Harnessing inexactness in scientific computing

Lecture 14: block low-rank matrices

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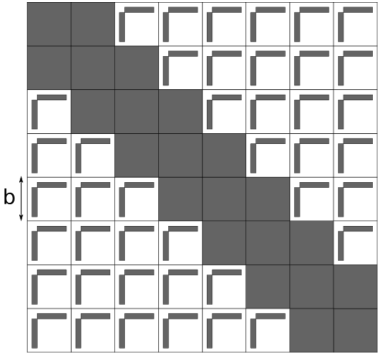
M2 course at ENS Lyon, 2024–2025

Slides available on course webpage



Introduction

Applications

Complexity

High performance implementation

Mixed precision

Multilevel BLR

Two exercises

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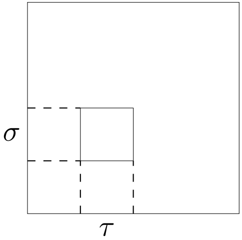
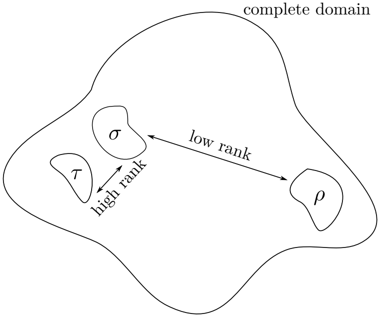
Two exercises

Data sparse matrices

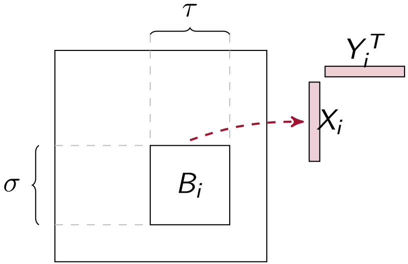
Data sparse matrices are not sparse but can be well approximated by "sparse data":



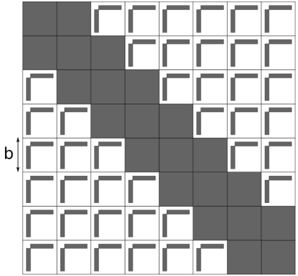


A block B represents the interaction
between two subdomains σ and τ.
Large distance $\Leftrightarrow$ low numerical rank

Block low-rank (BLR) matrices

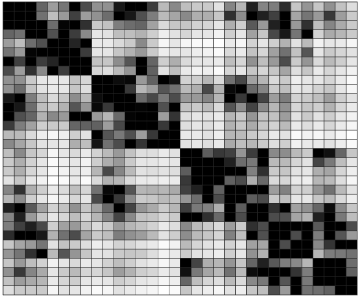


$\|B_i - X_i Y_i^T\| \leq \varepsilon \|A\|$



Block Low Rank

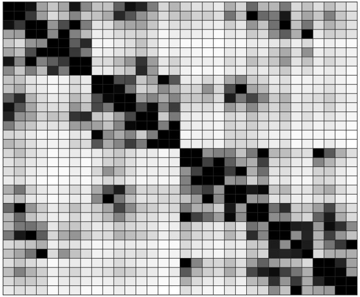
Block low-rank (BLR) matrices



Example of a BLR matrix (Schur complement of a 64^3 Poisson problem with block size 128)

- Diagonal blocks are full rank
- Off-diagonal ones are stored in low rank form if their ε-rank is small enough
- $\varepsilon = 10^{-15} \rightarrow 50\%$ entries kept

Block low-rank (BLR) matrices



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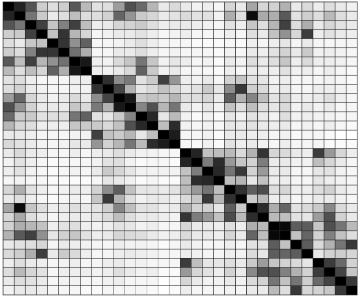

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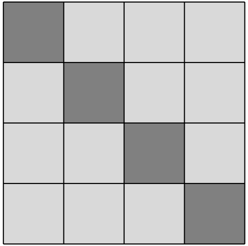
- $\varepsilon = 10^{-15} \rightarrow$ 50% entries kept
- $\varepsilon = 10^{-12} \rightarrow$ 36% entries kept
- $\varepsilon = 10^{-9} \rightarrow$ 23% entries kept

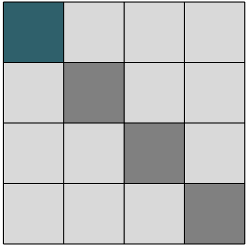
BLR LU factorization: FSCU variant

- How to adapt block LU factorization to exploit BLR structure?
- FSCU variant:



BLR LU factorization: FSCU variant

- How to adapt block LU factorization to exploit BLR structure?
- FSCU variant: Factor,



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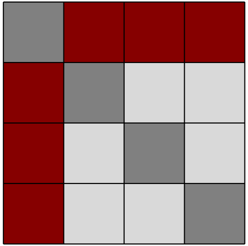

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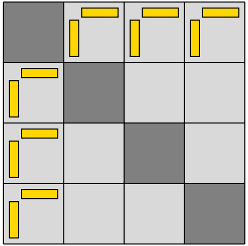

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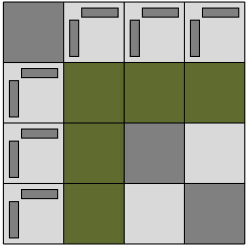

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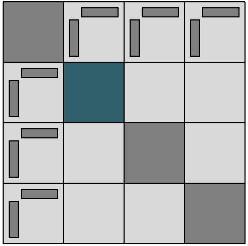

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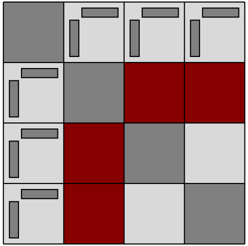

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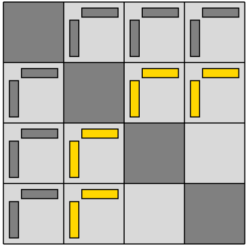

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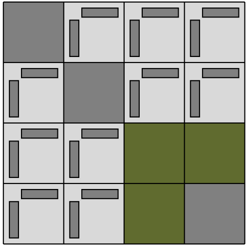

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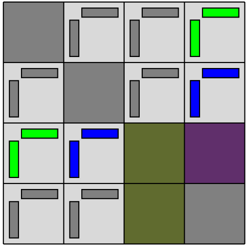

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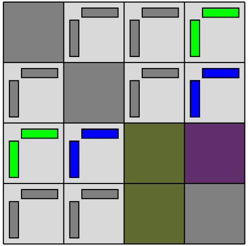

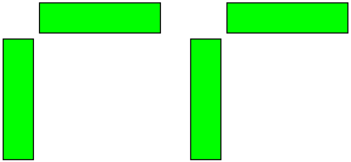

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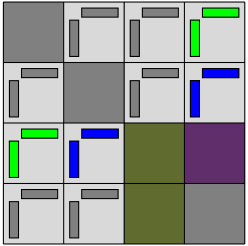

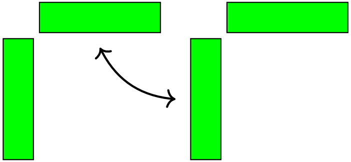

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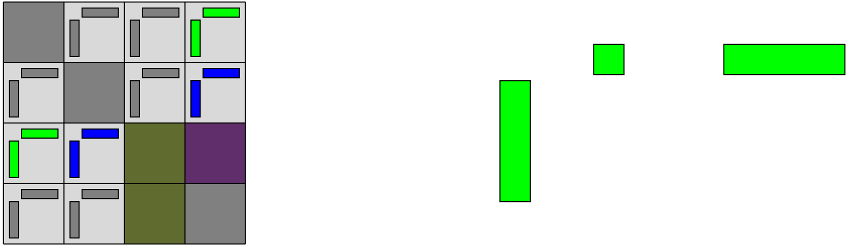

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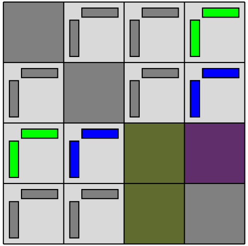

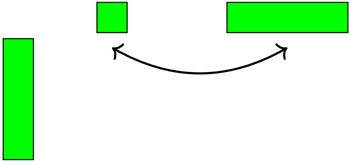

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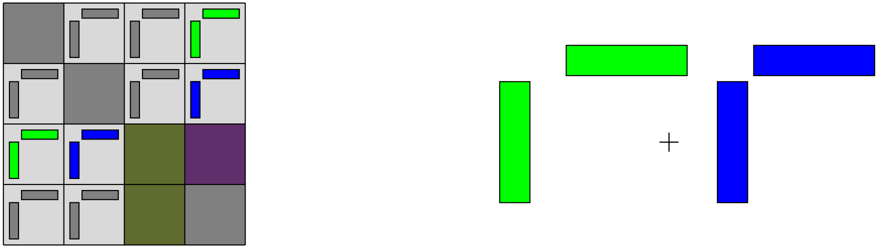

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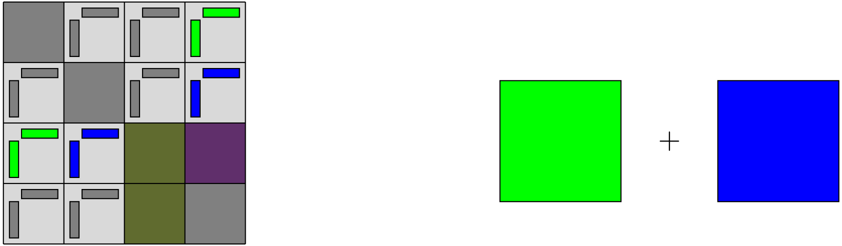

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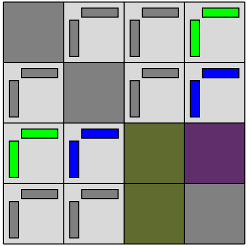
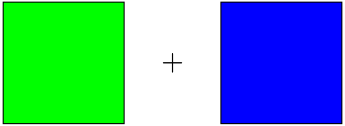
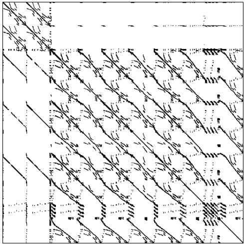


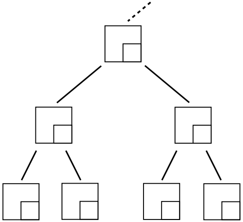


- Computed LU factors satisfy $\widehat{L}\widehat{U} = A + \Delta A$, $\|\Delta A\| \le c_n u \||\widehat{L}||\widehat{U}|\| + \varepsilon \|A\|$

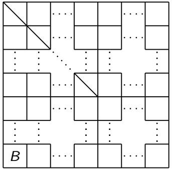
  Higham and M. (2021)



$\Longrightarrow$

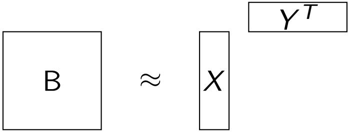


Elimination tree



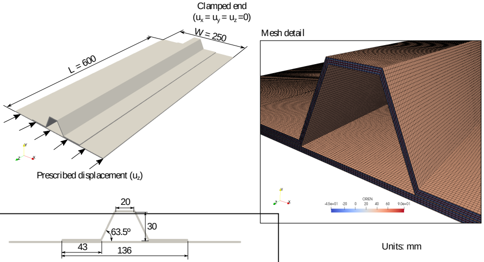
BLR clustering to build 2D block structure

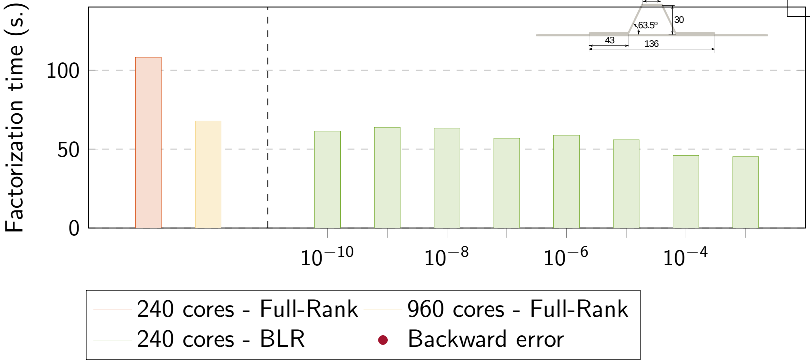
$\Longrightarrow$



SVD or RRQR $\Rightarrow$ X and Y s. t. $\|B - XY^T\| \leq \varepsilon$

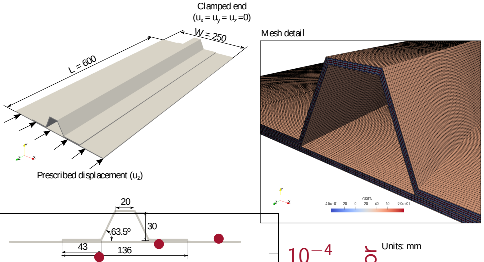
- structure subject to compression load
- matrix of order 10M

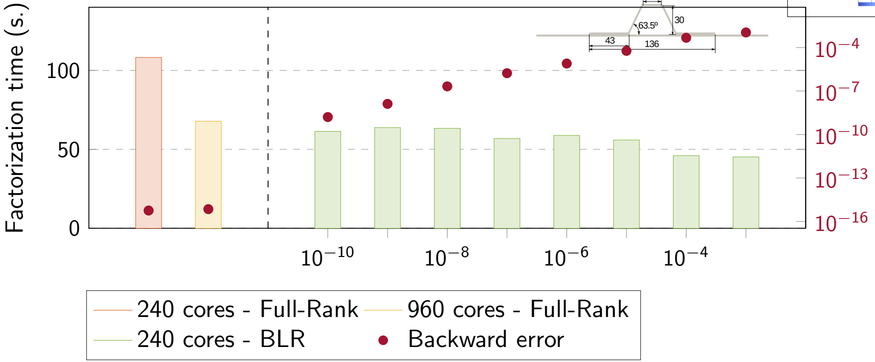




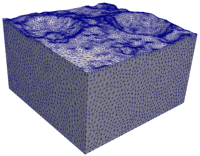
Structural mechanics: wind turbines (ALYA code)

- structure subject to compression load
- matrix of order 10M
- BLR backward error is in very good accordance with ε





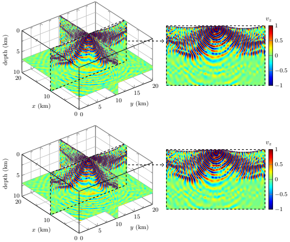
Surface topography



3D mesh (220k cells, $20{\times}20{\times}10$ km^3)

- surface topography: small cells
- below: larger cells and high order

Solution v_z at 3 Hz using Full-Rank (top) or BLR $\varepsilon{=}10^{-5}$ (bottom)



Matrix size (elastic equations, $f{=}3$ Hz, $3 \leq p \leq 6$): N=25M, NZ=5 859M

BLR compression:

	Full-Rank	BLR ($\varepsilon{=}10^{-5}$)
flops	1.1×10^{16}	3.6×10^{15} (34%)

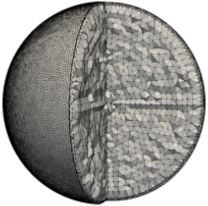
Time compression:

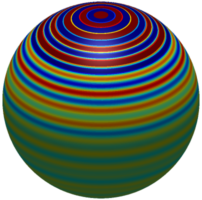
(HLRS cluster Stuttgart, using 40 nodes, 80 MPI, 32 threads/MPI)

Time (seconds)	Analysis	Facto.	Solve
MUMPS Full-Rank	11.7	2894	8.3
MUMPS BLR ($\varepsilon = 10^{-5}$)	13.2	1798	6.0

Helioseismology

Mesh and solution at 2 mHz for r=0.99. Cells near surface are very small (extreme properties)





Experiment with entire solar ball, r_{max}=1.0008, f=1 mHz

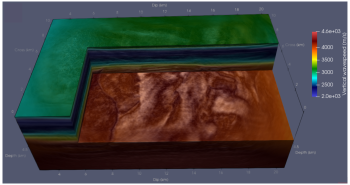
- required 40 nodes, 1 MPI per node (256 GB, 24 threads per node)
- BLR solver used, with $\varepsilon = 10^{-7}$
- Full-Rank estimate (12M, p=2-4): 3×10^{16} flops, memory $>$ **9 TiB**

#cells	p	#dofs	BLR flops (% of FR)	ana	fac	sol	Mem
12M	2-4	374M	4.7×10^{14} (2.0%)	500 s.	773 s.	20 s.	5.3 TiB
12M	3-4	381M	5.8×10^{14} (1.7%)	506 s.	999 s.	20 s.	5.3 TiB

- 50x BLR compression

Full-Waveform Inversion

- Adastra MUMPS4FWI project led by WIND team
- Application: Gorgon Model, reservoir 23km x 11km x 6.5km, grid size 15m, Helmholtz equation, 25-Hz
- Complex matrix, 531 Million dofs, storage(A)=220 GBytes;
- FR cost: flops for one LU factorization= 2.6×10^{18};
  Estimated storage for LU factors= 73 TBytes



(25-Hz Gorgon FWI velocity model)

FR (Full-Rank); BLR with $\varepsilon = 10^{-5}$; 48 000 cores (500 MPI $\times$ 96 threads/MPI)

FR: fp32; Mixed precision BLR: 3 precisions (32bits, 24bits, 16bits) for storage

LU size (TBytes)			Flops		Time BLR + Mixed (sec)			Scaled Resid.
FR	BLR	+mixed	FR	BLR+mixed	Analysis	Facto	Solve	BLR+mixed
73	34	26	2.6×10^{18}	0.5×10^{18}	446	5500	27	7×10^{-4}

in practice: hundreds to thousands of Solve steps (sparse right hand sides (sources))

Structural mechanics: pump of nuclear plant

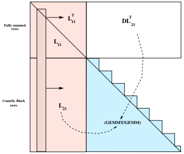
- Matrix from aero-acoustics, complex unsymmetric

N=4.1M, NZ=353M, flops(LU)= 2.6×10^{14} $\boxed{\text{pivots: 4 delayed, 415 off-diag}}$

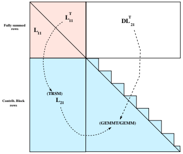
8 MPIx18 threads	Full-Rank		BLR ($\varepsilon = 10^{-8}$)	
Pivoting	std	off	std	off
Factor. time (s.)	273	241	164	114
Scaled residual	7×10^{-13}	1×10^{-11}	6×10^{-8}	2×10^{-7}

Pivoting off $\rightarrow$ improved BLR performance, residual still OK

std



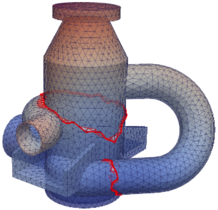
off



BLAS2&3

large BLAS 3

Structural mechanics: pump of nuclear plant

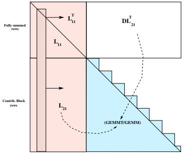


- Matrix from structural mechanics, real symmetric: pump (code_aster, EDF)

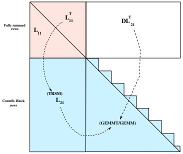
  N=5.4M, NZ=208M, flops(LDL^T)= 1.8×10^{13} | pivots: 79k delayed, 37k 2×2, 74k negative |

1MPIx18 threads	Full-Rank		BLR ($\varepsilon = 10^{-9}$)	
Pivoting	std	off	std	off
Factor. time (s.)	59.5	KO	43.9	KO
Scaled residual	1.9×10^{-15}		1.1×10^{-10}	

std

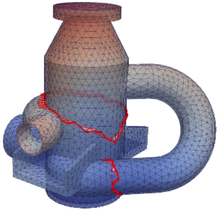


off



BLAS2&3

large BLAS 3



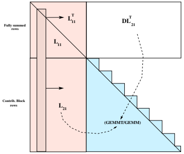
Relaxed pivoting: based on Duff and Pralet

- Matrix from structural mechanics, real symmetric: pump (code_aster, EDF)

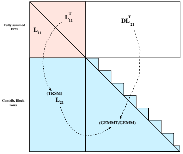
N=5.4M, NZ=208M, flops(LDL^T)= 1.8×10^{13} pivots: 79k delayed, 37k 2×2, 74k negative

1MPIx18 threads	Full-Rank			BLR ($\varepsilon = 10^{-9}$)		
Pivoting	std	off	relaxed	std	off	relaxed
Factor. time (s.)	59.5	KO	47.7	43.9	KO	31.4
Scaled residual	1.9×10^{-15}		1.9×10^{-15}	1.1×10^{-10}		1.3×10^{-10}

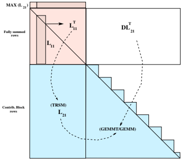
std



off



relaxed



BLAS2&3

large BLAS 3

Structural mechanics: pump of nuclear plant

- Matrix from aero-acoustics, complex unsymmetric

  N=4.1M, NZ=353M, flops(LU)= 2.6×10^{14} | pivots: 4 delayed, 415 off-diag |

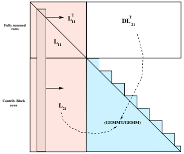
8 MPIx18 threads	Full-Rank			BLR ($\varepsilon = 10^{-8}$)		
Pivoting	std	off	relaxed	std	off	relaxed
Factor. time (s.)	273	241	**241**	164	114	**127**
Scaled residual	$7\text{x}10^{-13}$	$1\text{x}10^{-11}$	$1\text{x}10^{-12}$	$6\text{x}10^{-8}$	$2\text{x}10^{-7}$	$1\text{x}10^{-7}$

- Matrix from structural mechanics, real symmetric: pump (code_aster, EDF)

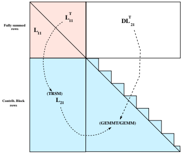
  N=5.4M, NZ=208M, flops(LDL^T)= 1.8×10^{13} | pivots: 79k delayed, 37k 2×2, 74k negative |

1MPIx18 threads	Full-Rank			BLR ($\varepsilon = 10^{-9}$)		
Pivoting	std	off	relaxed	std	off	relaxed
Factor. time (s.)	59.5	KO	47.7	43.9	KO	31.4
Scaled residual	$1.9\text{x}10^{-15}$		$1.9\text{x}10^{-15}$	$1.1\text{x}10^{-10}$		$1.3\text{x}10^{-10}$

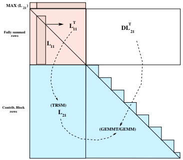
std



off



relaxed

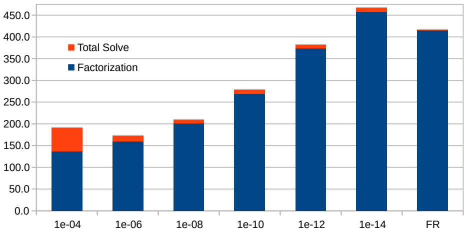


BLAS2&3

large BLAS 3

BLR as a preconditioner

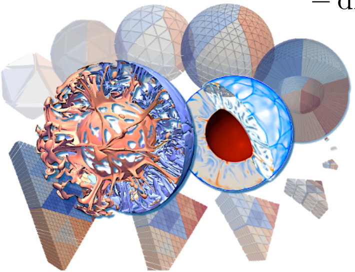
- Application in structural mechanics (ANSYS): highly nonlinear materials, 3D solid elements, matrix `Rubber RVE`
  N=3M, NZ=70M, flops(LDL^T)$= 9.8 \times 10^{14}$
- Conjugate Gradient preconditioned BLR LU:
  - Convergence criterion is scaled residual $\leq 10^{-10}$, time for analysis $\approx$ 45sec
  - CG with simple block-Jacobi preconditioner did not converge
  - Target computer: cluster with 28-core nodes based on Xeon E5-2690 v4-14 cores, 512GB



Solver(ε)	Size of L	Total (nbiter)
CG-BLR(10^{-4})	30GB	192(92)
CG-BLR(10^{-6})	51GB	173(13)
CG-BLR(10^{-8})	78GB	210 (4)
CG-BLR(10^{-10})	109GB	279 (3)
CG-BLR(10^{-12})	136GB	383 (1)
CG-BLR(10^{-14})	153GB	467 (1)
Full-Rank (FR)	157GB	417(0)

BLR in a multigrid solver

Mantle convection simulation:



$$
\begin{aligned}
-\operatorname{div}\left(\frac{\nu}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^\top)\right) + \nabla \mathbf{p} &= \mathbf{f} \quad \text{in } \Omega, \\
\operatorname{div}(\mathbf{u}) &= 0 \quad \text{in } \Omega, \\
\mathbf{u} &= \mathbf{g} \quad \text{on } \partial\Omega,
\end{aligned}
$$

- HHG (Hierarchical Hybrid Grids) geometric multigrid solver
- 6 levels with V-cycle and Uzawa smoother

→ compare BLR vs. PMINRES as coarse grid solvers

Buttari, Huber, Leleux, M., Ruede, Wohlmuth

BLR in a multigrid solver

n-fine	n-coarse
$1.21 \cdot 10^{11}$	$1.94 \cdot 10^{6}$

Time on the fine grid: 1200 s. (43200 cores, HLRS cluster Stuttgart)

Time on the coarse grid:

PMINRES	162.5 s.	$\Rightarrow$ not negligible
MUMPS Full-Rank	184.7 s.	
MUMPS BLR, $\varepsilon = 10^{-5}$	91.4 s.	
MUMPS BLR, $\varepsilon = 10^{-5}$ + single precision	83.6 s.	$\Rightarrow$ $2\times$ speedup

- PMINRES converges slowly $\Rightarrow$ coarse grid solution not negligible
- $2\times$ speedup on the coarse grid $\Rightarrow$ $\sim 6\%$ overall gain

Cost analysis of the involved steps

Let us consider two blocks A and B of size $b \times b$ and of rank bounded by r.

step	type	operation	cost
Factor	FR	$A \leftarrow LU$	$\mathcal{O}(b^3)$
Solve	FR-FR	$B \leftarrow BU^{-1}$	$\mathcal{O}(b^3)$
Compress	LR	$A \leftarrow \widetilde{A}$	$\mathcal{O}(b^2 r)$
Update	FR-FR	$C \leftarrow AB$	$\mathcal{O}(b^3)$
Update	LR-FR	$C \leftarrow \widetilde{A}B$	$\mathcal{O}(b^2 r)$
Update	FR-LR	$C \leftarrow A\widetilde{B}$	$\mathcal{O}(b^2 r)$
Update	LR-LR	$C \leftarrow \widetilde{A}\widetilde{B}$	$\mathcal{O}(b^2 r)$

This is not enough to compute the complexity $\Rightarrow$ we need to bound the number of FR blocks!

Admissible block partitions

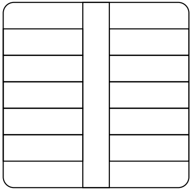
Admissibility of a block

An block $\sigma \times \tau$ is admissible if $\mathrm{dist}(\sigma,\tau) \geq \eta \max(\mathrm{diam}(\sigma), \mathrm{diam}(\tau))$.

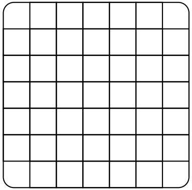
Admissibility of a block partition

A block partion $\mathcal{P}$ is admissible if there exists $q = O(1)$ such that

$$\begin{cases} \#\{\sigma, \quad \sigma \times \tau \in \mathcal{P} \text{ is not admissible}\} \leq q \\ \#\{\tau, \quad \sigma \times \tau \in \mathcal{P} \text{ is not admissible}\} \leq q \end{cases}$$



Non-Admissible



Admissible

Admissible block partitions

Key result

For any matrix, an admissible $\mathcal{P}$ can be built geometrically

Amestoy, Buttari, L'Excellent, M. (2017)

Admissible block partitions

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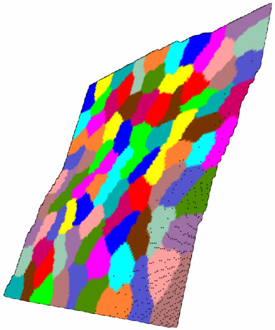

What about algebraic partitions?
For sparse problems, use the adjacency graph!

Root separator of a 128^3 Poisson problem clustered with SCOTCH via k-means Weisbecker (2015)

Memory complexity of the dense BLR factorization

We consider a dense $m \times m$ matrix with $m = pb$

The memory complexity to store the matrix can be computed as
$\mathcal{M}_{total}(b, p, r) = \mathcal{M}_{FR}(b, p) + \mathcal{M}_{LR}(b, p, r)$

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- Step 1: we have

$$\mathcal{M}_{FR}(b, p) = \mathcal{O}(pb^2)$$
$$\mathcal{M}_{LR}(b, p, r) = \mathcal{O}(p^2 br)$$

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- Step 2: assuming $b = \mathcal{O}(m^x)$ and $r = \mathcal{O}(m^\alpha)$, we have

$$\mathcal{M}_{total}(m, x, \alpha) = \mathcal{O}(m^{1+x} + m^{2-x+\alpha})$$

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$$\mathcal{M}_{total}(m, x, \alpha) = \mathcal{O}(m^{1+x} + m^{2-x+\alpha})$$

- Step 3: the optimal block size is $b^* = m^{(1+\alpha)/2}$ and the resulting optimal complexity is

$$\mathcal{M}_{opt}(m, r) = \mathcal{M}_{total}(m, x^*, \alpha) = \mathcal{O}(m^{3/2} r^{1/2})$$

Flop complexity of the dense BLR factorization

We consider a dense $m \times m$ matrix with $m = pb$

step	type	cost	number	$\mathcal{C}_{step}(b, p, r)$
Factor	FR	$\mathcal{O}(b^3)$	$\mathcal{O}(p)$	
Solve	FR-FR	$\mathcal{O}(b^3)$	$\mathcal{O}(p^2)$	
Compress	LR	$\mathcal{O}(b^2 r)$	$\mathcal{O}(p^2)$	
Update	FR-FR	$\mathcal{O}(b^3)$	$\mathcal{O}(p)$	
Update	LR-FR	$\mathcal{O}(b^2 r)$	$\mathcal{O}(p^2)$	
Update	LR-LR	$\mathcal{O}(b^2 r)$	$\mathcal{O}(p^3)$	

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Factor	FR	$\mathcal{O}(b^3)$	$\mathcal{O}(p)$	$\mathcal{O}(pb^3)$
Solve	FR-FR	$\mathcal{O}(b^3)$	$\mathcal{O}(p^2)$	$\mathcal{O}(p^2b^3)$
Compress	LR	$\mathcal{O}(b^2r)$	$\mathcal{O}(p^2)$	$\mathcal{O}(p^2b^2r)$
Update	FR-FR	$\mathcal{O}(b^3)$	$\mathcal{O}(p)$	$\mathcal{O}(pb^3)$
Update	LR-FR	$\mathcal{O}(b^2r)$	$\mathcal{O}(p^2)$	$\mathcal{O}(p^2b^2r)$
Update	LR-LR	$\mathcal{O}(b^2r)$	$\mathcal{O}(p^3)$	$\mathcal{O}(p^3b^2r)$

- Step 1: compute $\mathcal{C}_{step}(b,p,r) = \text{cost} \times \text{number}$

Flop complexity of the dense BLR factorization

We consider a dense $m \times m$ matrix with $m = pb$

step	type	cost	number	$\mathcal{C}_{step}(b,p,r)$	$\mathcal{C}_{step}(m,x,\alpha)$
Factor	FR	$\mathcal{O}(b^3)$	$\mathcal{O}(p)$	$\mathcal{O}(pb^3)$	$\mathcal{O}(m^{1+2x})$
Solve	FR-FR	$\mathcal{O}(b^3)$	$\mathcal{O}(p^2)$	$\mathcal{O}(p^2b^3)$	$\mathcal{O}(m^{2+x})$
Compress	LR	$\mathcal{O}(b^2r)$	$\mathcal{O}(p^2)$	$\mathcal{O}(p^2b^2r)$	$\mathcal{O}(m^{2+\alpha})$
Update	FR-FR	$\mathcal{O}(b^3)$	$\mathcal{O}(p)$	$\mathcal{O}(pb^3)$	$\mathcal{O}(m^{1+2x})$
Update	LR-FR	$\mathcal{O}(b^2r)$	$\mathcal{O}(p^2)$	$\mathcal{O}(p^2b^2r)$	$\mathcal{O}(m^{2+\alpha})$
Update	LR-LR	$\mathcal{O}(b^2r)$	$\mathcal{O}(p^3)$	$\mathcal{O}(p^3b^2r)$	$\mathcal{O}(m^{3-x+\alpha})$

- Step 1: compute $\mathcal{C}_{step}(b,p,r) = \text{cost} \times \text{number}$
- Step 2: compute $\mathcal{C}_{step}(m,x,\alpha)$ with $b = \mathcal{O}(m^x)$ and $r = \mathcal{O}(m^\alpha)$.

Flop complexity of the dense BLR factorization

We consider a dense $m \times m$ matrix with $m = pb$

step	type	cost	number	$\mathcal{C}_{step}(b,p,r)$	$\mathcal{C}_{step}(m,x,\alpha)$
`Factor`	`FR`	$\mathcal{O}(b^3)$	$\mathcal{O}(p)$	$\mathcal{O}(pb^3)$	$\mathcal{O}(m^{1+2x})$
`Solve`	`FR-FR`	$\mathcal{O}(b^3)$	$\mathcal{O}(p^2)$	$\mathcal{O}(p^2b^3)$	$\mathcal{O}(m^{2+x})$
`Compress`	`LR`	$\mathcal{O}(b^2r)$	$\mathcal{O}(p^2)$	$\mathcal{O}(p^2b^2r)$	$\mathcal{O}(m^{2+\alpha})$
`Update`	`FR-FR`	$\mathcal{O}(b^3)$	$\mathcal{O}(p)$	$\mathcal{O}(pb^3)$	$\mathcal{O}(m^{1+2x})$
`Update`	`LR-FR`	$\mathcal{O}(b^2r)$	$\mathcal{O}(p^2)$	$\mathcal{O}(p^2b^2r)$	$\mathcal{O}(m^{2+\alpha})$
`Update`	`LR-LR`	$\mathcal{O}(b^2r)$	$\mathcal{O}(p^3)$	$\mathcal{O}(p^3b^2r)$	$\mathcal{O}(m^{3-x+\alpha})$

- Step 1: compute $\mathcal{C}_{step}(b,p,r) = \text{cost} \times \text{number}$
- Step 2: compute $\mathcal{C}_{step}(m,x,\alpha)$ with $b = \mathcal{O}(m^x)$ and $r = \mathcal{O}(m^\alpha)$.
- Step 3: compute the total complexity (sum of all steps)

$$\mathcal{C}_{total}(m,x,\alpha) = \mathcal{O}(m^{3-x+\alpha} + m^{2+x})$$

Flop complexity of the dense BLR factorization

We consider a dense $m \times m$ matrix with $m = pb$

step	type	cost	number	$\mathcal{C}_{step}(b,p,r)$	$\mathcal{C}_{step}(m,x,\alpha)$
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Update	FR-FR	$\mathcal{O}(b^3)$	$\mathcal{O}(p)$	$\mathcal{O}(pb^3)$	$\mathcal{O}(m^{1+2x})$
Update	LR-FR	$\mathcal{O}(b^2r)$	$\mathcal{O}(p^2)$	$\mathcal{O}(p^2b^2r)$	$\mathcal{O}(m^{2+\alpha})$
Update	LR-LR	$\mathcal{O}(b^2r)$	$\mathcal{O}(p^3)$	$\mathcal{O}(p^3b^2r)$	$\mathcal{O}(m^{3-x+\alpha})$

- Step 1: compute $\mathcal{C}_{step}(b,p,r) =$ cost $\times$ number
- Step 2: compute $\mathcal{C}_{step}(m,x,\alpha)$ with $b = \mathcal{O}(m^x)$ and $r = \mathcal{O}(m^\alpha)$.
- Step 3: compute the total complexity (sum of all steps)

$$\mathcal{C}_{total}(m,x,\alpha) = \mathcal{O}(m^{3-x+\alpha} + m^{2+x})$$

- Step 4: the optimal block size is $b^* = m^{(1+\alpha)/2}$ and the resulting optimal complexity is $\mathcal{C}_{opt}(m,r) = \mathcal{C}_{total}(m,x^*,\alpha) = \mathcal{O}(m^{5/2}r^{1/2})$

Complexity of the sparse multifrontal BLR factorization

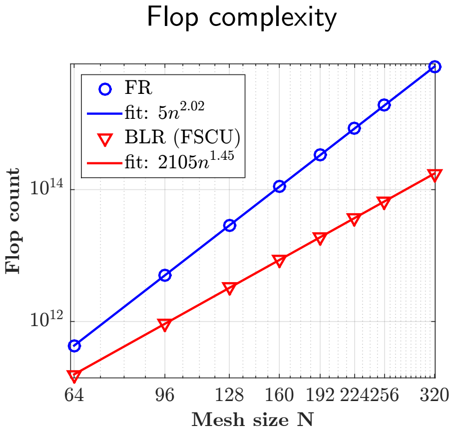
For a dense complexity $\mathcal{C}_{opt}(m, r)$, the sparse complexity is computed as

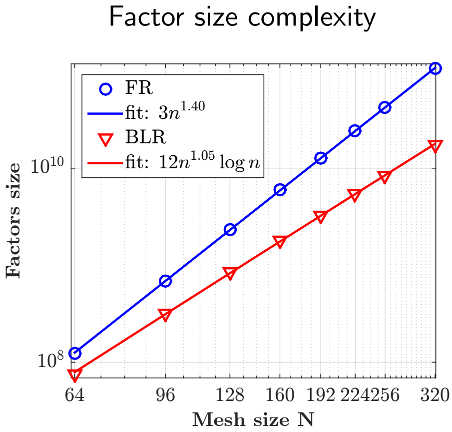
$$N \times N \text{ grid:} \quad \mathcal{C}_{mf} = \sum_{\ell=0}^{\log_2 N} 2^{2\ell} \mathcal{C}_{opt}\left(\frac{N}{2^\ell}\right),$$

$$N \times N \times N \text{ grid:} \quad \mathcal{C}_{mf} = \sum_{\ell=0}^{\log_4 N^2} 2^{3\ell} \mathcal{C}_{opt}\left(\frac{N^2}{2^{2\ell}}\right).$$

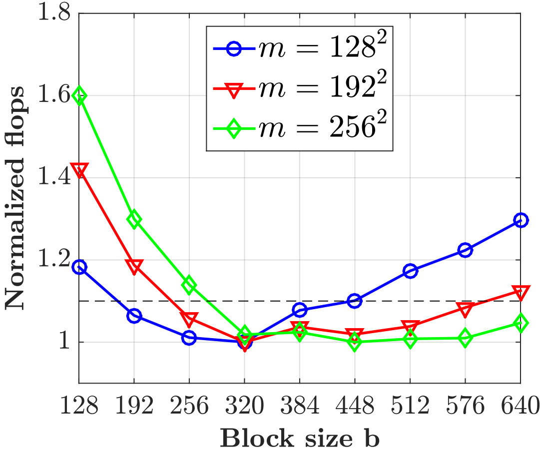
	operations (OPC)	factor size (NNZ)
	$N \times N$ grid	
FR	$\mathcal{O}(N^3)$	$\mathcal{O}(N^2 \log N)$
BLR	$\mathcal{O}(N^{5/2} r^{1/2})$	$\mathcal{O}(N^2)$
	$N \times N \times N$ grid	
FR	$\mathcal{O}(N^6)$	$\mathcal{O}(N^4)$
BLR	$\mathcal{O}(N^5 r^{1/2})$	$\mathcal{O}(N^3 \max(r^{1/2}, \log N))$

Experimental complexity on Poisson problem





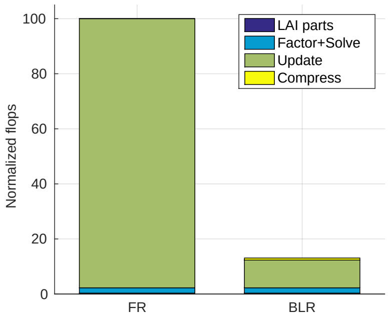
Influence of the block size b on the complexity



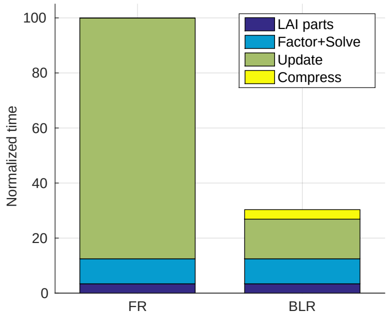
Analysis on the root node (of size $m = N^2$):

- large range of acceptable block sizes around the optimal b^* $\Rightarrow$ flexibility to tune block size for performance
- that range increases with the size of the matrix $\Rightarrow$ necessity to have variable block sizes

Sequential result



Normalized Flops

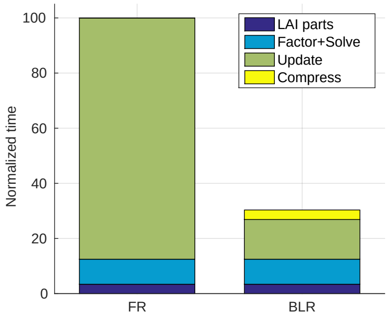


Normalized Time

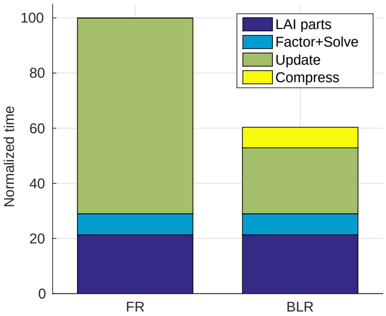
7.7 gain in flops only translated to a **3.3** gain in time: why?

- lower granularity of the Update
- higher relative weight of the FR parts
- inefficient Compress

Multithreaded result on 24 threads



Normalized Time (Seq.)

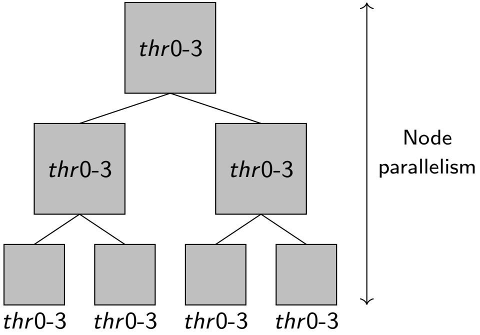


Normalized Time (MT)

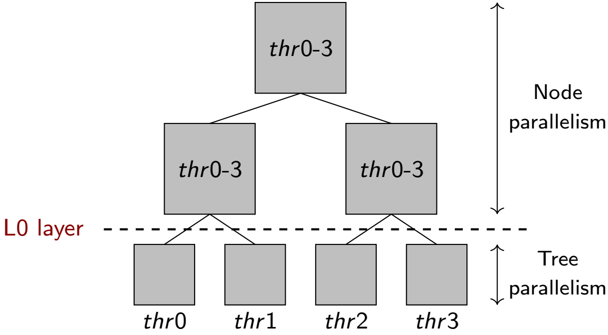
3.3 gain in sequential becomes **1.7** in multithreaded: why?

- LAI parts have become critical
- Update and Compress are memory-bound

Exploiting tree-based multithreading in MF solvers

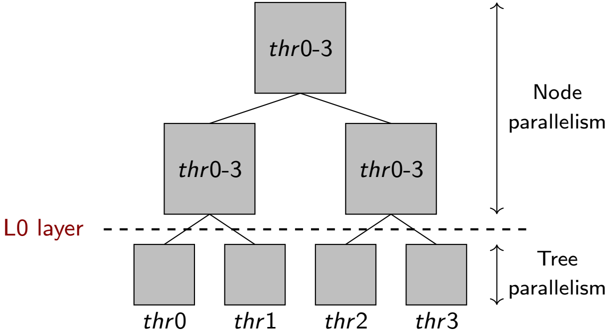


Exploiting tree-based multithreading in MF solvers



L'Excellent and Sid-Lakhdar (2014)

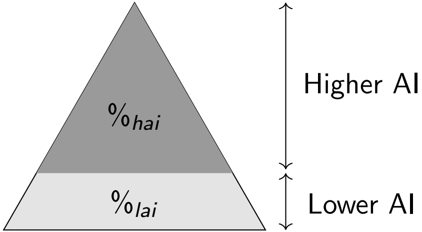
Exploiting tree-based multithreading in MF solvers



📄 L'Excellent and Sid-Lakhdar (2014)

$\Rightarrow$ how big an impact can tree-based multithreading make?

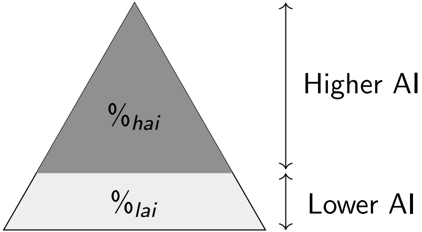
Impact of tree-based multithreading on BLR (24 threads)



	node only		node + tree	
	time	$\%_{lai}$	time	$\%_{lai}$
FR	509	21%		
BLR				

- In FR, top of the tree is dominant

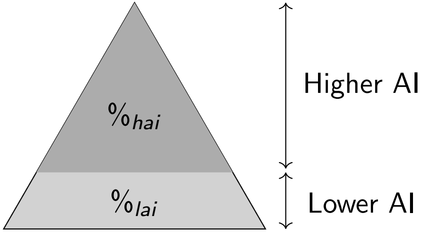
Impact of tree-based multithreading on BLR (24 threads)



	node only		node + tree	
	time	$\%_{lai}$	time	$\%_{lai}$
FR BLR	509	21%	424	13%

- In FR, top of the tree is dominant ⇒ tree MT brings little gain

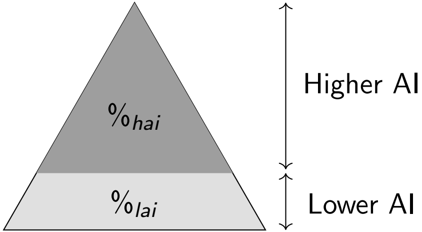
Impact of tree-based multithreading on BLR (24 threads)



	node only		node + tree	
	time	$\%_{lai}$	time	$\%_{lai}$
FR	509	21%	424	13%
BLR	307	35%		

- In FR, top of the tree is dominant $\Rightarrow$ tree MT brings little gain
- In BLR, bottom of the tree compresses less, becomes important

Impact of tree-based multithreading on BLR (24 threads)

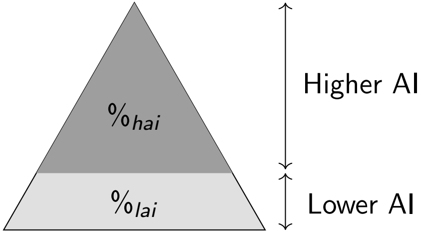


	node only		node + tree	
	time	$\%_{lai}$	time	$\%_{lai}$
FR	509	21%	424	13%
BLR	307	35%	221	24%

- In FR, top of the tree is dominant $\Rightarrow$ tree MT brings little gain
- In BLR, bottom of the tree compresses less, becomes important

$\Rightarrow$ **1.7** gain becomes **1.9** thanks to tree-based multithreading

Impact of tree-based multithreading on BLR (24 threads)



	node only		node + tree	
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BLR	307	35%	221	24%

- In FR, top of the tree is dominant $\Rightarrow$ tree MT brings little gain
- In BLR, bottom of the tree compresses less, becomes important

$\Rightarrow$ **1.7** gain becomes **1.9** thanks to tree-based multithreading

Theoretical speedup

		tree only	node only	node + tree
$N \times N \times N$ grid	FR	$\mathcal{O}(1)$	$\mathcal{O}(N^3)$	$\mathcal{O}(N^4)$
	BLR	$\mathcal{O}(1)$	$\mathcal{O}(N^2 r^{1/2})$	$\mathcal{O}(N^3 r^{1/2})$

Right-looking Vs. Left-looking analysis (24 threads)

	FR time		BLR time	
	RL	LL	RL	LL
Update	338	336	110	67
Total	424	421	221	175

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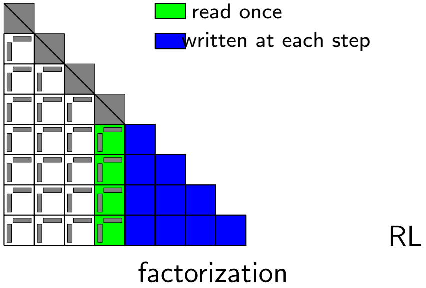

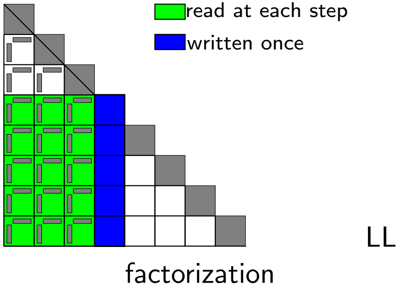

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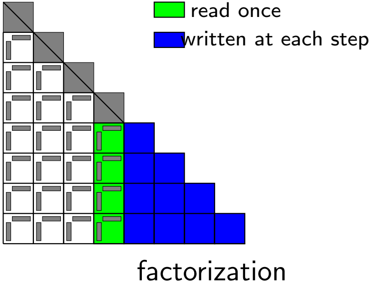
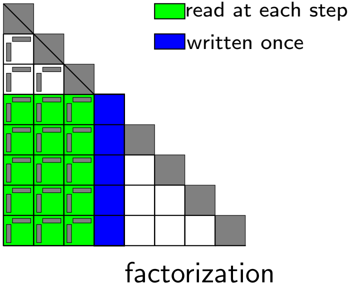


RL



LL

⇒ Lower volume of memory transfers in LL (more critical in MT)

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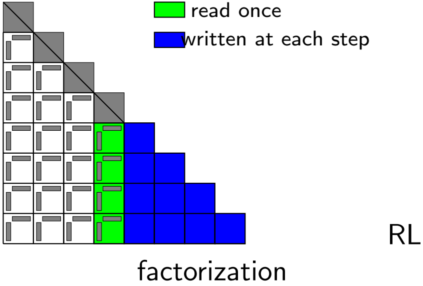
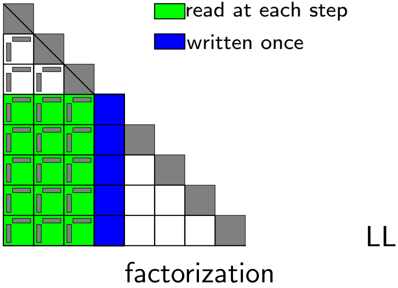
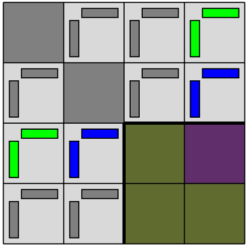


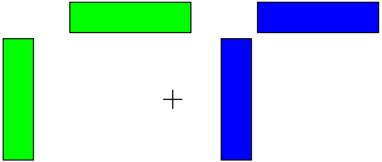


⇒ Lower volume of memory transfers in LL (more critical in MT)

Update is now less memory-bound: **1.9** gain becomes **2.4** in LL

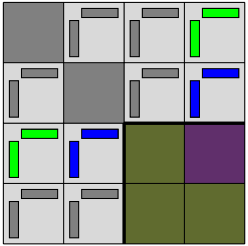
LUAR variant: accumulation and recompression

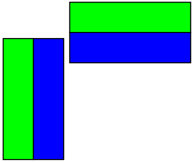




- FSCU (Factor, Solve, Compress, Update)
- FSCU+LUAR

LUAR variant: accumulation and recompression





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  - Better granularity in Update operations

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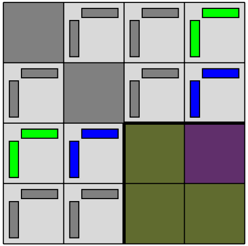

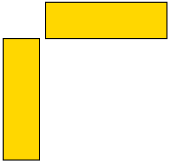

- FSCU (Factor, Solve, Compress, Update)
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  - Better granularity in Update operations
  - Potential recompression $\Rightarrow$ asymptotic complexity reduction?

    $\Rightarrow$ Designed and compared several recompression strategies

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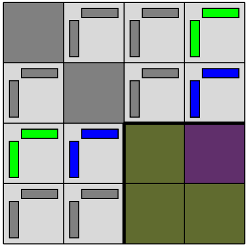

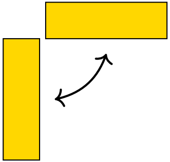

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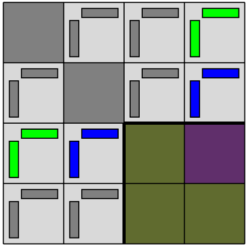

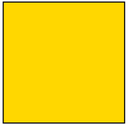

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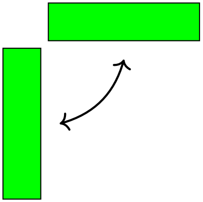
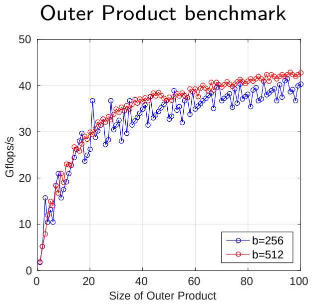
Performance of Outer Product with LUA(R) (24 threads)

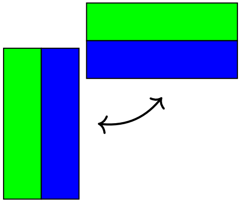
		LL	LUA	LUAR*
average size of Outer Product		16.5		
flops ($\times 10^{12}$)	Outer Product	3.8		
	Total	10.2		
time (s)	Outer Product	21		
	Total	175		

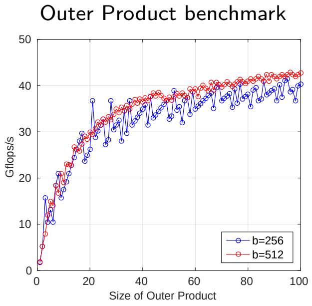




Performance of Outer Product with LUA(R) (24 threads)

		LL	LUA	LUAR*
average size of Outer Product		16.5	61.0	
flops ($\times 10^{12}$)	Outer Product	3.8	3.8	
	Total	10.2	10.2	
time (s)	Outer Product	21	14	
	Total	175	167	

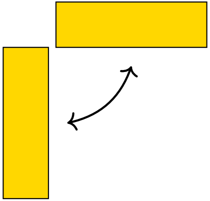




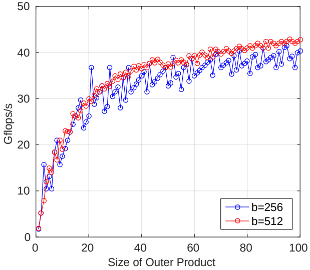
Performance of Outer Product with LUA(R) (24 threads)

		LL	LUA	LUAR*
average size of Outer Product		16.5	61.0	32.8
flops ($\times 10^{12}$)	Outer Product	3.8	3.8	1.6
	Total	10.2	10.2	8.1
time (s)	Outer Product	21	14	6
	Total	175	167	160

* All metrics include the Recompression overhead



Outer Product benchmark



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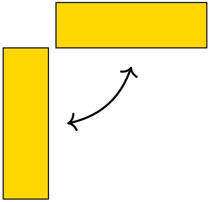
	Total	175	167	160

* All metrics include the Recompression overhead

Higher granularity and lower flops in Update:

$\Rightarrow$ **2.4** gain becomes **2.6**



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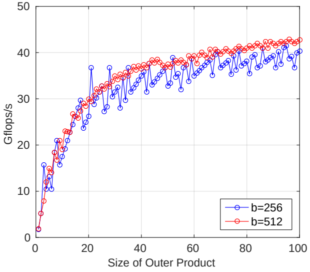

Impact of machine properties on BLR: roofline model

	specs		time (s) for BLR factorization		
	peak (GF/s)	bw (GB/s)	RL	LL	LUA
grunch (28 threads)	37	57	248	228	196
brunch (24 threads)	46	102	221	175	167

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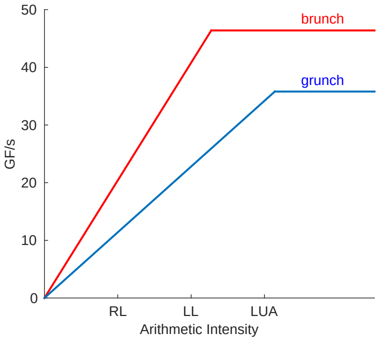
Arithmetic Intensity in BLR:

- LL > RL (lower volume of memory transfers)
- LUA > LL (higher granularities ⇒ more efficient cache use)



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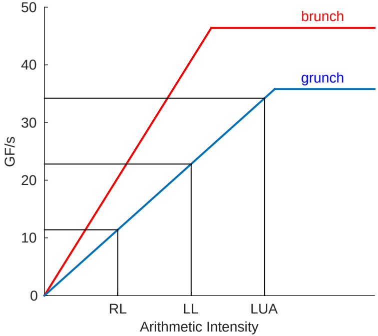

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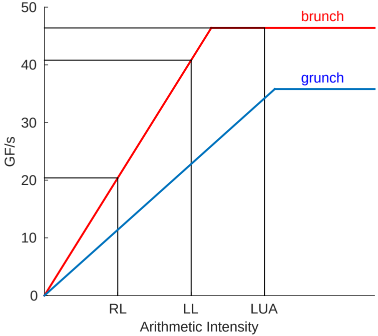
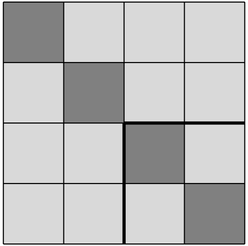


FCSU variant: compress before solve



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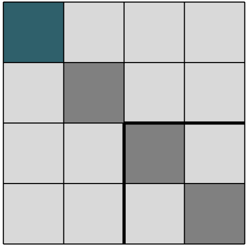

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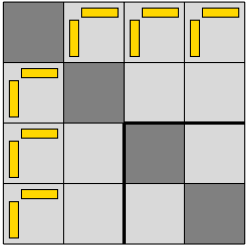

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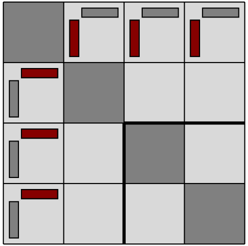

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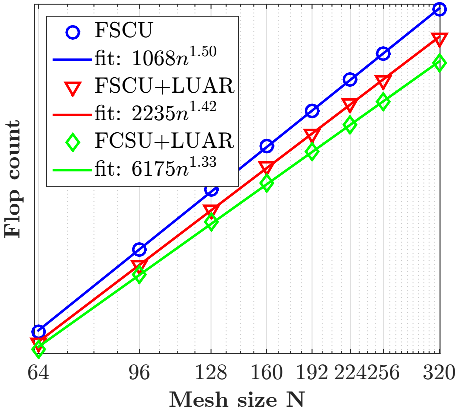
- FCSU(+LUAR)
  - Compress performed before Solve
  - Low-rank Solve ⇒ asymptotic complexity reduction?
  - On previous matrix: 160 → 111s ⇒ **2.6** gain becomes **3.7**

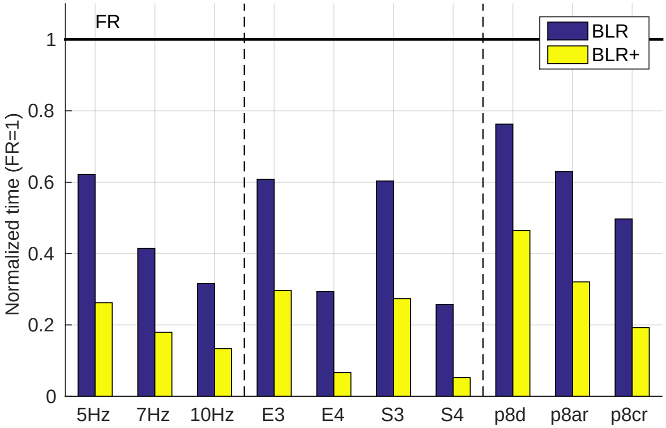
FCSU+LUAR improves asymptotic complexity! (see slide 57 for a proof ☺)

	FSCU	→ FCSU+LUAR
dense	$\mathcal{O}(m^{5/2} r^{1/2})$	$\to \mathcal{O}(m^2 r)$
sparse (3D)	$\mathcal{O}(N^5 r^{1/2})$	$\to \mathcal{O}(N^4 r)$

Experimental complexity



Multicore performance results (24 threads)



- "BLR": FSCU, right-looking, node only multithreading
- "BLR+": FCSU+LUAR, left-looking, node+tree multithreading

  Amestoy, Buttari, L'Excellent, M. (2019)

Combining (data) sparsity and low precisions

Two approaches: coarse and fine grain mixed precision

- **Coarse grain mixed precision:** Run baseline algorithm in low precision, refine the result to high precision
  - ☺ Simple and efficient, can rely on optimized libraries
  - ☹ Extra work for the refinement, not always guaranteed to work
- **Fine grain mixed precision:** Adapt the precision of each instruction/operation to achieve a given accuracy target
  - ☺ Optimal use of low precision, with guaranteed target accuracy
  - ☹ Much more intrusive, may be less efficient

Iterative refinement with BLR LU (coarse grain)

Error analysis: replace $\mathbf{u_f}$ by $\mathbf{u_f} + \varepsilon$ in the convergence conditions

Example on tminlet3M matrix
fp64 LU reference: time $\to$ 295.5 memory $\to$ 241.1

	time (s)		memory (GB)	
	LU-IR	GMRES-IR	LU-IR	GMRES-IR
FR	136.2	157.9	121.0	169.9

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$\varepsilon = 10^{-6}$	**88.3**	98.8	82.4	93.8

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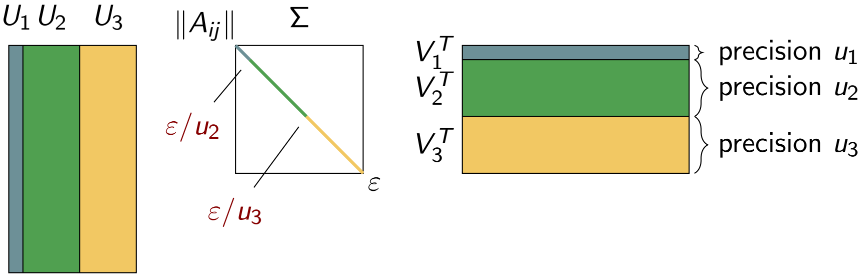
$\varepsilon = 10^{-8}$	149.7	165.3	114.0	161.9
$\varepsilon = 10^{-6}$	**88.3**	98.8	82.4	93.8
$\varepsilon = 10^{-4}$	—	105.6	—	**70.9**

- GMRES-IR allows to push BLR further!

  Amestoy, Buttari, Higham, L'Excellent, M., Vieublé (2023)

Adaptive precision low rank compression

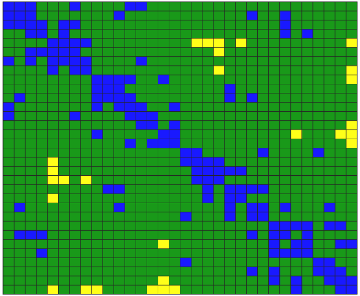


- **Adaptive precision compression:** partition U and V into q groups of decreasing precisions $u_1 \le \varepsilon < u_2 < \ldots < u_q$
- With p precisions and a partitioning such that $\|\Sigma_k\| \le \varepsilon\|A\|/u_k$, $\|A_{ij} - \widehat{U}_\varepsilon \Sigma_\varepsilon \widehat{V}_\varepsilon\| \lesssim (2p-1)\varepsilon\|A\|$
- If $\|A_{ij}\|/\|A\| \ll 1$, Σ_1 may be empty!

Adaptive precision BLR matrices

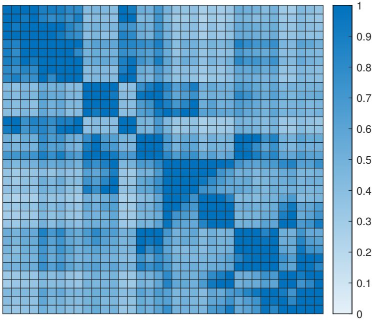
- If $\|A_{ij}\| \leq \varepsilon \|A\| / u_{\text{low}}$, block can be stored in precision u_{low}

(Poisson, $\varepsilon = 10^{-10}$)

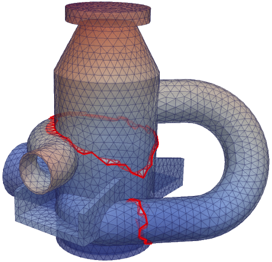


- **fp64**
- **fp32**
- **fp16**

Adaptive precision BLR compression



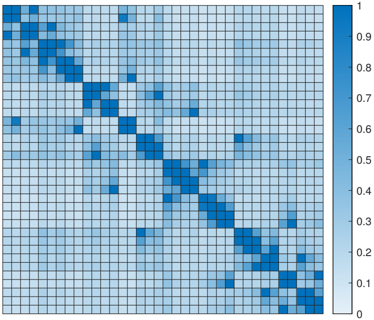
Normalized storage cost of each block



Matrix perf009d
(RIS pump from EDF)

100% entries in fp64

Adaptive precision BLR compression



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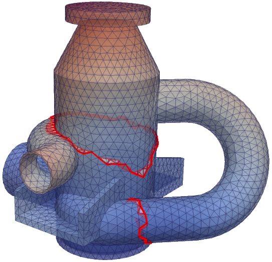


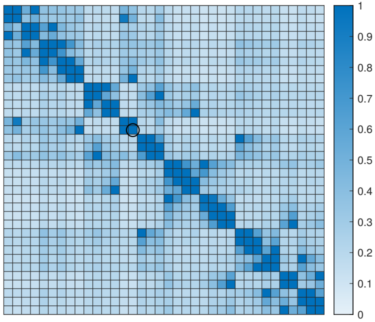
Matrix perf009d
(RIS pump from EDF)

100% entries in fp64

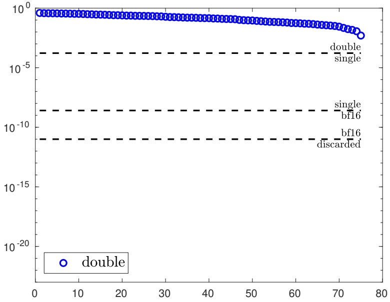
$$\rightarrow \begin{cases} 13\% \text{ in fp64} \\ 53\% \text{ in fp32} \\ 33\% \text{ in bfloat16} \end{cases}$$

$\Rightarrow 2\times$ storage reduction

Adaptive precision BLR compression



Normalized storage cost of each block



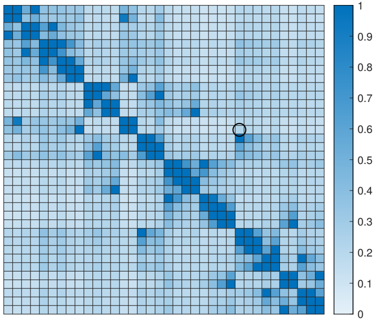
block (15,15)

100% entries in fp64

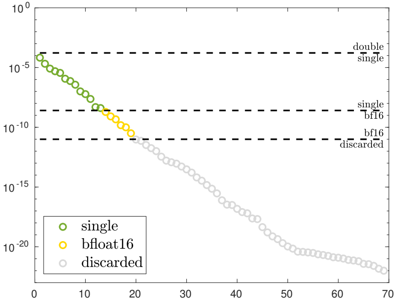
$$\rightarrow \begin{cases} 13\% \text{ in fp64} \\ 53\% \text{ in fp32} \\ 33\% \text{ in bfloat16} \end{cases}$$

$\Rightarrow 2\times$ storage reduction

Adaptive precision BLR compression



Normalized storage cost of each block



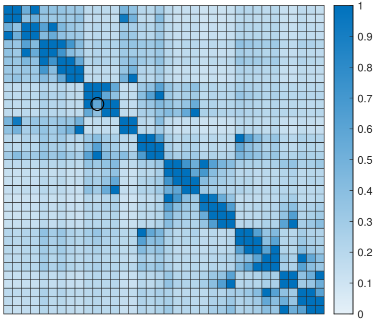
block (15,27)

100% entries in fp64

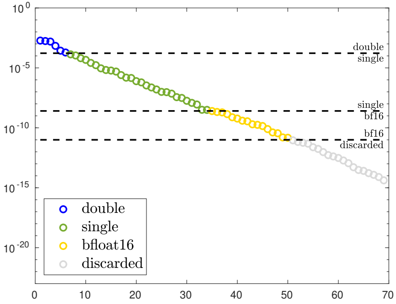
$$\to \begin{cases} 13\% \text{ in fp64} \\ 53\% \text{ in fp32} \\ 33\% \text{ in bfloat16} \end{cases}$$

$\Rightarrow$ $2\times$ storage reduction

Adaptive precision BLR compression



Normalized storage cost of each block



block (12,11)

100% entries in fp64

$$\rightarrow \begin{cases} 13\% \text{ in fp64} \\ 53\% \text{ in fp32} \\ 33\% \text{ in bfloat16} \end{cases}$$

$\Rightarrow$ 2$\times$ storage reduction

Low-rank admissibility condition
$k(m+n) \leq mn$ becomes

$$(\omega_1 k_1 + \omega_2 k_2 + \ldots + \omega_p k_p)(m+n) \leq mn$$

in mixed precision !

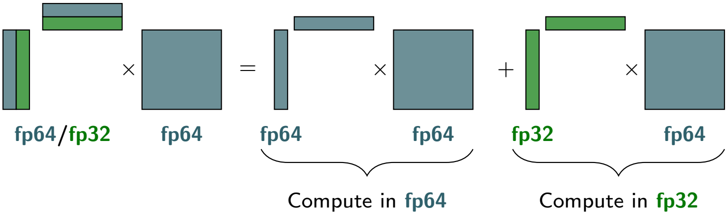
Adaptive precision BLR LU factorization

Stability of LU factorization: $\widehat{L}\widehat{U} = A + \Delta A$

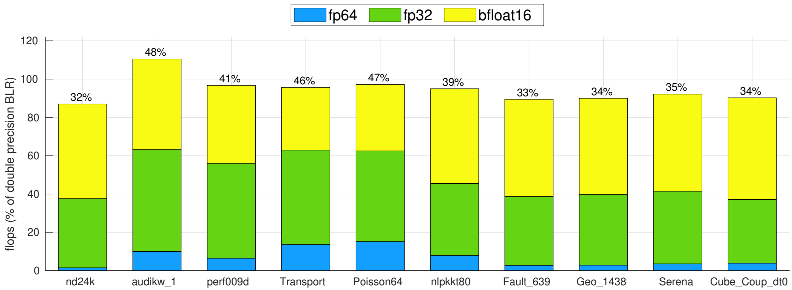
- **Standard LU** : $\|\Delta A\| \lesssim c_n u_1 \|A\|$
- **BLR LU** : $\|\Delta A\| \lesssim c'_n(\varepsilon + u_1)\|A\|$
- **Adaptive precision BLR LU** : $\|\Delta A\| \lesssim c''_n(\varepsilon + u_1)\|A\|$

  Amestoy, Boiteau, Buttari, Gerest, Jézéquel, L'Excellent, M. (2022)

Example of kernel: LR $\times$ matrix multiplication:



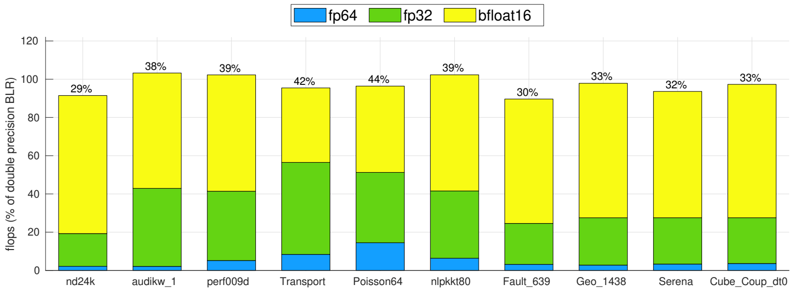
Adaptive precision BLR LU factorization



$$\varepsilon = 10^{-12}$$

Top of the bars: cost w.r.t. fp64 BLR, assuming
1 flop(fp64) = 2 flops(fp32) = 4 flops(bfloat16)

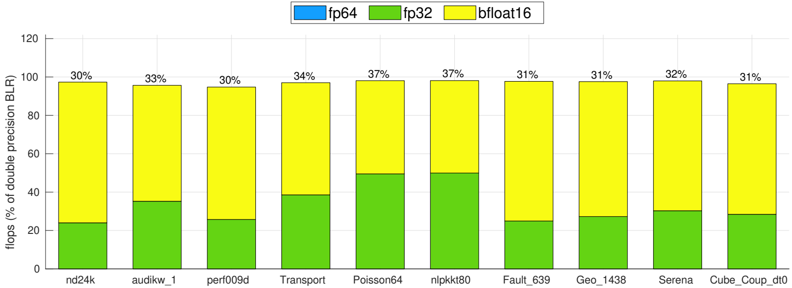
Adaptive precision BLR LU factorization



$\varepsilon = 10^{-9}$

Top of the bars: cost w.r.t. fp64 BLR, assuming
1 flop(fp64) = 2 flops(fp32) = 4 flops(bfloat16)

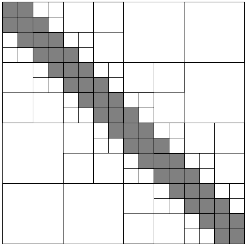
Adaptive precision BLR LU factorization



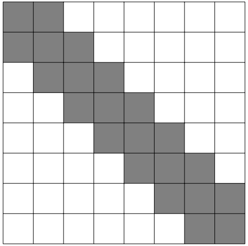
$$\varepsilon = 10^{-6}$$

Top of the bars: cost w.r.t. fp64 BLR, assuming
1 flop(fp64) = 2 flops(fp32) = 4 flops(bfloat16)

$\mathcal{H}$ and BLR matrices



$\mathcal{H}$ matrix Hackbusch (2015)



BLR matrix

- Theoretical complexity can be as low as $O(n)$
- Complex, hierarchical structure

- Theoretical complexity can be as low as $O(n^{4/3})$
- Simpler structure

BLR makes easier to preserve the numerical features of a direct solver and compromises well complexity, accuracy and performance

Nested dissection complexity formulas

$$\textbf{2D:} \quad \mathcal{C}_{sparse} = \sum_{\ell=0}^{\log N} 4^{\ell} \mathcal{C}_{dense}\left(\frac{N}{2^{\ell}}\right)$$

$$\textbf{3D:} \quad \mathcal{C}_{sparse} = \sum_{\ell=0}^{\log N} 8^{\ell} \mathcal{C}_{dense}\left(\frac{N^2}{4^{\ell}}\right)$$

Nested dissection complexity formulas

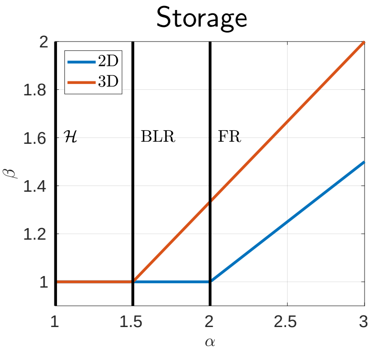
$$\textbf{2D:}\quad \mathcal{C}_{sparse} = \sum_{\ell=0}^{\log N} 4^{\ell}\,\mathcal{C}_{dense}\left(\frac{N}{2^{\ell}}\right) \quad \to \text{common ratio } 2^{2-\alpha}$$

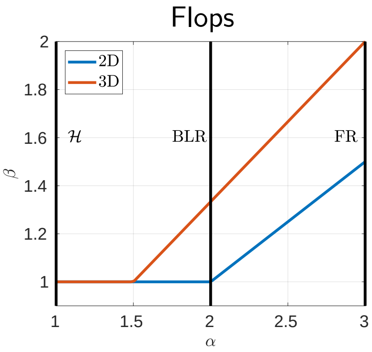
$$\textbf{3D:}\quad \mathcal{C}_{sparse} = \sum_{\ell=0}^{\log N} 8^{\ell}\,\mathcal{C}_{dense}\left(\frac{N^2}{4^{\ell}}\right) \quad \to \text{common ratio } 2^{3-2\alpha}$$

Assume $\mathcal{C}_{dense} = O(m^{\alpha})$. Then:

2D		3D	
	$\mathcal{C}_{sparse}(n)$		$\mathcal{C}_{sparse}(n)$
$\alpha > 2$	$O(n^{\alpha/2})$	$\alpha > 1.5$	$O(n^{2\alpha/3})$
$\alpha = 2$	$O(n \log n)$	$\alpha = 1.5$	$O(n \log n)$
$\alpha < 2$	$O(n)$	$\alpha < 1.5$	$O(n)$

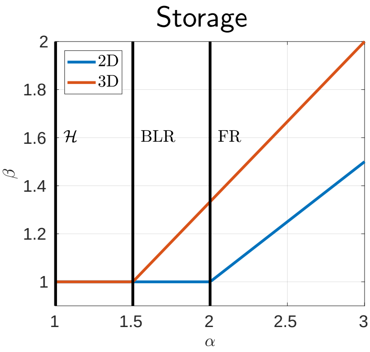
$$\mathcal{C}_{dense} = O(m^{\alpha}) \Rightarrow \mathcal{C}_{sparse} = O(n^{\beta})$$

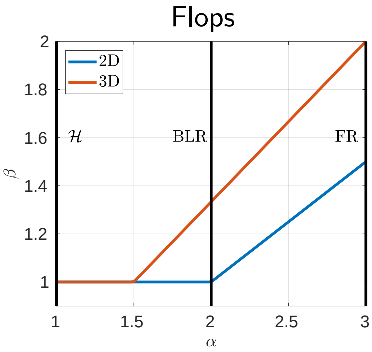




Bridging the gap between flat and hierarchical formats

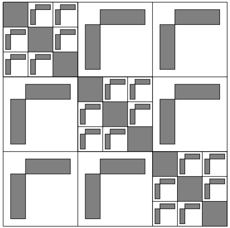
$$\mathcal{C}_{dense} = O(m^{\alpha}) \Rightarrow \mathcal{C}_{sparse} = O(n^{\beta})$$





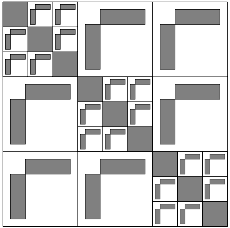
Key motivation: $\mathcal{C}_{dense} < O(m^2)$ (2D) or $O(m^{1.5})$ (3D) is enough to get $O(n)$ sparse complexity!

Complexity of the two-level BLR format



$$
\begin{aligned}
Storage &= cost_{LR} * nb_{LR} + cost_{BLR} * nb_{BLR} \\
&= O(br) * O((\frac{m}{b})^2) + O(b^{3/2} r^{1/2}) * O(\frac{m}{b}) \\
&= O(m^2 r / b + m(br)^{1/2}) \\
&= \mathbf{O(m^{4/3} r^{2/3})} \text{ for } b = (m^2 r)^{1/3}
\end{aligned}
$$

Complexity of the two-level BLR format



$$Storage = cost_{LR} * nb_{LR} + cost_{BLR} * nb_{BLR}$$
$$= O(br) * O((\frac{m}{b})^2) + O(b^{3/2}r^{1/2}) * O(\frac{m}{b})$$
$$= O(m^2 r/b + m(br)^{1/2})$$
$$= \mathbf{O(m^{4/3}r^{2/3})} \text{ for } b = (m^2 r)^{1/3}$$

Similarly, we can prove:

$$FlopLU = \mathbf{O(m^{5/3}r^{4/3})} \text{ for } b = (m^2 r)^{1/3}$$

		FR	BLR	2-BLR	...	$\mathcal{H}$
storage	dense	$O(m^2)$	$O(m^{1.5})$	$O(m^{1.33})$	...	$O(m \log m)$
	sparse	$O(n^{1.33})$	$O(n \log n)$	$O(n)$	...	$O(n)$
flop LU	dense	$O(m^3)$	$O(m^2)$	$O(m^{1.66})$	...	$O(m \log^3 m)$
	sparse	$O(n^2)$	$O(n^{1.33})$	$O(n^{1.11})$	...	$O(n)$

Multilevel BLR complexity

Main result

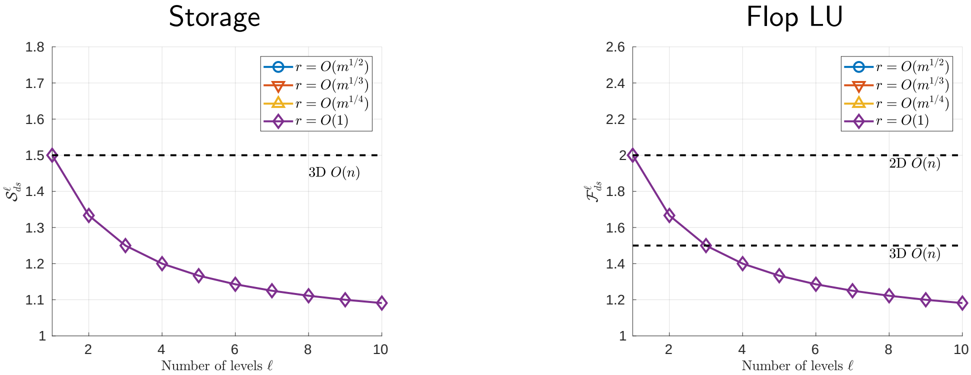
For $b = m^{\ell/(\ell+1)} r^{1/(\ell+1)}$, the $\ell-$level complexities are:

$$Storage = \mathbf{O(m^{(\ell+2)/(\ell+1)} r^{\ell/(\ell+1)})}$$
$$FlopLU = \mathbf{O(m^{(\ell+3)/(\ell+1)} r^{2\ell/(\ell+1)})}$$

Proof: by induction. Amestoy, Buttari, L'Excellent, M. (2019)

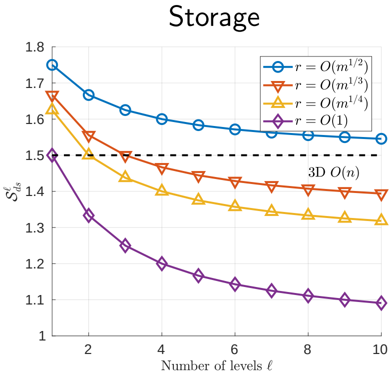
- Simple way to finely control the desired complexity
- Block size $b \propto O(m^{1-1/(\ell+1)}) \ll O(m)$
  $\Rightarrow$ larger blocks that can be efficiently processed in shared-memory

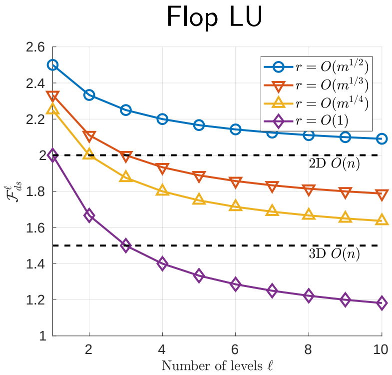
Influence of the number of levels ℓ



- If $r = O(1)$, can achieve $O(n)$ storage complexity with only two levels and $O(n \log n)$ flop complexity with three levels

Influence of the number of levels ℓ

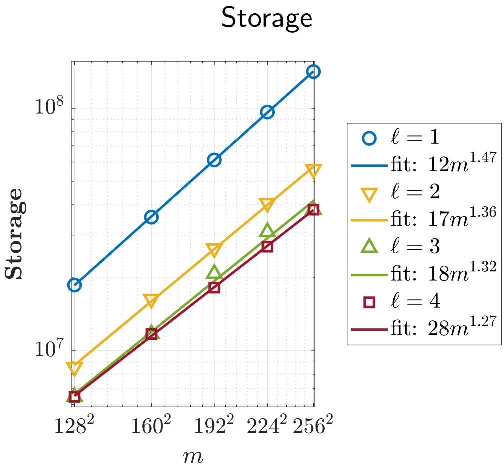


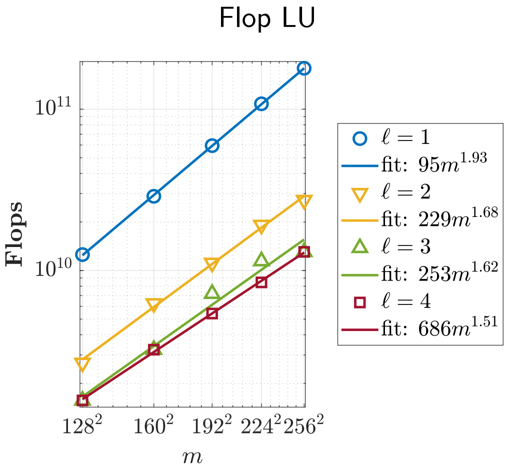


- If $r = O(1)$, can achieve $O(n)$ storage complexity with only two levels and $O(n \log n)$ flop complexity with three levels

- For higher ranks, improvement rate rapidly decreases:
the first few levels achieve most of the asymptotic gain

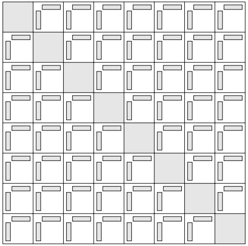
Experimental MBLR complexity (Poisson)



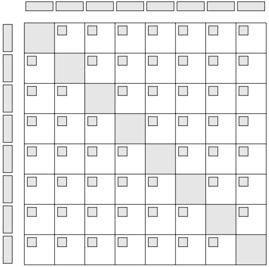


- Experimental complexity in relatively good agreement with theoretical one
- Asymptotic gain decreases with levels

The BLR^2 format

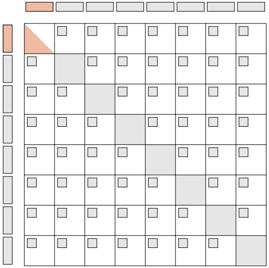


The BLR^2 format



- Common basis of size $s \geq r$ for all the blocks in a row/column

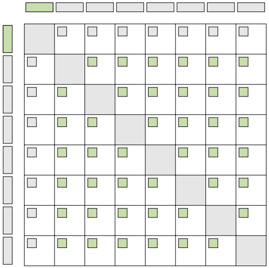
The BLR^2 format



- Solve: only involves the common pivotal row and column bases

- Common basis of size $s \geq r$ for all the blocks in a row/column

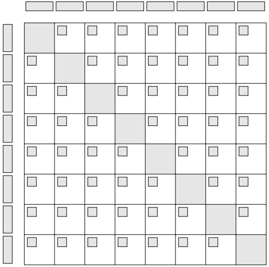
The BLR^2 format



- Solve: only involves the common pivotal row and column bases
- Update: only involves the common pivotal row and column bases and coupling matrices

- Common basis of size $s \geq r$ for all the blocks in a row/column

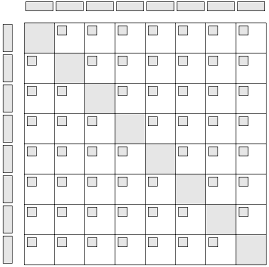
The BLR^2 format



- Solve: only involves the common pivotal row and column bases
- Update: only involves the common pivotal row and column bases and coupling matrices

- Common basis of size $s \geq r$ for all the blocks in a row/column
- If $s = \mathcal{O}(1)$ storage complexity is $\mathcal{O}(n)$ and flops complexity is $\mathcal{O}(n^{1.2})$

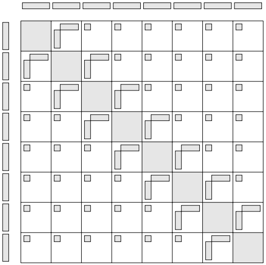
The BLR^2 format



- Solve: only involves the common pivotal row and column bases
- Update: only involves the common pivotal row and column bases and coupling matrices

- Common basis of size $s \geq r$ for all the blocks in a row/column
- If $s = \mathcal{O}(1)$ storage complexity is $\mathcal{O}(n)$ and flops complexity is $\mathcal{O}(n^{1.2})$
- In practice s is usually larger

The BLR^2 format



- Solve: only involves the common pivotal row and column bases
- Update: only involves the common pivotal row and column bases and coupling matrices

- Common basis of size $s \geq r$ for all the blocks in a row/column
- If $s = \mathcal{O}(1)$ storage complexity is $\mathcal{O}(n)$ and flops complexity is $\mathcal{O}(n^{1.2})$
- In practice s is usually larger
- Keep high-rank blocks off the common basis $\rightarrow$ substantial storage gains but complex factorization
- Ashcraft, Buttari, M. (2021) (one of the possible research papers to be read for the evaluation)

Pen & paper exercise (4 points)

- Goal: prove the reduced $\mathcal{O}(m^2 r)$ complexity of the FCSU+LUAR variant given on slide 37
- The accumulated updates always recompress to rank r no matter how many updates have been accumulated
- Suggested steps:
  - What is the cost of the FR-LR solve operation? How many times do we perform it?
  - What is the cost of the Recompress operation? How many times do we perform it?
  - Add these two new operations in the table on slide 23. What else changes in the table?
  - Recompute the optimal complexity as previously.

Practical exercise (4 points)

- Goal: implement BLR LU factorization and assess storage, flops and time gains w.r.t. matrix size and ε accuracy
- Already provided:
  - FR factorization (`FR_factorization.m`)
  - Basic kernels and utilitary routines
  - Main test launcher (`test.m`)
  - BLR factorization template, initialized identical to FR factorization (`BLR_factorization.m`) $\Rightarrow$ this is the file you need to modify
- 3 test matrices given, root separator of a 3D Poisson problem of dimensions $N \times N \times N$. Can change value of N (30, 50, or 70) in `test.m`
- Choice of BLR LU variant left up to you (vanilla FSCU is certainly the simplest)