



# Sparse supernodal solver using block low-rank compression: Design, performance and analysis

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# Sparse supernodal solver using block low-rank compression: Design, performance and analysis

November 21th, 2019 - JOREK development meeting - Cadarache

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## Context - PhD of Gregoire Pichon and Esragul Korkmaz

Current sparse direct solvers for 3D problems of size  $n$

- $\Theta(n^2)$  time complexity
- $\Theta(n^{\frac{4}{3}})$  memory complexity
- BLAS Level 3 operations with computations on blocks

Low-rank compression in sparse direct solvers

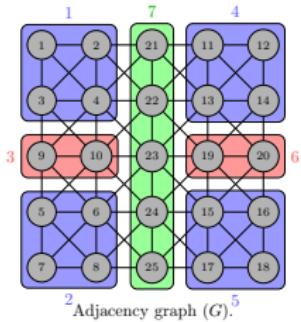
- Compress diagonal and off-diagonal blocks
- Use different compression formats: BLR,  $\mathcal{H}$ , HODLR, HSS,  $\mathcal{H}^2$ ..
- Recently introduced in many solvers: MUMPS, PASTIX, STRUMPACK and many others

Objective of this talk: study low-rank clustering strategies to enhance blocks compressibility in the Block Low-Rank (BLR) case

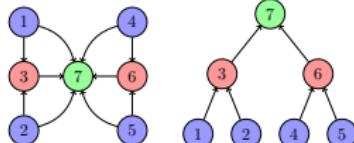
# Symbolic Factorization

## 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

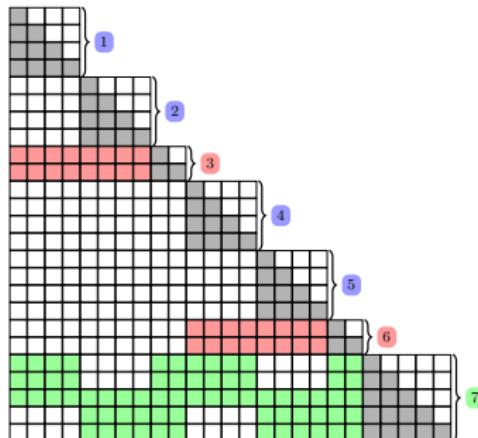


Adjacency graph ( $G$ ).



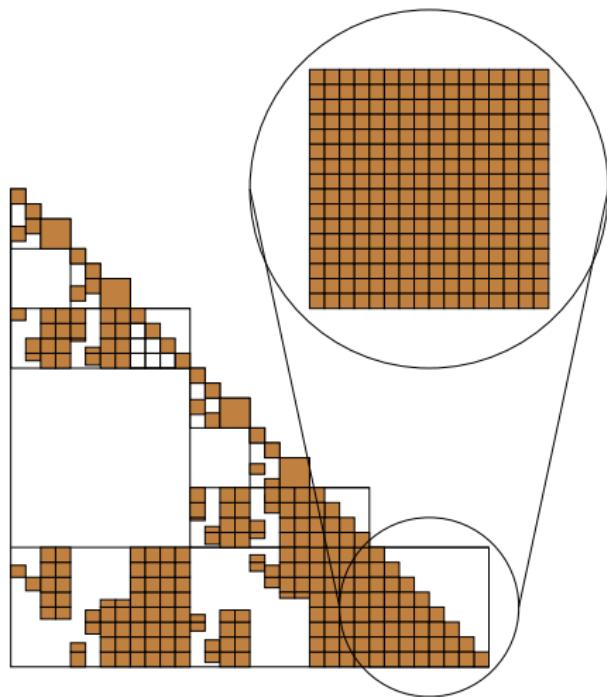
Quotient graph ( $G^*/P$ )  
 $= (G/P)^*$

Elimination tree ( $T$ ).



Factorized matrix ( $L$ ).

# BLR compression – Symbolic factorization



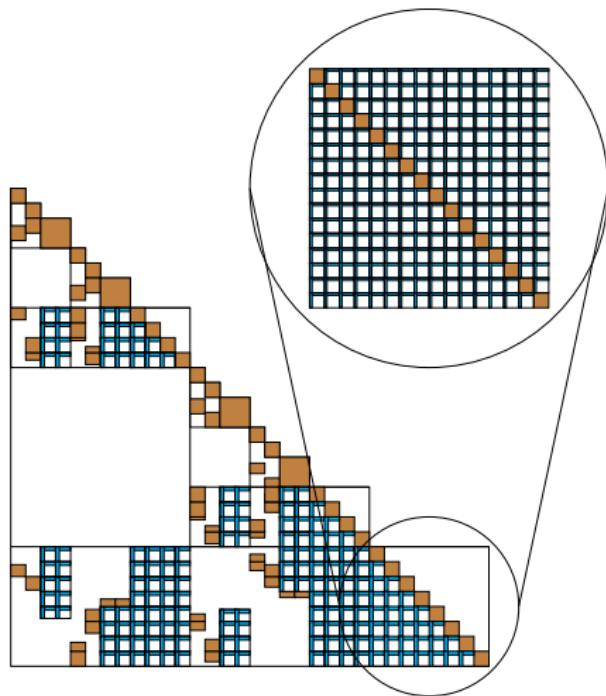
## Approach

- Large supernodes are split
- It increases the level of parallelism

## Operations

- Dense diagonal blocks
- TRSM are performed on dense off-diagonal blocks
- GEMM are performed between dense off-diagonal blocks

# BLR compression – Symbolic factorization



## Approach

- Large supernodes are split
- Large off-diagonal blocks are **low-rank**

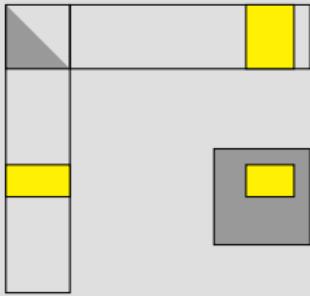
## Operations

- Dense diagonal blocks
- TRSM are performed on **low-rank** off-diagonal blocks
- GEMM are performed between **low-rank** off-diagonal blocks

## Summary of the possible updates

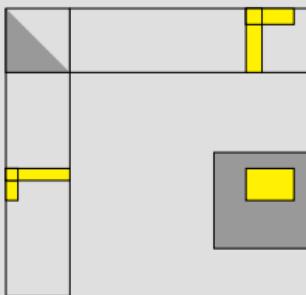
Cost of applying a  $m \times n$  update to a  $M \times N$  block.

Full rank



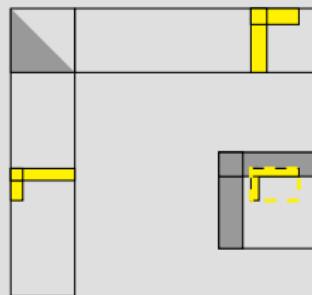
- A single GEMM kernel
- Cost depends on  $mn$

Just-In-Time  
(non-fully structured)



- Serie of small GEMM kernels
- Cost depends on  $mn$

Minimal Memory  
(fully structured)



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

Can we reduce the number small updates, especially for fully structured case?

# Compression kernels

Kernel	Complexity
Singular Value Decomposition (SVD)	$\Theta(mn^2)$
Rank-Revealing QR (RRQR)	$\Theta(mnr)$
RRQR with randomization	$\Theta(mnr)$
ACA, BDLR, CUR	$\Theta((m + n)r)$

## Properties

- SVD provides the best ranks at a given accuracy with  $\| \cdot \|_2$
- RRQR keeps a control of accuracy, but efficiency is poor due to pivoting
- Randomization techniques are suitable to perform a rank- $r$  approximation but may be costly for computing an accurate representation
- The accuracy of ACA/BDLR/CUR is problem dependent

## Experimental setup

Machine: 2 INTEL Xeon  $E5 - 2680v3$  at 2.50 GHz

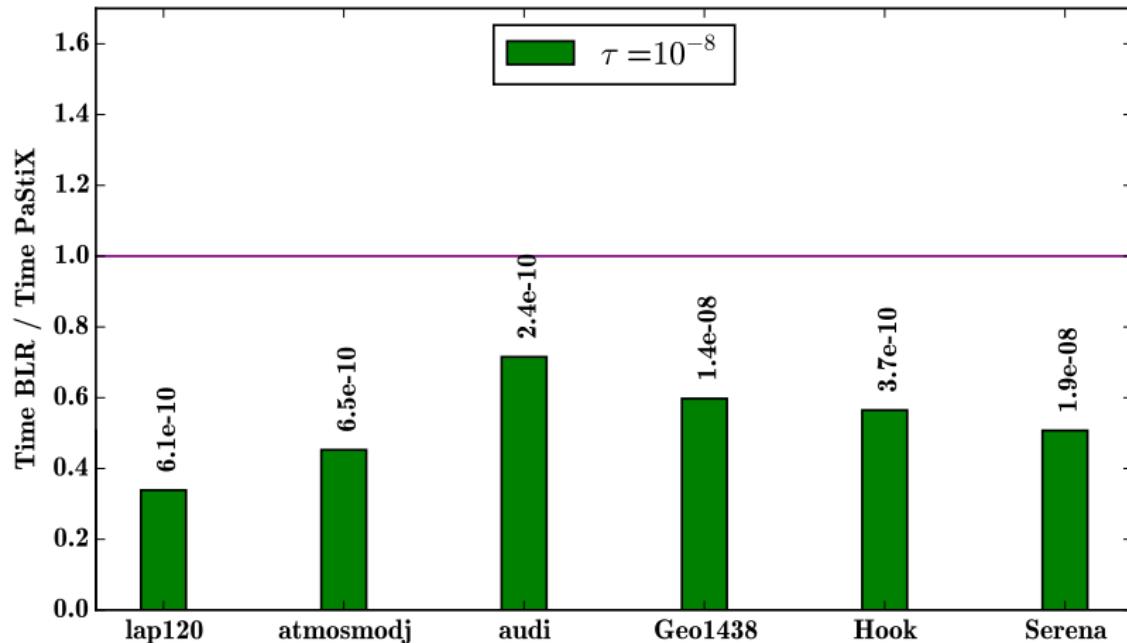
- 128 GB
- 24 threads
- Parallelism is obtained following PASTIX static scheduling for multi-threaded architectures (PARSEC version will be discussed later)

## Entry parameters

- Tolerance  $\tau$ : absolute parameter (normalized for each block)
- Compression method is RRQR
- Blocking sizes: between 128 and 256 in following experiments

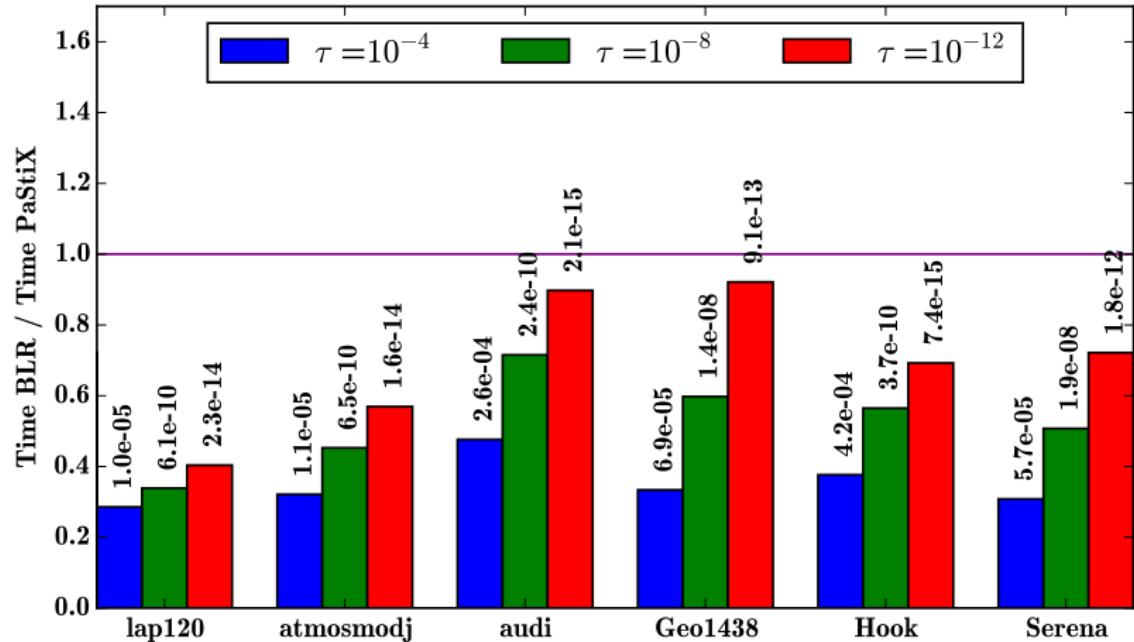
Matrix	Fact.	Size	Field
<b>lap120</b>	$LDL^t$	$120^3$	Poisson problem
<b>Atmosmodij</b>	$LU$	1 270 432	atmospheric model
<b>Audi</b>	$LL^t$	943 695	structural problem
<b>Geo1438</b>	$LL^t$	1 437 960	geomechanical model of earth
<b>Hook</b>	$LDL^t$	1 498 023	model of a steel hook
<b>Serena</b>	$LDL^t$	1 391 349	gas reservoir simulation

## Performance of RRQR/Just-In-Time wrt full-rank version



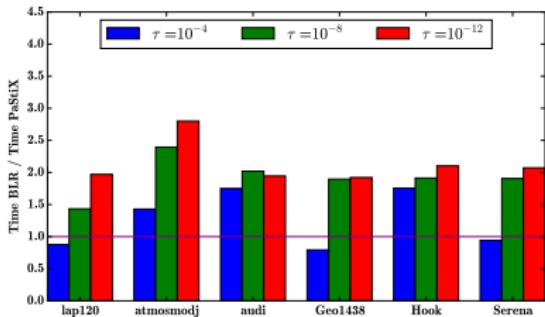
Factorization time reduced by a factor of 2 for  $\tau = 10^{-8}$

## Performance of RRQR/Just-In-Time wrt full-rank version



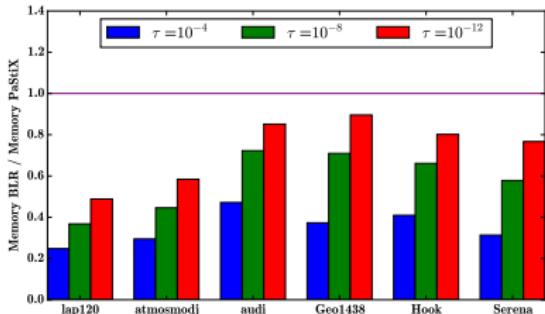
Factorization time reduced by a factor of 2 for  $\tau = 10^{-8}$

# Behavior of RRQR/Minimal Memory wrt full-rank version



## Performance

- Increase by a factor of 1.9 for  $\tau = 10^{-8}$
- Better for a lower accuracy



## Memory peak

- Reduction by a factor of 1.7 for  $\tau = 10^{-8}$
- Close to the results obtained using SVD

## Related work

### BLR

**MUMPS** BLR compression in a multifrontal solver with dense assembly, which can perform pivoting

### Hierarchical

**H-LIB** Hierarchical matrices for sparse by Hackbusch et al. which does not exploit all structural zeroes

**Hmat-OSS** A. Falco's thesis that uses hierarchical matrices together with a symbolic factorization

**CHOLMOD** Supernodal solver using randomization with fixed rank

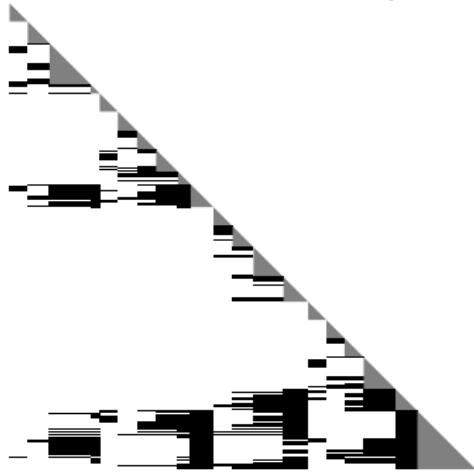
**STRUMPACK** HSS by Ghysels et al. with randomized sampling

### Many other solvers

- Weak admissibility: HODLR, HSS
- Nested bases: HSS,  $\mathcal{H}^2$
- Often used as preconditioners

# Ordering for sparse matrices

One can reorder separators without modifying the fill-in



Symbolic factorization of a  $8 \times 8 \times 8$  Laplacian

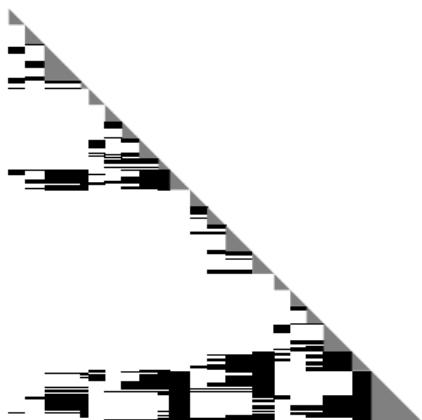
## Enhance ordering

- Modify the partitioning process to enhance compressibility
- Reorder unknowns within a separator:
  - ▶ To enhance clustering within the separator
  - ▶ To enhance the coupling part

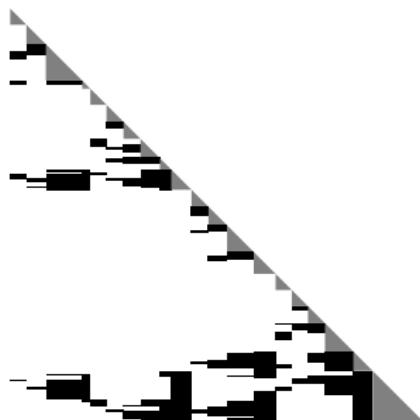
# Reordering to minimize the number of off-diagonal blocks

## Proposition

- Ordering of separators to minimize the number of off-diagonal blocks
- Does not impact memory consumption or the number of operations
- Increase granularity
  - ▶ Reduce the number of low-rank updates
  - ▶ Enhance the use of heterogeneous architectures (GPUs, Xeon Phi)



Without reordering (RCM)



With reordering

## Reordering results

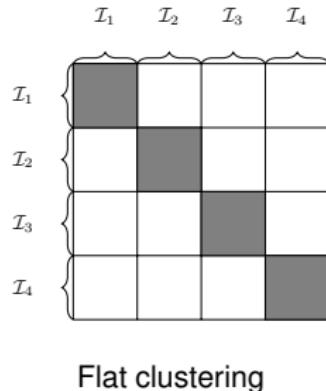
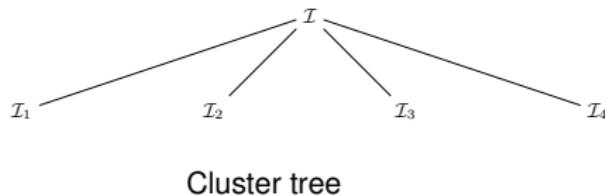
### Summary

- Reduce the number of off-diagonal blocks and thus the overhead associated with low-rank updates
- Lead to larger data blocks suitable for modern architectures
- Always increase performance wrt SCOTCH

Architecture	Nb. units	Mean gain	Max gain
Westmere	12 cores	2%	6%
Xeon E5	24 cores	7%	13%
Fermi	12 cores + 1 to 3 M2070	10%	20%
Kepler	24 cores + 1 to 4 K40	15%	40%
Xeon Phi	64 cores	20%	40%

Performance gain for the full-rank factorization when using PARSEC runtime system with TSP instead of SCOTCH

## BLR clustering for a dense matrix



Flat clustering

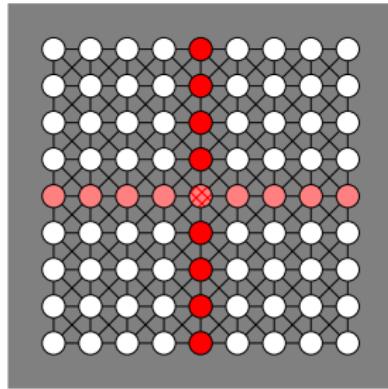
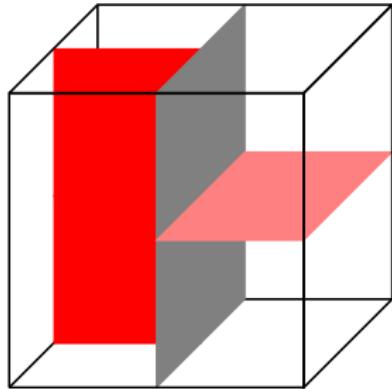
$$\sigma \times \tau \text{ is admissible} \iff \max(\text{diam}(\sigma), \text{diam}(\tau)) \leq \eta \text{ dist}(\sigma, \tau)$$

Can be computed with the knowledge of geometry; otherwise, k-way partitioning can be used for clustering separators

## Towards sparse ordering dedicated to low-rank

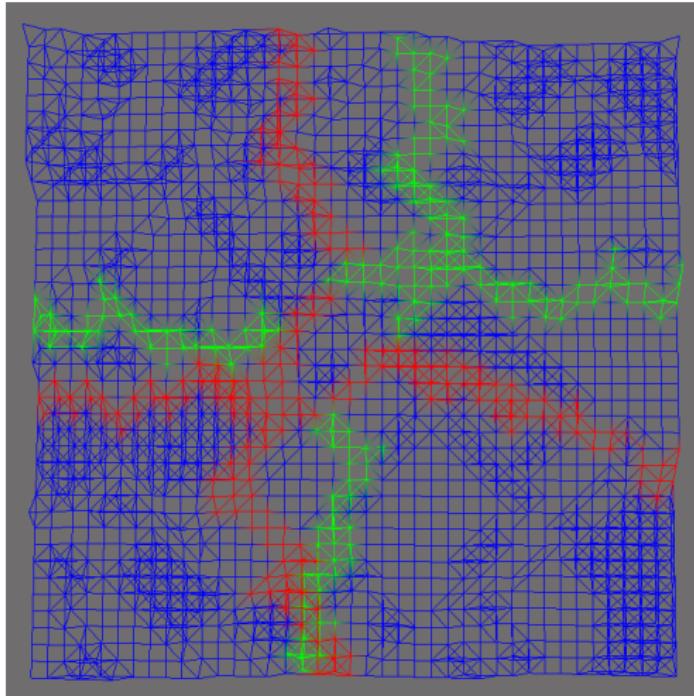
### Nested dissection

1. Partition  $V = A \cup B \cup C$
2. Order  $C$  with larger indices:  $V_A < V_C$  and  $V_B < V_C$
3. Apply the process recursively on  $A$  and  $B$



As  $A$  and  $B$  are processed independently, their interaction with  $C$  is not the same, even for a perfect nested dissection of a  $N \times N \times N$  cube

## Example on a cube partitioned with SCOTCH



First separator of a  $40 \times 40 \times 40$  Laplacian partitioned with SCOTCH

## Suitable clustering strategy

Let us consider the last separator  $A_{22}$  and its interactions with previous supernodes  $A_{11}$ :

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

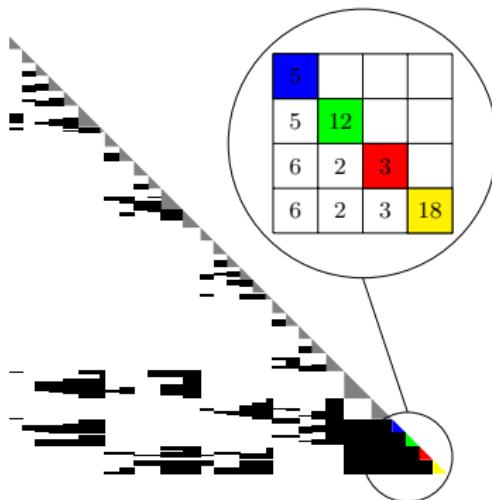
### Existing approaches

- K-way partitioning orders correctly  $A_{22}$
- The reordering strategy reduces the number of off-diagonal blocks in  $A_{12}$  and  $A_{21}$

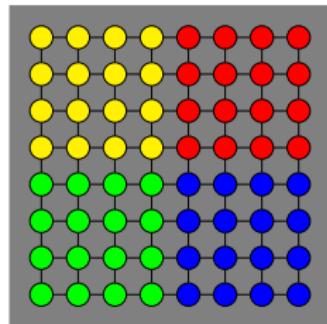
We introduce a new strategy to couple the advantages of both approaches, with suitable structure for both intra and inter separators blocks

## Clustering techniques: existing solutions

- k-way partitioning (dense, multifrontal)



(a) Symbolic factorization

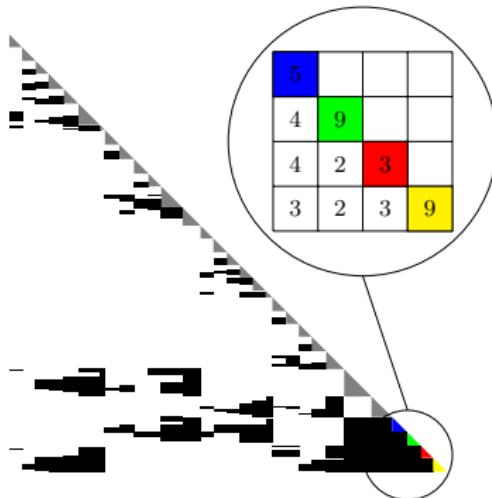


(b) First separator clustering

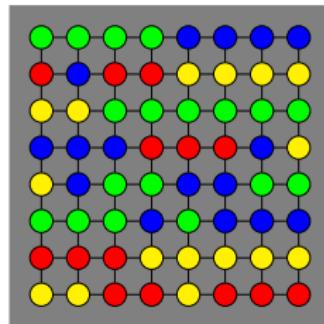
$8 \times 8 \times 8$  Laplacian partitioned using SCOTCH and k-way clustering on the first separator

## Clustering techniques: existing solutions

- k-way partitioning (dense, multifrontal)
- 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

## New heuristic based on projections

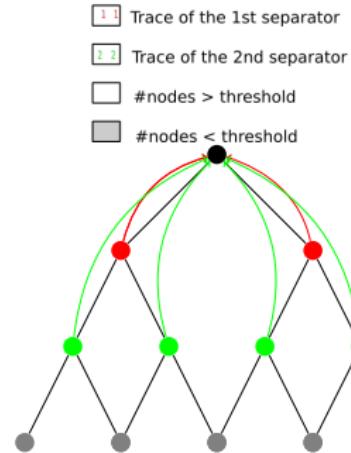
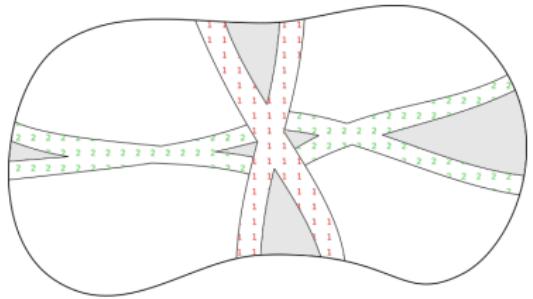
Pre-selected vertices of a separator are vertices connected to a close child in the elimination tree

For each separator we have:

$$A_{22} = \begin{pmatrix} A_{kk} & A_{ks} \\ A_{sk} & A_{ss} \end{pmatrix}$$

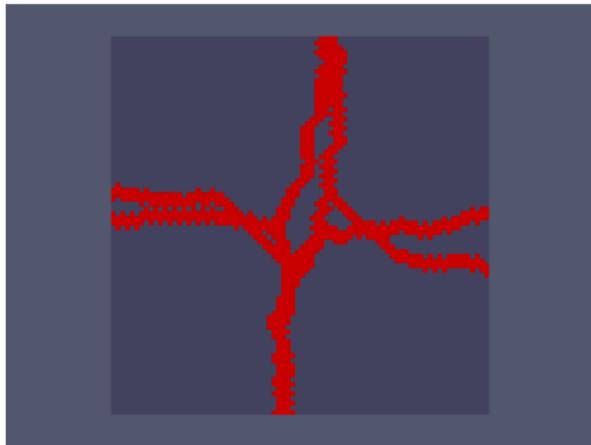
where  $A_{ss}$  corresponds to pre-selected vertices.

Only interactions between non pre-selected vertices  $A_{kk}$  are compressed



## Example - $80 \times 80 \times 80$ Laplacian matrix

Interactions with pre-selected vertices (in red) are not compressed

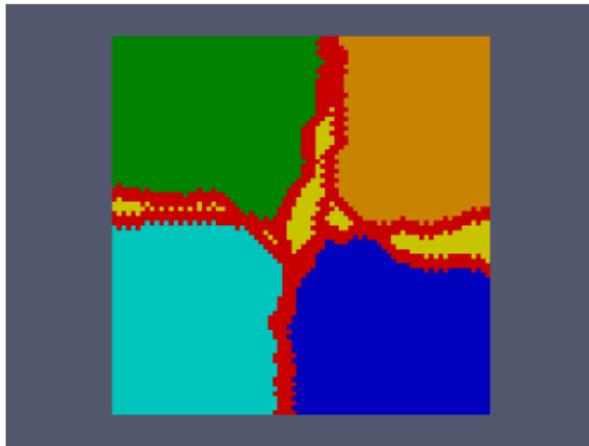


1. Compute pre-selected vertices

Projections heuristic on last separator of size  
 $80 \times 80$

## Example - $80 \times 80 \times 80$ Laplacian matrix

Interactions with pre-selected vertices (in red) are not compressed

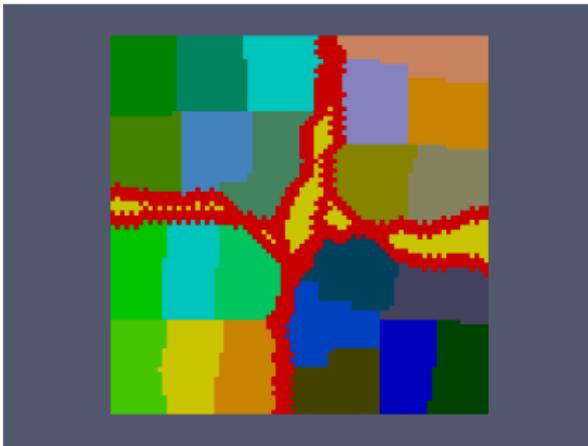


1. Compute pre-selected vertices
2. Isolate connected components
3. Merge small components

Projections heuristic on last separator of size  
 $80 \times 80$

## Example - $80 \times 80 \times 80$ Laplacian matrix

Interactions with pre-selected vertices (in red) are not compressed



Projections heuristic on last separator of size  
 $80 \times 80$

1. Compute pre-selected vertices
2. Isolate connected components
3. Merge small components
4. Apply k-way partitioning on large components
5. Perform TSP reordering on each cluster

# Experimental setup

## Architecture

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

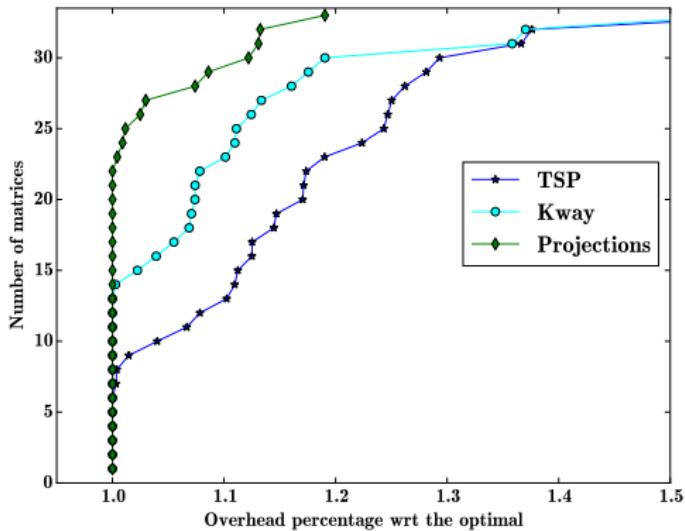
## Set of matrices

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

## Strategies studied for the PaStiX solver

- Reordering with TSP
- K-way partitioning using SCOTCH + TSP on each cluster
- The new Projections strategy + TSP on each cluster

## Performance profile of the factorization time

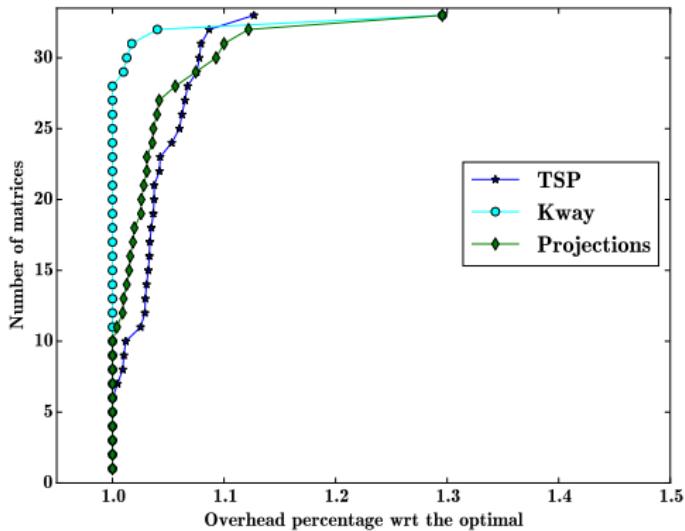


### Method

- For each matrix, percentage wrt the best method
- Percentage are sorted increasingly
- A curve close to  $x = 1$  is close to optimal

**Minimal Memory** (fully structured with low-rank updates), with  $\tau = 10^{-8}$

## Performance profile of the memory consumption



### Method

- For each matrix, percentage wrt the best method
- Percentage are sorted increasingly
- A curve close to  $x = 1$  is close to optimal

**Minimal Memory** (fully structured with low-rank updates), with  $\tau = 10^{-8}$

# Clustering summary

## Ordering strategies

- Both reordering and k-way are limited to form suitable clusters
- Pre-selection of some unknowns allows to obtain well-separated clusters and to exhibit non-compressible operations

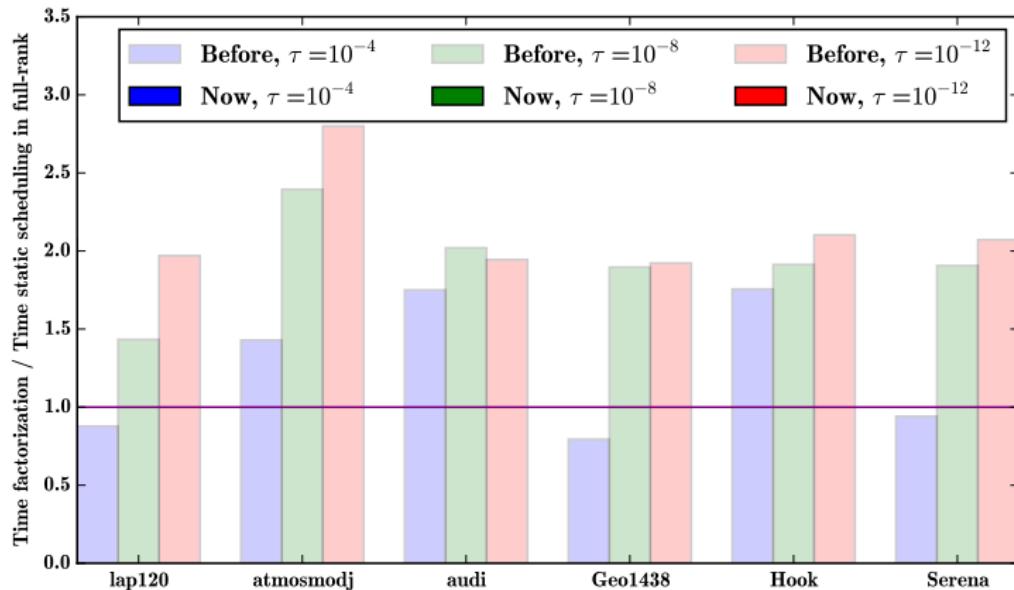
## Impact on preprocessing stats

- Ordering time controlled: 70% overhead with respect to SCOTCH ordering
- Slight increase in the number of off-diagonal blocks: mean 1.05, max 1.35 for both **K-way** and **Projections** strategies

## Conclusion

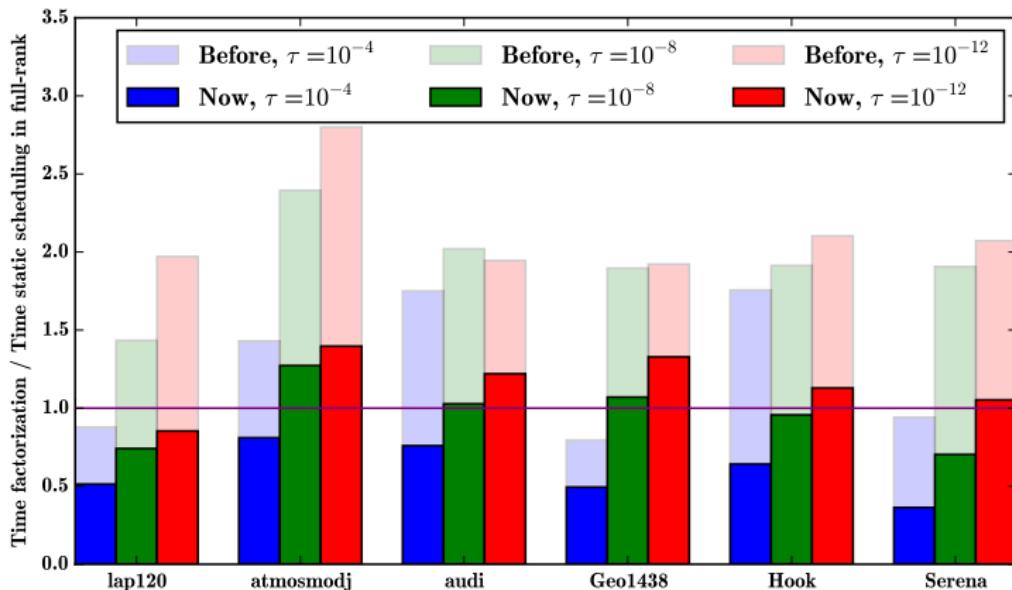
- Somewhat similar to ILU(k) to select more important data
- When moving to hierarchical matrices, the cluster trees may not be binary trees

# Behavior of RRQR/Minimal Memory with PARSEC and Projections



Adding Projections and the use of PARSEC runtime system reduces factorization time

# Behavior of RRQR/Minimal Memory with PARSEC and Projections



Adding Projections and the use of PARSEC runtime system reduces factorization time

# HORSE: Practical application (S. Lanteri - ANR TECSER)

## Method

- Introduce an hybrid variable to solve a system smaller than the one obtained through DG
- Perform Domain-Decomposition to solve this system
- Use a direct solver for subdomains

Solve 3D frequency-domain Maxwell's equations

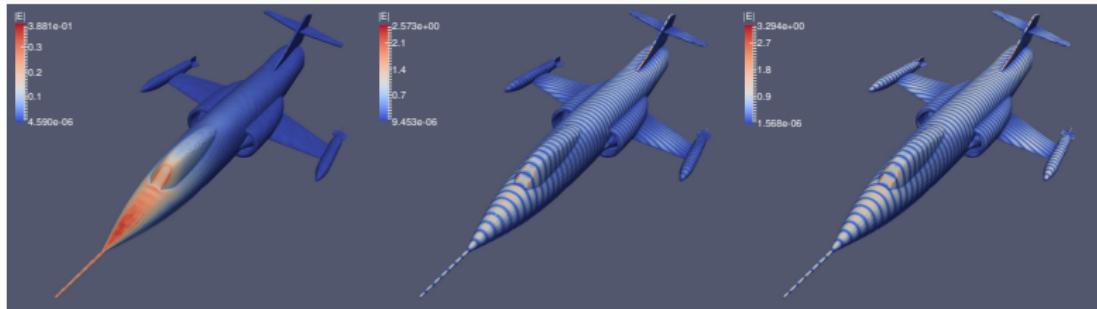
- $i\omega\epsilon_r \mathbf{E} - \mathbf{curl} \mathbf{H} = -\mathbf{J}$ , in  $\Omega$
- $i\omega\mu_r \mathbf{H} + \mathbf{curl} \mathbf{E} = 0$ , in  $\Omega$
- $\mathbf{n} \times \mathbf{E} = 0$ , on  $\Gamma_m$
- $\mathbf{n} \times \mathbf{E} + \mathbf{n} \times (\mathbf{n} \times \mathbf{H}) = \mathbf{n} \times \mathbf{E}^{\text{inc}} + \mathbf{n} \times (\mathbf{n} \times \mathbf{H}^{\text{inc}})$ , on  $\Gamma_a$

# HORSE: Hybridizable DG method in 3D

Scattering of a plane wave by a jet

- Unstructured tetrahedral mesh: 1,645,874 elements / 3,521,251 faces
- Frequency: 600 MHz, Wavelength:  $\lambda \simeq 0.5$  m, Penalty parameter:  $\tau = 1$

HDG method	# DoF $\Delta$ field	# DoF EM field
HDG- $\mathbb{P}_1$	21,127,506	39,500,976
HDG- $\mathbb{P}_2$	42,255,012	98,752,440
HDG- $\mathbb{P}_3$	70,425,020	197,504,880



Contour line of  $|\mathbf{E}|$  - HDG- $\mathbb{P}_1$  to HDG- $\mathbb{P}_3$

# Experimental setup

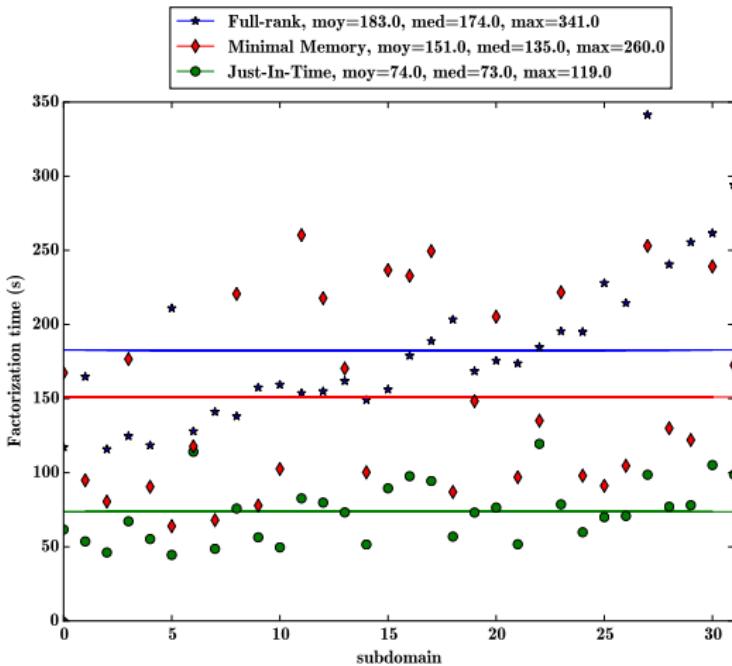
## Study case

- Jet with  $\mathbb{P}_2$  interpolation
- 42 255 012 unknowns for  $\Lambda$
- A single factorization is performed on each subdomain
- There may be several solves for iterative refinement between subdomains

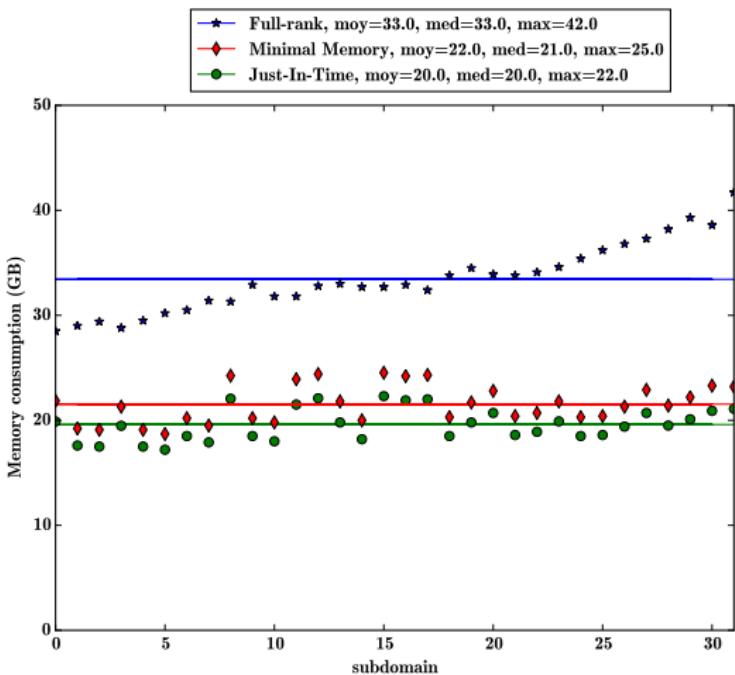
## Machine

- Occigen: 24-cores nodes with 128 GB
- Each MPI process is hold on a socket with 12 cores
- In next experiments, we use 32, 48 or 64 subdomains
- Subdomains are ordered accordingly to the number of operations for the complete factorization

## Factorization on each subdomain – 32 processes with $\tau = 1e - 4$



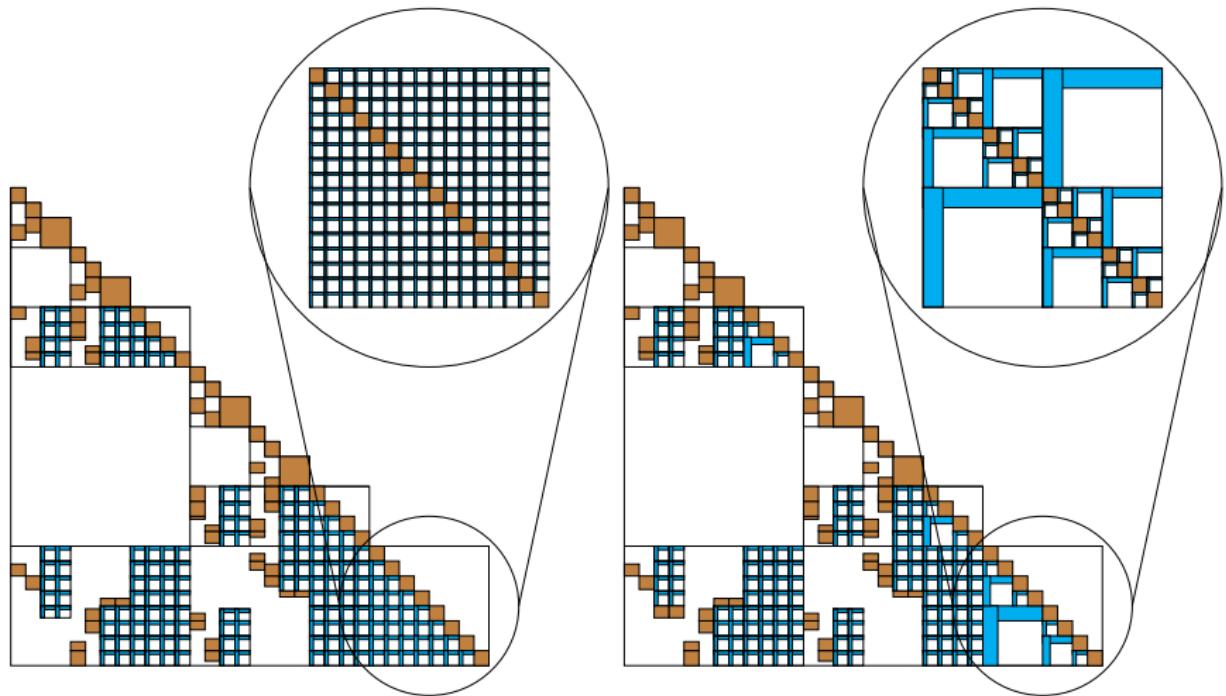
## Memory Consumption on each subdomain – 32 processes with $\tau = 1e - 4$



# Impact on HORSE

Subs	$\tau$	Method	Fact(s)	Nb. of iters	Refinement (s)	HDGM (s)	Memory (GB)
32	1e-4	-	Full-rank	526.0	9	254.5	814.0
		Just-In-Time	209.3	9	164.8	<b>405.8</b>	41.7 (22.3)
		Minimal-Memory	516.7	15	273.2	822.0	<b>24.5</b>
	1e-8	Just-In-Time	325.2	9	192.9	550.4	41.7 (29.4)
		Minimal-Memory	600.1	9	193.2	825.8	30.5
48	1e-4	-	Full-rank	237.3	8	118.6	374.6
		Just-In-Time	112.2	9	106.1	<b>237.1</b>	24.9 (14.1)
		Minimal-Memory	229.3	13	159.7	407.5	<b>15.3</b>
	1e-8	Just-In-Time	171.5	8	105.8	296.1	24.9 (18.1)
		Minimal-Memory	319.4	8	109.8	447.9	18.8
64	1e-4	-	Full-rank	179.8	9	104.7	298.3
		Just-In-Time	79.7	10	91.1	<b>184.1</b>	17.4 (10.0)
		Minimal-Memory	138.1	13	120.7	272.2	<b>11.0</b>
	1e-8	Just-In-Time	124.6	9	90.0	228.2	17.4 (12.9)
		Minimal-Memory	239.2	9	91.5	344.5	13.7

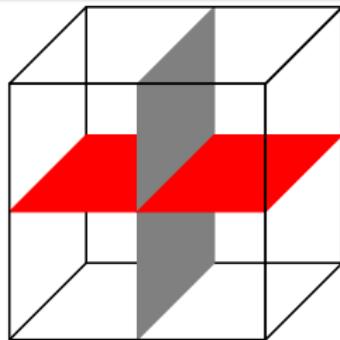
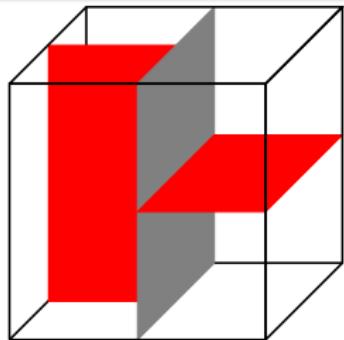
## Future works: HODLR compression



## Future works: align separators

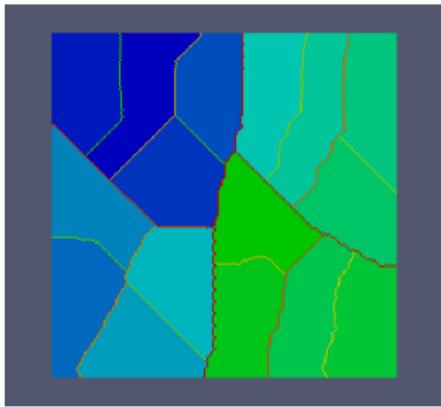
### Constraint partitioning process

- Align separators to form clusters during the nested dissection process
- Preliminary work using fixed vertices
- When partitioning  $G = A \cup B \cup C$ , ensure that the children interaction with  $C$  is symmetric to have similar contribution pattern

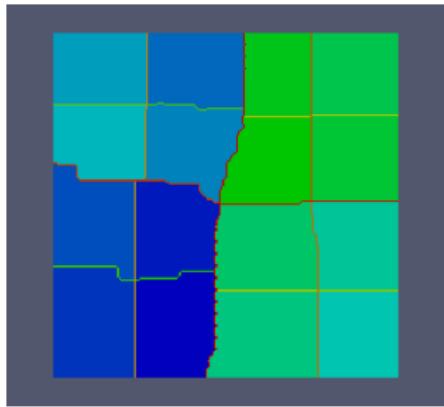


# Result on a $200^2$ Laplacian

With SCOTCH



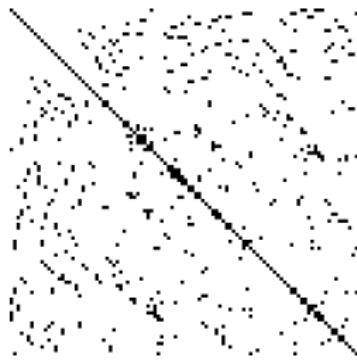
With **ALIGNATOR**



## PASTIX 6.0.1

<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 integrated in master branch with clustering strategies
- Cholesky,  $LDL$  and  $LU$  factorizations
- GMRES, CG, BiCG iterative refinements



## LR2LR kernel using SVD

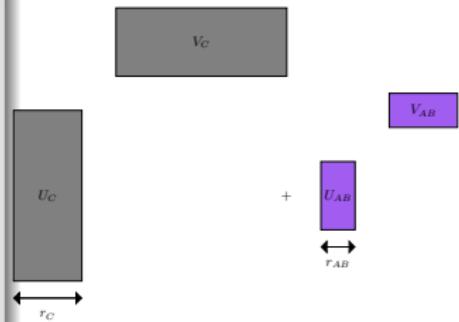
A low-rank structure  $U_C V_C^t$  receives a low-rank contribution  $U_{AB} V_{AB}^t$

### Recompression algorithm

$$U_C V_C^t + U_{AB} V_{AB}^t = ([U_C, U_{AB}]) \times ([V_C, V_{AB}])^t$$

- QR:  $[U_C, U_{AB}] = Q_1 R_1$
- QR:  $[V_C, V_{AB}] = Q_2 R_2$
- SVD:  $R_1 R_2^t = u \sigma v^t$

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



The complexity of this operation depends on the dimensions of the target  $C$   
Slightly more complex algorithm for RRQR, that still requires zeroes padding

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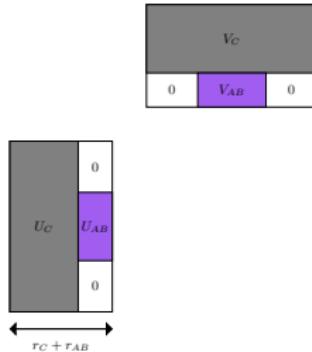
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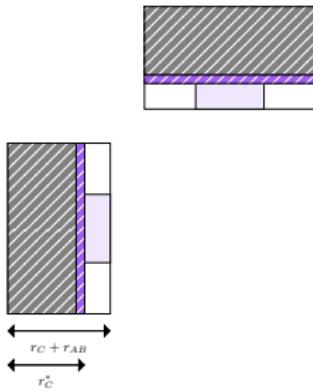
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The complexity of this operation depends on the dimensions of the target  $C$   
Slightly more complex algorithm for RRQR, that still requires zeroes padding



## LR2LR kernel using RRQR

A low-rank structure  $u_1 v_1^t$  receives a low-rank contribution  $u_2 v_2^t$ .  
 $u_1$  and  $u_2$  are orthogonal matrices

### Algorithm

$$A = u_1 v_1^t + u_2 v_2^t = ([u_1, u_2]) \times ([v_1, v_2])^t$$

Orthogonalize  $u_2$  with respect to  $u_1$  :

$$u_2^* = u_2 - u_1(u_1^t u_2) \quad \Theta(m r_1 r_2)$$

Form new orthogonal basis, and normalize each column :

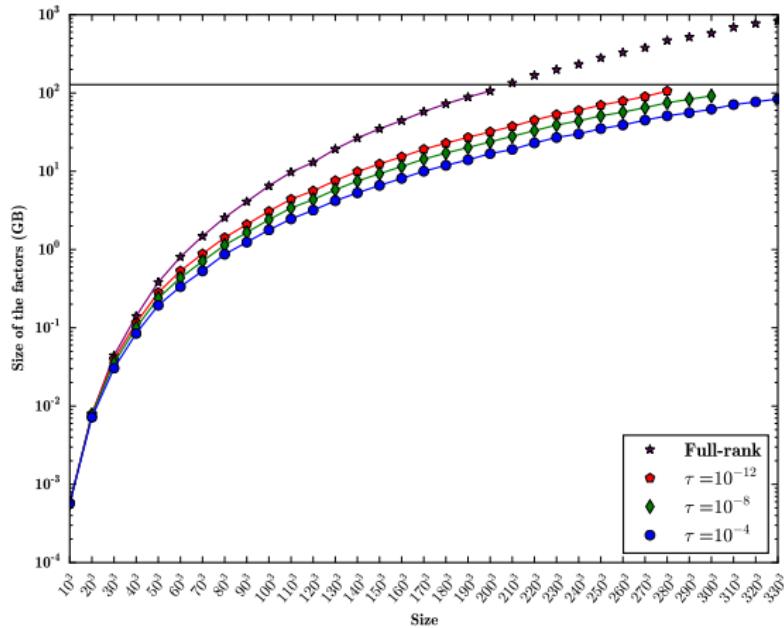
$$[u_1, u_2] = [u_1, u_2^*] \times \begin{pmatrix} I & u_1^t u_2 \\ 0 & I \end{pmatrix}$$

Apply a RRQR on :

$$\begin{pmatrix} I & u_1^t u_2 \\ 0 & I \end{pmatrix} \times ([v_1, v_2])^t$$

RRQR with truncation in  $\Theta(n(r_1 + r_2)r_1^*)$ . Less stable?

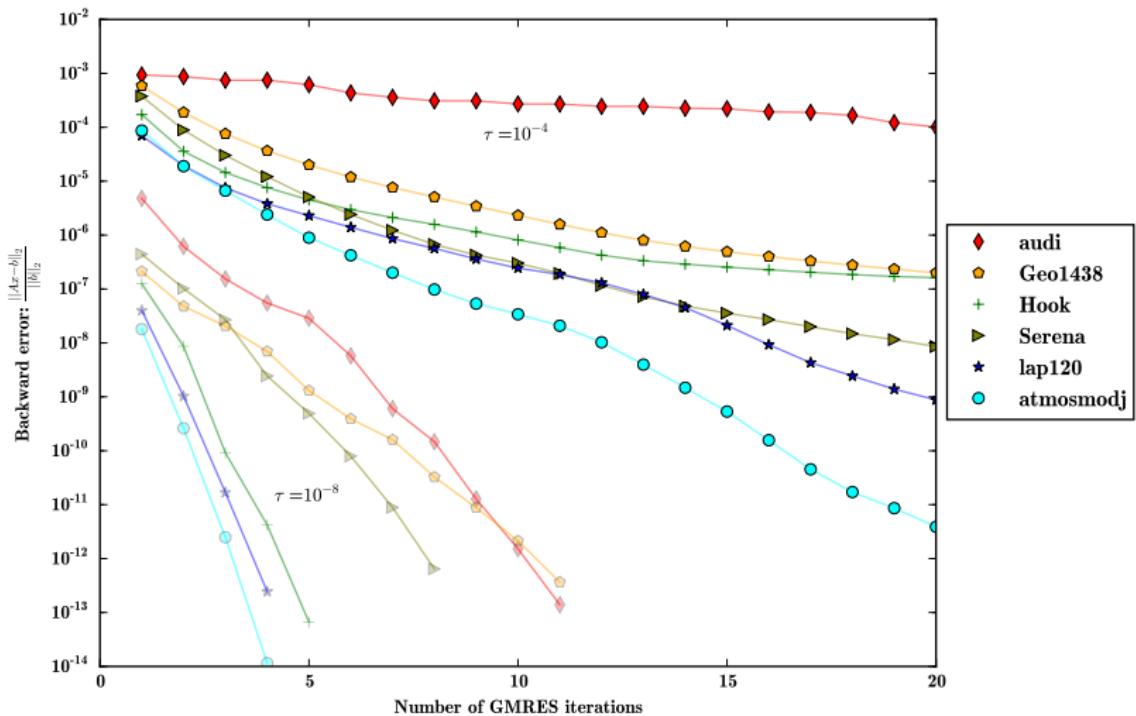
# Scaling on Laplacians: memory consumption RRQR/Minimal Memory



## Results

- Maximum consumption of 128 GB
- Problem of size  $200^3 = 8M$  with full-rank
- Problem of size  $330^3 = 36M$  with  $10^{-4}$  tolerance

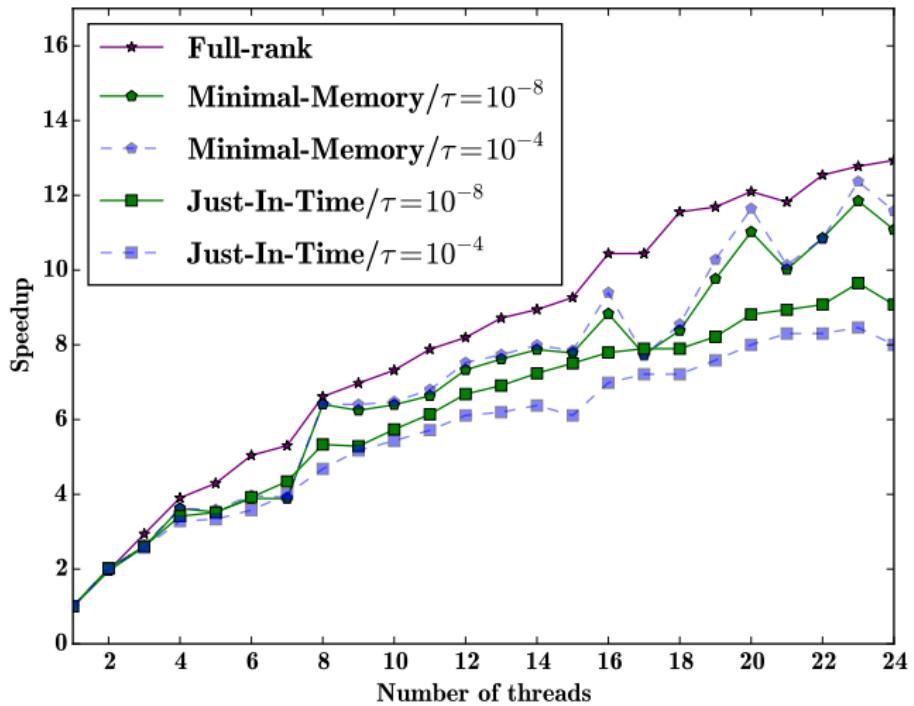
# Convergence of RRQR/Minimal Memory



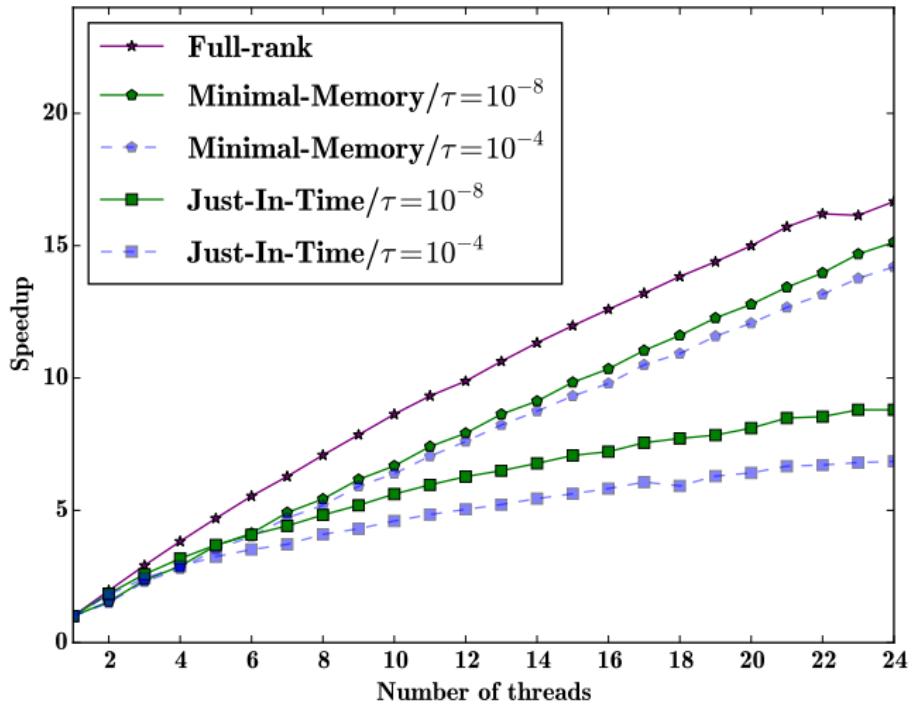
# Costs distribution on the Atmosmodj matrix with $\tau = 10^{-8}$

	Full-rank	Just-In-Time		Minimal Memory	
		SVD	RRQR	SVD	RRQR
<b>Factorization time (s)</b>					
Compression	-	4.1e+02	3.4e+01	1.8e+02	5.6e+00
Block factorization (GETRF)	7.2e-01	7.4e-01	7.3e-01	7.8e-01	7.6e-01
Panel solve (TRSM)	1.7e+01	6.9e+00	7.4e+00	7.6e+00	7.9e+00
Update					
Formation of contribution	-	-	-	9.9e+01	4.2e+01
Addition of contribution	-	-	-	3.0e+03	7.3e+02
Dense update (GEMM)	4.6e+02	1.3e+02	9.7e+01	2.8e+01	2.4e+01
<b>Total</b>	<b>4.7e+02</b>	<b>5.5e+02</b>	<b>1.4e+02</b>	<b>3.6e+03</b>	<b>8.1e+02</b>
<b>Solve time (s)</b>					
	6.3e+00	1.9e+00	3.0e+00	<b>1.5e+00</b>	3.2e+00
<b>Factor final size (GB)</b>					
	16.3	6.95	7.49	<b>6.85</b>	7.31
<b>Memory peak for the factors (GB)</b>					
	16.3	16.3	16.3	<b>6.85</b>	7.31

## Parallelism / static scheduling



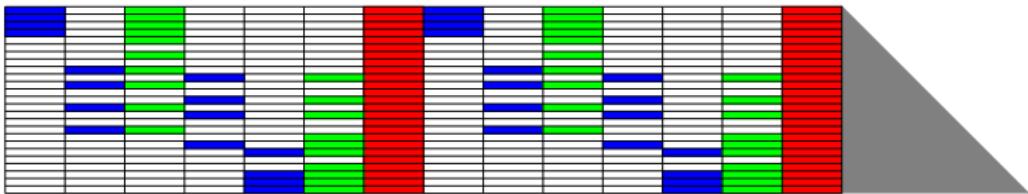
## Parallelism / Parsec



# Modeling of the problem

## Proposition

- Define a distance between rows: the number of differences between off-diagonal blocks
- Express the problem as a Traveling Salesman Problem (TSP) to sort rows in order to minimize the overall distance
- Use heuristics to perform TSP with low complexity



# Modeling of the problem

## Proposition

- Define a distance between rows: the number of differences between off-diagonal blocks
- Express the problem as a Traveling Salesman Problem (TSP) to sort rows in order to minimize the overall distance
- Use heuristics to perform TSP with low complexity

1				
2				
3	+1	+1	+0	+0
4				

	1	2	3	4
1	0	-	-	-
2	3	0	-	-
3	3	2	0	-
4	1	4	2	0

## Improvements with $\tau = 10^{-8}$ on a set of six matrices

Variant	Just-In-Time		Minimal Memory		
	Time PARSEC	Time static	Time PARSEC	Time static	Memory
strong admissibility	0.52	0.62	1.24	2.28	0.52
+ k-way	<b>0.49</b>	0.55	1.17	1.94	<b>0.48</b>
+ projections	0.50	0.55	1.19	1.90	0.50
+ ratio set to 0.5	0.51	0.56	<b>0.96</b>	1.43	0.54
+ ratio set to 0.25	0.50	0.55	1.19	1.89	0.50

## Towards sparse ordering dedicated to low-rank

### Nested dissection

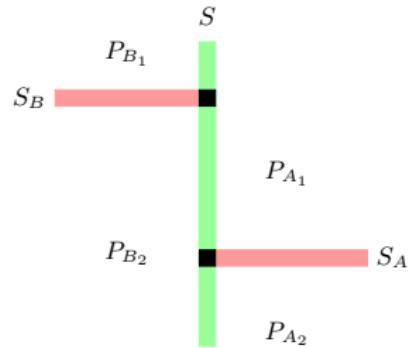
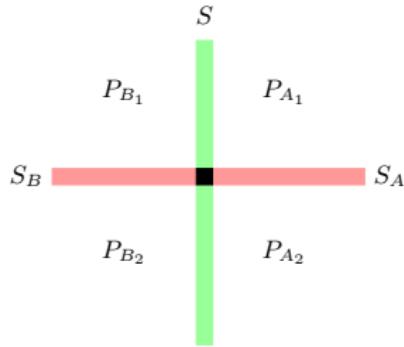
1. Partition  $V = A \cup B \cup S$ , such as any path from  $A$  to  $B$  goes through  $S$
2. Order  $S$  with larger numbers:  $V_A < V_B < V_S$
3. Apply the process recursively on  $A$  and  $B$

As  $A$  and  $B$  are processed independently, their contribution on  $S$  is not symmetric

### Current solutions in sparse low-rank solvers

- Find low-rank clustering by applying a k-way partitioning on each separator (Mumps, Strumpack)
- Reordering strategy to cluster close contributions (PaStiX, and cf. previous talk)

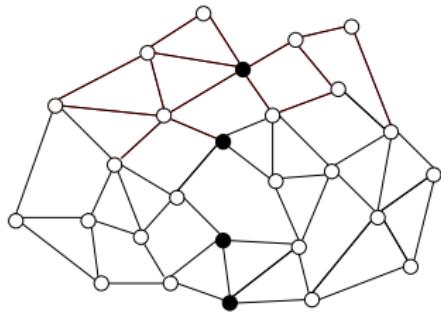
## Simple representation of the problem on a 2D graph



- 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

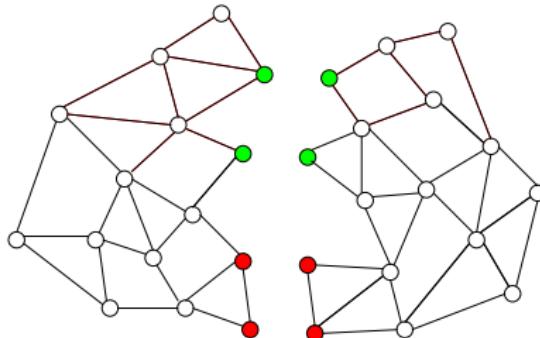
- Double interaction: between  $S$  and  $S_A$  and between  $S$  and  $S_B$  in the original graph
- Three “large” interaction blocks during the factorization

## Fixed vertices



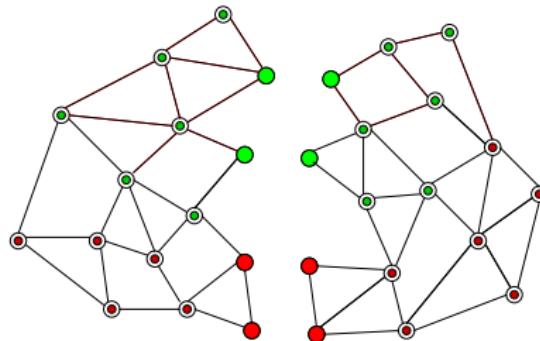
- Regular nested dissection on  $G = A \cup B \cup C$ .

## Fixed vertices



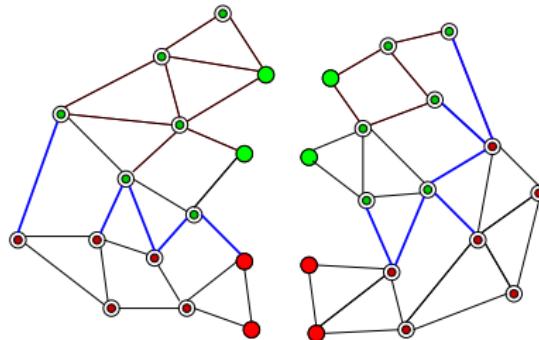
- Recursion with the halo on  $A \cup C$  and  $B \cup C$ .
- $C$  vertices are bi-partitioned into green and red vertices.

## Fixed vertices



- The partition of  $C$  is extended to both  $A \cup C$  and  $B \cup C$ .

## Fixed vertices



- We got a new edge separator for both subgraphs.
- Turn those separators into vertex separators.