Bridging the gap between flat and hierarchical low-rank matrix formats

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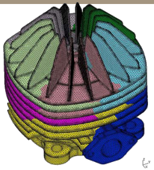
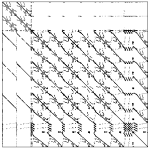
Structured Matrix Days, Lyon, 14-15 May 2018

 $\rightarrow$  $\rightarrow$ 

Linear system $Ax = b$

Often a keystone in scientific computing applications
(discretization of PDEs, step of an optimization method, ...)

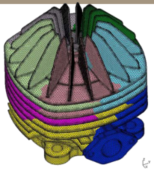
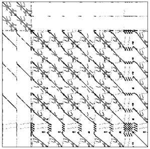
Direct methods

Factorize $A = LU$ and solve $LUx = b$

- ☺ Numerically reliable
- ☹ Computational cost

Theo Mary (contact: theo.mary@manchester.ac.uk)

Context

 $\rightarrow$  $\rightarrow$ 

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Objective:
reduce the cost of direct methods ...
...while maintaining their numerical reliability

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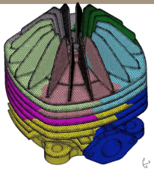
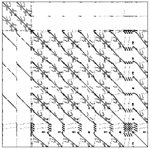
 $\rightarrow$  $\rightarrow$ 

Large scale applications

- Target size is $n \sim 10^9$ for sparse $\Rightarrow$ $m \sim 10^6$ for dense
- $O(m^2)$ storage complexity and $O(m^3)$ flop complexity
  $m \sim 10^6 \Rightarrow$ TeraBytes of storage and ExaFlops of computation!

$\Rightarrow$ Need to reduce the asymptotic complexity

Large scale systems

- Increasingly large numbers of cores available

$\Rightarrow$ Need to design parallel algorithms

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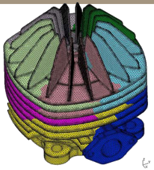
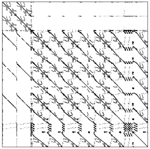
 $\rightarrow$  $\rightarrow$ 

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These two objectives are not always compatible

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Outline

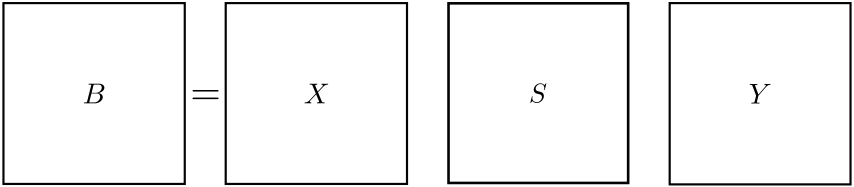
1. Introduction
   - The $\mathcal{H}$ format: very good complexity
   - The BLR format: very good parallelism
2. Motivation
   - Why we need a new format to bridge the gap
3. The MBLR format
   - Complexity analysis
   - Numerical results
4. Conclusion

Preprint

P. Amestoy, A. Buttari, J.-Y. L'Excellent, and T. Mary, *Bridging the gap between flat and hierarchical low-rank matrix formats: the multilevel BLR format*, submitted (2018).

Introduction

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



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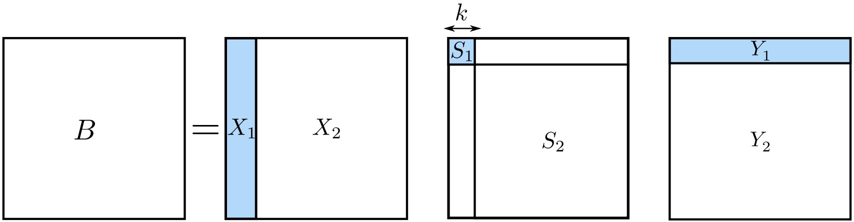

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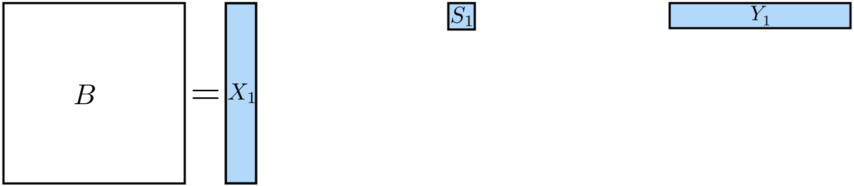

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$\tilde{B} = X_1 S_1 Y_1$ is a low-rank approximation to B: $\|B - \tilde{B}\|_2 \le \varepsilon$

Low-rank matrices

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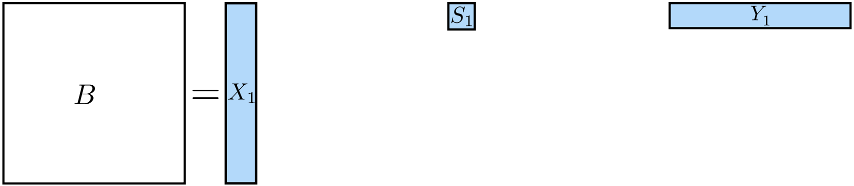

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$\tilde{B} = X_1 S_1 Y_1$ is a low-rank approximation to B: $\|B - \tilde{B}\|_2 \le \varepsilon$

Storage savings: $b^2/2bk = b/2k$
Similar flops savings when used in most linear algebra kernels

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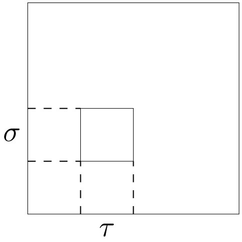
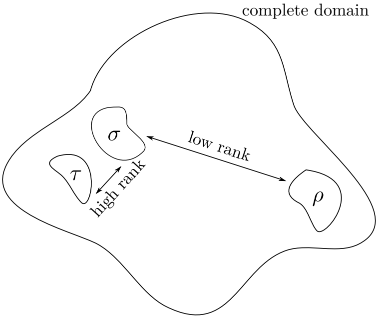
Low-rank blocks

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





A block B represents the interaction between two subdomains σ and τ.
Small diameter and far away $\Rightarrow$ low numerical rank.

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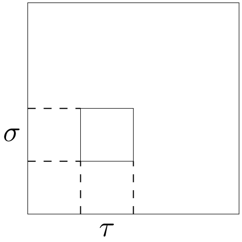

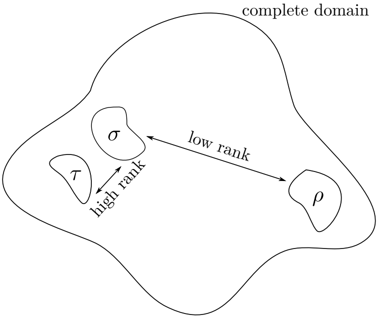

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How to choose a good block partitioning of the matrix?

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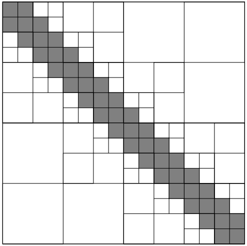

$\mathcal{H}$-matrix

- Nearly linear complexity
- Complex, hierarchical structure

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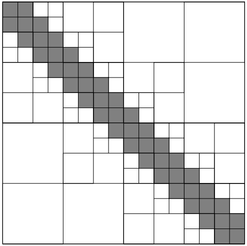
$\mathcal{H}$ and BLR matrices



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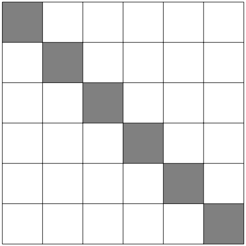

BLR matrix

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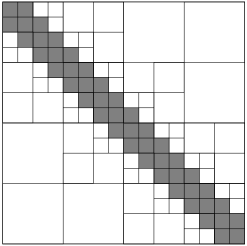
- Superlinear complexity
- Simple, flat structure

$\mathcal{H}$ and BLR matrices



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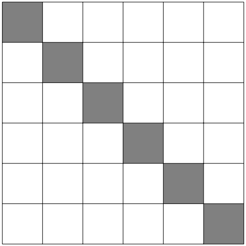

BLR matrix

- Superlinear complexity
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BLR is a comprise between complexity and performance:

- Small blocks $\Rightarrow$ can fit on single shared-memory node
- No global order between blocks $\Rightarrow$ flexible data distribution
- Easy to handle numerical pivoting

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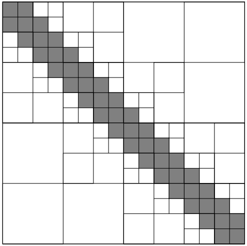
$\mathcal{H}$ and BLR matrices



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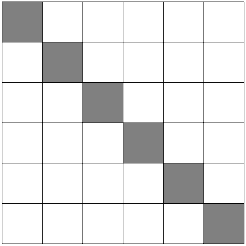

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Can we find an even better comprise?

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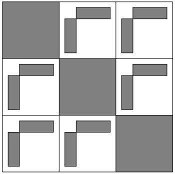
Motivation

Computing the BLR complexity

Assume all off-diagonal blocks are low-rank. Then:



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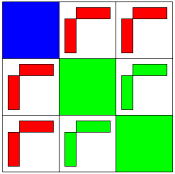

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$$\begin{aligned}
FlopLU &= cost_{getrf} * nb_{getrf} + cost_{trsm} * nb_{trsm} + cost_{gemm} * nb_{gemm} \\
&= O(b^3) * O(\frac{m}{b}) + O(b^2 r) * O((\frac{m}{b})^2) + O(br^2) * O((\frac{m}{b})^3) \\
&= O(mb^2 + m^2 r + m^3 r^2 / b^2) \\
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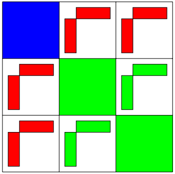

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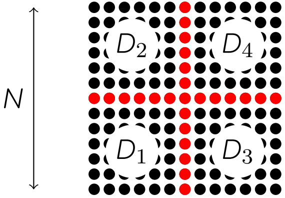
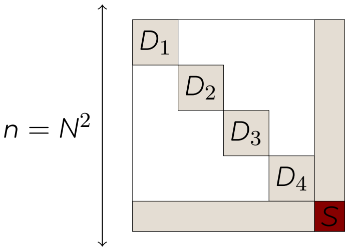
Result holds if a **constant** number of off-diag. blocks is full-rank.

P. Amestoy, A. Buttari, J.-Y. L'Excellent, and T. Mary, *On the Complexity of the Block Low-Rank Multifrontal Factorization*, SIAM J. Sci. Comput. (2017).

From dense to sparse: nested dissection





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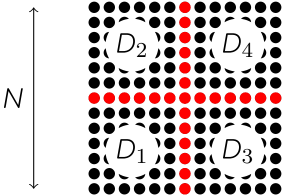

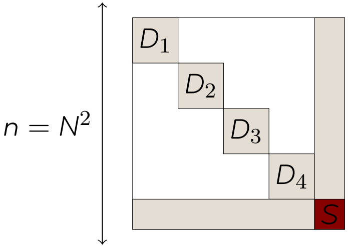

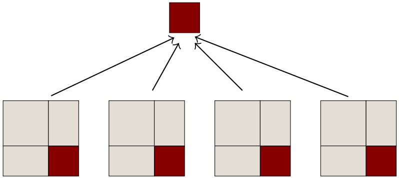

Proceed recursively to compute separator tree

Factorizing a sparse matrix amounts to factorizing a sequence of dense matrices

$\Rightarrow$

sparse complexity is directly derived from dense one

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Nested dissection complexity formulas

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

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Nested dissection complexity formulas

2D: $\mathcal{C}_{sparse} = \sum_{\ell=0}^{\log N} 4^{\ell} \mathcal{C}_{dense}(\frac{N}{2^{\ell}})$ $\rightarrow$ common ratio $2^{2-\beta}$

3D: $\mathcal{C}_{sparse} = \sum_{\ell=0}^{\log N} 8^{\ell} \mathcal{C}_{dense}(\frac{N^2}{4^{\ell}})$ $\rightarrow$ common ratio $2^{3-2\beta}$

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

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

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

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Bridging the gap between flat and hierarchical formats

	Storage			Flop LU		
	$\mathcal{C}_{dense}$	$\mathcal{C}_{sparse}$ 2D	$\mathcal{C}_{sparse}$ 3D	$\mathcal{C}_{dense}$	$\mathcal{C}_{sparse}$ 2D	$\mathcal{C}_{sparse}$ 3D
FR	$O(m^2)$	$O(n \log n)$	$O(n^{4/3})$	$O(m^3)$	$O(n^{3/2})$	$O(n^2)$
BLR	$O(m^{3/2})$	$O(n)$	$O(n \log n)$	$O(m^2)$	$O(n \log n)$	$O(n^{4/3})$
$\mathcal{H}$	$O(m \log m)$	$O(n)$	$O(n)$	$O(m \log^2 m)$	$O(n)$	$O(n)$

Motivation:

- 2D flop and 3D storage complexity: can we find a simple way to improve just a little $\mathcal{C}_{dense}$?
- 3D flop complexity: still a large gap between BLR and $\mathcal{H}$

We propose a multilevel BLR format to bridge the gap

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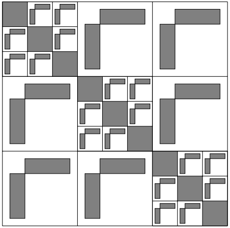
The MBLR format

Complexity of the two-level BLR format

Assume all off-diagonal blocks are low-rank. Then:



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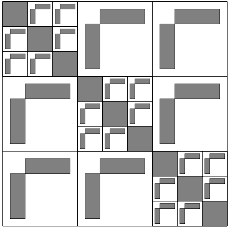

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Similarly, we can prove:

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

Result holds if a **constant** number of off-diag. blocks is BLR.

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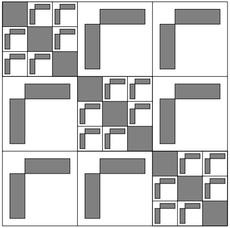

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		FR	BLR	2-BLR	...	$\mathcal{H}$
storage	dense	$O(m^2)$	$O(m^{1.5})$	$O(m^{1.33})$	...	$O(m \log m)$
	sparse	$O(n^{1.33})$	$O(n \log n)$	$O(n)$	...	$O(n)$
flop LU	dense	$O(m^3)$	$O(m^2)$	$O(m^{1.66})$	...	$O(m \log^3 m)$
	sparse	$O(n^2)$	$O(n^{1.33})$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

Multilevel BLR complexity

Main result

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

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

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

Proof: by induction. $\square$

- Simple way to finely control the desired complexity
- Block size $b \propto O(m^{\ell/(\ell+1)}) \ll O(m)$
  $\Rightarrow$ may be efficiently processed in shared-memory
- Number of blocks per row/column $\propto O(m^{1/(\ell+1)}) \gg O(1)$
  $\Rightarrow$ flexibility to distribute data in parallel

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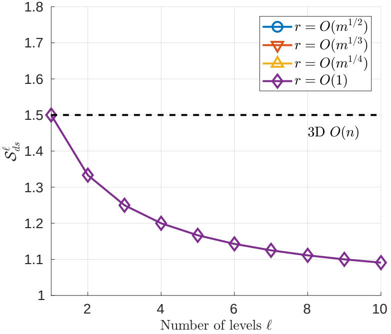
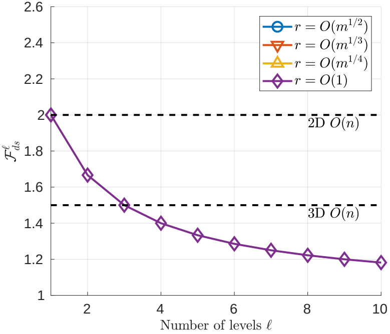
Storage



Flop LU



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

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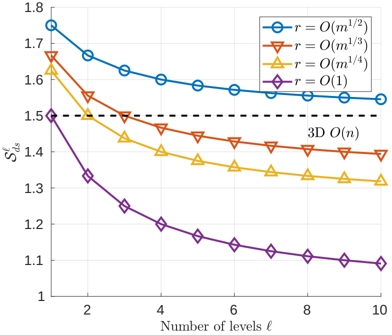
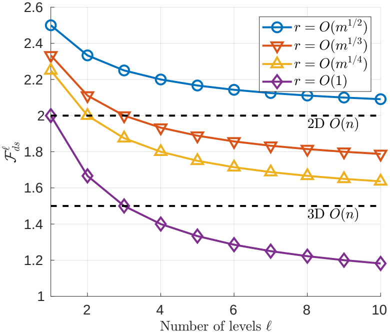
Influence of the number of levels ℓ

Storage



Flop LU



- 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, optimal sparse complexity is not attainable with constant ℓ **but** improvement rate is rapidly decreasing: **the first few levels achieve most of the asymptotic gain**

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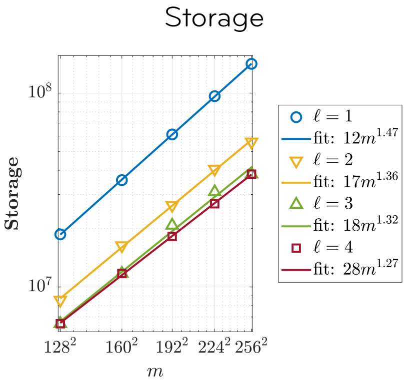
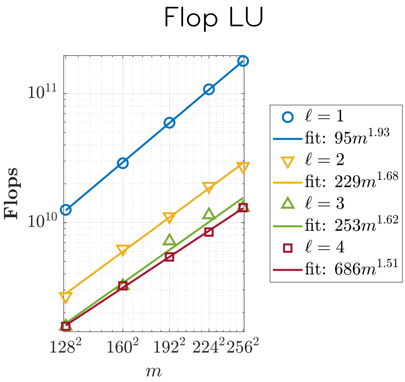
Numerical experiments (Poisson)





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

Conclusion

Conclusions and perspectives

A new multilevel format to...

- Finely control desired complexity between BLR's and $\mathcal{H}$'s
- Strike a balance between BLR's simplicity and $\mathcal{H}$'s complexity
- Trade off $\mathcal{H}$'s nearly linear dense complexity and still achieve $\mathcal{C}_{sparse} = O(n)$

Future work: high-performance implementation

- Implementation of the MBLR format in a parallel, algebraic, general purpose sparse solver (e.g. MUMPS)

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Thank you for your attention

Slides and paper available here:

personalpages.manchester.ac.uk/staff/theo.mary/