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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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\textsuperscript{b}Stanford University
**Introduction**

Current sparse direct solver for 3D problems

- $\Theta(n^2)$ time complexity
- $\Theta(n^{\frac{4}{3}})$ 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 \((T)\).
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 $uv^t$
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
   1.2 Compress off-diagonal blocks belonging to the supernode
   1.3 Apply a TRSM on LR blocks (cheaper)
   1.4 LR update on dense matrices (\( LR2GE \) extend-add)

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

Compress $L$

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   1.3 LR update on dense matrices (*LR2GE* extend-add)

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*

**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*

**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)**
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Strategy *Minimal Memory*

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   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
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 $u_Cv_C^t$
- $u_{AB}v_{AB}^t = (u_A(v_A^tv_B))u_B^t$ or $u_{AB}v_{AB}^t = u_A((v_A^tv_B)u_B^t)$
- Eventually, recompression of $(v_A^tv_B)$
LR2LR kernel using SVD

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

Algorithm

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

- 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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Behaviour of RRQR/Minimal Memory

Performance

Memory footprint
Performance of RRQR/Just-In-Time

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

Time BLR / Time PaStiX

G. Pichon – Sparse Supernodal Solver exploiting Low-Rankness Property
Convergence of RRQR/Minimal Memory

$\tau = 10^{-4}$

$\tau = 10^{-8}$

Backward error: $\frac{|Ax-b|}{|b|}$

Number of refinement iterations

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

G. Pichon – Sparse Supernodal Solver exploiting Low-Rankness Property
Scaling on Laplacians: Memory Consumption
RRQR/Minimal Memory

Factors size, full rank
Factors size, $\tau = 10^{-4}$
Factors size, $\tau = 10^{-8}$
Factors size, $\tau = 10^{-12}$

Size

Memory consumption (GB)

Factors size, full rank
Factors size, $\tau = 10^{-4}$
Factors size, $\tau = 10^{-8}$
Factors size, $\tau = 10^{-12}$

100
110
120
130
140
150
160
170
180
190
200
210
220
230

G. Pichon – Sparse Supernodal Solver exploiting Low-Rankness Property
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.