# Block Low-Rank Multifrontal Solvers: complexity, performance, and scalability

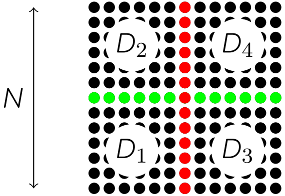
P. Amestoy[*,1] A. Buttari[*,2] J.-Y. L'Excellent[†,3] T. Mary[*,4]

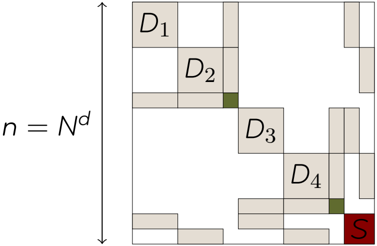
[*]Université de Toulouse [†]ENS Lyon
[1]INPT-IRIT [2]CNRS-IRIT [3]INRIA-LIP [4]UPS-IRIT

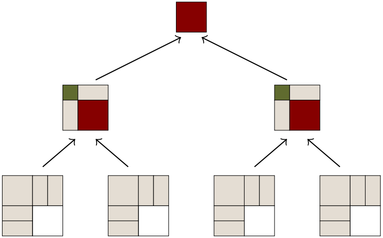
Sparse Days, 6-8 Sep. 2017, Toulouse

# Introduction

# Multifrontal Factorization with Nested Dissection



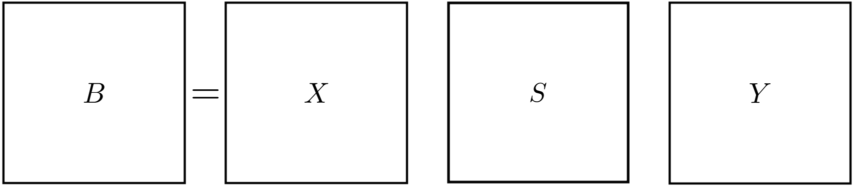



**3D problem complexity**

→ Flops: $O(n^2)$, mem: $O(n^{4/3})$

# Low-rank matrices

Take a dense matrix $B$ of size $b \times b$ and compute its SVD $B = XSY$:



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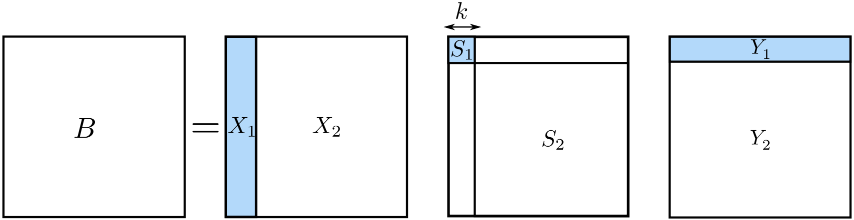


$$B = X_1 S_1 Y_1 + X_2 S_2 Y_2 \quad \text{with} \quad S_1(k,k) = \sigma_k > \varepsilon,\ S_2(1,1) = \sigma_{k+1} \leq \varepsilon$$

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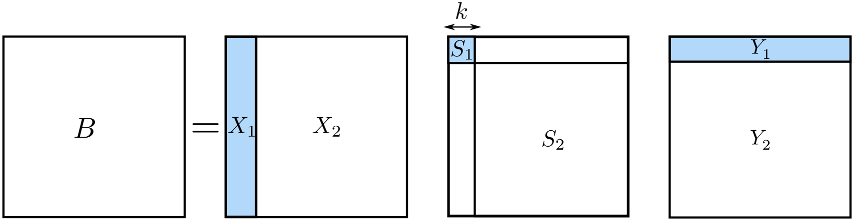


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If $\tilde{B} = X_1 S_1 Y_1 \quad \text{then} \quad \|B - \tilde{B}\|_2 = \|X_2 S_2 Y_2\|_2 = \sigma_{k+1} \leq \varepsilon$

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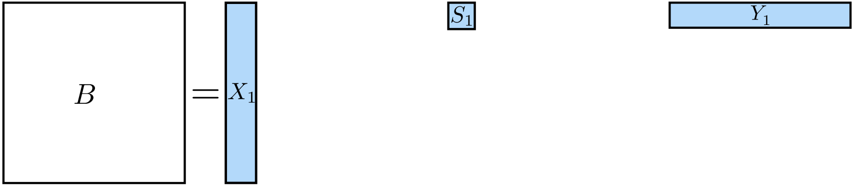


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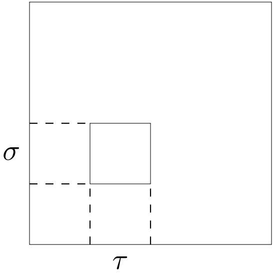
If $\tilde{B} = X_1 S_1 Y_1$ then $\|B - \tilde{B}\|_2 = \|X_2 S_2 Y_2\|_2 = \sigma_{k+1} \leq \varepsilon$

If the singular values of $B$ decay very fast (e.g. exponentially) then $k \ll b$ even for very small $\varepsilon$ (e.g. $10^{-14}$) $\Rightarrow$ memory and CPU consumption can be reduced considerably with a controlled loss of accuracy ($\leq \varepsilon$) if $\tilde{B}$ is used instead of $B$

# Low-rank matrix formats

Frontal matrices are not low-rank but in some applications they exhibit low-rank blocks




A block $B$ represents the interaction between two subdomains $\sigma$ and $\tau$.
If they have a small diameter and are far away their interaction is weak $\Rightarrow$ rank is low.

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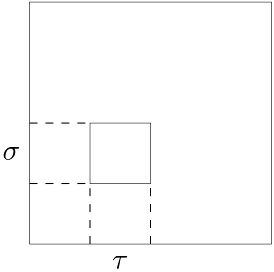


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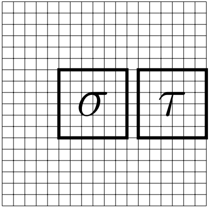


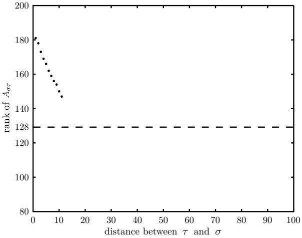

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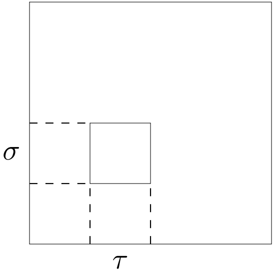


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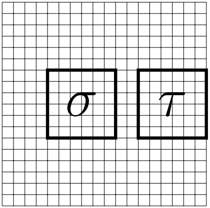


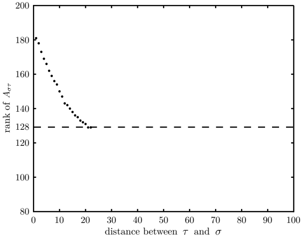

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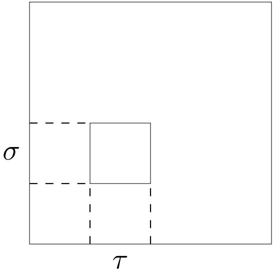


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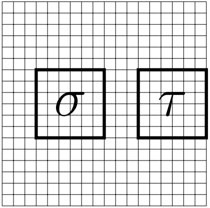


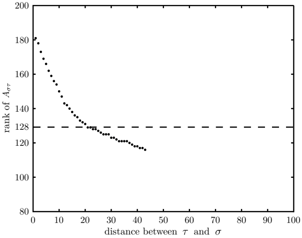


 

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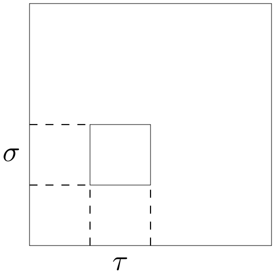


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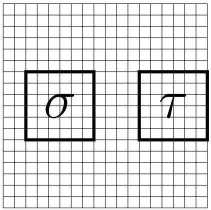


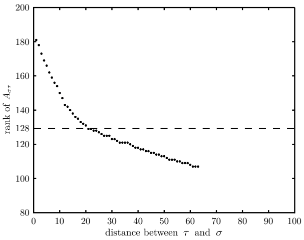

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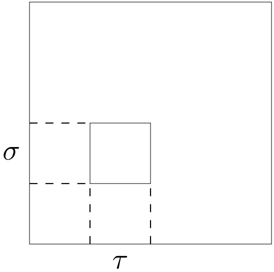


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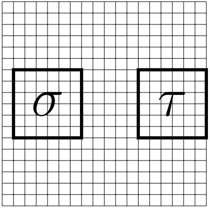


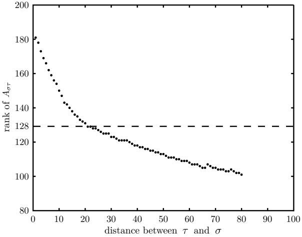

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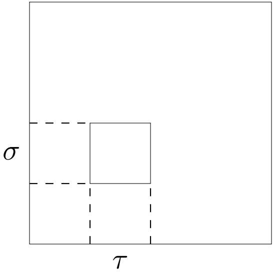


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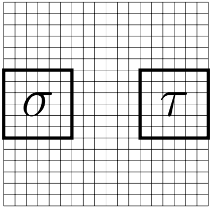
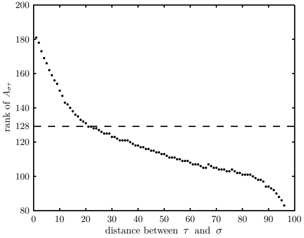
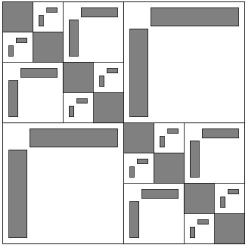
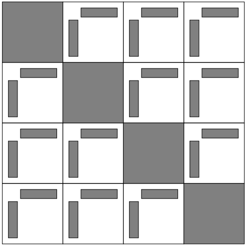


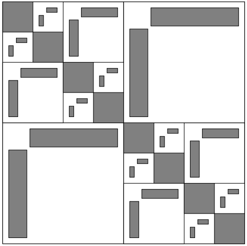
# $\mathcal{H}$ and BLR matrices



$\mathcal{H}$-matrix



BLR matrix



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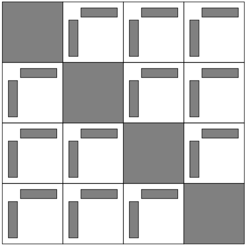

BLR matrix

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

- Theoretical complexity?
  $\Rightarrow O(n^{4/3})$, as we will prove
- Simple structure

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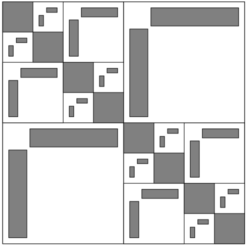

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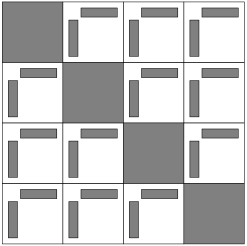

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**Find a good comprise between complexity and performance**

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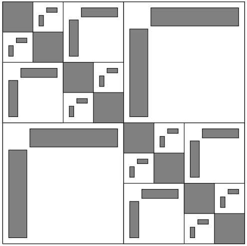

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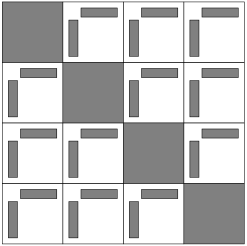

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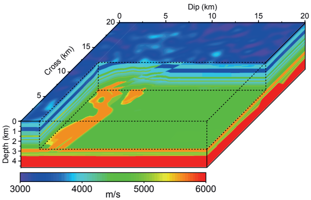
**Find a good comprise between complexity and performance**

$\Rightarrow$ Ongoing collaboration with STRUMPACK team (LBNL) to compare BLR and hierarchical formats

# Applications



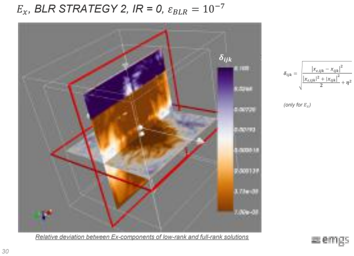

3D Seismic Modeling
Helmholtz equation
Single complex (c) arithmetic
Unsymmetric *LU* factorization
Required accuracy: $\varepsilon = 10^{-3}$
Credits: SEISCOPE

| matrix | n | nnz | flops | storage |
|---|---|---|---|---|
| 5Hz | 2.9M | 70M | 65.0 TF | 59.7 GB |
| 7Hz | 7.2M | 177M | 404.2 TF | 205.0 GB |
| 10Hz | 17.2M | 446M | 2.6 PF | 710.8 GB |

Full-Rank statistics

- Amestoy, Brossier, Buttari, L'Excellent, Mary, Métivier, Miniussi, and Operto. *Fast 3D frequency-domain full waveform inversion with a parallel Block Low-Rank multifrontal direct solver: application to OBC data from the North Sea*, Geophysics, 2016.

# Experimental Setting: Matrices (2/3)




3D Electromagnetic Modeling

Maxwell equation

Double complex (z) arithmetic

Symmetric $LDL^T$ factorization

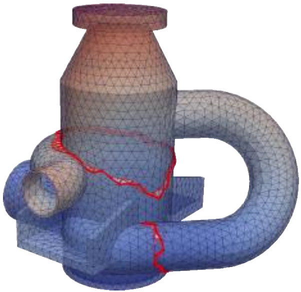
Required accuracy: $\varepsilon = 10^{-7}$

Credits: EMGS

| matrix | n | nnz | flops | storage |
|---|---|---|---|---|
| E3 | 2.9M | 37M | 57.9 TF | 77.5 GB |
| E4 | 17M | 226M | 1.8 PF | 1.7 TB |
| S3 | 3.3M | 43M | 78.0 TF | 94.6 GB |
| S4 | 21M | 266M | 2.5 PF | 2.1 TB |

Full-Rank statistics

- Shantsev, Jaysaval, de la Kethulle de Ryhove, Amestoy, Buttari, L'Excellent, and Mary. *Large-scale 3D EM modeling with a Block Low-Rank multifrontal direct solver*, Geophysical Journal International, 2017.



3D Structural Mechanics

Double real (d) arithmetic

Symmetric $LDL^T$ factorization

Required accuracy: $\varepsilon = 10^{-9}$

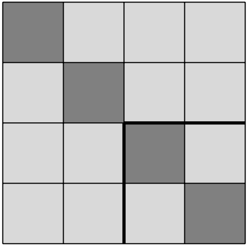
Credits: Code_Aster (EDF)

| matrix | n | nnz | flops | storage |
|---|---|---|---|---|
| perf008d | 1.9M | 81M | 101.0 TF | 52.6 GB |
| perf008ar | 3.9M | 159M | 377.5 TF | 129.8 GB |
| perf008cr | 7.9M | 321M | 1.6 PF | 341.1 GB |
| perf009ar | 5.4M | 209M | 23.4 TF | 40.2 GB |

Full-Rank statistics

# The Block-Low Rank Factorization

# Standard BLR factorization: FSCU



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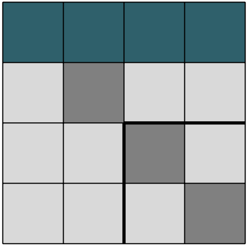

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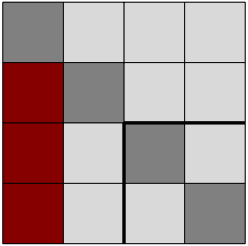

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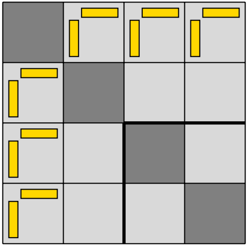

- FSCU (Factor, Solve, Compress,

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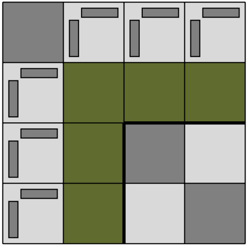

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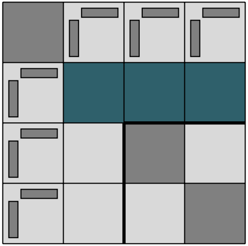

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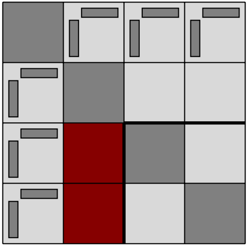

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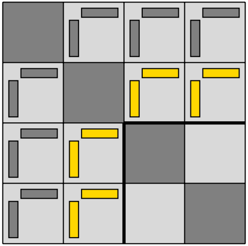

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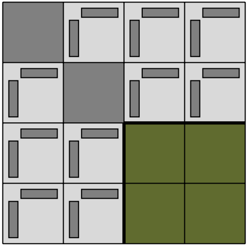

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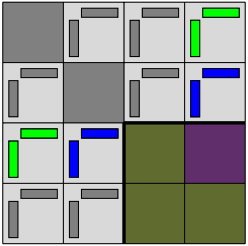

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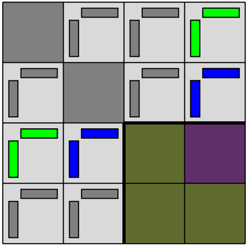

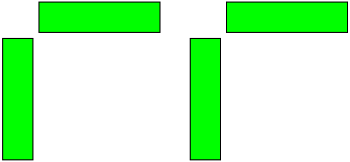

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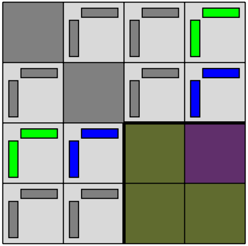

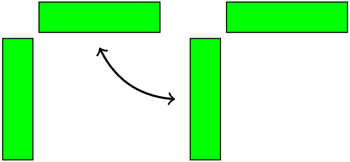

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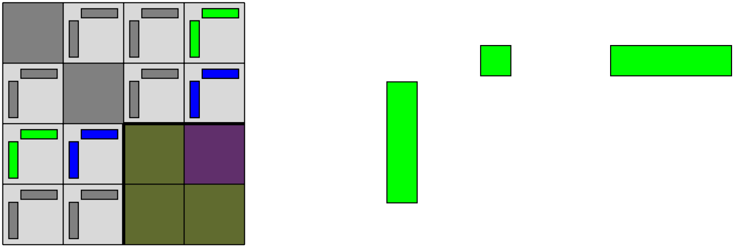

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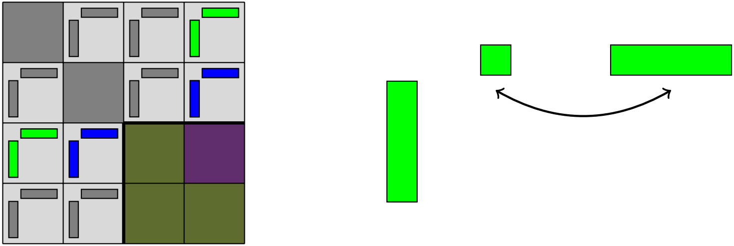

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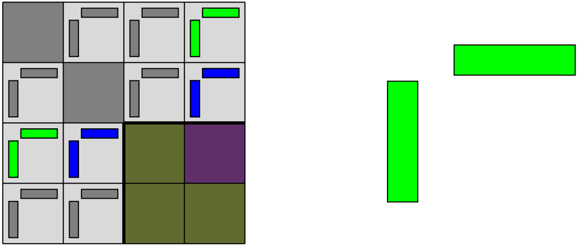

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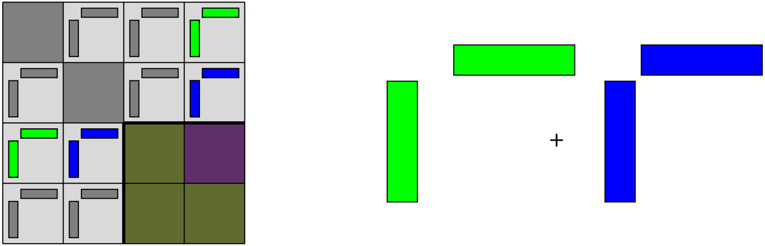


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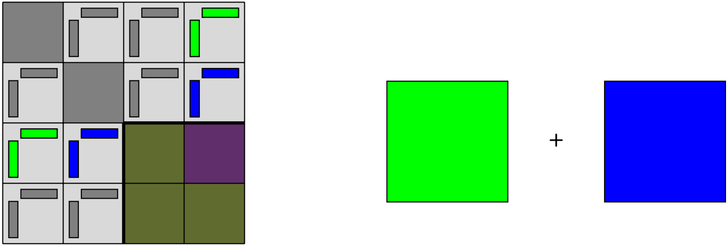


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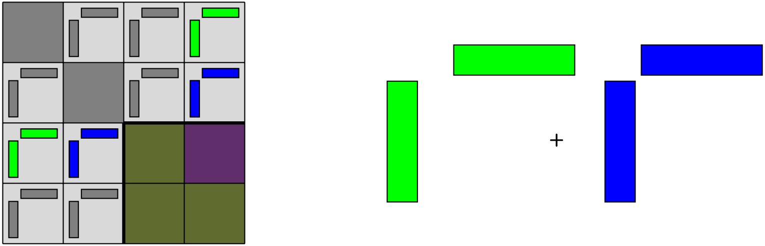

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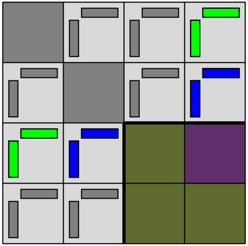

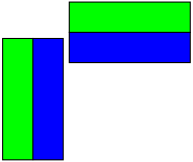

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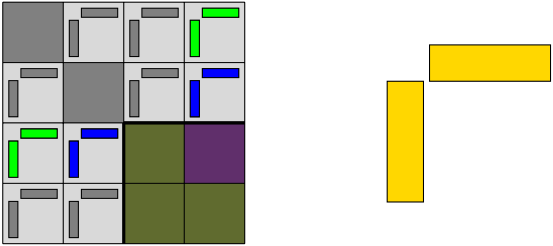

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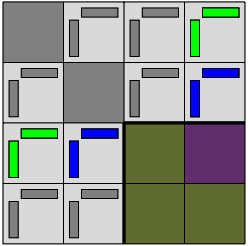

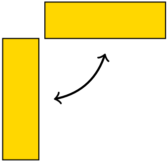

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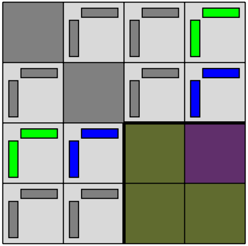

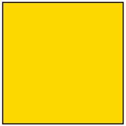

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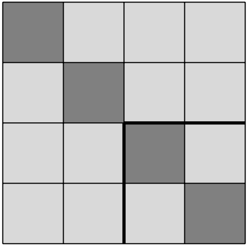

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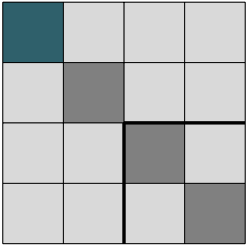

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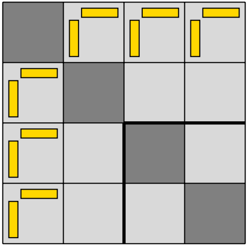

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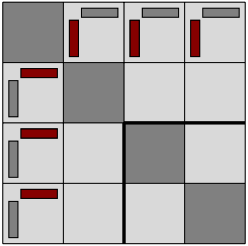

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# Complexity of the factorization

# $\mathcal{H}$ vs. BLR complexity

Until recently, BLR complexity was unknown.
Can we use $\mathcal{H}$ theory on BLR matrices?

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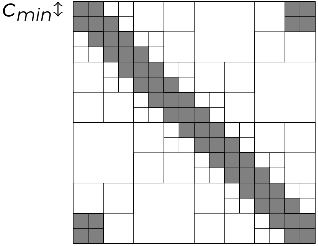

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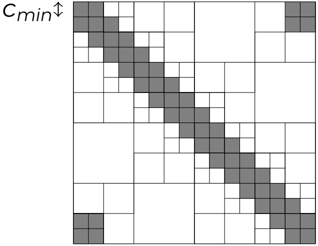


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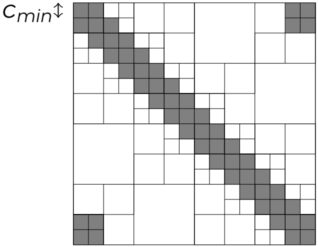

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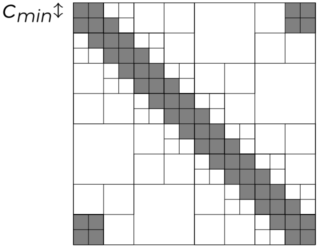


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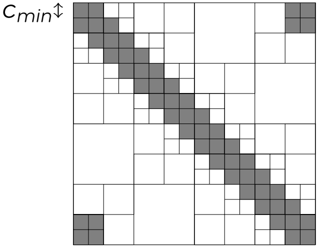


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- $\mathcal{H}$ theory applied to BLR does not give a satisfying result
- Solution: extend the theory by bounding the number of full-rank blocks
  - Amestoy, Buttari, L'Excellent, and Mary. *On the Complexity of the Block Low-Rank Multifrontal Factorization*, SIAM SISC, 2016.

# Complexity of multifrontal BLR factorization

| | operations (OPC) | | factor size (NNZ) | |
|---|---|---|---|---|
| | $r = O(1)$ | $r = O(N)$ | $r = O(1)$ | $r = O(N)$ |
| FR | $O(n^2)$ | $O(n^2)$ | $O(n^{\frac{4}{3}})$ | $O(n^{\frac{4}{3}})$ |
| BLR | $O(n^{\frac{4}{3}}) - O(n^{\frac{5}{3}})$ | $O(n^{\frac{5}{3}}) - O(n^{\frac{11}{6}})$ | $O(n \log n)$ | $O(n^{\frac{7}{6}} \log n)$ |
| $\mathcal{H}$ | $O(n \log n)$ | $O(n^{\frac{4}{3}} \log n)$ | $O(n \log n)$ | $O(n^{\frac{7}{6}} \log n)$ |

in the 3D case (similar analysis possible for 2D)

Important properties: with both $r = O(1)$ or $r = O(N)$

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**How to convert complexity reduction into performance gain?**

# Performance on Multicores

# Experimental Setting

Experiments are done on the brunch shared-memory machine of the LIP laboratory of Lyon:

- Four Intel(r) 24-cores Broadwell @ 2,2 GHz
- Peak per core is 35.2 GF/s
- Total memory is 1.5 TB

# Getting Gflops/s out of the BLR factorization

Follow the **FR/BLR ratio** on matrix S3

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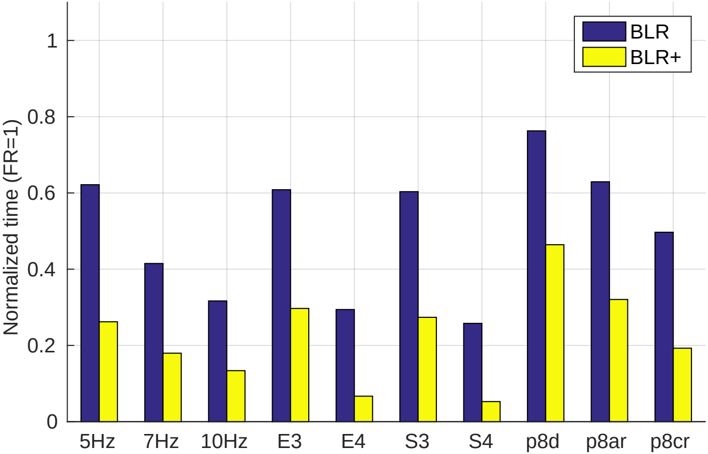
- Compress before Solve (FCSU) ⇒ **3.6 ratio**

# Multicore performance results (24 threads)




- Amestoy, Buttari, L'Excellent, and Mary. *Performance and Scalability of the Block Low-Rank Multifrontal Factorization on Multicore Architectures*, submitted to ACM TOMS, 2017.

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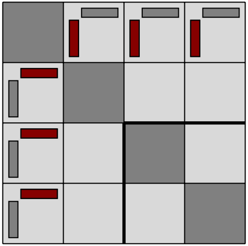

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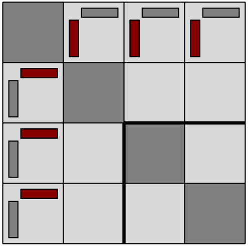

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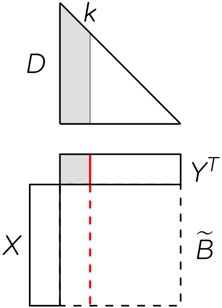
- FCSU(+LUAR)
  - Restricted pivoting, e.g. to diagonal blocks $\Rightarrow$ **not acceptable in many applications**
  - Low-rank Solve $\Rightarrow$ complexity reduction: $O(n^{\frac{11}{6}}) \rightarrow O(n^{\frac{4}{3}})$

# Compress before Solve + pivoting: CFSU variant

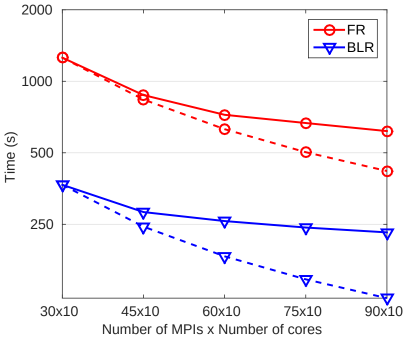



How to assess the quality of pivot $k$?
We need to estimate $\|\widetilde{B}_{:,k}\|_{max}$:
$\|\widetilde{B}_{:,k}\|_{max} \leq \|\widetilde{B}_{:,k}\|_2 = \|XY^T_{k,:}\|_2 = \|Y^T_{k,:}\|_2$,
assuming $X$ is orthonormal (e.g. RRQR, SVD).

| matrix | residual | | | flops (% FR) | | |
|---|---|---|---|---|---|---|
| | FSCU | FCSU | CFSU | FSCU | FCSU | CFSU |
| af_shell10 | 2e-06 | 5e-06 | 4e-06 | 29.9 | 22.7 | 22.7 |
| Lin | 4e-05 | 4e-05 | 4e-05 | 24.0 | 18.5 | 18.5 |
| mario002 | 2e-06 | fail | 1e-06 | 82.8 | – | 72.2 |
| perf009ar | 3e-13 | 1e-01 | 9e-11 | 26.0 | 22.7 | 22.1 |

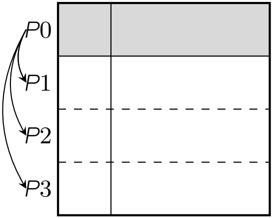
# Distributed-memory BLR factorization

# Strong scalability analysis

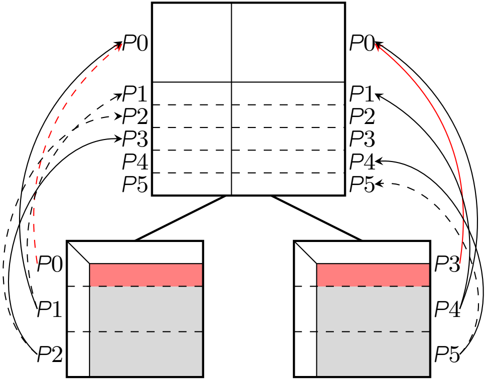



- Flops reduced by $12.8$ but volume of communications only by $2.2 \Rightarrow$ higher relative weight of communications
- Load unbalance (ratio between most and less loaded processes) increases from $1.28$ to $2.57$

# Communication analysis

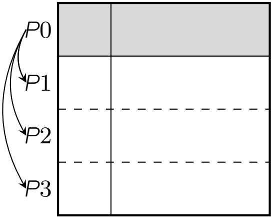



*LU* messages




CB messages

# Communication analysis

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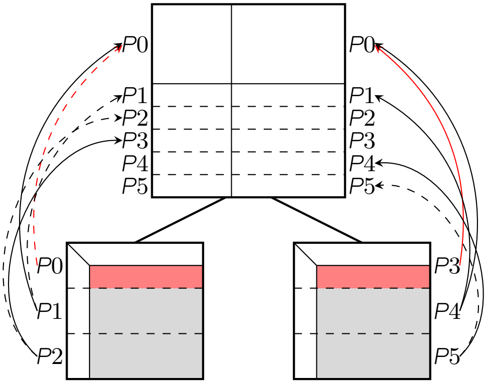
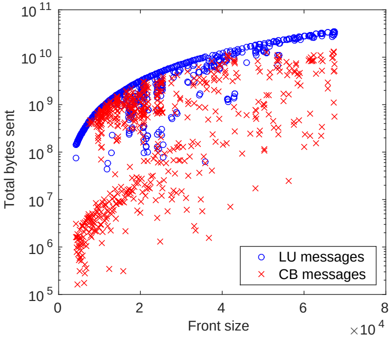



CB messages

- Volume of *LU* messages is reduced in BLR (compressed factors)
- Volume of CB messages can be reduced by compressing the CB $\Rightarrow$ but it is an overhead cost

# Communication analysis




- FR case: *LU* messages dominate

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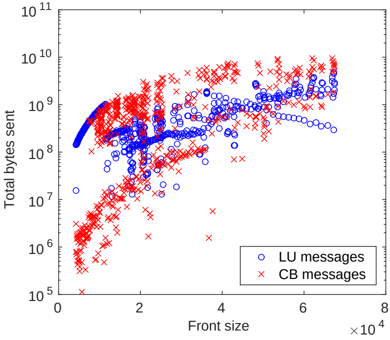


- FR case: *LU* messages dominate
- BLR case: CB messages dominate ⇒ underwhelming reduction of comms.

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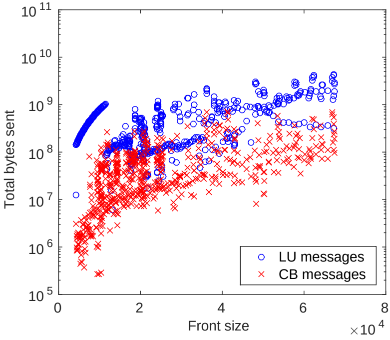
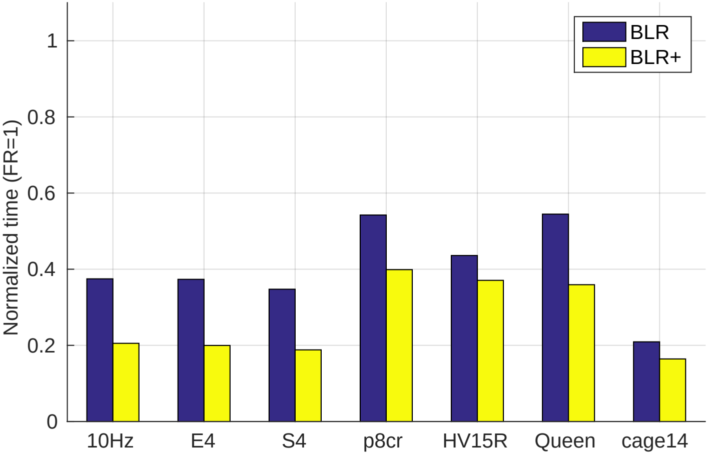



- FR case: *LU* messages dominate
- BLR case: CB messages dominate $\Rightarrow$ underwhelming reduction of comms.

$\Rightarrow$ CB compression allows for truly reducing the comms. Represents an overhead cost but may lead to speedups depending on network speed w.r.t. processor speed

# Distributed performance results ($90 \times 10$ cores)




$\Rightarrow$ promising preliminary results, much work left to do!

# Conclusion

# References and acknowledgements

## Software

- MUMPS 5.1.0

## Publications


- Amestoy, Buttari, L'Excellent, and Mary. *On the Complexity of the Block Low-Rank Multifrontal Factorization*, SIAM SISC, 2017.
- Amestoy, Buttari, L'Excellent, and Mary. *Performance and Scalability of the Block Low-Rank Multifrontal Factorization on Multicore Architectures*, submitted to ACM TOMS, 2017.
- Amestoy, Brossier, Buttari, L'Excellent, Mary, Métivier, Miniussi, and Operto. *Fast 3D frequency-domain full waveform inversion with a parallel Block Low-Rank multifrontal direct solver: application to OBC data from the North Sea*, Geophysics, 2016.
- Shantsev, Jaysaval, de la Kethulle de Ryhove, Amestoy, Buttari, L'Excellent, and Mary. *Large-scale 3D EM modeling with a Block Low-Rank multifrontal direct solver*, Geophysical Journal International, 2017.


## Acknowledgements


- LIP and CALMIP for providing access to the machines
- EMGS, SEISCOPE, and EDF for providing the matrices

Thanks!

Questions?

# Backup Slides

1. **`Poisson`**: $N^3$ grid with a 7-point stencil with $u = 1$ on the boundary $\partial\Omega$

$$\Delta u = f$$

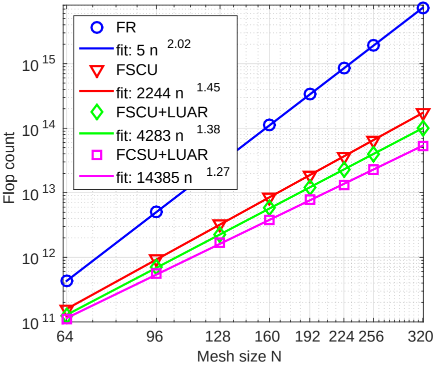
2. **`Helmholtz`**: $N^3$ grid with a 27-point stencil, $\omega$ is the angular frequency, $v(x)$ is the seismic velocity field, and $u(x, \omega)$ is the time-harmonic wavefield solution to the forcing term $s(x, \omega)$.

$$\left(-\Delta - \frac{\omega^2}{v(x)^2}\right) u(x, \omega) = s(x, \omega)$$

$\omega$ is fixed and equal to $4$Hz.

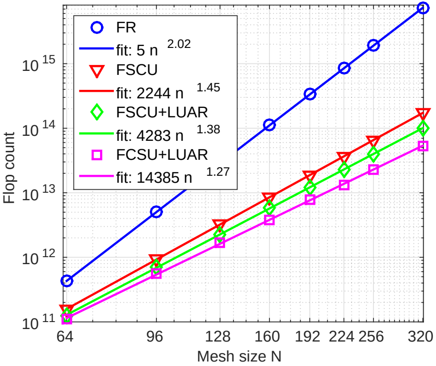
# Experimental MF flop complexity: Poisson ($\varepsilon = 10^{-10}$)

Nested Dissection ordering (geometric)

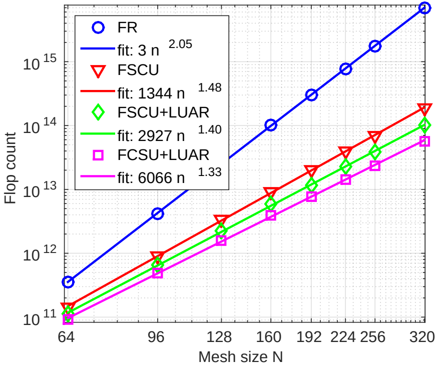



- good agreement with theoretical complexity ($O(n^2)$, $O(n^{1.67})$, $O(n^{1.55})$, and $O(n^{1.33})$)

Nested Dissection ordering (geometric)



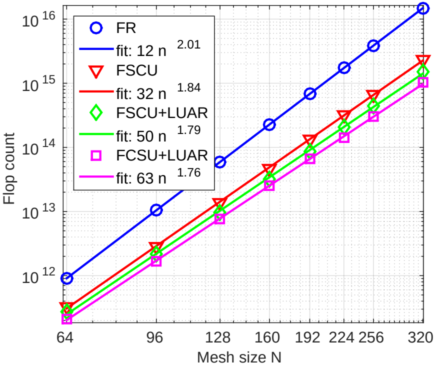

METIS ordering (purely algebraic)



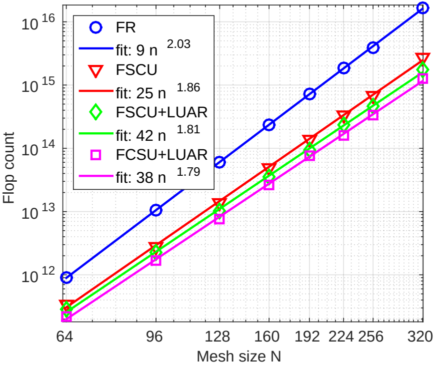

- good agreement with theoretical complexity ($O(n^2)$, $O(n^{1.67})$, $O(n^{1.55})$, and $O(n^{1.33})$)
- remains close to ND complexity with METIS ordering

# Experimental MF flop complexity: Helmholtz ($\varepsilon = 10^{-4}$)

Nested Dissection ordering (geometric)



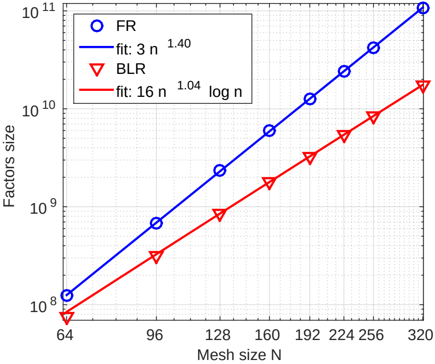

METIS ordering (purely algebraic)



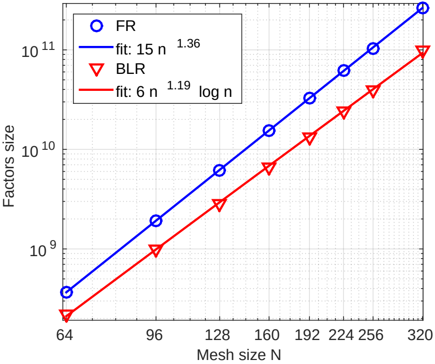

- good agreement with theoretical complexity ($O(n^2)$, $O(n^{1.83})$, $O(n^{1.78})$, and $O(n^{1.67})$)
- remains close to ND complexity with METIS ordering

# Experimental MF complexity: factor size

NNZ (Poisson)




NNZ (Helmholtz)



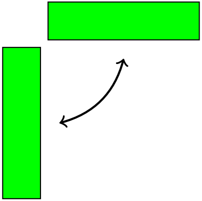

- good agreement with theoretical complexity (FR: $O(n^{1.33})$; BLR: $O(n \log n)$ and $O(n^{1.17} \log n)$)

# Experimental Setting: Machines

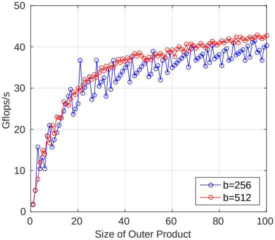
Experiments are done on the shared-memory machines of the LIP laboratory of Lyon:

1. **`brunch`**
   - Four Intel(r) 24-cores Broadwell @ 2,2 GHz
   - Peak per core is 35.2 GF/s
   - Total memory is 1.5 TB

2. **`grunch`**
   - Two Intel(r) 14-cores Haswell @ 2,3 GHz
   - Peak per core is 36.8 GF/s
   - Total memory is 768 GB



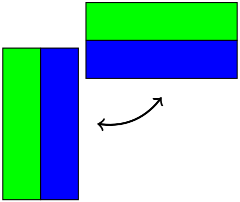
Double complex (z) performance benchmark of Outer Product



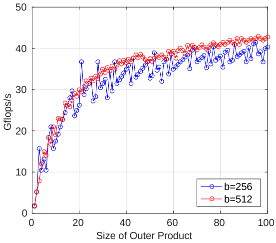

| | | LL | LUA | LUAR* |
|---|---|---|---|---|
| average size of Outer Product | | 16.5 | 61.0 | 32.8 |
| flops ($\times 10^{12}$) | Outer Product | 3.76 | 3.76 | 1.59 |
| | Total | 10.19 | 10.19 | 8.15 |
| time (s) | Outer Product | 21 | 14 | 6 |
| | Total | 175 | 167 | 160 |

* All metrics include the Recompression overhead

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



Double complex (z) performance benchmark of Outer Product




| | | LL | LUA | LUAR* |
|---|---|---|---|---|
| average size of Outer Product | | 16.5 | 61.0 | 32.8 |
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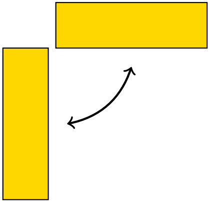
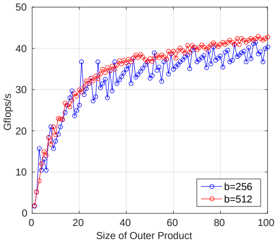


Double complex (z) performance benchmark of Outer Product

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