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To cite this version:
Grégoire Pichon, Eric Darve, Mathieu Faverge, Pierre Ramet, Jean Roman. Sparse Supernodal Solver exploiting Low-Rankness Property. Sparse Days 2017, Sep 2017, Toulouse, France. hal-01585622

HAL Id: hal-01585622
https://inria.hal.science/hal-01585622
Submitted on 2 Oct 2017

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Sparse Supernodal Solver exploiting Low-Rankness Property

September 6th, 2017 - Sparse Days

Grégoire Pichon\textsuperscript{a}, Eric Darve\textsuperscript{b}, Mathieu Faverge\textsuperscript{a}, Pierre Ramet\textsuperscript{a}, Jean Roman\textsuperscript{a}

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Introduction

Current sparse direct solver for 3D problems

- $\Theta(n^2)$ time complexity
- $\Theta(n^{4/3})$ memory complexity
- BLAS 3 operations

Block Low-Rank solver

- Large blocks are compressed into a low-rank form
- Operations keep untouched the global behaviour of PASTIX
- Minimal Memory strategy allows to save memory
- Just-In-Time strategy allows to reduce time-to-solution

Objective: build an algebraic low-rank solver following the supernodal approach of PASTIX, with block-data structures
Symbolic Factorization

General approach

1. Build a partition with the nested dissection process
2. Compress information on data blocks
3. Compute the block elimination tree using the block quotient graph

Adjacency graph \((G)\)

Quotient graph \((G^*/P) = (G/P)^*\)

Elimination tree \((T)\)

Factorized matrix \((L)\)
Numerical Factorization

Algorithm to eliminate the column block $k$:

1. **Factorize** the diagonal block (POTRF/GETRF)
2. **Solve** off-diagonal blocks in the current column (TRSM)
3. **Update** the trailing matrix with the column’s contribution (GEMM)

Parallelism:
- Right-Looking
- Left-Looking
Large off-diagonal are low-rank, in the form $uv^t$. 

Block-Low-Rank Compression – Symbolic Factorization
### Some Related Works

**Block Low-Rank solvers**

- BLR-MUMPS introduced an approach focused on reducing the time to solution which is close to our *Just-In-Time* strategy
- LSTC developed compression/recompression techniques in a dense context

**Other approaches for sparse**

- Strumpack HSS by Ghysels et al. utilizes randomized sampling to perform an efficient extend-add
- HODLR by Darve et al. uses pre-selection of rows and columns (BDLR)
- $\mathcal{H}$-LU by Hackbusch et al. does not fully exploit the symbolic factorization
Block-Low-Rank Algorithm

Approach
- Large supernodes are partitioned into a set of smaller supernodes
- Large off-diagonal blocks are represented as low-rank blocks

Operations
- Diagonal blocks are dense
- TRSM are performed on low-rank off-diagonal blocks
- GEMM are performed between low-rank off-diagonal blocks. It creates contributions to dense or low-rank blocks: this is the extend-add problem

Compression techniques
- SVD, RRQR for now
- Possible extension to any algebraic method: ACA, randomized techniques...
**Strategy Just-In-Time**

**Compress \( L \)**

1. Eliminate each column block
   1.1 Factorize the dense diagonal block
       Compress off-diagonal blocks belonging to the supernode
   1.2 Apply a TRSM on LR blocks (cheaper)
   1.3 LR update on dense matrices (\( LR2GE \) extend-add)

2. Solve triangular systems with low-rank blocks
Strategy *Just-In-Time*

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2. Solve triangular systems with low-rank blocks
Strategy *Minimal Memory*

**Compress \( A \)**

1. Compress large off-diagonal blocks in \( A \) (exploiting sparsity)
2. Eliminate each column block
   - 2.1 Factorize the dense diagonal block
   - 2.2 Apply a TRSM on LR blocks (cheaper)
   - 2.3 LR update on LR matrices (\( LR2LR \) extend-add)
3. Solve triangular systems with LR blocks
Strategy *Minimal Memory*

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1. Compress large off-diagonal blocks in $A$ (exploiting sparsity)
2. Eliminate each column block
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3. Solve triangular systems with LR blocks
Comparison of both strategies

Memory consumption

- **Minimal Memory** strategy really saves memory
- **Just-In-Time** strategy reduces the size of $L'$ factors, but supernodes are allocated dense at the beginning: no gain in pure right-looking

Low-Rank extend-add

- **Minimal Memory** strategy requires expensive extend-add algorithms to update (recompress) low-rank structures with the $LR2LR$ kernel
- **Just-In-Time** strategy continues to apply dense update at a smaller cost through the $LR2GE$ kernel
Focus on the *LR2LR* kernel

- Update of $C$ with contribution from blocs $A$ and $B$
- The low-rank matrix $u_{AB}v_{AB}^t$ is added to $u_Cv_C^t$
- $u_{AB}v_{AB}^t = (u_A(v_A^t v_B))u_B^t$ or $u_{AB}v_{AB}^t = u_A((v_A^t v_B)u_B^t)$
- Eventually, recompression of $(v_A^t v_B)$
**LR2LR kernel using SVD**

A low-rank structure $u_C v_C^t$ receives a low-rank contribution $u_{AB} v_{AB}^t$.

**Algorithm**

\[
A = u_C v_C^t + u_{AB} v_{AB}^t = ([u_C, u_{AB}]) \times ([v_C, v_{AB}])^t
\]

- QR: $[u_C, u_{AB}] = Q_1 R_1 \Theta(m(r_C + r_{AB})^2)$
- QR: $[v_C, v_{AB}] = Q_2 R_2 \Theta(n(r_C + r_{AB})^2)$
- SVD: $R_1 R_2^t = u\sigma v^T \Theta((r_C + r_{AB})^3)$

\[
A = (Q_1 u\sigma) \times (Q_2 v)^t
\]

Optimizations using RRQR to reduce complexity to $\Theta(n(r_C + r_{AB})r_C^*)$
Experimental setup

Machine: 2 INTEL Xeon E5 – 2680v3 at 2.50 GHz
- 128 GB
- 24 threads

3D Matrices from The SuiteSparse Matrix Collection
- *Audi*: structural problem (943 695 dofs)
- *Atmosmodj*: atmospheric model (1 270 432 dofs)
- *Geo1438*: geomechanical model of earth (1 437 960 dofs)
- *Hook*: model of a steel hook (1 498 023 dofs)
- *Serena*: gas reservoir simulation (1 391 349 dofs)
- + Laplacian: Poisson problem (7-points stencil)

Parallelism is obtained following PASTIX static scheduling for multi-threaded architectures
# Parameters

## Entry parameters
- Tolerance $\tau$: absolute parameter (normalized for each block)
- Compression method: SVD or RRQR
- Compression strategy: *Minimal Memory* or *Just-In-Time*
- Blocking sizes: between 128 and 256 in following experiments

## Strategy *Minimal Memory*
- Blocks are compressed at the beginning
- Each contribution implies a recompression

## Strategy *Just-In-Time*
- Blocks are compressed just before a supernode is eliminated
- Those blocks are never uncompressed
Costs distribution on the Atmosmodj matrix with $\tau = 10^{-8}$

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</table>
Behaviour of RRQR/Minimal Memory

![Graphs showing performance and memory footprint comparisons for different datasets and values of τ.](image)

**Performance**

**Memory footprint**
Performance of RRQR/Just-In-Time

\[ \tau = 10^{-4} \quad \tau = 10^{-8} \quad \tau = 10^{-12} \]

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Time BLR / Time PaStiX</th>
</tr>
</thead>
<tbody>
<tr>
<td>lap120</td>
<td>0.45</td>
</tr>
<tr>
<td>atmosmodj</td>
<td>0.62</td>
</tr>
<tr>
<td>audi</td>
<td>0.89</td>
</tr>
<tr>
<td>Geo1438</td>
<td>1.00</td>
</tr>
<tr>
<td>Hook</td>
<td>0.88</td>
</tr>
<tr>
<td>Serena</td>
<td>0.85</td>
</tr>
</tbody>
</table>
Convergence of RRQR/Minimal Memory

\[ \tau = 10^{-4} \]

\[ \tau = 10^{-8} \]

Backward error: \( \|Ax - b\|_2 \)
\( \|b\|_2 \)

Number of refinement iterations

0 5 10 15 20

10^{-14}
10^{-13}
10^{-12}
10^{-11}
10^{-10}
10^{-9}
10^{-8}
10^{-7}
10^{-6}
10^{-5}
10^{-4}
10^{-3}
10^{-2}

\text{audi}
\text{Geo1438}
\text{Hook}
\text{Serena}
\text{lap120}
\text{atmosmodj}
Scaling on Laplacians: Memory Consumption
RRQR/Minimal Memory

Factors size, full rank
Factors size, $\tau = 10^{-4}$
Factors size, $\tau = 10^{-8}$
Factors size, $\tau = 10^{-12}$
Ongoing work with E. Esnard and M. Predari

- Single interaction between $S$ and $S_A \cup S_B$ in the original graph
- Two large interaction blocks $P_{A_1} \cup P_{B_1}$ and $P_{A_2} \cup P_{B_2}$ during the factorization

- Double interaction: between $S$ and $S_A$ and between $S$ and $S_B$ in the original graph
- Three “large” interaction blocks during the factorization
Example on a $200^2$ Laplacian

Scotch ordering

Aligned ordering
Conclusion

**Block Low-Rank solver**
- Allows to see how to use the symbolic structure and the extend-add issues in a supernodal context
- The version presented follows the parallelism of PASTIX
- On-going work to implement efficiently this approach over the PARSEC runtime system

**Ordering strategies**
- Study of a nested dissection designed to increase compressibility
- Add pre-selection to isolate data which is not compressible, and thus reduce the overhead of trying to compress uncompressed blocks
PASTIX 6.0.0alpha is now available!
http://gitlab.inria.fr/solverstack/pastix

- Support shared memory with different schedulers:
  - sequential
  - static scheduler
  - PaRSEC runtime system
- Low-rank support
- Cholesky and LU factorizations

Thank you.