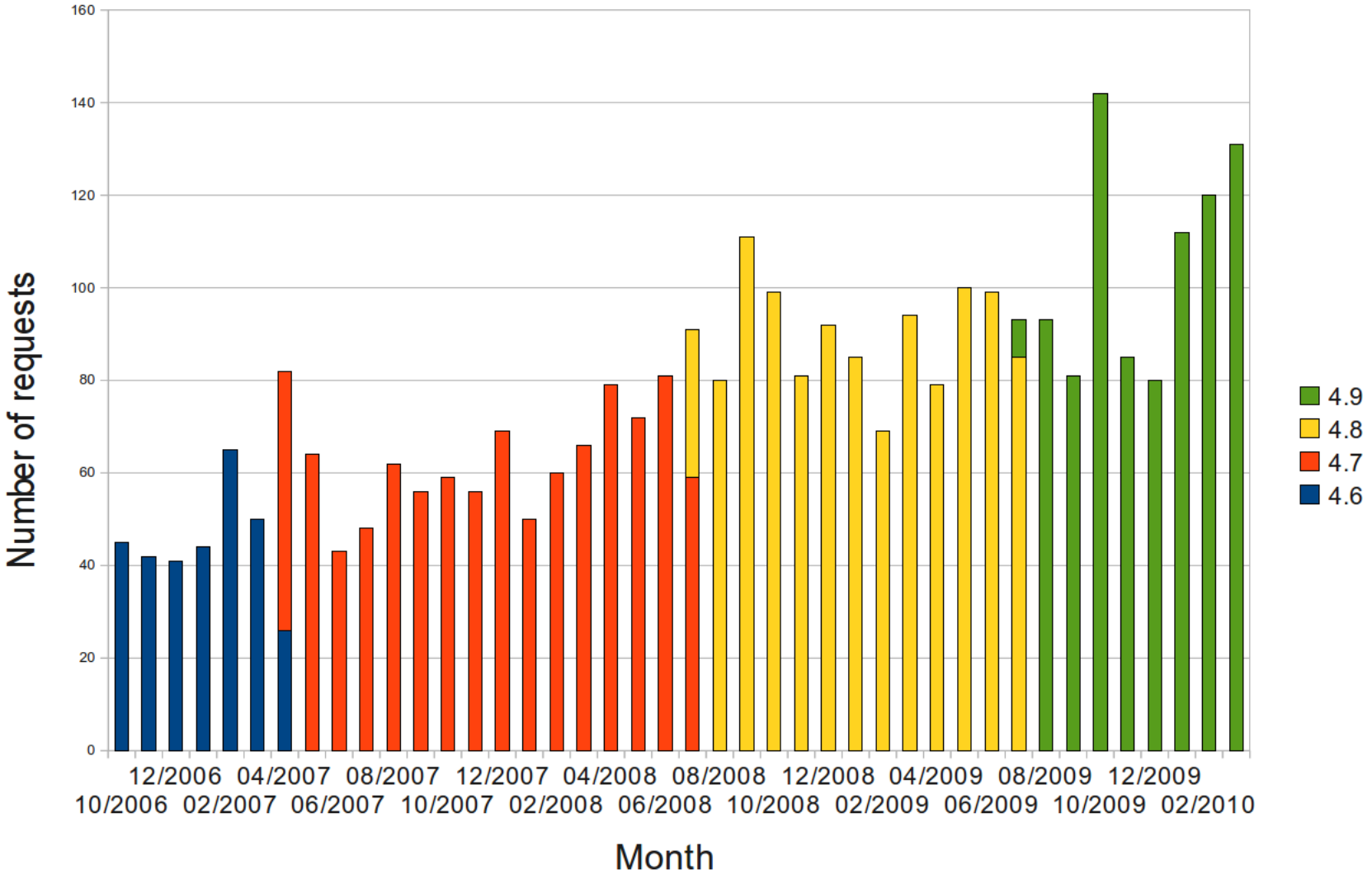


`SuperLU_DIST`

- Current version mainly MPI-based, not so advanced on thread-management (compared to, e.g., Pastix)

News since last users'day (Oct. 2006)

Download requests forms filled on the MUMPS website



MUMPS Team since since last users'day (2006)

Permanent members in 2006

Patrick Amestoy (N7-IRIT, Toulouse)

Jean-Yves L'Excellent (INRIA-LIP, Lyon)

Abdou Guermouche (LABRI, Bordeaux)

Bora Uçar (CNRS-LIP, Lyon)

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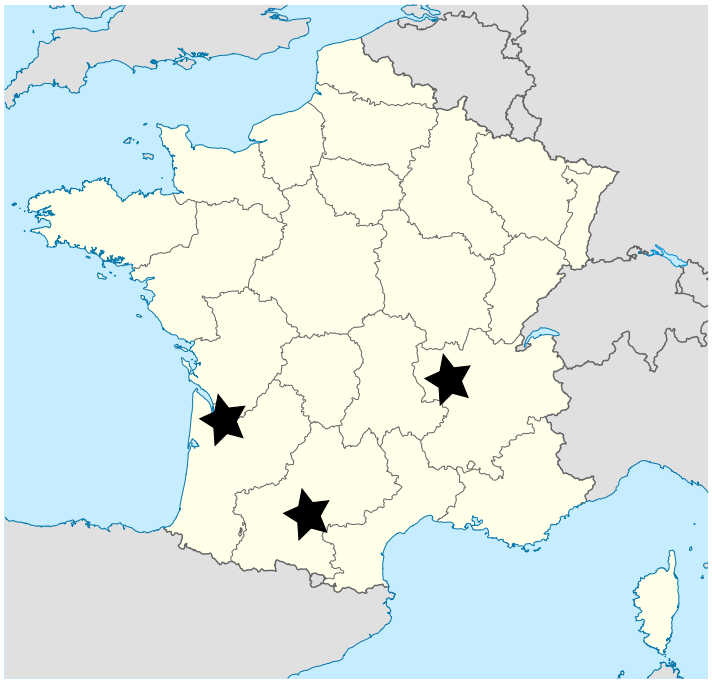

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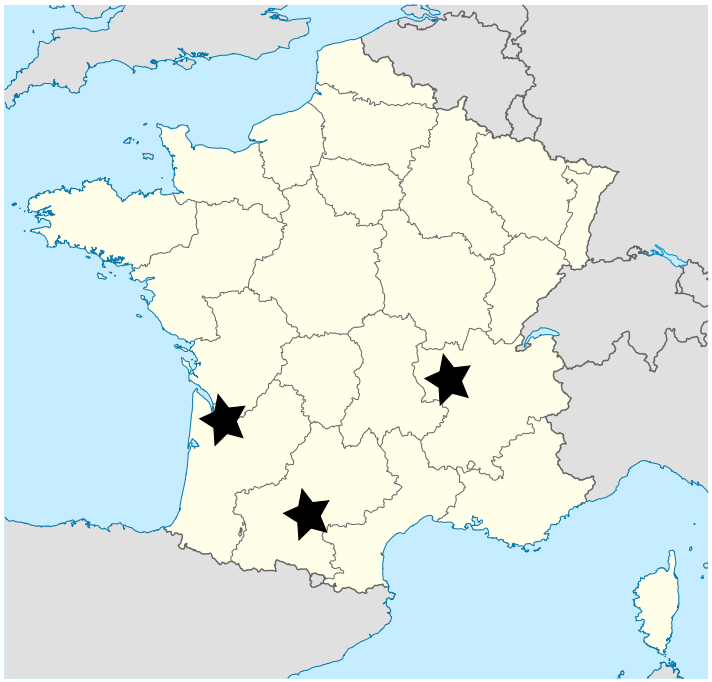

MUMPS Team since since last users'day (2006)

- Post-docs Indranil Chowdhury (May 2009–March 2010)
  Alfredo Buttari (Jan. 2008-Oct. 2008)
  Bora Uçar (Jan. 2007-Dec. 2008)

- Engineers Aurélia Fèvre (INRIA, 2005-2007)
  Philippe Combes (CNRS, Dec. 2007-Dec. 2008)
  Maurice Brémond (INRIA, Oct. 2009-Oct. 2012)$^{new!}$
  Guillaume Joslin (INRIA, Oct.2009-Oct. 2011)$^{new!}$

- PhD. Students Emmanuel Agullo (ENS Lyon, 2005-2008)
  Mila Slavova(CERFACS, Toulouse, 2005-2009)
  François-Henry Rouet (INPT-IRIT, Toulouse)$^{new!}$

- Master Student Clément Weisbecker (INPT-IRIT, Toulouse) $^{new!}$

Main projects and contracts since 2006

Main projects and contracts

- France-Berkeley project (2008-2009)
- Collaboration with the SEISCOPE consortium (2006-2008)
- Contracts with Samtech S.A. (2005-2006, then 2008-2010)
- French-Israeli Multicomputing project (2009-2010)
- ANR Solstice project (2007-2010), partners : INRIA, CERFACS, INPT-IRIT, CEA-CESTA, EADS IW, EDF, CNRS-CNRM-LA.
- Starting INRIA "Action of Technological Development" (2009-2012)

News since last users'day (Oct. 2006)

Out-of-core storage : 2 PhD completed

- Emmanuel AGULLO (ENS Lyon, 2005-2008) **On the Out-of-core Factorization of Large Sparse Matrices**
- Mila Slavova (CERFACS, Toulouse, 2005-2009) **Parallel triangular solution in the out-of-core multifrontal approach**

→ See talk by A. Guermouche before lunch "Recent Features : Out-of-Core"

Computing inverse entries of a sparse matrix

- PhD François-Henry Rouet (INPT, started Sept.2009) → See talk by F.-H. Rouet and Bora Uçar "Recent Features : Computation of a matrix inverse in MUMPS" tomorrow morning
- F.-H. Rouet also reconsiders scalability issues on large numbers of processors (→ See talk by A. Guermouche reporting preliminary work of E. Agullo during his PhD)

News since last users'day (cont')

- Parallel analysis and parallel scalings
  → see talk by Alfredo Buttari and Bora Uçar this afternoon

- Research around detection of null-space basis and null-space basis computations
  → see talk by Xavier Vasseur tomorrow morning

- Use of MUMPS in Block-Cimmino hybrid solvers
  → discuss with Daniel Ruiz, Ronan Guivarch and Mohamed Zenadi

- Code for QR factorization and least square problems
  → see talk by Alfredo Buttari tomorrow afternoon

News since last users'day (cont')

- Strong connections with the GRID-TLSE project
  → see talk by TLSE team tomorrow afternoon

- Hybrid MPI + OpenMP version of MUMPS
  - Indranil Chowdhury (May 2009–March 2010)
  - Some promising results
  - Work to be pursued

Other activities and specific developments

All this is nice... but how can it work ?
Two key issues :

I. Software Engineering

- MUMPS is a research code more than 15-year old
- Software engineering not so easy in the context of academic research
- Some recent initiatives :
  - 1-year funding by CNRS (2008) : Philippe Combes
    - taught us good software engineering practices, cvs to svn migration, with a trunk and release branches, new makefiles and Shell scripts for release generation+night tests, ...
  - Starting project "Action of Technological Development" funded by INRIA → see last talk today by Maurice Brémond and Guillaume Joslin

Other activities and specific developments

All this is nice... but how can it work ?
Two key issues :

2. Development of MUMPS

1. continuous improvements of our algorithms and code (mapping, ordering, communications, pivoting) according to users' feedback on specific classes of matrices or machines
2. for each research aspect we (developers) must :
   - make it available in software (interface, validation, documentation)
   - ensure compatibility with existing combinations of functionalities (example : out-of-core + panels + distributed frontal matrices + asynchronous pipelined factorizations + various types of factorizations + pivoting)
   - integrate, validate and maintain students' work

Examples of developments (cont')

- 64-bit integers to address large internal arrays (requested by users but also needed to show the interest of out-of-core or parallel analysis on large challenging problems)

- out-of-core factorization using a panel-oriented scheme

		I/O granularity for Factors	
Matrix	#procs	Written by fronts	Written by panels
AUDIKW_1	1	1067.1	12.8
AUDIKW_1	32	155.5	12.8
CONV3D64	1	3341.5	40.2
CONV3D64	32	757.6	40.2

Size of I/O Buffers (MB) with asynchronous I/O's

Examples of developments (cont')

Reduce memory for asynchronous communication buffers

- Idea : send messages by packets that fit in a smaller buffer
- Cost : more synchronizations (receiver must receive data before we can send the next packet)

Matrix	Communication scheme	
	Large buffers	Small buffers
AUDIKW_1	264	4.2
CONV3D64	286	16.1

Size of the communication buffers (MB) with 32 processors

Examples of developments (cont')

- Work on optimization matrices from ESI Group

	Time for analysis (8 processors)
Before	1724 seconds
After	24 seconds

- Redesign parts of the mapping algorithm ("Epicure" matrix from EDF)

	Factors	InCore Memory (in MB)	
	Min/Max	Avg	Max
Before	0.06	1,753	2,883
After	0.70	1,634	2,019

	Factor. time (seconds)				
Nprocs MPI	2	4	8	16	32
Before	337	229	132	86	52
After	316	163	103	53	33

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Summary

- MUMPS functionalities, performance, memory usage have improved a lot since the last users'day
- The MUMPS team and the users' community have both grown
- Our TODO list on the development side keeps increasing, priorities defined according to collaborations, contracts and research projects
- Enjoy the meeting and discussions

Other speakers not cited before

- Invited

  Cleve Ashcraft (LSTC, USA)
  Evgenii Rudnyi (CADFEM, Germany)
  Heidi Thornquist (Sandia National Labs, USA)

- Other users

  Leo Gonzalez (Univ. Polytécnica Madrid)
  Michel Fournié (UPS, Toulouse)
  Antoine Petitet (ESI Group)

- Collaborators through contracts/projects

  Samtech contract :
  Jean-Pierre Delsemme (Samtech)
  ANR Solstice project :
  François Pellegrini (LaBRI)
  Olivier Boiteau and Fabrice Zaoui (EDF)
  Guillaume Sylvand (EADS IW)
  Seiscope :
  Stéphane Operto (CNRS, Geoazur)
  French-Israeli Multicomputing project :
  Yuri Feldman and Alexandre Gelfgat (Tel Aviv Univ.)