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

June 28th, 2018 - PMAA

Grégoire Pichon<sup>a</sup>, Eric Darve<sup>b</sup>, Mathieu Faverge<sup>a</sup>, Pierre Ramet<sup>a</sup>, Jean Roman<sup>a</sup>

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## Context

### PaStiX library

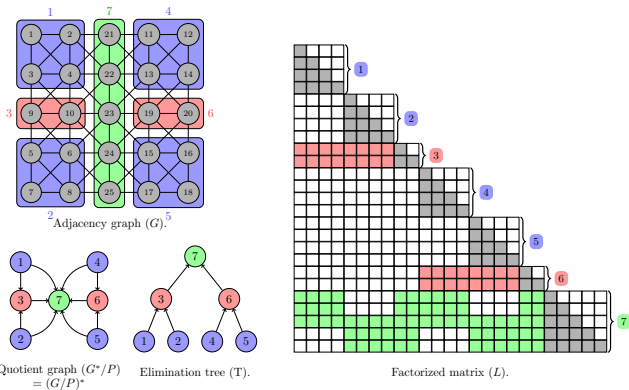
- Sparse direct solver with supernodal method
- Right-looking scheduling strategy
- Block low-rank support:
  - ▶ Large blocks are compressed into a low-rank form
  - ▶ Similar global behavior to the full-rank solver
  - ▶ *Minimal Memory* strategy to save memory
  - ▶ *Just-In-Time* strategy to reduce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

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

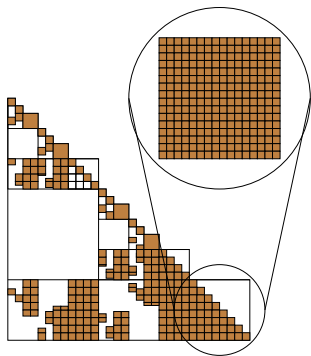
# Symbolic Factorization

## 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



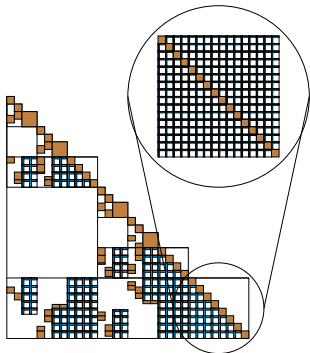
## From full-rank to low-rank



### 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)

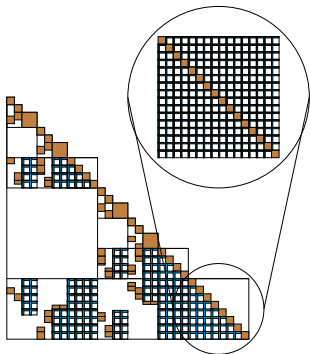
## From full-rank to low-rank



### *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

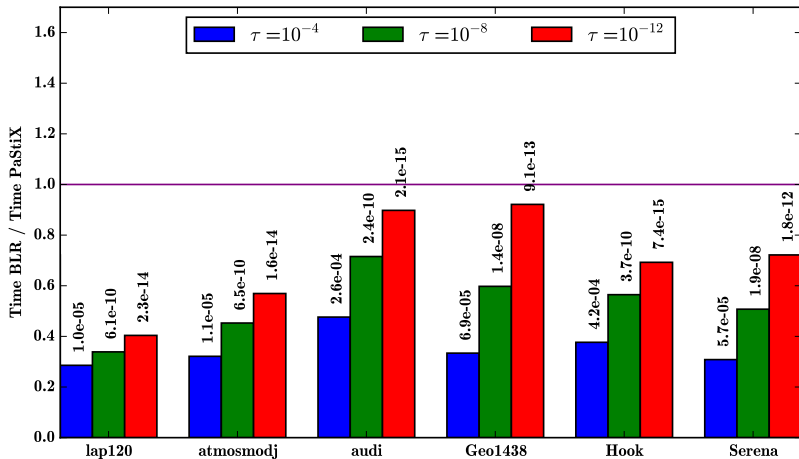
## From full-rank to low-rank



### Minimal Memory algorithm

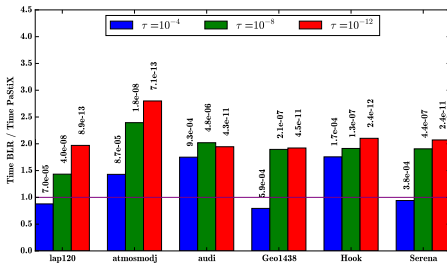
- Compress all off-diagonal blocks
  - For each column-block / supernode:
    1. **Factorize** the diagonal block (POTRF/GETRF)
    2. **Solve** low-rank off-diagonal blocks in the current column (TRSM)
    3. **Update** the trailing matrix (LR2LR)
- 
- Reduce the memory peak of the solver
  - LR2LR updates may be too costly for *small* cases

## Performance of RRQR/*Just-In-Time*

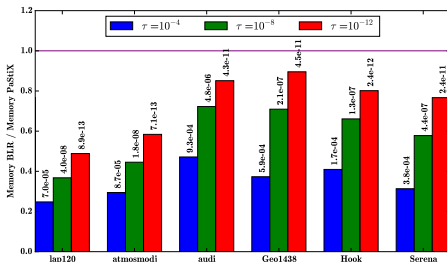




# Performance of RRQR/Minimal Memory

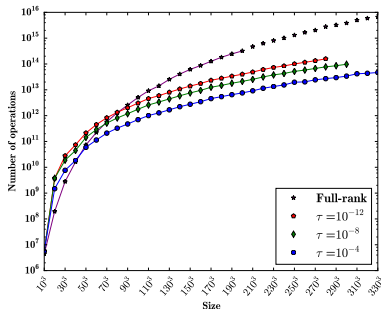
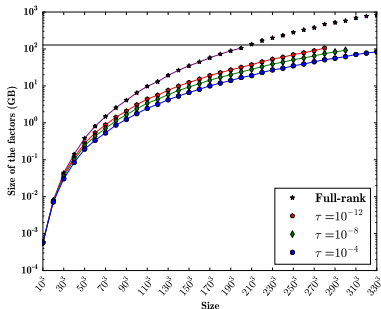


Factorization time



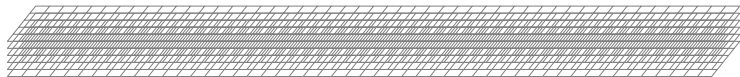
Memory footprint

# Scalability of *Minimal Memory* strategy on Laplacian matrices



- 128GB of memory
- Up to 8M unknowns in full-rank
- Up to 36M unknowns with  $\tau = 10^{-4}$

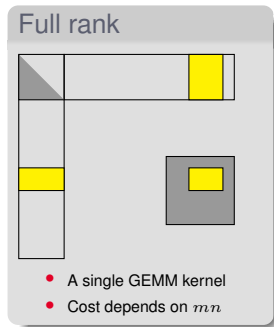
## Up to what limit?



- 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

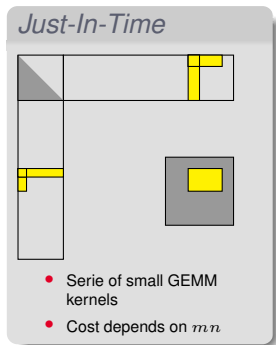
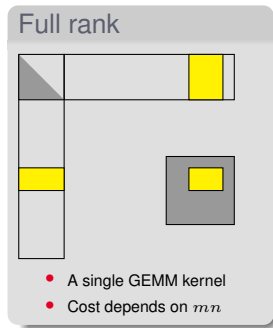
## Summary of the updates

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



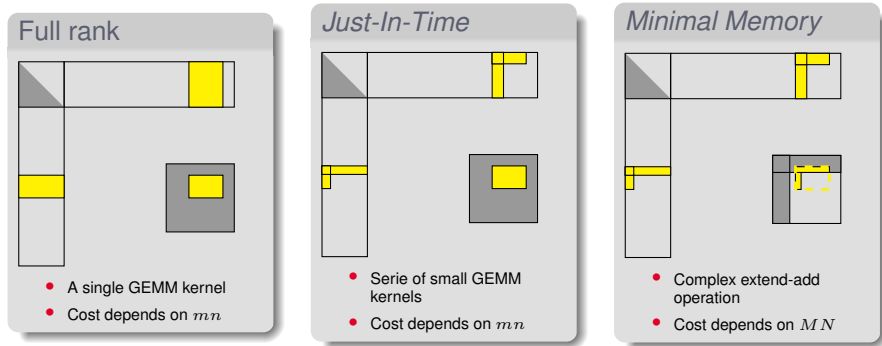
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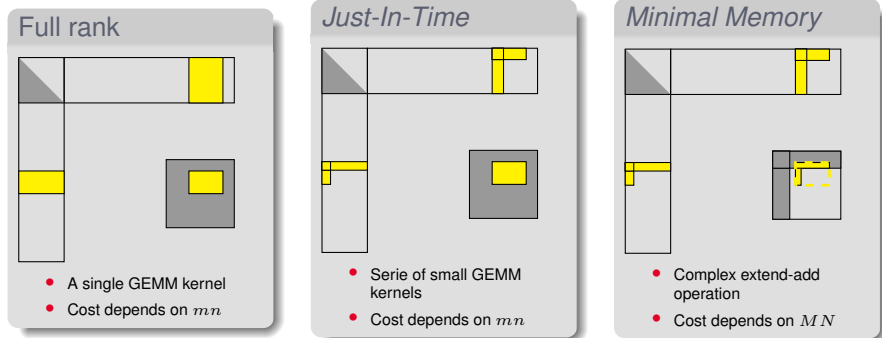
## Summary of the updates

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



## Summary of the updates

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



Can we reduce the number of those problematic updates?

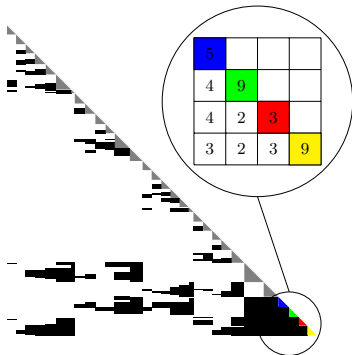
# 1

## Block Low-Rank clustering techniques

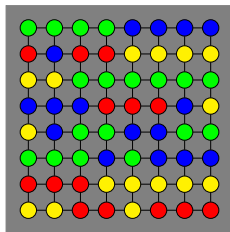


## Clustering techniques: existing solutions

- Supernode reordering techniques (supernodal)



(a) Symbolic factorization

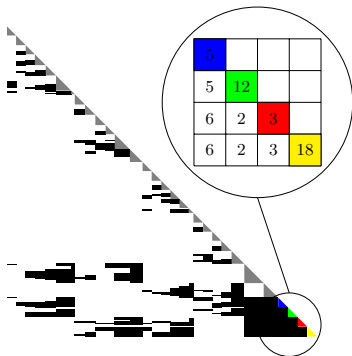


(b) First separator clustering

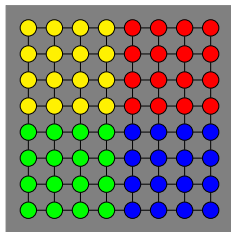
$8 \times 8 \times 8$  Laplacian partitioned using SCOTCH and Reordering clustering on the first separator

## Clustering techniques: existing solutions

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



(a) Symbolic factorization



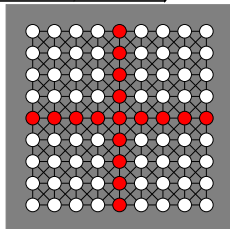
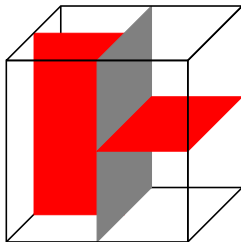
(b) First separator clustering

$8 \times 8 \times 8$  Laplacian partitioned using SCOTCH and k-way clustering on the first separator

## How to take benefit from both algorithms?

Pre-selection to detect 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  $ILU(k)$  factorizations



## How to take benefit from both algorithms?

*Hierarchical Interpolative Factorization for Elliptic Operators: Differential Equations*, Kenneth L. Ho and Lexing Ying, 2014.

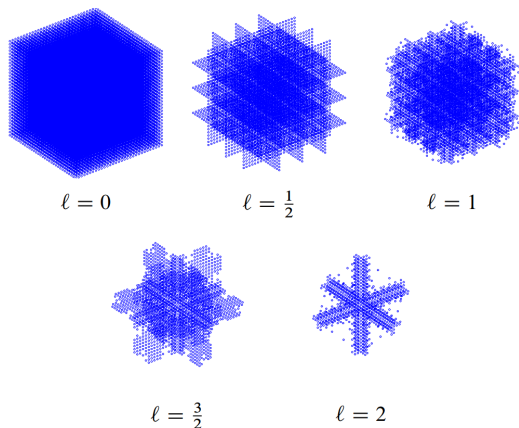


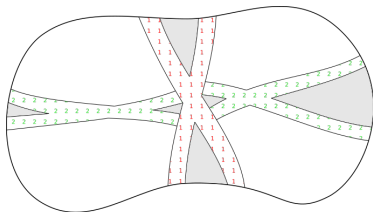
FIGURE 4.2. Active DOFs at each level  $l$  of HIF-DE in 3D.





## New heuristic based on projections

`ComputeProjections(nblvl, distp, width)`

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.



-  Trace of the 1st separator
-  Trace of the 2nd separator
-  #nodes > threshold
-  #nodes < threshold

## New heuristic based on projections

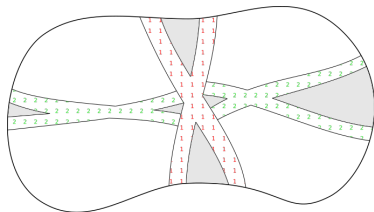
ComputeProjections(*nblvl*, *distp*, *width*)

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 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



- Trace of the 1st separator
- Trace of the 2nd separator
- #nodes > threshold
- #nodes < threshold

## Proposed algorithm for the clustering of supernodes

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### Algorithm 1 Cluster a supernode

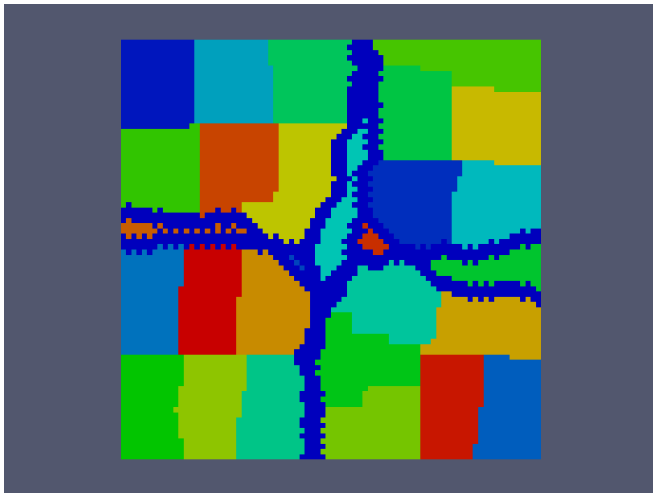
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```
1: ConnectSupernode( dist )
2: ComputeProjections( levels, distp, width )
3: IsolateConnectedComponents()
4: For each connected component  $C$  Do
5:   If  $|C| < threshold$  Then
6:     Merge  $C$  into pre-selected vertices
7:   Else
8:     Kway()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

---

Projections are performed on separators of size larger than  $16 \times MAX\_BLOCKSIZE$ , to obtain at least four large connected subparts that will be split into four parts using kway.

## Example - $80^3$ Laplacian matrix





# 2

## 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

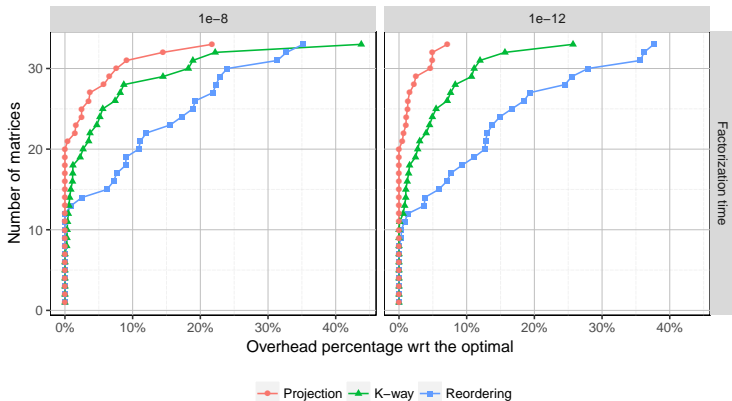
### BLR solver

- 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

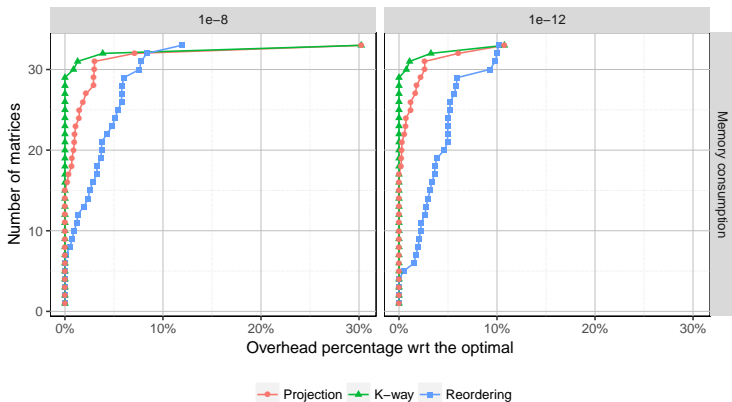
### Pre-selection

- Graphs are reconnected using distance 1 in the Halo
- Selected vertices are obtained with `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.

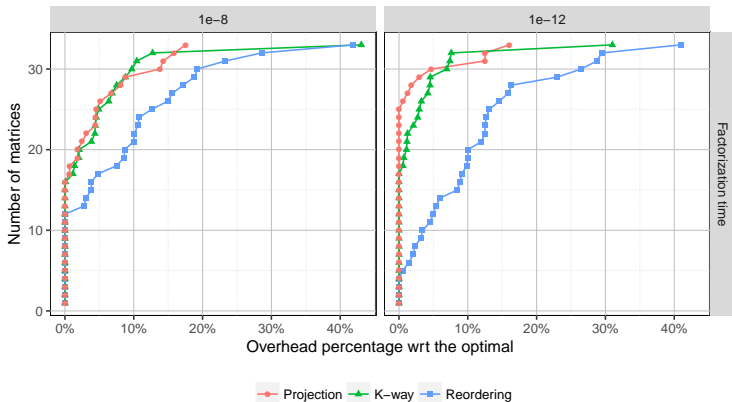
# Performance profile of the factorization time – *Minimal Memory*



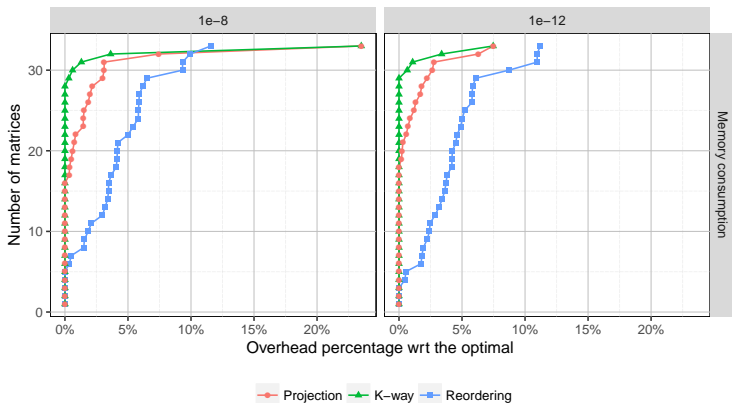
# Performance profile of the memory consumption – *Minimal Memory*



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



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



# 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



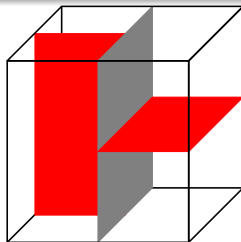
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## Future works

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



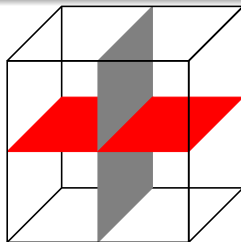
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## PASTIX 6.1.0

<http://gitlab.inria.fr/solverstack/pastix>

- 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.