Patrick Amestoy (INPT(ENSEEIHT)-IRIT), Abdou Guermouche (Univ. de Bordeaux), Jean-Yves L'Excellent (Inria-LIP-ENS Lyon)
Outline

Sparse direct methods

a MUltifrontal Massively Parallel Solver (MUMPS)

Data analysis: software requests, website, mail exchanges

MUMPS Usersdays 2010: Wish list

Programme of the workshop
Sparse direct methods

a MUltifrontal Massively Parallel Solver (MUMPS)

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Programme of the workshop
Sparse direct solvers

Discretization of a physical model (e.g., finite elements) $\rightarrow$ Solution of sparse systems $Ax = b$

*Often the most expensive part in numerical simulation codes*

Sparse direct methods to solve $Ax = b$:

- Decompose $A$ under the form $LU, LDL^t$ or $LL^t$
- Solve the triangular systems $Ly = b$, then $Ux = y$

Black box?

- Default (automatic/adaptive) setting of options often available
- Knowledge and setting of the *preprocessing* and algorithmic options can help the user to improve:
  - size of $L, U$ factors and memory needed
  - operation count and computational time
  - numerical accuracy
Influence of preprocessing on factorization

Matrix lhr01.rua, Chemical process simulation

Original \((A = lhr01)\)  \hspace{1cm}  Preprocessed \(A'\)  \hspace{1cm}  Factor \(A' = L'U'\)

Modified problem: \(A'x' = b'\) with \(A' = PD_rAQD_cP^t\)

<table>
<thead>
<tr>
<th>NonZeros in (A)</th>
<th>NonZeros in (LU(PD_rAQD_cP^t))</th>
<th>NonZeros in (LU(PAP^t))</th>
</tr>
</thead>
<tbody>
<tr>
<td>18K</td>
<td>136K</td>
<td>1 017K</td>
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</table>
Complexity of sparse direct methods

<table>
<thead>
<tr>
<th></th>
<th>2D</th>
<th>3D</th>
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<tbody>
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<td>( N \times N ) grid</td>
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<td>( \Theta(N^3) )</td>
</tr>
<tr>
<td>Nonzeros in factors</td>
<td>( \Theta(N^2 \log N) )</td>
<td>( \Theta(N^4) )</td>
</tr>
<tr>
<td>Floating-point ops</td>
<td>( \Theta(N^3) )</td>
<td>( \Theta(N^6) )</td>
</tr>
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</table>

3D example in earth science: acoustic wave propagation, 27-point finite difference grid

Current goal [Operto Virieux]:
\( LU \) on complete earth

Extrapolation on a \( 1000 \times 1000 \times 1000 \) grid:
15 exaflops, 200 Tbytes for factors, 32 TBytes for active memory!
Too big (but we are far from exploiting all cores of exascale computers)
Complexity of sparse direct methods

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Evolution of computers and applications needs ⇒ considerable efforts on algorithms and code development

- **Parallel algorithm issues**: synchronization avoidance, mapping irregular data structures, scheduling for memory/for performance, memory scalability, out-of-core storage, heterogeneous architectures, checkpointing and resilience

- **Numerical issues**: numerical accuracy, low-rank compression of dense submatrices, hybrid iterative-direct solvers, application-specific solvers

- **Code development**: develop and combine complex features, experimentation/analysis/validation tools, software engineering
Objectives of this workshop

- Present some facets of the **algorithmic, numerical and software work** in the context of the MUMPS project/solver

- Share experience

- Identify users expectations (software evolution, new features)

- Discuss future research tracks and future of MUMPS
Outline

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Programme of the workshop
MUMPS (MUltifrontal Massively Parallel Solver)

Initially funded by European project PARASOL (1996-1999)

Platform for research

- Research projects, PhD thesis
- Hybrid direct-iterative methods, ... 

Competitive software package used worldwide

- Co-developed in Toulouse, Lyon-Grenoble, Bordeaux by CERFACS, CNRS, ENS Lyon, INPT, Inria, Univ. Bordeaux
- Latest release: MUMPS 4.10.0, May 2011, \( \approx 250,000 \) lines of C and Fortran code
- Integrated within commercial and open-source packages (e.g., Samcef from Samtech, Actran from Free Field Technologies, Code_Aster from EDF, PAM-Crash from ESI, IPOPT, Petsc, Trilinos, Debian packages, ...).
Permanent members:

Patrick Amestoy (INPT-IRIT, Toulouse)
Jean-Yves L’Excellent (INRIA-LIP, Lyon)
Abdou Guermouche (LABRI, Bordeaux)
Bora Uçar (CNRS-LIP, Lyon)
Alfredo Buttari (CNRS-IRIT, Toulouse)

Engineers:

Maurice Brémond (INRIA, Grenoble)
Chiara Puglisi (CERFACS-IRIT joint lab)
Guillaume Joslin (CERFACS-IRIT joint lab)

PhD Students:

Clément Weisbecker (INPT, Toulouse)
Mohamed Sid-Lakhdar (ENS-Lyon)
Florent Lopez (UPS, Toulouse)

Former Phd Students (current location):

J. Koster (Uppsala U.), C. Voemel (ETH Zurich)
S. Pralet (Bull), E. Agullo (INRIA)
M. Slavova (Sogeti), F.-H. Rouet (LBNL)
2000-2013: Research through PhD’s

Ph.D. students connected to the project:

- F. Lopez, UPS
- W. Sid-Lakhdar, ENS Lyon
- C. Weisbecker, INPT-EDF
- F.-H. Rouet, INPT
- M. Slavova, CERFACS
- E. Agullo, ENS Lyon
- S. Pralet, CERFACS
- A. Guermouche, ENS Lyon
- C. Voemel, CERFACS

Some research themes: Preprocessing and orderings, Numerical pivoting and accuracy, Numerical features, Memory usage and task scheduling, Shared-memory parallelism

Closely related to MUMPS: Experiment and validate research

Initial versions:

22 internal PARASOL releases: 02/98 (asynchronous LU), 06/98 (SPD), 09/98 (general symmetric), 02/99 (element-entry), 03/99 (distributed entry), 05/99 (Schur complement)

**MUMPS 4.0.4 (09/1999):** Final version PARASOL (first public domain version)

**MUMPS 4.1.6 (03/2000):** First stabilized and freely distributed release


- All precisions/arithmetic (“SDCZ”)
- More orderings (AMF, QAMD, Metis, PORD)
- Limit scheduling decisions with candidate processors (memory estimates based on worst-case distribution PhD C. Voemel)
- Multiple Right-Hand Sides (or RHS)
Software evolutions (2003-2007)

<table>
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<tr>
<th>MUMPS 4.5 (2005)</th>
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</thead>
<tbody>
<tr>
<td>• 2D block-cyclic Schur complement</td>
</tr>
<tr>
<td>• Symmetric indefinite matrices (PhD S. Pralet)</td>
</tr>
<tr>
<td>• Sparse multiple Right-Hand Sides</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>MUMPS 4.6 (2006) and MUMPS 4.7 (2007)</th>
</tr>
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<tbody>
<tr>
<td>• Tree traversals to reduce memory usage (PhD A. Guermouche)</td>
</tr>
<tr>
<td>• Hybrid scheduler – performance under memory constraints (estimates based on average distribution PhDs A. Guermouche and S. Pralet)</td>
</tr>
<tr>
<td>• Reduced RHS on an interface and use of partial solution</td>
</tr>
<tr>
<td>• Detection of zero pivots (singular matrices)</td>
</tr>
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</table>
## Software evolutions (2007-)

### MUMPS 4.8 (2008)
- Parallel scaling for distributed matrices (Post-doc B. Uçar)
- Memory reductions (communication buffers and in-place assembly)
- Out-of-core (PhDs E. Agullo and M. Slavova)

### MUMPS 4.9 (2009) and MUMPS 4.10 (2011)
- Parallel Analysis (Post-doc A. Buttari) 64-bit addressing
- Compute selected entries of $A^{-1}$ (PhD M. Slavova and F.-H. Rouet)
- Compute determinant (collaboration with A. Salzman)

Next release MUMPS 5.0 (described in afternoon talk)
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Programme of the workshop
Software download requests

- **Period**: 2002-2012; 8 major releases; 8839 requests
- *Mumps_Solver also* redistributed in many packages
- Each download request includes:
  
  - First Name:
  - Last Name:
  - e-mail:
  - Institution:
  - Country:
  - Platform(s):
  - Type of matrices:
  - Area/Type of activity:
## Data sets used for our analysis (II)

### Website visits (google-analytics)

- **Period**: 2011-2012; 54,284 visits
- Each visit reports:
  - country,
  - region,
  - city,
  - and time of visit

### MUMPS users’ mailing list (mumps-users)

- Dataset of mails between users: 2,753 mail exchanges over 6 years.

### MUMPS exchanges developers ↔ users

- 8,677 mail exchanges over last 10 years
- Contents not analyzed yet
Software requests

World Map (8839 requests)

Figure: Map of the software requests in the world since December 2002
Software requests

Area of activities

requests from release 4.2 to 4.6.4 (from Dec/2002 to April/2007)

requests from release 4.7 to 4.8 (from April/2007 to July/2009)

requests from release 4.9 to 4.10 (from July/2009 to Dec/2012)

Interesting to notice the evolution of “Optimization” over the releases
Software requests

Number of requests

Requests per day

MUMPS releases

20/30 MUMPS Users Group Meeting — Clamart, France, May 29-30, 2013
Visits on our website

World Map (54284 visits)

Figure: Map of the visits from the countries since November 2010
10939 visits from USA

Figure: Map of the visits from USA by states since November 2010
Visits on our website

2103 visits from California

Figure: Map of the California visits by cities since November 2010
Main topics of exchanges between users

Figure: Mails between users (2007 - 2012)
Outline

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MUMPS Usersdays 2010: Wish list

Programme of the workshop
Few major research tracks

- **Hybrid parallelism** to address complex architectures based on distributed memory nodes with multicore/multi GPU processors.
- **Low-rank multifrontal Solver** for specific problems (elliptic PDEs)
- **Sparse QR factorization**
- **Hybrid direct-iterative methods to address larger problems**
- **Reproducibility/deterministic executions**
### Few major research tracks

- **Hybrid parallelism** Phd thesis and talks of W. Sid Lakdhar (2011-) on multicore and F. Lopez (2012-) on heterogeneous architectures

- **Low-rank multifrontal Solver** talk and PhD thesis of C. Weisbecker (2010-2013) on Block-Low-Rank method

- **Sparse QR factorization** qr_mumps v. 1.0 (01/08/2012) talk by A. Buttari, talk and PhD thesis of F. Lopez

- **Hybrid direct-iterative methods** talk and PhD thesis of M. Zenadi (2010-2013) on Block-Cimmino method

- Reproducibility/deterministic executions
Few critical issues

- **Solution Phase** performance (time and memory)
  - Improve size of workspace and performance in case of multiple Right-Hand Sides (RHS)
  - Sparse RHS and Solution (sequential and parallel)

- **Memory scalability and quality of memory estimates**

- **Orderings for specific problems** such as augmented (Lagrangian) problems
### Few critical issues

**Solution Phase** PhD F.-H. Rouet; MUMPS 5.0 talk and release
- Improve size of workspace and performance in case of multiple Right-Hand Sides (RHS)
- Sparse RHS and Solution (sequential and parallel)

**Memory scalability and quality of memory estimates** PhDs E. Agullo (2005-2008) and F.-H. Rouet (2009-2012), talk by F.-H. Rouet on memory-aware mappings

**Ordering for specific problems**, preliminary work conducted by B. Uçar
New or improved features

- **Exploit sparsity** of Right-Hand Sides (RHS)
- **Factors-free factorization and determinant**
- **Restart Mode**
- **Inertia** was not compatible with Scalapack on Root
### New or improved features

- **Exploit sparsity** of Right-Hand Sides (RHS), PhD thesis of T. Slavova (2006-2009) and F.-H. Rouet (2009-2012), see MUMPS 5.0 talk and release
- **Factors-free factorization and determinant**: available in next release
- **Restart Mode**: preliminary version in next release, see talk by G. Joslin and M. Brémond
- Inertia was not compatible with Scalapack on Root
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Programme of the workshop
Programme

MUMPS Usersdays Wednesday 29 and Thursday 30 May 2013
Centre R&D EDF, Clamart

Wednesday 29 May

9.30 - 10.00 Registration and welcome coffee
10.00 - 10.15 Welcome by EDF and presentation of the 2 day meeting
10.15 - 11.00 Patrick Amestoy (INPT(ENSEEIHT)-IRIT), Abdou Guermouche (Univ. de Bordeaux), Jean-Yves L’Excellent (Inria-LIP-ENS Lyon)
MUMPS overview
11.00 - 11.30 Olivier Boiteau (EDF, France)
Partnership EDF-MUMPS, a fruitful win-win story
11.30 - 12.15 François-Henry Rouet (Lawrence Berkeley National Laboratory, USA)
Robust memory-aware mappings for parallel multifrontal factorizations
12.15 - 12.45 Antoine Petitet (ESI Group, France)
Feedback on The Utilization of MUMPS in ESI’s products
Lunch
14.30 - 15.15 Clément Weisbecker (Université de Toulouse, INPT(ENSEEIHT)-IRIT, France)
Block Low-Rank (BLR) approximations to improve multifrontal sparse solvers
15.15 - 15.45 François Pellegrini (ENSEIRB-LaBRI, France)
Shared memory parallel algorithms in Scotch 6
Coffee Break
16.15 - 16.45 Eveline Rosseel (FFT, Belgium)
Performing acoustic, vibro-acoustic and aero-acoustic computations using MUMPS
16.45 - 17.15 Wissam Sid-Lakhdar (École Normale Supérieure de Lyon, France)
Evolution of MUMPS towards multicore architectures
17.15 - 18.00 Patrick Amestoy (INPT(ENSEEIHT)-IRIT), Abdou Guermouche (Univ. de Bordeaux), Jean-Yves L’Excellent (Inria-LIP-ENS Lyon)
Introducing MUMPS 5.0 and discussions
19.30 - 22.00 Banquet at “L’Ardoise”
Thursday 30 May

9.00 - 9.30  Jean-Pierre Delsemme (LMSINTL, Belgium)
Recent Progress of Parallel SAMCEF with MUMPS

9.30 - 10.00 Alfredo Buttari (CNRS-IRIT, France)
qr_mumps: a multithreaded, multifrontal QR solver

10.00 - 10.30 Florent Lopez (Université de Toulouse, INPT(ENSEEIHT)-IRIT, France)
Towards a multifrontal QR factorization for heterogeneous architectures over runtime systems

Coffee Break

11.00 - 11.30 Guillaume Sylvand (EADS Innovation Works, France)
Application of sparse matrices and H-matrices at EADS Innovation Works

11.30 - 12.00 Maurice Brémond (INRIA, France),
Guillaume Joslin (CERFACS-IRIT common laboratory, France)
Some engineering issues in the MUMPS project

12.00 - 12.30 Romain Brossier (SEISCOPE Consortium, France)
Frequency-domain seismic modeling with the MUMPS sparse direct solver: application to the imaging of the earth’s interior.

12.30 - 13.00 Mohamed Zenadi (INPT(ENSEEIHT)-IRIT)
A hybrid iterative solver based on Block-Cimmino method

Lunch

14.00 - 16.00 Round Table: User requirements and closing

Credits

This event is supported by:
EDF CERFACS INPT-ENSEEIHT IRIT CNRS INRIA