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Supernodes ordering to enhance Block Low-Rank compression in sparse direct solvers

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## Context

### PaStiX library

- Sparse direct solver with supernodal method
- Right-looking scheduling strategy
- Block low-rank support:
  - Large blocks are compressed into a low-rank form
  - Similar global behavior to the full-rank solver
  - *Minimal Memory* strategy to save memory
  - *Just-In-Time* strategy to reduce time-to-solution

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**Objective of this talk**: study low-rank clustering strategies to enhance blocks compressibility
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
From full-rank to low-rank

Full-rank algorithm

- For each column-block / supernode:
  1. **Factorize** the diagonal block (POTRF/GETRF)
  2. **Solve** off-diagonal blocks in the current column (TRSM)
  3. **Update** the trailing matrix (GEMM)
From full-rank to low-rank

Just-In-Time algorithm

- For each column-block / supernode:
  1. **Factorize** the diagonal block (POTRF/GETRF)
  2. **Compress** off-diagonal blocks
  3. **Solve** low-rank off-diagonal blocks in the current column (TRSM)
  4. **Update** the trailing matrix (LR2FR)

- Reduce the time to solution
- Memory peak is as large as full-rank
From full-rank to low-rank

**Minimal Memory algorithm**

- Compress all off-diagonal blocks
- For each column-block / supernode:
  1. **Factorize** the diagonal block (POTRF/GETRF)
  2. **Solve** low-rank off-diagonal blocks in the current column (TRSM)
  3. **Update** the trailing matrix (LR2LR)

- Reduce the memory peak of the solver
- LR2LR updates may be too costly for small cases
Performance of RRQR/Just-In-Time

Time BLR / Time PaStiX

\(\tau = 10^{-4}\) \(\tau = 10^{-8}\) \(\tau = 10^{-12}\)

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Performance of RRQR/Minimal Memory

Factorization time

Memory footprint

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Scalability of *Minimal Memory* strategy on Laplacian matrices

- 128GB of memory
- Up to 8M unknowns in full-rank
- Up to 36M unknowns with \( \tau = 10^{-4} \)
Up to what limit?

- 96 cores machine with 3TB of memory
- $100 \times 100 \times 100K$ mesh
- Full-rank would have required $11TB$ of memory
- With $\tau = 10^{-4}$:
  - Only $2TB$ of memory for the coefficients
  - Less than 6 hours to factorize
  - $10^{-8}$ solution with 15 iterations of iterative refinement
Summary of the updates

Cost of applying a $m \times n$ update to a $M \times N$ block.

Full rank

- A single GEMM kernel
- Cost depends on $mn$
Summary of the updates

Cost of applying a $m \times n$ update to a $M \times N$ block.

**Full rank**
- A single GEMM kernel
- Cost depends on $mn$

**Just-In-Time**
- Serie of small GEMM kernels
- Cost depends on $mn$
Summary of the updates

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**Minimal Memory**
- Complex extend-add operation
- Cost depends on $MN$
Summary of the updates

Cost of applying a $m \times n$ update to a $M \times N$ block.

Full rank
- A single GEMM kernel
- Cost depends on $mn$

Just-In-Time
- Serie of small GEMM kernels
- Cost depends on $mn$

Minimal Memory
- Complex extend-add operation
- Cost depends on $MN$

Can we reduce the number of those problematic updates?
1

Block Low-Rank clustering techniques
Clustering techniques: existing solutions

- Supernode reordering techniques (supernodal)

8 × 8 × 8 Laplacian partitioned using SCOTCH and Reordering clustering on the first separator
Clustering techniques: existing solutions

- Supernode reordering techniques (supernodal)
- k-way partitioning (dense, multifrontal)

(a) Symbolic factorization  
(b) First separator clustering

$8 \times 8 \times 8$ Laplacian partitioned using SCOTCH and k-way clustering on the first separator
How to take benefit from both algorithms?

Pre-selection to detect uncompressed vertices

- Pre-select unknowns that represent close interactions and will not be compressible
- Idea of Boundary Distance Low-Rank (BDLR) introduced by Darve et al.
- For instance, pre-select interactions between a father and its direct children
- Hypothesis similar to ILU($k$) factorizations
How to take benefit from both algorithms?


**Figure 4.2.** Active DOFs at each level $\ell$ of HIF-DE in 3D.
New heuristic based on projections

Let's consider a supernode and the $nblvl$ levels below in the elimination tree, with the constraint that nodes are issued from nested dissection, and not from minimum-fill as it happens at the bottom of the elimination tree.

- Each vertex of the separator being clustered is pre-selected iff it is a neighbor to one of the children at a distance $distp$.
- The trace is then enlarged with neighbors within the separator at a distance $width$, similarly to BDLR.

ComputeProjections($nblvl, distp, width$)
ComputeProjections( $nblvl$, $distp$, $width$ )

Let's consider a supernode and the $nblvl$ levels below in the elimination tree, with the constraint that nodes are issued from nested dissection, and not from minimum-fill as it happens at the bottom of the elimination tree.

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- The trace is then enlarged with neighbors within the separator at a distance $width$, similarly to BDLR.

How to control the number of pre-selected vertices?

- Ensure that this number is low wrt to the total number of vertices of a separator: $\#selected < \alpha \sqrt{n}$
- Ensure that it creates at least two non-connected components.
Proposed algorithm for the clustering of supernodes

**Algorithm 1** Cluster a supernode

1: ConnectSupernode( dist )
2: ComputeProjections( levels, distp, width )
3: IsolateConnectedComponents()
4: **For** each connected component \( C \) **Do**
5: \[ \text{If } |C| < \text{threshold} \text{ Then} \]
6: \[ \text{Merge } C \text{ into pre-selected vertices} \]
7: \[ \text{Else} \]
8: \[ \text{Kway()} \]
9: \[ \text{Reordering()} \]
10: \[ \text{End If} \]
11: **End For**
12: Reordering() of pre-selected vertices

Projections are performed on separators of size larger than \( 16 \times MAX\_BLOCKSIZE \), to obtain at least four large connected subparts that will be split into four parts using kway.
Example - $80^3$ Laplacian matrix
Numerical Experiments
Experimental setup

Architecture
- 2 Intel Xeon E5 – 2680v3 at 2.50 GHz (24 threads)
- 128 GB

Matrices
- 33 square matrices from the SuiteSparse Matrix Collection
- real or complex
- $50K \leq N \leq 5M$
- $nb_{ops} > 1TFlops$

Solver
- PASTIX solver with SCOTCH ordering
- Static scheduling
Parameters

BLR solver

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

Pre-selection

- Graphs are reconnected using distance 1 in the Halo
- Selected vertices are obtained with $\text{ComputeProjections}(3,1,1)$
- Projections are performed on supernodes of size larger than 16 times the blocking size parameters.
- K-way is configured to get partition fitting the blocking size parameters
- Connected components smaller than the minimal size for low-rank compression are merged into the pre-selected vertices set.
Performance profile of the factorization time – *Minimal Memory*

![Graph showing performance profile](image)

- Overhead percentage wrt the optimal
- Number of matrices
- Factorization time

Options for reordering:
- Projection
- K-way
- Reordering

Parameters:
- $10^{-8}$
- $10^{-12}$
Performance profile of the memory consumption – *Minimal Memory*

![Graph showing the performance profile of memory consumption](image)

- **Projection**
- **K-way**
- **Reordering**

**Graph Details**:
- X-axis: Overhead percentage wrt the optimal
- Y-axis: Number of matrices
- Two scenarios illustrated: $1 \times 10^{-8}$ and $1 \times 10^{-12}$

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Performance profile of the factorization time – *Just-In-Time*

![Graph showing performance profile of factorization time](image-url)
Performance profile of the memory consumption – Just-In-Time

![Graph showing memory consumption profile](image-url)
Conclusion

Ordering strategies

• Both reordering and k-way are limited to form suitable clusters
  ▶ reordering does not allow a good compression of separators
  ▶ k-way compresses well the separators, but does not take into account updates

• Pre-selection of some unknowns allows to obtain well-separated clusters and to exhibit non-compressible operations

• We demonstrated it is suitable for reducing time-to-solution with only a small memory consumption increase
Conclusion

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Future works

• Align separators to form clusters during the nested dissection process
• Preliminary work using fixed vertices
Conclusion

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Future works

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• Preliminary work using fixed vertices
Support shared memory with different schedulers:
  ▶ sequential
  ▶ static scheduler
  ▶ PARSEC/STARPU runtime systems with experimental GPU support

Low-rank support

Cholesky, $LDL$ and $LU$ factorizations

GMRES, CG, BiCG iterative refinements

Thank you.