MUMPS overview and recent features

MUMPS group:
CERFACS, CNRS, ENS-Lyon, INRIA, INPT, Univ. Bordeaux

Contents of the presentation:

- MUMPS overview, history, statistics on usage, research links
- Main recent features, software releases
- MUMPS User days 2017
Discretization of a physical problem (e.g. Code_Aster, finite elements)

Solution of sparse systems

\[ AX = B \]

Often the most expensive part in numerical simulation codes

Sparse direct methods:

- Analyse graph of matrix, permutation, memory estimates
- Factor \( A = LU \) (\( LDL^t \) if \( A \) symmetric) using Gaussian elimination
- Triangular solve: \( LY = B \), then \( UX = Y \)

Sometimes preferred to iterative methods for their robustness and ability to solve efficiently multiple/successive right-hand sides.
MUMPS: a MUltifrontal Massively Parallel Solver

Solve $A \mathbf{x} = \mathbf{b}$,

$A$ is a large sparse matrix, and $\mathbf{b}$ is dense or sparse
on multiprocessor architectures

<table>
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- 2000: First “public domain” version of MUMPS
- 2013: Third edition of MUMPS User Group Meeting (EDF-Clamart)
- 2014: Consortium of MUMPS users
  Founding members: CERFACS, INPT, Inria, ENS-Lyon, Bordeaux University
- 2015: MUMPS 5.0.0, first CeCILL-C version of MUMPS
MUMPS consortium

... to ensure software sustainability and development


- Manager: Inria; President of Executive Committee: INP Toulouse
- **Membership agreement** stipulates Member’s rights:
  - experiment with versions in advance (latest upgrades, beta releases)
  - exert an influence over future developments and the interface of new features
  - appoint a representative to annual meeting of the Consortium Committee
  - priority access to developers: support, advice, performance analysis which may give rise to a specific study agreement
- **Members (10):**
  - EDF, Altair, Michelin, LSTC (USA), SISW-Siemens (Belgium), FFT-MSC Soft. (Belgium), ESI Group, Total, SAFRAN, Lawrence Berkeley Nat. Lab. (USA)

Membership fees → funding for PhD and engineers
• Co-developed in France (Toulouse, Lyon, Bordeaux) by CERFACS, CNRS, ENS Lyon, INPT, Inria, Bordeaux Univ.
  ○ Address wide classes of problems: various types of matrices/formats, numerical pivoting, many numerical features
  ○ Asynchronous approach to parallelism

• Software package used worldwide in academic research, R&D departments, and also through
  ○ commercial software: (Samcef from Samtech/Siemens, Actran from Free Field Technologies/MSC, PAM-Crash from ESI-Group, Flux from Altair, OptiStruct from Altair, COMSOL MultiPhysics from COMSOL, . . .).
  ○ open-source and research packages: Code_Aster (EDF), IPOPT, Petsc, Trilinos, FreeFEM++, OpenSEES, SOPALE, Kwant, . . .
  ○ Linux distributions: Debian, CentOS, . . .
Software download requests: countries around the world

requests 4.2 - 4.6.4 (Dec 2002 - Apr 2007)
requests 4.7 - 4.8 (Apr 2007 - Jul 2009)
requests 4.9 - 4.10 (Jul 2009 - Feb 2015)
requests 5.0 - 5.1 (Feb 2015 - May 2017)

See requests from the US, Germany, Japan, China
World maps

- 14,232 download requests from Dec 2002 to May 2017 from our website

- 177,612 visitors (112,090 unique visits) on our website from Nov 2010 to May 2017
Software download requests: Application Fields

requests 4.2 - 4.6.4 (Dec 2002 - April 2007)

requests 4.7 - 4.8 (April 2007 - July 2009)

requests 4.9 - 4.10 (July 2009 - Feb 2015)

requests 5.0 - 5.1 (Feb 2015 - May 2017)
• 550 subscribers, \( \sim 1 \) message per day on average

**Main topics of exchanges between users (2013-2017)**

- Sequential
- Large
- Parallel
- Memory
- Numerically
- Building
- MPI-Free
-make
- Large
- Entries
- Interface
- ICNTL
- Solve
- Solution
- Max
- Computing
- Analysis
- Distributed
- Running
- Examples
- Many
- Fortran
- Bit
- Using
- Intel
- Wrong
- Errors
- Problems
- Installation
- Integer
- Number
- While
- Send
- Avoid
- Compile
- Question
- Available
- Code
- Factorization
- Singular
- Simple
- Performance
- Communicators
- Hand
- Related
- Out-of-Core
- MPI
• Robust Memory-Aware Mappings (memory scalability and quality of memory estimates) (PhD Agullo, ENS Lyon, 2005-2008 and Rouet, INPT-IRIT, 2009-2012)

• Shared and distributed memory parallelism on NUMA clusters (initiated with PhD Sid-Lakdhar, ENS Lyon, 2011-2014)

• Synchronisation avoidance and deadlock prevention, in context of dynamic distributed scheduling with asynchronous p2p & collective communications (initiated with PhD’s Rouet and Sid-Lakhdar)
• **Block Low-Rank (BLR):**
  algebraic solver based on BLR approximation (**PhDs Weisbecker, INPT-IRIT, EDF funding, 2010-2013 and Mary, UPS-IRIT, 2014-2017**);
  ◦ Collab. O. Boiteau (EDF), C. Ashcraft (LSTC, Livermore, USA)
    → See talk by Théo Mary (Toulouse University)
  ◦ Application to geophysics applications (SEISCOPE, EMGS)
    → See talk by Daniil Shantsev (EMGS, Norway)

• **Performance of solution phase** (**PhDs Rouet INPT-IRIT, 2009-2012 and Moreau, ENS Lyon, 2015-**): entries of $A^{-1}$, exploit sparsity of right-hand sides/partial solution, performance of (BLR) solve, . . .
  → See talk by Gilles Moreau this afternoon

• **Continuous collaborations and feedback from applications**
  ... crucial for MUMPS future research and developments
Scientific themes for recent papers:

- Amestoy, Buttari, L’Excellent, Mary: Implementation, Performance, scalability of multithreaded BLR, ACM TOMS (submitted)
- Amestoy, Brossier, Buttari, L’Excellent, Mary, Métivier, Miniussi, Operto: Application and performance of BLR to 3D full waveform inversion: Geophysics, 2016

Strong interaction with software work: M. Durand, G. Joslin, C. Puglisi (Inria, supported by MUMPS consortium)

performance tuning, scalability studies, parallel performance with respect to other solvers, multithreading, reduce memory consumption, validation on real-life applications, development/stabilization of new features, follow-up applications feedback/consortium/users’ community, user support, etc.
Software history (1996-2013)

• 22 internal PARASOL releases, 1996→ MUMPS 4.0.4 (1999): $LU$, $LDLT^T$, elemental input, distributed matrix input, Schur complement

• MUMPS 4.1.6 (2000): first freely distributed stabilized release!

• MUMPS 4.2 beta (2002), MUMPS 4.3 (2003): “SDCZ” arithmetics, many orderings (Scotch, Pord, Metis, AMD, QAMD, AMF), candidate processors (PhD Voemel), multiple Right-Hand sides (RHS), inertia

• MUMPS 4.5 (2005): progress on symmetric indefinite matrices (PhD Pralet), 2D block-cyclic Schur complement, first API for sparse RHS, distributed solution

• MUMPS 4.6 (2006), MUMPS 4.7 (2007): hybrid scheduling (PhD’s Guermouche+Pralet), reduced/condensed RHS, detection of zero pivots

• MUMPS 4.8 (2008): Parallel scalings (postdoc Uçar), memory reductions, out-of-core (PhD’s Agullo+Slavova)

• MUMPS 4.9 (2009), MUMPS 4.10 (2011): Parallel analysis (postdoc Buttari), 64-bit addressing for factors, $A^{-1}$ entries (PhD’s Slavova+Rouet), determinant (collaboration A. Salzman)
Software releases since last User Days
MUMPS 5.0.0 (2015): a major release

- First version under Cecill-C license
- **Userguide** considerably improved/redesigned
- New features:
  - First version with **OpenMP** directives (significant performance gains)
  - Forward elimination during factorization, use workspace from user, deterministic parallel analysis, . . .
  - **Solve phase revisited** (memory scalability and performance)
- Evolutions: MUMPS 5.0.1, MUMPS 5.0.2 (stabilization of 5.0.0 and performance improvements for specific matrices)
- Received positive feedback from users, e.g.:
  - “You know, you’ve made a huge contribution to the scientific community here. A modern, parallel sparse linear solver that runs on pretty much any platform is enormously useful.”
  - “The OpenMP is definitely faster overall, especially with larger problems with a few hundred thousand nonzeros and up”
MUMPS 5.0.0 vs MUMPS 4.10.0: user feedback

- Computation of $A^{-1}B$ ($B$ sparse) by blocks of 32: **72 MPI processes**

<table>
<thead>
<tr>
<th></th>
<th>Factorization (seconds)</th>
<th>Solve (seconds)</th>
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</thead>
<tbody>
<tr>
<td>MUMPS 4.10.0</td>
<td>158.9</td>
<td>13923.3</td>
</tr>
<tr>
<td>MUMPS 5.0.0</td>
<td>60.3</td>
<td>9806.0</td>
</tr>
</tbody>
</table>

- Time for factorization (shift and invert method, numerical issues). **360 cores (36 MPI and 10 threads/MPI).**

<table>
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<tr>
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<th>Factorization Phase (LU) (seconds)</th>
<th>(LDLT) (seconds)</th>
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</thead>
<tbody>
<tr>
<td>MUMPS 4.10.0</td>
<td>568</td>
<td>652</td>
</tr>
<tr>
<td>MUMPS 5.0.0</td>
<td>388</td>
<td>294</td>
</tr>
</tbody>
</table>
• A release with two new major features:
  ◦ 64-bit integers where needed (O(NZ) data on top of O(|L|) data)
    • Specifications guided by industrial partners, backward-compatible,
    • Metis, Scotch, PORD → 64-bit integers (32-bit also possible)
    • full 64-bit integer version also possible but more resource consuming
      → See presentation by Kostas Sikelis (Altair)
  ◦ First public version with low-rank compression (i.e. BLR) (work
    initiated in 2010!) → See presentation by Théo Mary on
      Block-Low-Rank and HSS multifrontal solvers
• Many other issues concerning robustness and performance (e.g., of
  solve phase with many RHS) → See presentation by Marie Durand

... and quite a lot of ongoing work ...
## Timings in seconds on 900 cores

(90 MPI x 10 threads)

<table>
<thead>
<tr>
<th>EOS computer, CALMIP mesocenter (<a href="https://www.calmip.univ-toulouse.fr/">https://www.calmip.univ-toulouse.fr/</a>)</th>
<th>Full Rank</th>
<th>Block Low Rank</th>
</tr>
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<tbody>
<tr>
<td>5.1.1</td>
<td>FR +</td>
<td>5.1.1</td>
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</table>

### 3D Full Waveform Inversion (Helmholtz equations)

- **N=17 M**
- **BLR precision** $\epsilon_{BLR} = 10^{-3}$
- FR: 937 seconds, BLR: 548 seconds

### 3D Electromagnetism (Maxwell equations)

- **N=21 M**
- **BLR precision** $\epsilon_{BLR} = 10^{-7}$
- FR: 2587 seconds, BLR: 1255 seconds

### 3D Structural Mechanics

- **N=8 M**
- **BLR precision** $\epsilon_{BLR} = 10^{-9}$
- FR: 722 seconds, BLR: 266 seconds

→ See closing presentation today “MUMPS perspectives and discussions”
Objectives:

• Bring together some MUMPS users from both academia and industry and MUMPS developers (61 participants from 10 countries)

• Have time for discussions and informal exchanges

• Present some aspects of MUMPS activities by MUMPS group members / share users’ feedback and experience with MUMPS → cf. next 2 slides

• And also:
  ○ benefit from experts knowledge on impact of computer evolutions:
    → presentation by François Courteille (NVIDIA, France) this afternoon
    → presentation by Patrick Demichel (HPE, France) tomorrow
  ○ share experience with other developers of sparse solvers:
    • sparse direct solver “MF2” → presentation by Bob Lucas tomorrow
    • domain decomposition methods (often using direct methods):
      → presentation by Pierre Jolivet (CNRS, France) tomorrow
      → presentation by Augustin Parret-Fréaud (SAFRAN, France) tomorrow
General presentations/discussions:
  Overview and recent features (now)
  MUMPS perspectives (last talk today)
  Closing discussion (tomorrow afternoon)

Members on permanent academic positions:
  Patrick Amestoy (INPT-IRIT, Toulouse)
  Jean-Yves L’Excellent (Inria-LIP, Lyon)
  Abdou Guermouche (LaBRI, Bordeaux)
  Alfredo Buttari (CNRS-IRIT, Toulouse) → qr_mumps: a runtime-based Sequential Task Flow parallel solver (this afternoon)

Engineers:
  Guillaume Joslin (MUMPS Consortium, Inria, Lyon)
  Chiara Puglisi (MUMPS Consortium, Inria, Toulouse)
  Marie Durand (MUMPS Consortium, Inria, Lyon) → Discussion of MUMPS parallel performance in multithreaded environments (this morning)

PhD Students:
  Théo Mary (UPS, Toulouse) → On the comparison of sparse multifrontal hierarchical and Block Low-Rank solvers (this morning)
  Gilles Moreau (MUMPS Consortium, MILyon) → Recent advances on the solution phase of direct solvers with multiple sparse right-hand sides (this afternoon)
• Olivier Boiteau (EDF, France): Use of MUMPS in EDF codes (thermomechanics, material structure, electromagnetics, hydrodynamics)

• Kostas Sikelis (Altair, Greece): Comparison of 32bit vs 64bit integer MUMPS in Optistruct (linear and nonlinear structural and thermal analysis, . . .)

• Daniil Shantsev (EMGS, Norway): Large-scale 3D Controlled source EM modeling with a Block Low-Rank MUMPS solver

• Eveline Rosseel (FFT-MSC Software Belgium): Improving (aero/vibro-)acoustic simulations using MUMPS - Evaluation of Block Low-Rank factorizations

• Rémy Perrin-Bit (Altair, France): Brief history of time in FLUX (Electromagnetic and thermal simulations)

• Luis E. García Castillo (University Carlos III of Madrid, Spain): Higher-Order Finite Element Code for Electromagnetic Simulation

• Yuri Feldman (Ben-Gurion University, Israel): Two phase flow simulations based on Immersed boundary method, by utilizing MUMPS solver
Enjoy those two days!

MUMPS User Days
Thursday, June 1st and Friday, June 2nd, 2017
Inria centre, Montbonnot Saint-Martin (near Grenoble, France)

Programme

Thursday, June 1st

8.30 - 8.45  Registration and welcome coffee
8.45 - 9.00  Welcome and presentation of the two day meeting
9.00 - 9.30  Patrick Amestoy (INPT-ENSEEIHT)-IRIT), Abdou Guermouche (Univ. de Bordeaux), Jean-Yves L’Excellent (Inria-LIP-ENS Lyon)
MUMPS overview and recent features
9.30 - 10.00  Olivier Boiteau (EDF Lab Paris-Saclay, France)
Feedback in the use of MUMPS in EDF codes
10.00 - 10.30  Théo Mary (University of Toulouse, France)
On the comparison of sparse multifrontal hierarchical and Block Low-Rank solvers
10.30 - 11.00  Coffee Break
11.00 - 11.30  Eveline Rosseel (FFT-Msc_Software, Belgium)
Improving aero/vibro-acoustic simulations using MUMPS: evaluation of Block Low-Rank factorizations
11.30 - 12.00  Marie Durand (MUMPS Consortium/Inria, France)
Discussion of MUMPS parallel performance in multithreaded environments
12.00 - 12.30  Kostas Sikelis (Altair, Greece)
Comparison of 32bit vs 64bit integer MUMPS in Optistruct
12.30 - 14.30  Lunch
14.30 - 15.00  Danil Shantsev (EMGS, Norway)
Large-scale 3D Controlled source EM modeling with a Block Low-Rank MUMPS solver
15.00 - 15.30  Gilles Moreau (MUMPS Consortium/LabEx MILYON/Inria, France)
Recent advances on solution phase of sparse solvers with multiple RHS
15.30 - 16.00  Break
16.00 - 16.30  Alfredo Buttari (CNRS, France)
gr_mumps: a runtime-based Sequential Task Flow parallel solver
16.30 - 17.00  François Courteille (NVIDIA, France)
Programming heterogeneous architecture with libraries: a survey of NVIDIA linear algebra libraries
17.00 - 17.30  Patrick Amestoy (INPT-ENSEEIHT)-IRIT), Abdou Guermouche (Univ. de Bordeaux), Jean-Yves L’Excellent (Inria-LIP-ENS Lyon)
MUMPS 5.1, perspectives and discussions
19.30 - 22.00  Banquet at “Le Garage” (134 Chemin de l’étoile 383330 Montbonnot)

Friday, June 2nd

9.00 - 9.30  Bob Lucas (LSTC, USA)
Block Low-Rank approximations in LS-DYNA
9.30 - 10.00  Augustin Parret-Fréaud (SAFRAN, France)
Robust domain decomposition methods for high performance computation of industrial structures
10.00 - 10.30  Pierre Jolivet (CNRS, France)
MUMPS on thousands of cores: feedback on the use of direct solvers in domain decomposition methods
10.30 - 11.00  Coffee Break
11.00 - 11.30  Rémy Perrin-Bit (Altair, France)
Brief history of time in Flux
11.30 - 12.00  Luis E. Garcia Castillo (University Carlos III of Madrid, Spain)
Higher-Order Finite Element Code for Electromagnetic Simulation on HPC Environments
12.00 - 12.30  Patrick Demichel (HPE, France)
The Machine and genZ Implications for extreme scale solver problems
12.30 - 14.00  Lunch
14.00 - 14.30  Yuri Feldman (Ben-Gurion University, Israel)
Two phase flow simulations based on Immersed boundary method, by utilizing MUMPS solver
14.30 - 15.00  Closing session (MUMPS team)

Credits

This event is supported by:

INPT ENSEEIHT  Inria  MUMPS Consortium  IRIT

Labex MILYON

23/52 MUMPS User Days — Montbonnot, June 1-2, 2017
Discussion of MUMPS parallel performance in multithreaded (MT) environments

Marie Durand
(Inria-MUMPS Consortium)
Performance study

Presentation of the study

- focus on the factorization phase (few results on solve)
- a lot of matrices tested
- comparison with direct solvers dedicated to MT environments
  ○ MKL Pardiso
  ○ HSL ma86, HSL ma87
- MUMPS evaluated over several #MPI × #OpenMP threads
- LIP grunch computer: 2x14 cores @2.30GHz - Intel Xeon E5-2695 v3
MUMPS vs others - scalability study

3D Structural Mechanics - N=1.9 M - NRHS=128
LIP grunch computer - 2x14 cores @2.30Gz - Intel Xeon E5-2695 v3

- MUMPS 5.0.1
- HSL MA86
- MKL Pardiso

Acceleration wrt MUMPS 5.0.1

Number of OpenMP Threads
Each point corresponds to a matrix and to the best time obtained on each configuration of cores.
Using MUMPS in a shared memory environment

Factorization phase - MUMPS 5.0 (Early 2016)
LIP grunch computer - 2x14 cores @ 2.30GHz - Intel Xeon E5-2695 v3

Speedup ($T_1/T_p$) vs. Number of OpenMP threads per MPI

- 3D structural mechanics
- Fluorem RM07R
- GHS_psdef apache2
- Geoazur 2D 2024
### Generic points

- 2D problems require tree-based parallelism: use MPI if possible

- For 3D problems in MT, the number of MPI can be reduced
Getting more parallelism: the tree-based multithreading

MUMPS 5.1.1: Node parallelism (MPI, OpenMP), tree parallelism (MPI only)

Node parallelism

thr0-3

thr0-3

thr0-3

thr0-3

thr0-3

Node parallelism
Getting more parallelism: the tree-based multithreading

in future MUMPS (FR++): tree parallelism (MPI, OpenMP)

---

**FR++: Tree-Based Multithreading**

- work based on W. M. Sid-Lakhdar’s PhD thesis (defended in 2014)
- under the Layer, sub-trees are distributed to threads
- above the Layer, threads work together on each node
Importance of the tree-based multithreading

- Computationally Intensive
- Not Computationally Intensive

<table>
<thead>
<tr>
<th>1 thread</th>
<th>time</th>
<th>%nci</th>
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<tbody>
<tr>
<td>FR</td>
<td>62660s (1)</td>
<td>1%</td>
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3D Poisson; $n = 256^3$ (16M); $\varepsilon = 10^{-6}$; *PhD W. Sid Lakhdar (2014)
**Importance of the tree-based multithreading**

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<tr>
<td>BLR</td>
<td>7823s (8)</td>
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<td></td>
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| 3D Poisson; $n = 256^3$ (16M); $\varepsilon = 10^{-6}$ | *PhD W. Sid Lakhdar (2014) |

*Computationally Intensive*  
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<tr>
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<td>time</td>
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<td>FR</td>
<td>62660s (1)</td>
<td>1%</td>
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- **Computationally Intensive**
- **Not Computationally Intensive**

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<th>28 threads + tree-based MT*</th>
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<td>time</td>
<td>%(_{n\text{ci}})</td>
<td>time</td>
</tr>
<tr>
<td>FR</td>
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<td>1%</td>
<td></td>
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<td>557s (7)</td>
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3D Poisson; \(n = 256^3\) (16M); \(\varepsilon = 10^{-6}\); *PhD W. Sid Lakhdar (2014)
## Importance of the tree-based multithreading

![Computationally Intensive vs Not Computationally Intensive Diagram]

### Computationally Intensive

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<td>FR</td>
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</tr>
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<td>BLR</td>
<td>7823s (8)</td>
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</tr>
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3D Poisson; $n = 256^3$ (16M); $\varepsilon = 10^{-6}$; *PhD W. Sid Lakhdar (2014)
Improvement of LDLT factorization for multithreaded configurations

Evolution of the factorization execution time - 3D Structural mechanics
LIP brunch computer - 4x24 cores @2.20GHz - Intel Xeon E7-8890 v4

Execution time [s]

- 1 x 1
- 1 x 8
3D Structural Mechanics - N=1.9 M - NRHS=128
LIP grunch computer - 2x14 cores @2.30Gz - Intel Xeon E5-2695 v3

Acceleration wrt MUMPS 5.0.1(T1)

Number of OpenMP Threads
Multi RHS solve phase (NRHS=128)
Geoazur 2D 2048 with internal granularity increase
LIP brunch computer - 4x24 cores @2.20GHz - Intel Xeon E7-8890 v4
2D problems

- switch to MUMPS 5.1.1
- improvement increasing internal granularity
- if multiple RHS, increasing the blocking factor may help
Conclusion

We just spoke about

- MUMPS with respect to other MT solvers ⇒ not so bad
- what could speed up a lot the factorization and the solve part
  - ⇒ tree-based multithreading

We haven’t spoken about

- the analysis part!
- other non computationally intensive parts
  - matrix distribution and scaling (up to 30% of the factor time on some classes of matrices)
  - memory management
  - frontal matrix assembling
MUMPS perspectives and discussions MUMPS group
CERFACS, CNRS, ENS-Lyon, INRIA, INPT, University of Bordeaux

Present and discuss ongoing work that might influence future versions and give new possibilities/perspective to users

Outline

• Preamble: recent work since MUMPS 5.1.1
• Perspectives on Block Low-Rank (BLR)
• BLR memory issues and BLR solve
• Ongoing work
Nodes of parallel computers often have multi/many cores. Good usage of such computers may mix MPI based parallelism with shared memory programming paradigms

- **To enhance performance** we are working on:
  - Strategies to map MPI tasks on processors
  - Dynamic scheduling, multithreading
  - Multi-level blocking for performance and communication
  - Processing the elimination tree for performance
  - Increase of BLAS3 usage in case pivoting is not requested

- **Aggressive optimization** setting has been designed
  → referred to as **MUMPS FR +**
### Timings in seconds

<table>
<thead>
<tr>
<th>Electromagnetism, M1ms1</th>
<th>N=0.5 M</th>
<th>[\text{MPI} \times \text{threads}]</th>
<th>[\text{FR} + ]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 \times 1</td>
<td>1080</td>
<td>1080</td>
<td></td>
</tr>
<tr>
<td>1 \times 28</td>
<td>109</td>
<td>108</td>
<td></td>
</tr>
<tr>
<td>28 \times 1</td>
<td>125</td>
<td>88</td>
<td></td>
</tr>
<tr>
<td>[\text{RES}_\infty]</td>
<td></td>
<td>[1 \times 10^{-5}]</td>
<td></td>
</tr>
</tbody>
</table>

**Advanced FR + → gains when using MPI**
What about multithreading and BLR?

- gain in flops (black line) does not fully translate into gain in time
- average multithreaded efficiency lower in LR than in FR

⇒ improve efficiency of operations and multithreading with variants
More Performance?

FR ++: Tree-Based Multithreading (see M. Durand’s talk)

- work based on W. M. Sid-Lakhdar’s PhD thesis (defended in 2014)

MUMPS is compared here to MKL Pardiso referred to as Pard

### Timings in seconds - unsymmetric single precision complex

<table>
<thead>
<tr>
<th>Matrix M1ms1</th>
<th>Matrix M1ms2</th>
<th>Matrix M3ms1</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Pard</strong></td>
<td><strong>MUMPS</strong></td>
<td><strong>MUMPS</strong></td>
</tr>
<tr>
<td><strong>FR +</strong></td>
<td><strong>FR ++</strong></td>
<td><strong>FR +</strong></td>
</tr>
<tr>
<td><strong>FR ++</strong></td>
<td><strong>FR ++</strong></td>
<td><strong>FR ++</strong></td>
</tr>
</tbody>
</table>

Using 1 or 28 OpenMP Threads – No BLR

<table>
<thead>
<tr>
<th>2x14 cores @ 2.30GHz - Intel Xeon E5-2695 v3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pard</td>
</tr>
<tr>
<td>FR +</td>
</tr>
<tr>
<td>1 369</td>
</tr>
<tr>
<td>28 21</td>
</tr>
</tbody>
</table>

- on this class of matrices: performance limited by sequential parts (scaling, matrix distribution)
**Multithreading non computationally intensive parts**

<table>
<thead>
<tr>
<th></th>
<th>FR+ 1 core</th>
<th>FR+ 28 cores</th>
<th>FR++ 28 cores</th>
</tr>
</thead>
<tbody>
<tr>
<td>Factorization</td>
<td>274</td>
<td>57</td>
<td>20</td>
</tr>
<tr>
<td>Scaling+preparation</td>
<td>10</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>Total JOB=2</td>
<td>284</td>
<td>67</td>
<td>30</td>
</tr>
</tbody>
</table>

This will become even critical in the future

**Even more critical in BLR**

<table>
<thead>
<tr>
<th></th>
<th>FR</th>
<th>BLR</th>
<th>BLR (with FR ++)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S3 (3D EM modelling), times in seconds, 28 cores</td>
<td>585</td>
<td>324</td>
<td>239</td>
</tr>
</tbody>
</table>

More generally, multithread all non computationally intensive parts will become even more critical in the future.
Perspectives on Block Low-Rank feature

Expose part of recent work presented in T. Mary’s talk


- Amestoy, Buttari, L’Excellent, and Mary. *Block Low-Rank Multifrontal Factorization on Multicore Architectures*, Submitted to ACM Transactions on Mathematical Software.

- **Left-looking factorization:**
  lower volume of memory transfers in BLR

- **Low-rank Updates with Accumulation** (so called LUA):
  increases the GFlops/s rate of the low-rank based update operations.

- Compression is performed before the solve steps:
  additional reduction in the number of operations

→ referred to as **BLR †** (it includes **FR ‡‡**)

43/52
Results on complete set of problems on 24 threads

Normalized time (FR=1)

FR
FR++
BLR
BLR++

44/52 MUMPS User Days — Montbonnot, June 1-2, 2017
BLR memory issues and BLR solve

Factors: Working mem.
L, U: Front CB

State: FR children have produced a CB (FR subtrees finished)
BLR memory issues and BLR solve

Factors Working mem.
L, U front CB

State: Memory for parent reserved
BLR memory issues and BLR solve

factors Working mem. L, U front CB

State: Parent assembled (children CB consumed)
BLR memory issues and BLR solve

- factors
- Working mem.
- L, U
- FR
- LR
- State: Parent assembled (children CB consumed)
BLR memory issues and BLR solve

Factors Working mem.
L, U front CB

State: FR factorization of parent
BLR memory issues and BLR solve

Factors Working mem.
L, U front CB

State: Stacked FR factors and FR CB

Matrix from SEISCOPE 10Hz (3D seismic imaging, N: 17M, NNZ: 446M)

<table>
<thead>
<tr>
<th>Factor size/proc</th>
<th>FR</th>
<th>BLR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 proc</td>
<td>711 GB</td>
<td></td>
</tr>
<tr>
<td>90 procs</td>
<td></td>
<td>8 GB</td>
</tr>
</tbody>
</table>

Memory efficiency: perfect for factors
BLR memory issues and BLR solve

Matrix from SEISCOPE 10Hz (3D seismic imaging, N: 17M, NNZ: 446M)

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</thead>
<tbody>
<tr>
<td>1 proc</td>
<td>711 GB</td>
<td>175 GB</td>
</tr>
<tr>
<td>90 procs</td>
<td>8 GB</td>
<td>2 GB</td>
</tr>
</tbody>
</table>

\textbf{Memory efficiency:} perfect for factors
BLR memory issues and BLR solve

Reminding current BLR characteristics (MUMPS 5.1):

- Memory not reduced
- Compression used to accelerate factorization
- Factors in full-rank (approximated) form stored in memory for current FR solve to work

BLR solve

- Reduce memory usage:
  - keep BLR factors during factorization (for use during solve)
  - Memory used: Working memory (tend to OOC size with compression)
    + FR factors of small fronts + BLR factors
- Reduce flops/memory accesses during solve
BLR-related memory issues (factorization)

Matrix from SEISCOPE 10Hz (3D seismic imaging, \(N: 17M, \text{NNZ: 446M}\))

<table>
<thead>
<tr>
<th>Factors/proc</th>
<th>Working mem./proc</th>
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<tbody>
<tr>
<td></td>
<td>FR</td>
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<tr>
<td>1 proc</td>
<td>711 GB</td>
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</tr>
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</table>

Memory efficiency: perfect for factors; bad for working memory (12/90)
BLR-related memory issues (factorization)

Factors/proc | Working mem./proc
---|---
FR | BLR
1 proc | 711 GB | 175 GB | 87 GB | 9 GB
90 procs | 8 GB | 2 GB | 7 GB | 1 GB

Memory efficiency: perfect for factors; bad for working memory (12/90)
Good news: working memory has greater potential for compression
BUT at the cost of an increase in compression flops
BLR-related memory issues (factorization)

Factors Working mem.
L, U front CB

Matrix from SEISCOPE 10Hz (3D seismic imaging, \textbf{N: 17M, NNZ: 446M})

<table>
<thead>
<tr>
<th></th>
<th>Total</th>
<th>Within fronts</th>
<th>Between fronts</th>
</tr>
</thead>
<tbody>
<tr>
<td>FR</td>
<td>5.1 TB</td>
<td>3.0 TB</td>
<td>2.0 TB</td>
</tr>
<tr>
<td>BLR (5.1.1)</td>
<td>2.3 TB</td>
<td>0.3 TB</td>
<td>2.0 TB</td>
</tr>
<tr>
<td>BLR (if compressed CB)</td>
<td>0.5 TB</td>
<td>0.3 TB</td>
<td>0.2 TB</td>
</tr>
</tbody>
</table>

Volume of communication (90 MPI procs)
Factors and CB blocks can be compressed BUT compression factor not known in advance!

- Provide memory estimates at analysis?

Compression of CBs
- offers a great potential but at the cost of extra compression
- could also reduce communication volume
- To be understood: how to compromise flops increase and memory reduction objectives
Much active research and perspectives

- Performance related
  - Performance of the solution phase
  - Improve quality of memory estimates
  - Improve parallel efficiency

- BLR-related
  - New BLR variants, improved compression and further reduce complexity (collaboration with LSTC)
  - Comparisons with HSS (LBNL collab.)
  - MPI/OpenMP performance and scalability
  - Exploit BLR format during solution phase and compress memory during factorization

- Performance of solution phase
  - Sometimes critical (electromagnetism, geophysics, DD, . . .)
  - MPI/OpenMP scalability (e.g. mapping of factors for solve?)
  - Sparsity of right-hand sides: flops reduction versus parallelism?

Work often related to the PhD thesis of T. Mary and G. Moreau
Closing Session
Concluding remarks

Statistics about workshop

- **61 participants** (Belgium, France, Greece, Israel, Italy, Norway, Saudi Arabia, South Africa, Spain, USA), 45 have participated to the banquet
  - 39 industrials
  - 22 academics

- **18 talks** (MUMPS overview and recent features, 2 talks from MUMPS PhD students, 9 talks from industrials, 3 from public researchers using MUMPS, 2 talks from MUMPS team, Perspectives and discussion)

Next MUMPS usersday

- Change format (talks, duration) ?
- When and Where ?

51/52
Merci à Inria pour son accueil

Merci aux organisateurs:
Marie Durand, Guillaume Joslin, Chiara Puglisi