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

June 28th, 2018 - PMAA

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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

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

Adjacency graph ($G$).

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

Elimination tree (T).

Factorized matrix ($L$).
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

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

Time BLR / Time PaStiX

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

<table>
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<td>1.8e-12</td>
</tr>
</tbody>
</table>

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Performance of RRQR/Minimal Memory

Factorization time

Memory footprint
Scalability of *Minimal Memory* strategy on Laplacian matrices

- 128GB of memory
- Up to 8$M$ unknowns in full-rank
- Up to 36$M$ 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
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**Just-In-Time**
- Serie of small GEMM kernels
- Cost depends on $mn$
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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)

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

Pre-selection to detect uncompressible 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(κ) factorizations
How to take benefit from both algorithms?


![Diagram](image)

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

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.

- 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.
New heuristic based on projections

ComputeProjections\left(nblvl, distp, width\right)

Lets 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.

How to control the number of pre-selected vertices?

- Ensure that this number if 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: If $|C| < threshold$ Then
6: Merge $C$ into pre-selected vertices
7: Else
8: Kway()
9: Reordering()
10: End If
11: End For
12: Reordering() of pre-selected vertices

Projections are performed on separators of size larger than $16 \times MAX\_BLOCK\_SIZE$, 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 \texttt{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 the performance profile of factorization time](image)

- **x-axis**: Overhead percentage wrt the optimal
- **y-axis**: Number of matrices
- **Legend**:
  - Red: Projection
  - Green: K-way
  - Blue: Reordering

The graph compares the overhead percentage against the number of matrices for different factorization times (1e-8 and 1e-12). It illustrates the efficiency and overhead characteristics of different reordering methods and the impact of varying factorization times on the performance profile.
Performance profile of the memory consumption – **Minimal Memory**

![Graph showing performance profile of memory consumption]

- **Overhead percentage wrt the optimal**
- **Number of matrices**
- **Memory consumption**

- **1e−8**
- **1e−12**

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

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

![Graph showing performance profile of factorization time](image)

- **Y-axis:** Number of matrices
- **X-axis:** Overhead percentage wrt the optimal
- **Legend:**
  - Red: Projection
  - Green: K-way
  - Blue: Reordering

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Performance profile of the memory consumption – *Just-In-Time*

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

- **Overhead percentage wrt the optimal**
- **Number of matrices**
- **Memory consumption**

- **1e-8**
- **1e-12**

Different curves represent different methods:
- **Projection**
- **K-way**
- **Reordering**
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
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Future works

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

- Align separators to form clusters during the nested dissection process
- 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.