Combining sparse approximate factorizations with mixed precision iterative refinement

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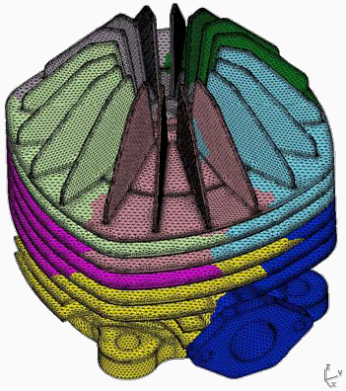
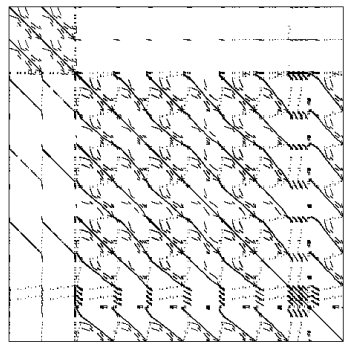
Joint work with : Patrick Amestoy, Alfredo Buttari, Jean-Yves L'Excellent, Nicholas J. Higham, Théo Mary

ISC 2022

Sparse Direct Solver

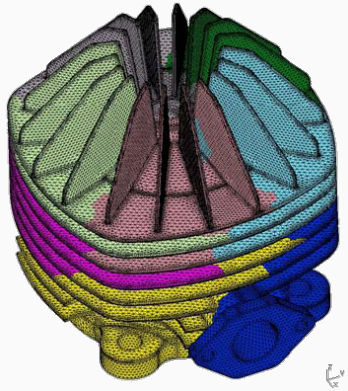
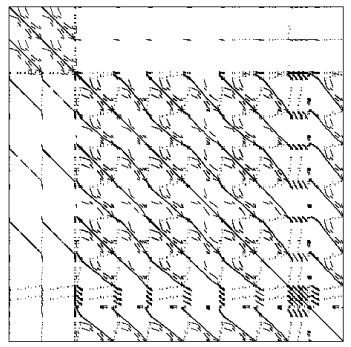

Large Sparse Linear System $Ax = b$

At the foundations of many scientific computing applications (discretization of PDEs, step of an optimzation method, ...).

Direct solver properties

- Pros : Robust, easy to use, accurate.
- Cons : Compute and memory intensive, limited scalability.

Sparse Direct Solver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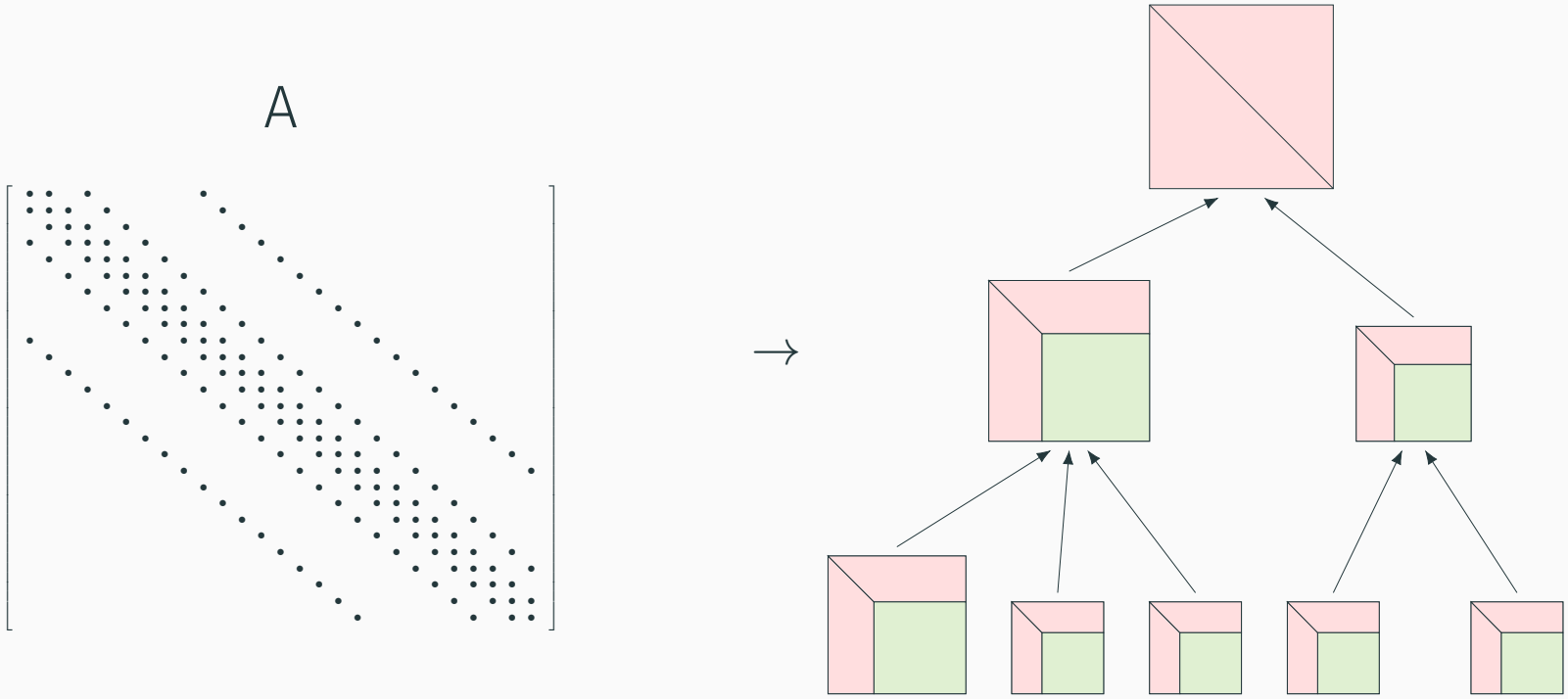
Direct solver properties

- Pros : Robust, easy to use, accurate.
- Cons : Compute and memory intensive, limited scalability.

$\Rightarrow$ **Reduce the complexity :** Numerical approximations, low arithmetic precisions.

Multifrontal Sparse Direct Factorization

A sparse factorization can be decomposed into a series of factorizations of dense matrices (fronts) :



- The red parts are the LU entries, the green part are temporary data.
- In multifrontal factorization the total memory consumption is higher than the factors in memory. The difference is called the active memory overhead.

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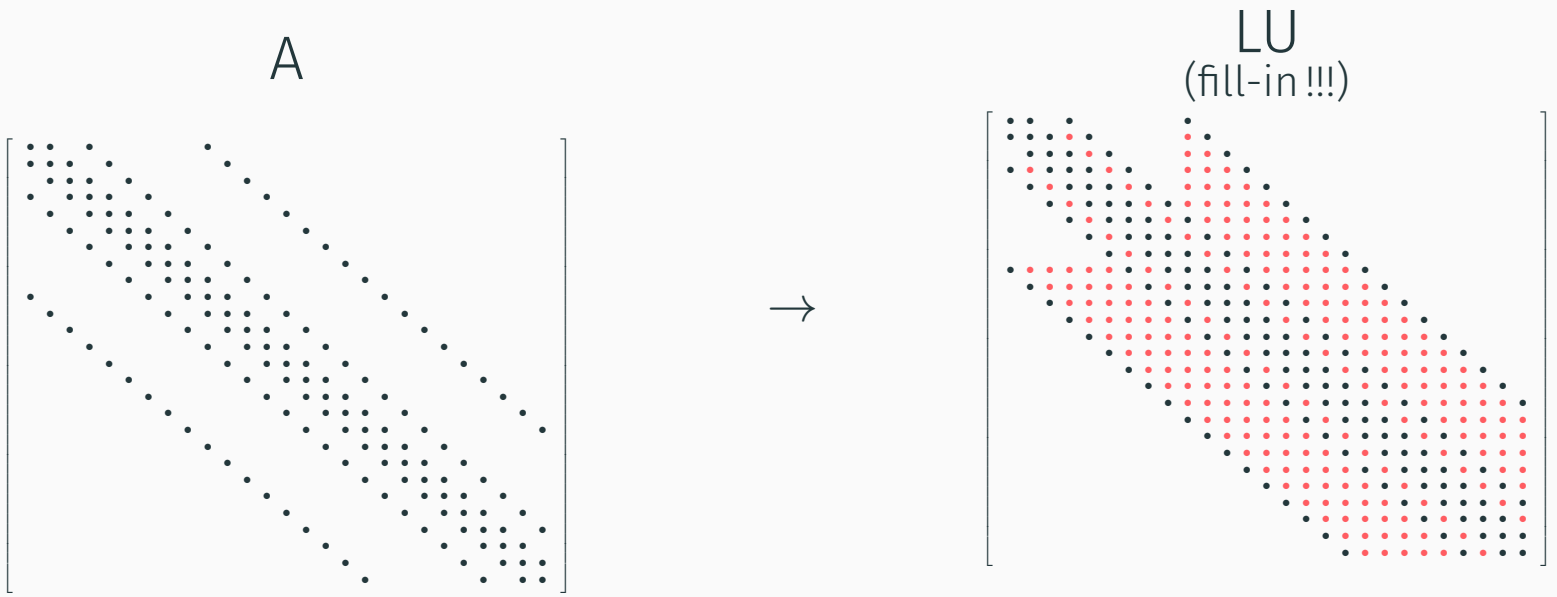

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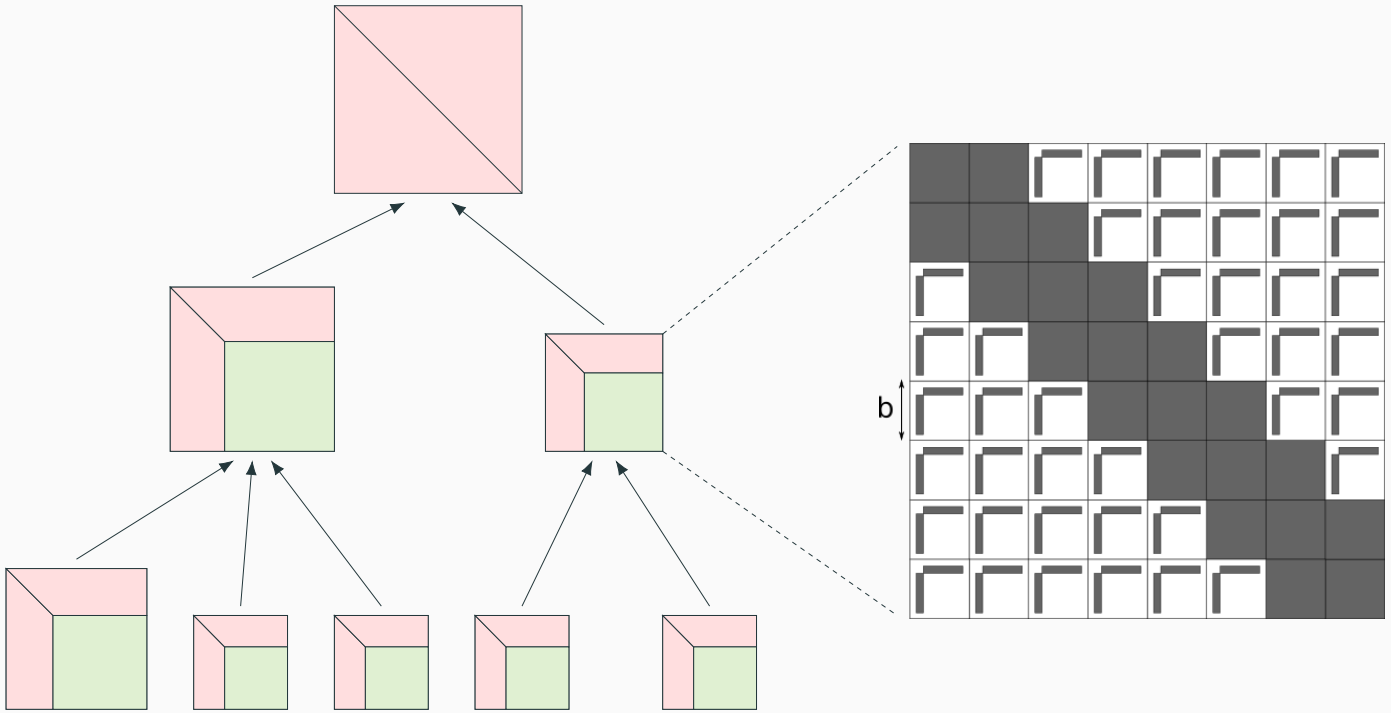
Numerical approximations : Block-Low-Rank

Block-Low-Rank[1] **:** Decompose the dense matrices into regular blocks of size b. Try to compress each block with a low rank approximation at precision ϵ_{BLR}.



1. Théo Mary, *Block Low-Rank multifrontal solvers : complexity, performance, and scalability*, 2017

Numerical approximations : Block-Low-Rank

Block-Low-Rank : Decompose the dense matrices into regular blocks of size b. Try to compress each block with a low rank approximation at precision ϵ_{BLR}.

	Flops	Memory
Classic	$O(n^2)$	$O(n^{\frac{4}{3}})$
BLR	$O(n^{\frac{4}{3}})$	$O(n \log(n))$

Complexities on cubic domain

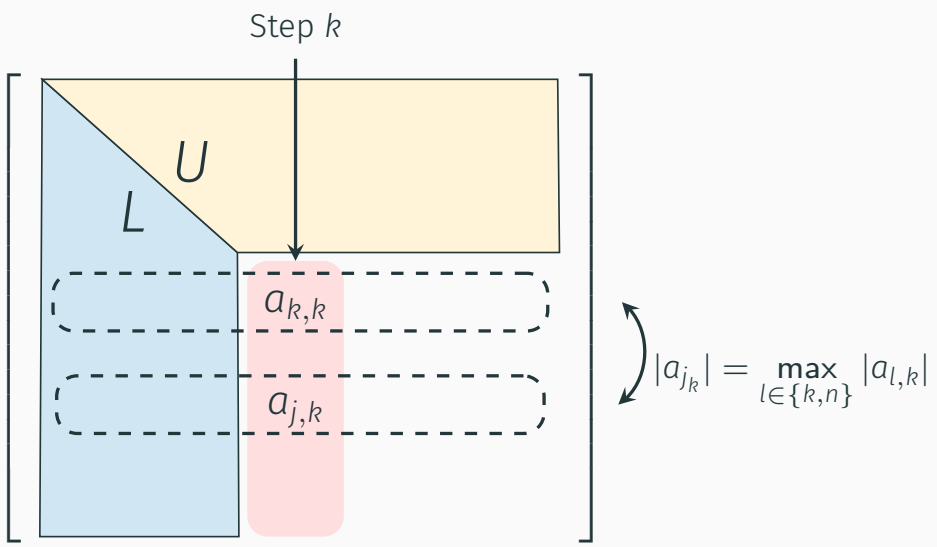
Pros :

- ➤ Reduction of asymptotic complexity...
- ➤ ... which is translated in time and memory savings !

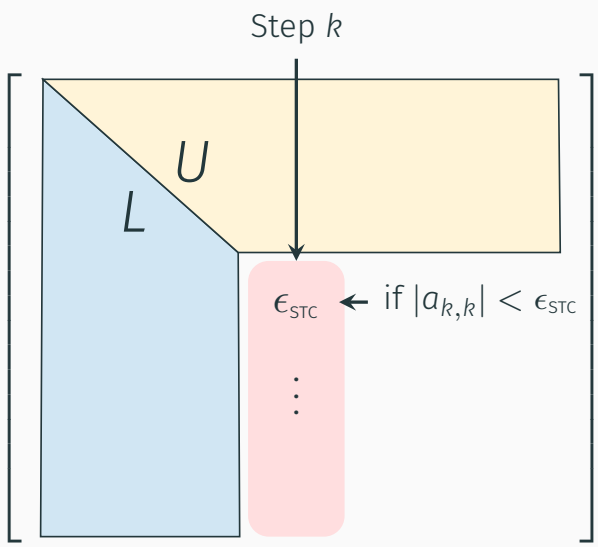
Cons :

- ➤ Introduce a perturbation ϵ_{BLR}.
- ➤ Compression is problem dependent.

Numerical approximations : Static pivoting



Partial Pivoting



Static Pivoting [2]

Pros :

- ➤ No pivot search overhead.
- ➤ No synch communications for pivoting.
- ➤ Keep the ordering of the analysis.

Cons :

- ➤ Large ϵ_{STC} less accuracy.
- ➤ Low ϵ_{STC} less stability.

2. X. S. Li and J. W. Demmel, *A Scalable Sparse Direct Solver Using Static Pivoting*, 1998

Why using numerical approximations?

The philosophy is to deliberately approximate the computations in order to improve the performance at the cost of introducing a perturbation.

- The perturbed problem should be close to the original one and...
- should reduce time and/or memory!
- Sometimes the bigger the perturbations the bigger the savings (e.g. BLR).

BUT big perturbations = low accuracy

Mixed-precision iterative refinement for direct solvers

Algorithm Iterative refinement

1 : Compute the LU factorization $A = \hat{L}\hat{U}$ (u_f)
2 : Solve $Ax_0 = b$ (u_f)
3 : **while not** converged **do**
4 : Compute $r_i = b - Ax_i$ (u_r)
5 : Solve $Ad_i = r_i$. (u_s)
6 : Compute $x_{i+1} = x_i + d_i$ (u)
7 : **end while**

The strategy is to accelerate with low precisions the factorization and recover a good accuracy with higher precisions on the correction iterations.

Mixed-precision iterative refinement for direct solvers

Algorithm Iterative refinement : **LU-IR3** [a]

1 : Compute the LU factorization $A = \hat{L}\hat{U}$ (u_f)
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4 : Compute $r_i = b - Ax_i$ (u_r)
5 : Solve $Ad_i = r_i$ by $d_i = \hat{U}^{-1}\hat{L}^{-1}r_i$. (u_f)
6 : Compute $x_{i+1} = x_i + d_i$ (u)
7 : **end while**

We can change the solver used for the correction equation :

➤ LU-IR3 : the classical form of refinement for direct solvers.

a. E. Carson and N. J. Higham, *Accelerating the solution of linear systems by iterative refinement in three precisions*, 2018

Mixed-precision iterative refinement for direct solvers

Algorithm Iterative refinement : **GMRES-IR5** [a]

1 : Compute the LU factorization $A = \hat{L}\hat{U}$ (u_f)
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5 : Solve $\widetilde{A}d_i = \hat{U}^{-1}\hat{L}^{-1}Ad_i = \hat{U}^{-1}\hat{L}^{-1}r_i$ by GMRES at precision (u_g) with matrix vector products with $\widetilde{A}$ at precision (u_p).
6 : Compute $x_{i+1} = x_i + d_i$ (u)
7 : **end while**

We can change the solver used for the correction equation :

➤ GMRES-IR5 : a more robust form capable of tackling higher condition number $\kappa(A)$.

a. Amestoy, Buttari, Higham, L'Excellent, Mary, and Vieublé, *Five-Precision GMRES-based iterative refinement*, 2021

Mixed-precision iterative refinement for direct solvers

Algorithm Iterative refinement : **GMRES-IR5**

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7 : **end while**

$\Rightarrow$ We want to use iterative refinement to improve the accuracy of sparse approximate solvers !

Question : What are the specificities of IR with sparse approximate solvers ?

Specificities with sparse factorization

Algorithm Iterative refinement : complexities Dense VS Sparse

1 : Compute the LU factorization $A = \hat{L}\hat{U}$	$\mathcal{O}(n^3)$	$\mathcal{O}(n^2)$	(u_f)
2 : Solve $Ax_0 = b$	$\mathcal{O}(n^2)$	$\mathcal{O}(n^{4/3})$	(u_f)
3 : **while not** converged **do**			
4 : Compute $r_i = b - Ax_i$	$\mathcal{O}(n^2)$	$\mathcal{O}(n)$	(u_r)
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Fill-in in sparse direct solvers, i.e. $\mathbf{NNZ}(A) \ll \mathbf{NNZ}(LU)$!

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7 : **end while**			

Fill-in in sparse direct solvers, i.e. $\mathbf{NNZ}(A) \ll \mathbf{NNZ}(LU)$!

➤ SpMV much cheaper than solve $\Rightarrow$ $u_r \ll u$ has limited impact on performance (even for $u_r =$ fp128).

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7 : **end while**			

Fill-in in sparse direct solvers, i.e. $\mathbf{NNZ}(A) \ll \mathbf{NNZ}(LU)$!

➤ Memory space of A in u_r negligible compared with the LU factors in $u_f \Rightarrow$ LU-IR3 stores LU factors in precision u_f, direct solver stores in precision u, then LU-IR3 saves memory !

Specificities with sparse factorization

Algorithm Iterative refinement : complexities Dense VS Sparse			
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Fill-in in sparse direct solvers, i.e. $\mathbf{NNZ}(A) \ll \mathbf{NNZ}(LU)$!

➤ If no cast on the fly, GMRES-IR5 needs to store the factors in u_p.
GMRES-IR5 saves memory on the active memory even if $u_p = u$!

Specificities with approximate factorization

Algorithm LU-IR3 : complexities Sparse VS Approximations [a]

1 :	Compute the LU factorization $A = \hat{L}\hat{U}$	$\mathcal{O}(n^2)$	$\mathcal{O}(n^\alpha)$	$(u_f\rho_n + \epsilon)$
2 :	Solve $Ax_0 = b$	$\mathcal{O}(n^{4/3})$	$\mathcal{O}(n^\beta)$	$(u_f\rho_n + \epsilon)$
3 :	**while not** converged **do**			
4 :	Compute $r_i = b - Ax_i$	$\mathcal{O}(n)$	$\mathcal{O}(n)$	(u_r)
5 :	Solve $Ad_i = r_i$ by $d_i = \hat{U}^{-1}\hat{L}^{-1}r_i$.	$\mathcal{O}(n^{4/3})$	$\mathcal{O}(n^\beta)$	$(u_f\rho_n + \epsilon)$
6 :	Compute $x_{i+1} = x_i + d_i$	$\mathcal{O}(n)$	$\mathcal{O}(n)$	(u)
7 :	**end while**			

- Where $2 \geq \alpha$ and $4/3 \geq \beta$.
- Where ϵ refers to the perturbation introduced, and ρ_n is the growth factor ($\approx$ difference of scale between the values of A and its factors L and U).

a. Amestoy, Buttari, Higham, L'Excellent, Mary, and Vieublé, *Combining sparse approximate factorizations with mixed precision iterative refinement*, 2022

Error analysis with numerical approximations

Theorem (Convergence conditions)

Let $Ax = b$ be solved by LU-IR3 or GMRES-IR5 using an approximate LU factorization. Then the forward error will converge provided that

$$(u_f \rho_n + \epsilon)\kappa(A) \ll 1 \qquad (LU - IR3)$$

$$(u_g + u_p \rho_n \kappa(A))(u_f \rho_n + \epsilon)^2 \kappa(A)^2 \ll 1 \qquad (GMRES - IR5)$$

Where ϵ refers to the perturbation introduced, and ρ_n is the growth factor ($\approx$ difference of scale between the values of A and its factors L and U).

Remark : This theorem applies for generic numerical approximations, it includes static pivoting and BLR.

Implemented parallel methods

Solver	u_f	u	u_r	u_g	u_p	$\max(\kappa(A))$ $(\epsilon = 0)$	forward error
DMUMPS	fp64 LU standard solver					—	$\kappa(A) \times 10^{-16}$
LU-IR	S	D	D	—	—	2×10^{7}	$\kappa(A) \times 10^{-16}$
GMRES-IR	S	D	D	D	D	1×10^{10}	$\kappa(A) \times 10^{-16}$

➤ We use the **multifrontal sparse solver** MUMPS for factorization and LU solve operations.

➤ LU-IR and GMRES-IR use **single precision (fp32) factorization** to accelerate. When using **BLR and/or static pivoting** we name the variants (BLR/STC)-(GMRES/LU)-IR.

Matrix set

Name	N	NNZ	Arith.	Sym.	$\kappa(A)$	Fact. (flops)	Slv. (flops)
ElectroPhys10M	1.02E+07	1.41E+08	R	1	1.10E+01	4E+14	9E+10
DrivAer6M	6.11E+06	4.97E+07	R	1	9.40E+05	6E+13	3E+10
Queen_4147	4.14E+06	3.28E+08	R	1	4.30E+06	3E+14	6E+10
tminlet3M	2.84E+06	1.62E+08	C	0	2.70E+07	1E+14	2E+10
perf009ar	5.41E+06	2.08E+08	R	1	3.70E+08	2E+13	2E+10
elasticity-3d	5.18E+06	1.16E+08	R	1	3.60E+09	2E+14	5E+10
lfm_aug5M	5.52E+06	3.71E+07	C	1	5.80E+11	2E+14	5E+10
CarBody25M	2.44E+07	7.06E+08	R	1	8.60E+12	1E+13	3E+10
thmgas	5.53E+06	3.71E+07	R	0	8.28E+13	1E+14	4E+10

Set of **industrial** and SuiteSparse matrices.

➤ The matrices are **ordered in increasing $\kappa(A)$**, the higher $\kappa(A)$ is, the slower the convergence (if reached at all).

Matrix set

Name	N	NNZ	Arith.	Sym.	$\kappa(A)$	Fact. (flops)	Slv. (flops)
ElectroPhys10M	1.02E+07	1.41E+08	R	1	1.10E+01	4E+14	9E+10
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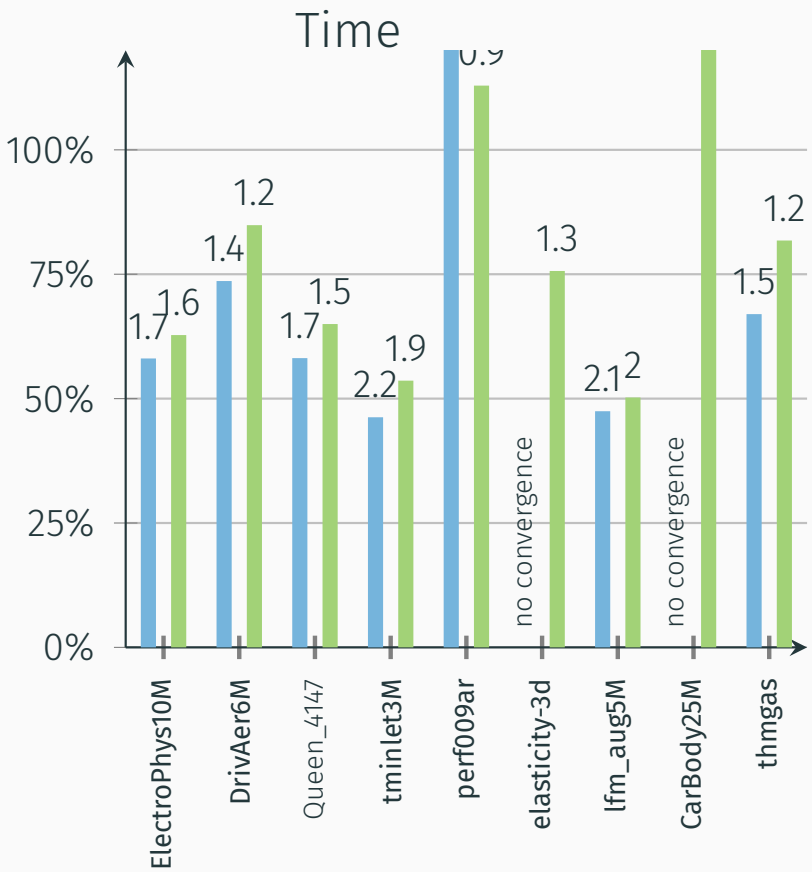
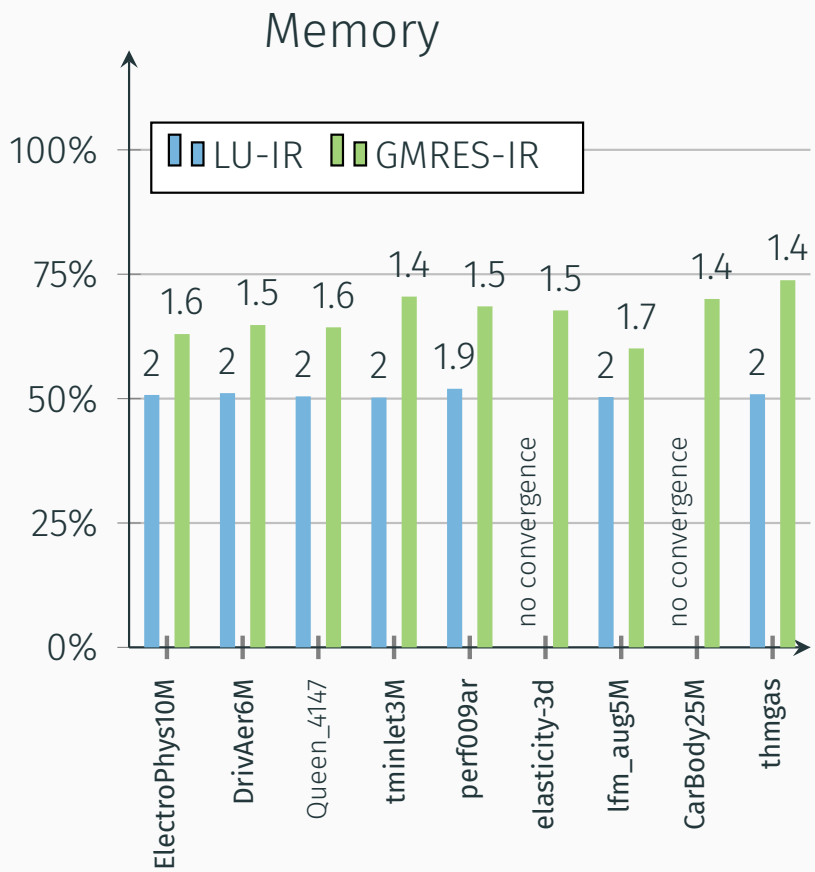
tminlet3M	2.84E+06	1.62E+08	C	0	2.70E+07	1E+14	2E+10
perf009ar	5.41E+06	2.08E+08	R	1	3.70E+08	2E+13	2E+10
elasticity-3d	5.18E+06	1.16E+08	R	1	3.60E+09	2E+14	5E+10
lfm_aug5M	5.52E+06	3.71E+07	C	1	5.80E+11	2E+14	5E+10
CarBody25M	2.44E+07	7.06E+08	R	1	8.60E+12	1E+13	3E+10
thmgas	5.53E+06	3.71E+07	R	0	8.28E+13	1E+14	4E+10

Set of **industrial** and SuiteSparse matrices.

➤ We run on OLYMPE supercomputer nodes (two Intel 18-cores Skylake/node), 1 node (2MPI×18threads) or 2 nodes (4MPI×18threads) depending on the matrix size.

Time and memory performance w.r.t. DMUMPS





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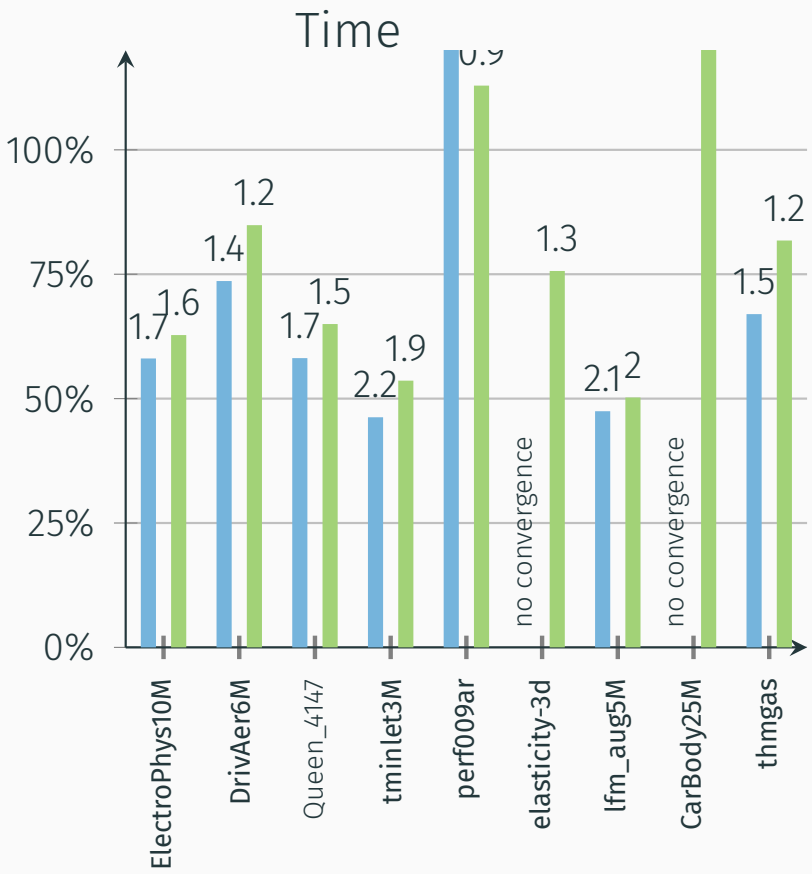
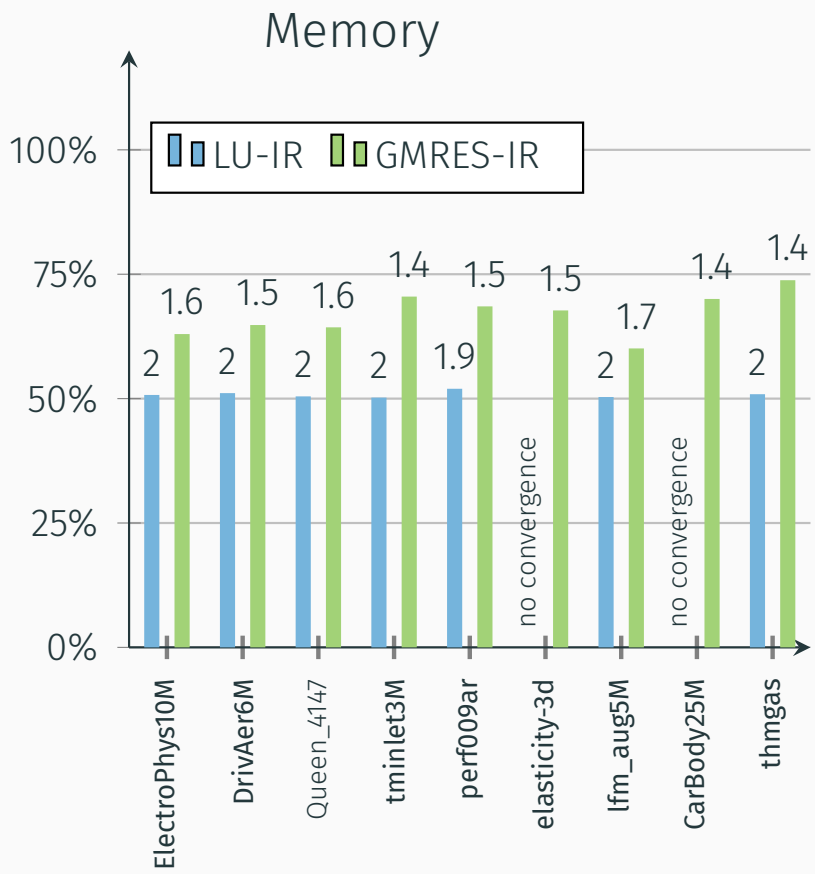
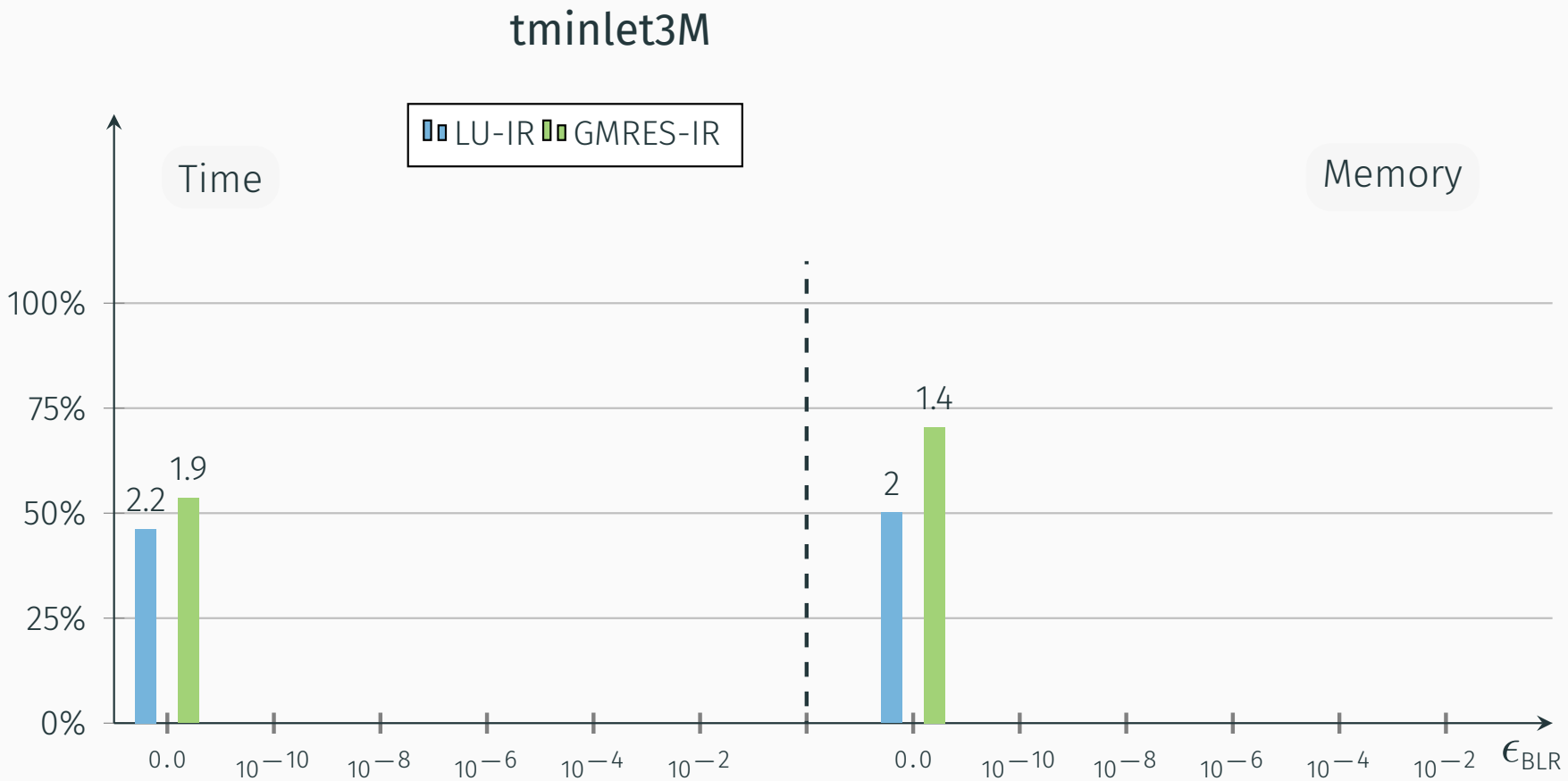




- LU-IR up to 2× faster.
- GMRES-IR slower (requires more LU solves), but more robust on $\kappa(A)$.

- LU-IR consumes 2× less memory!
- GMRES-IR consumes at best 1.7× less despite factors in double ⇒ save active memory.

Time and memory performance with BLR w.r.t. DMUMPS



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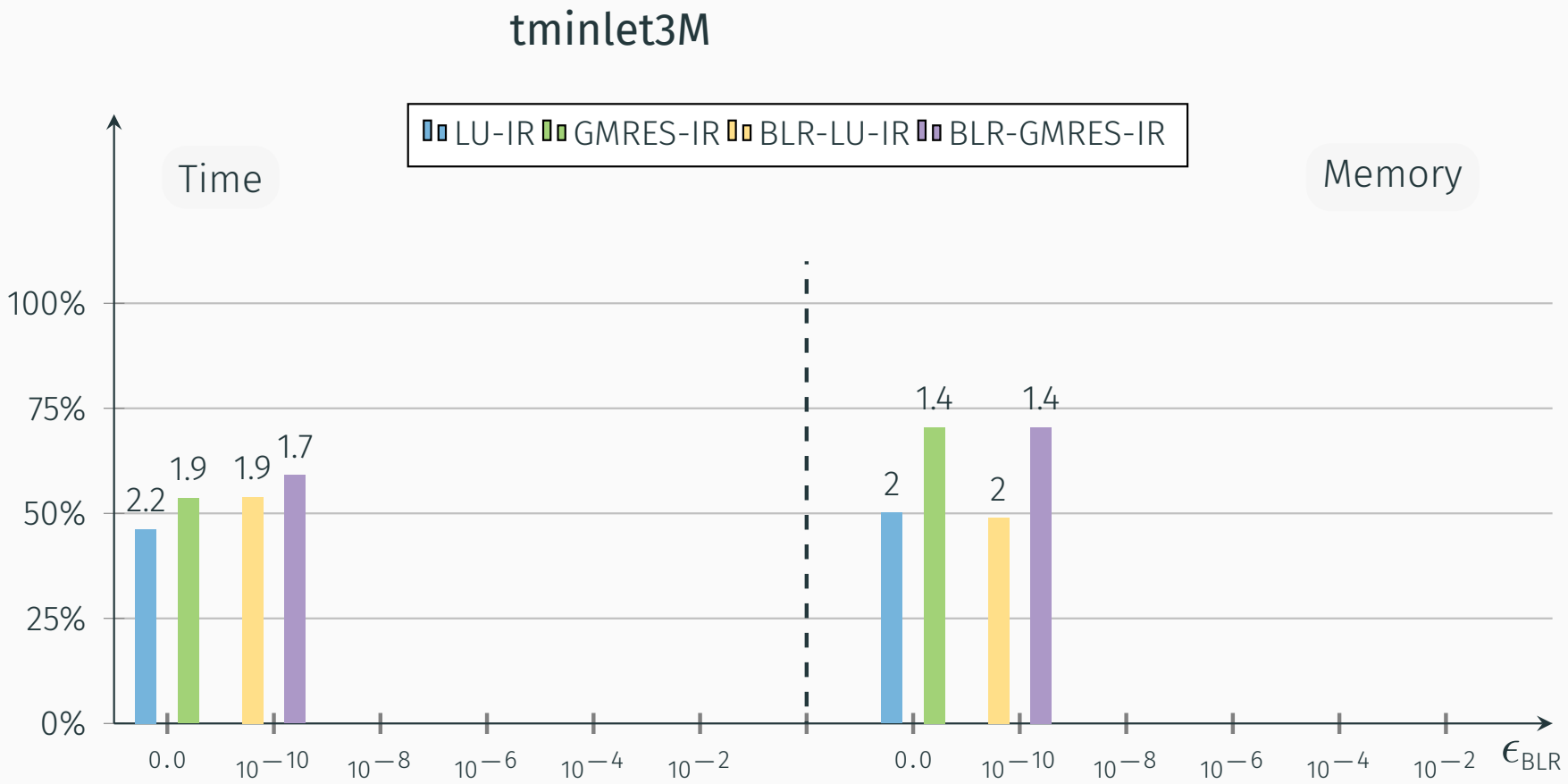

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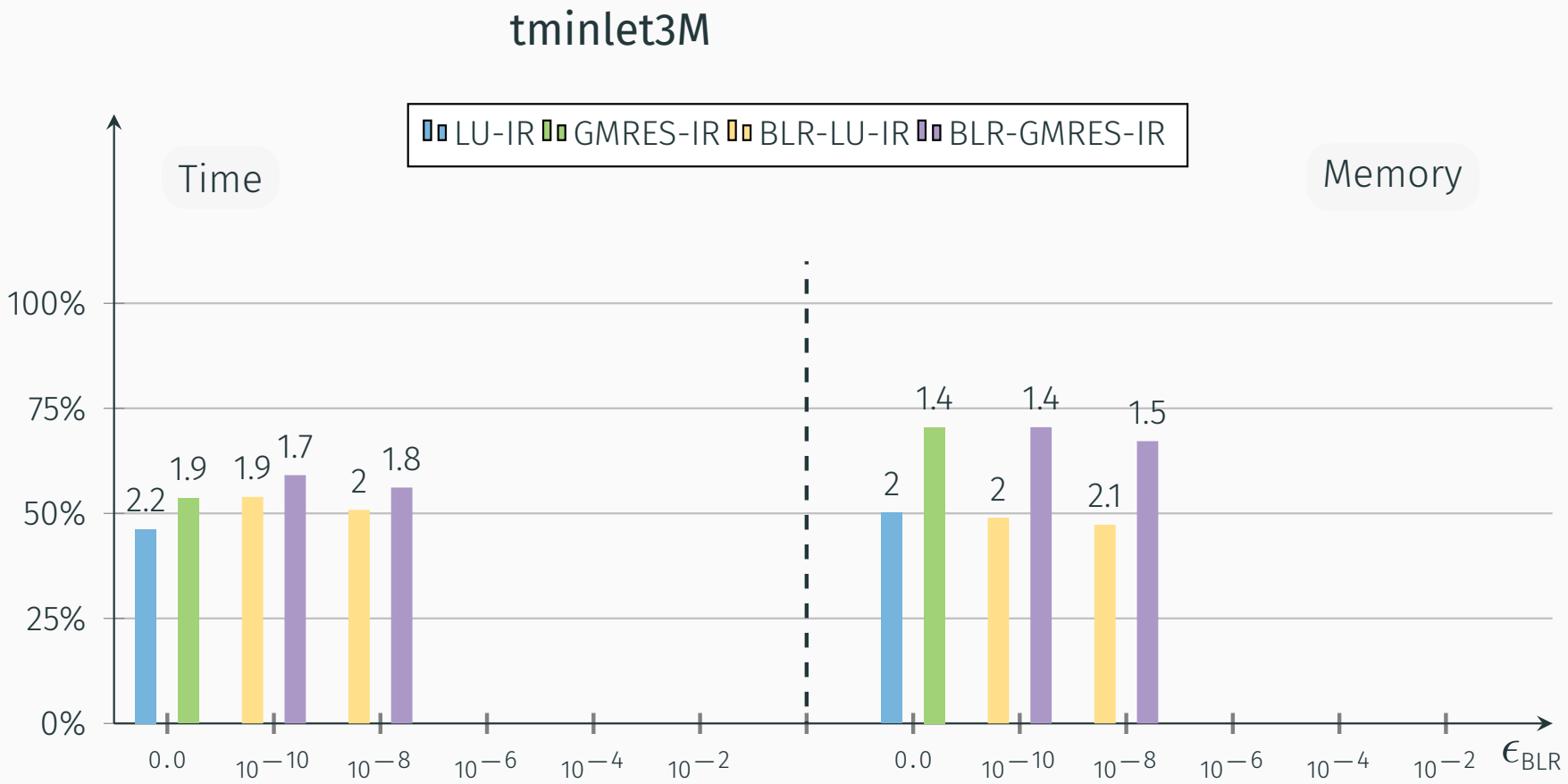

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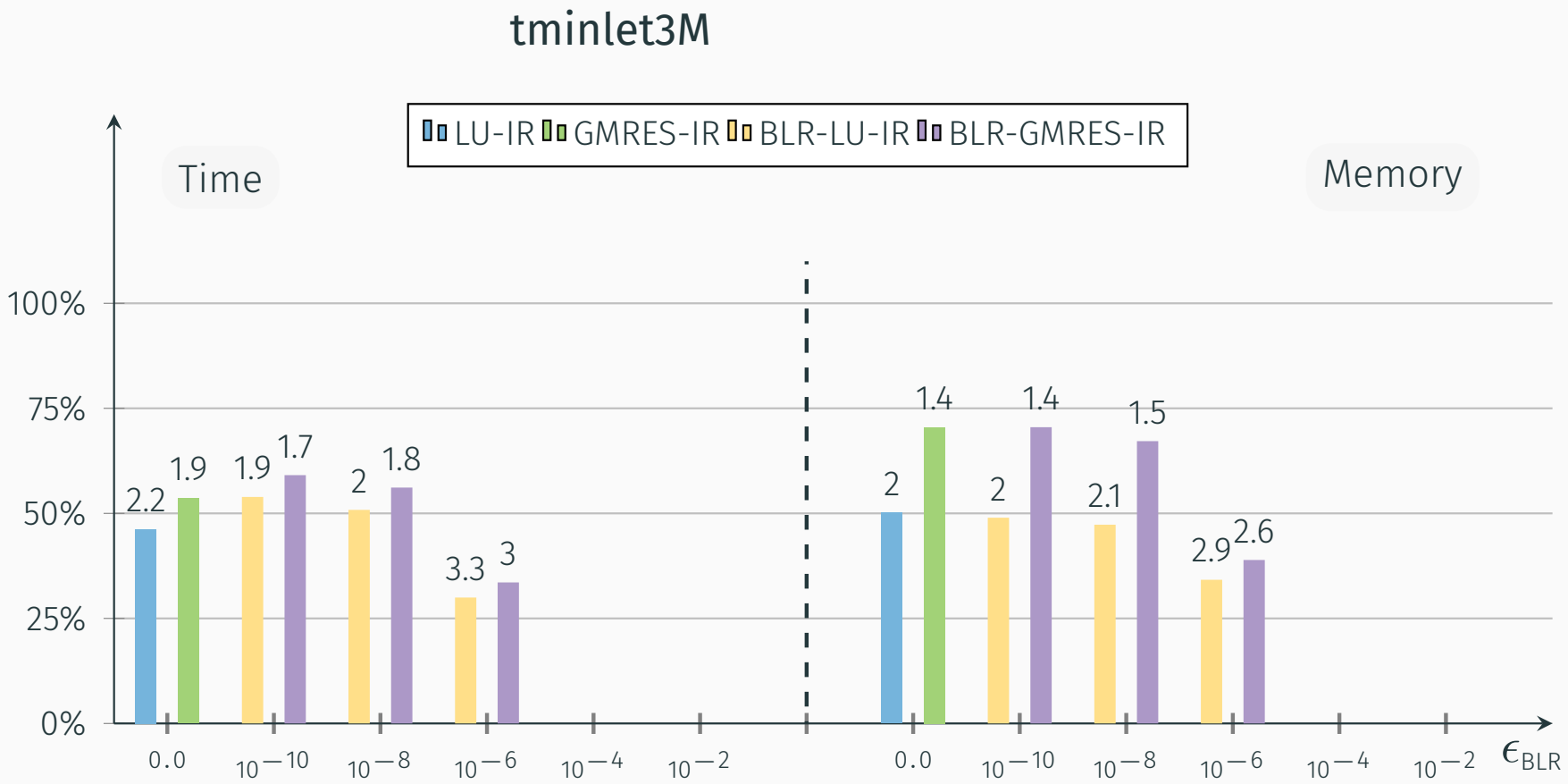

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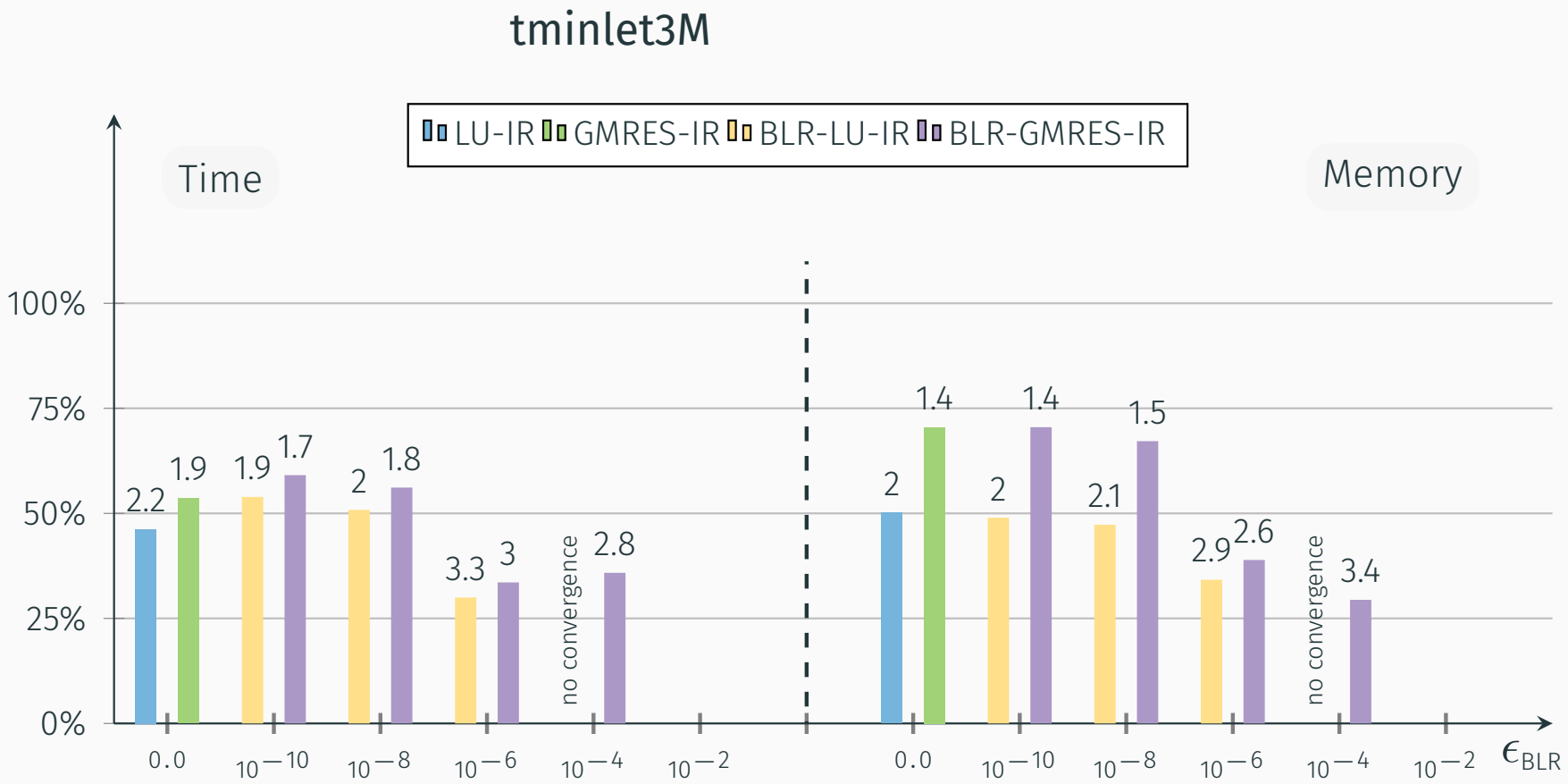

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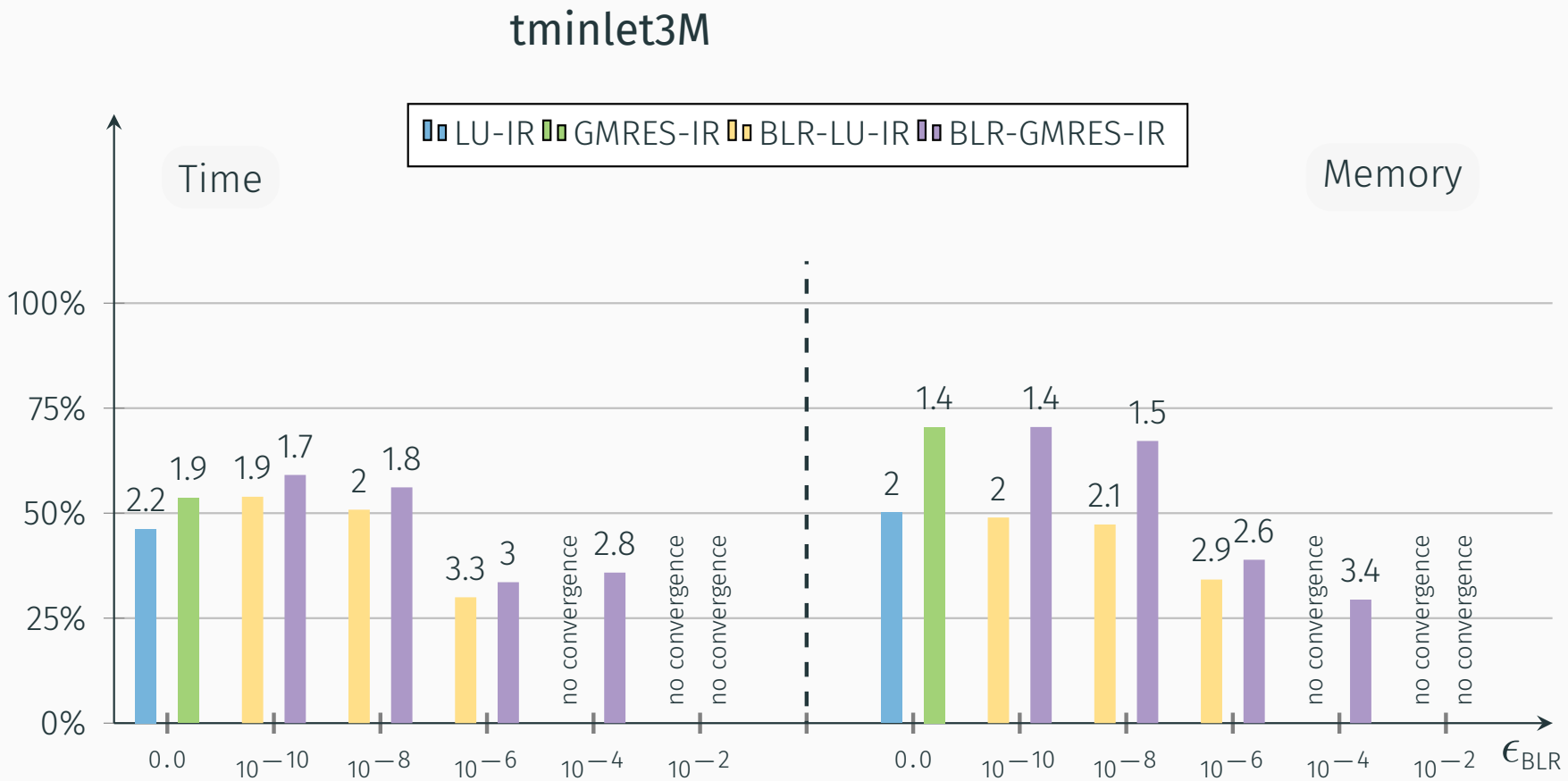
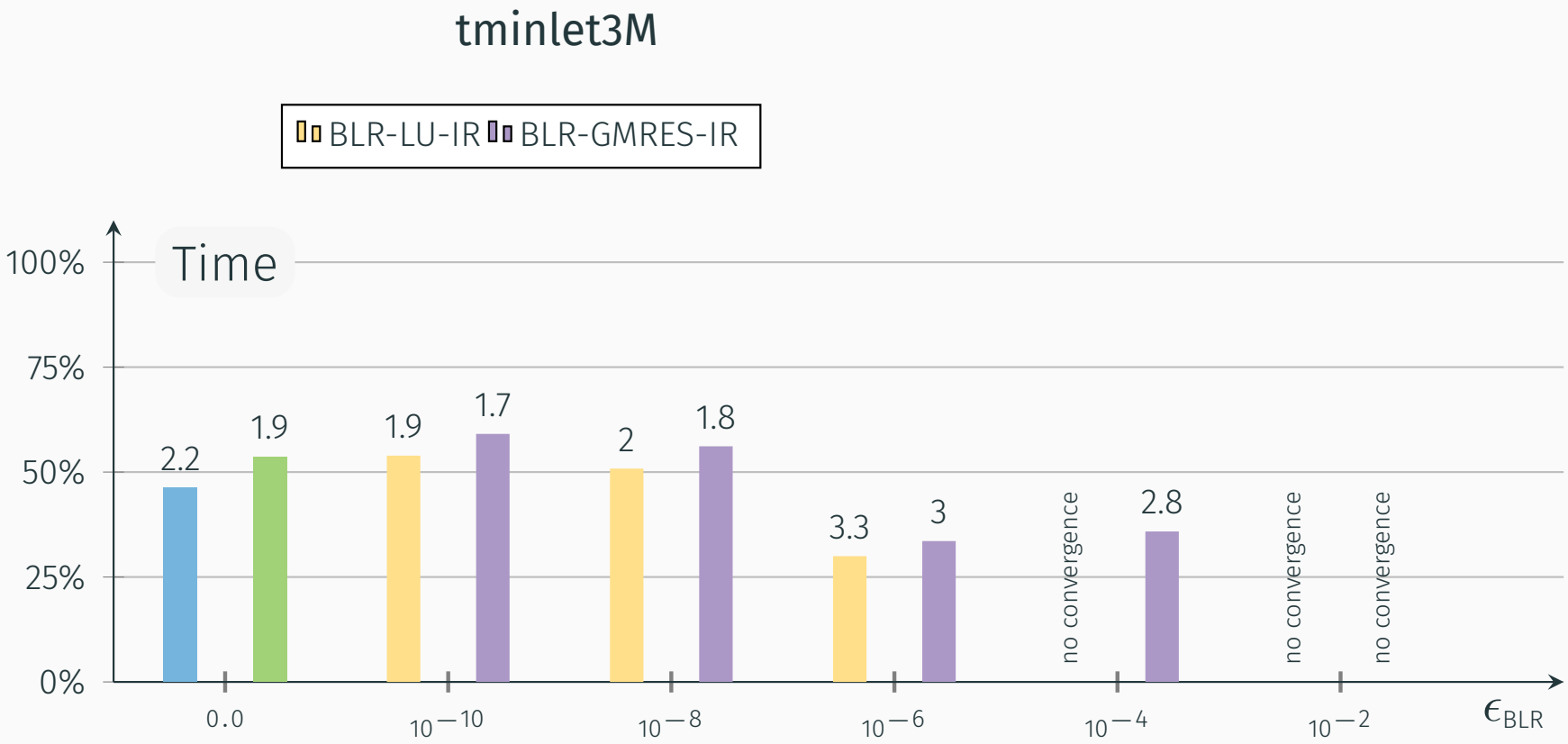


Time performance with BLR + static pivoting w.r.t. DMUMPS



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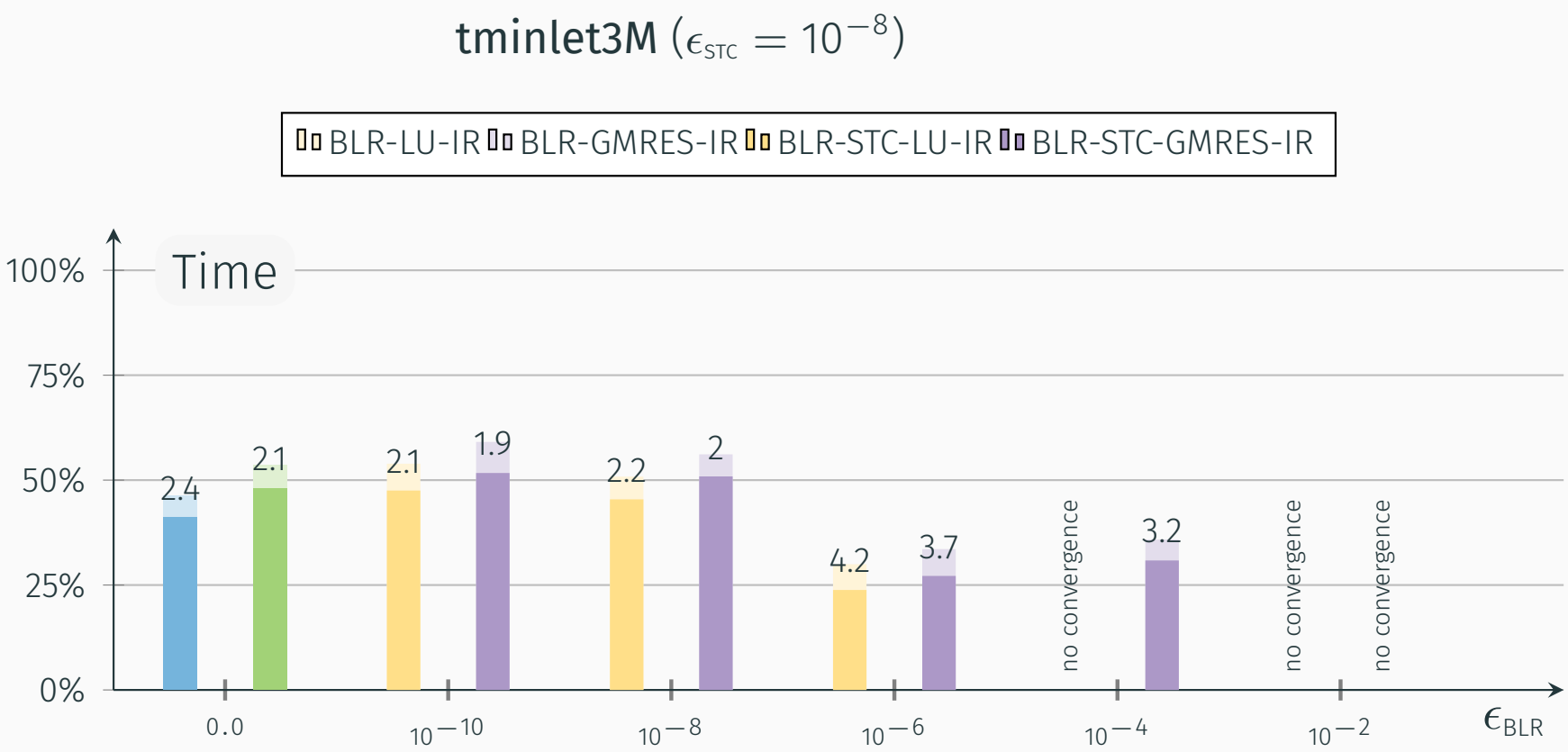
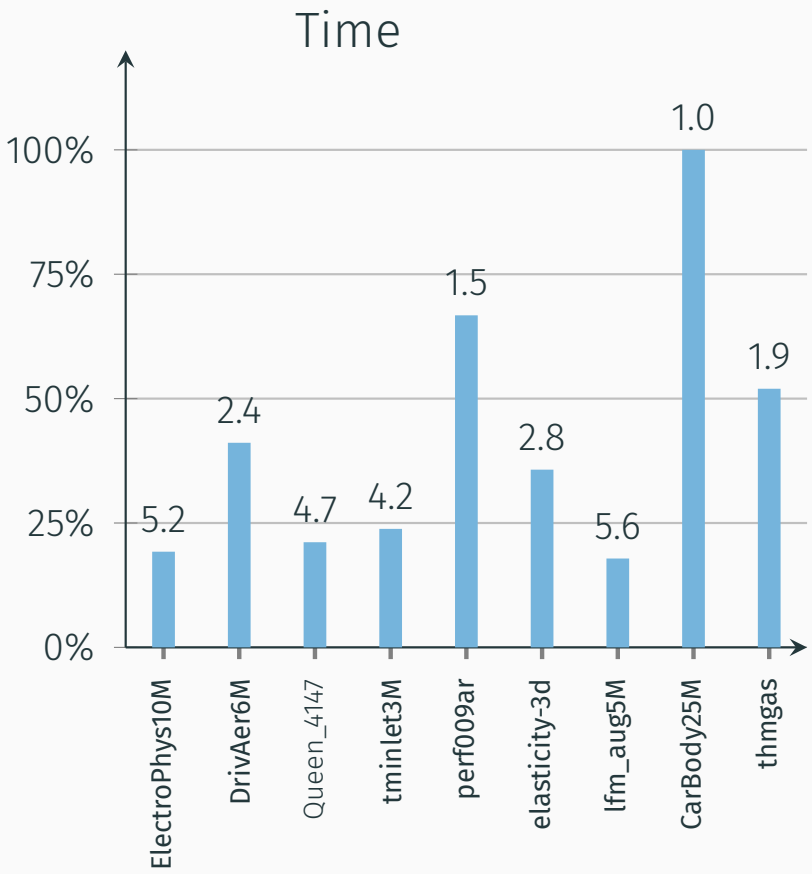
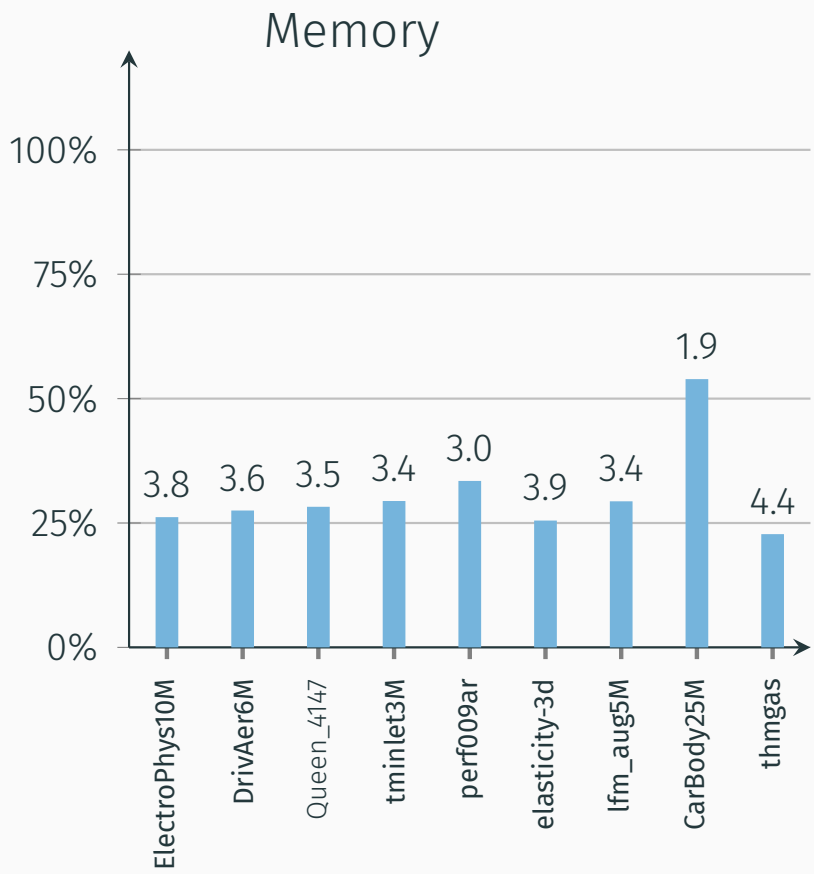


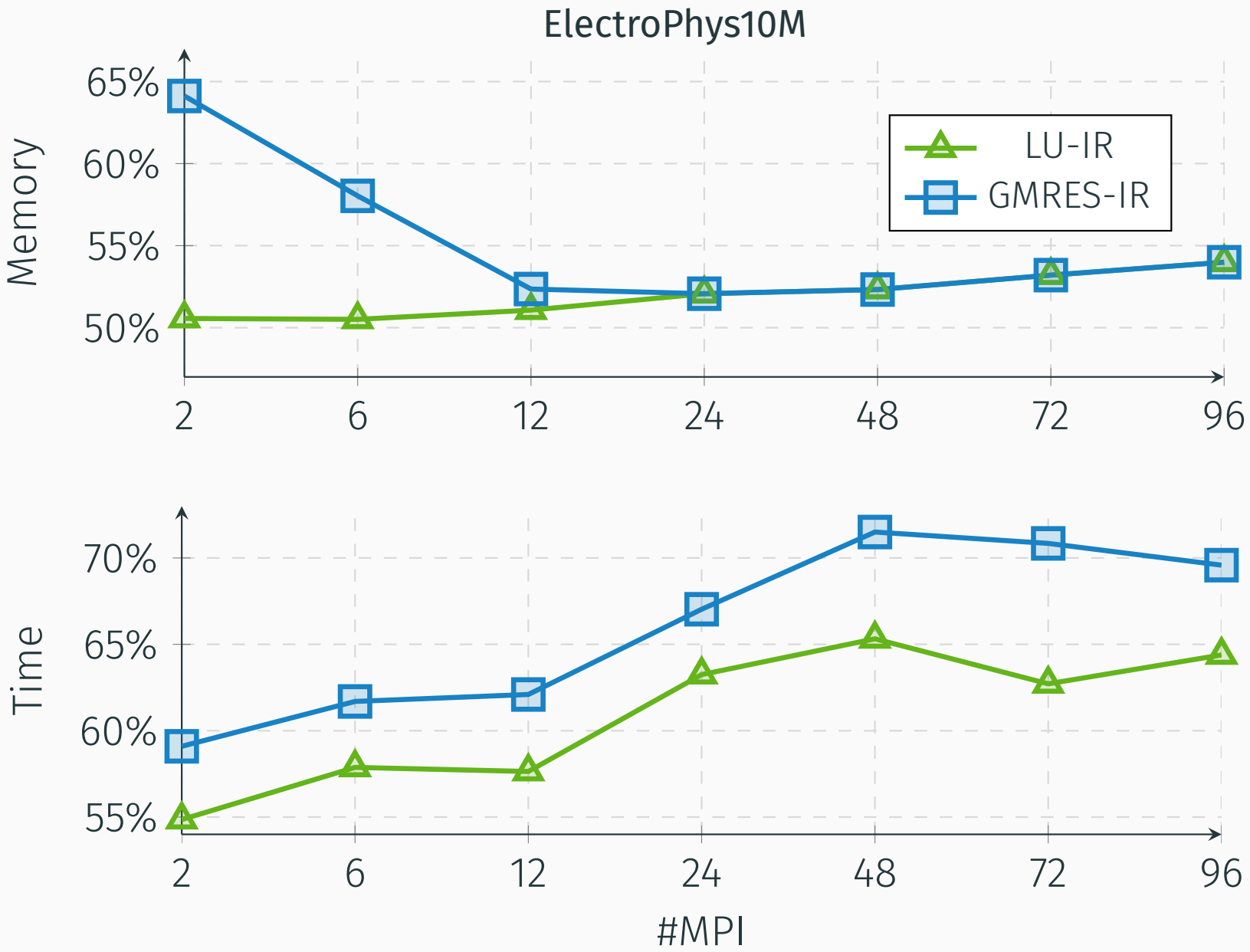
Gather it all : Best time and memory w.r.t. DMUMPS





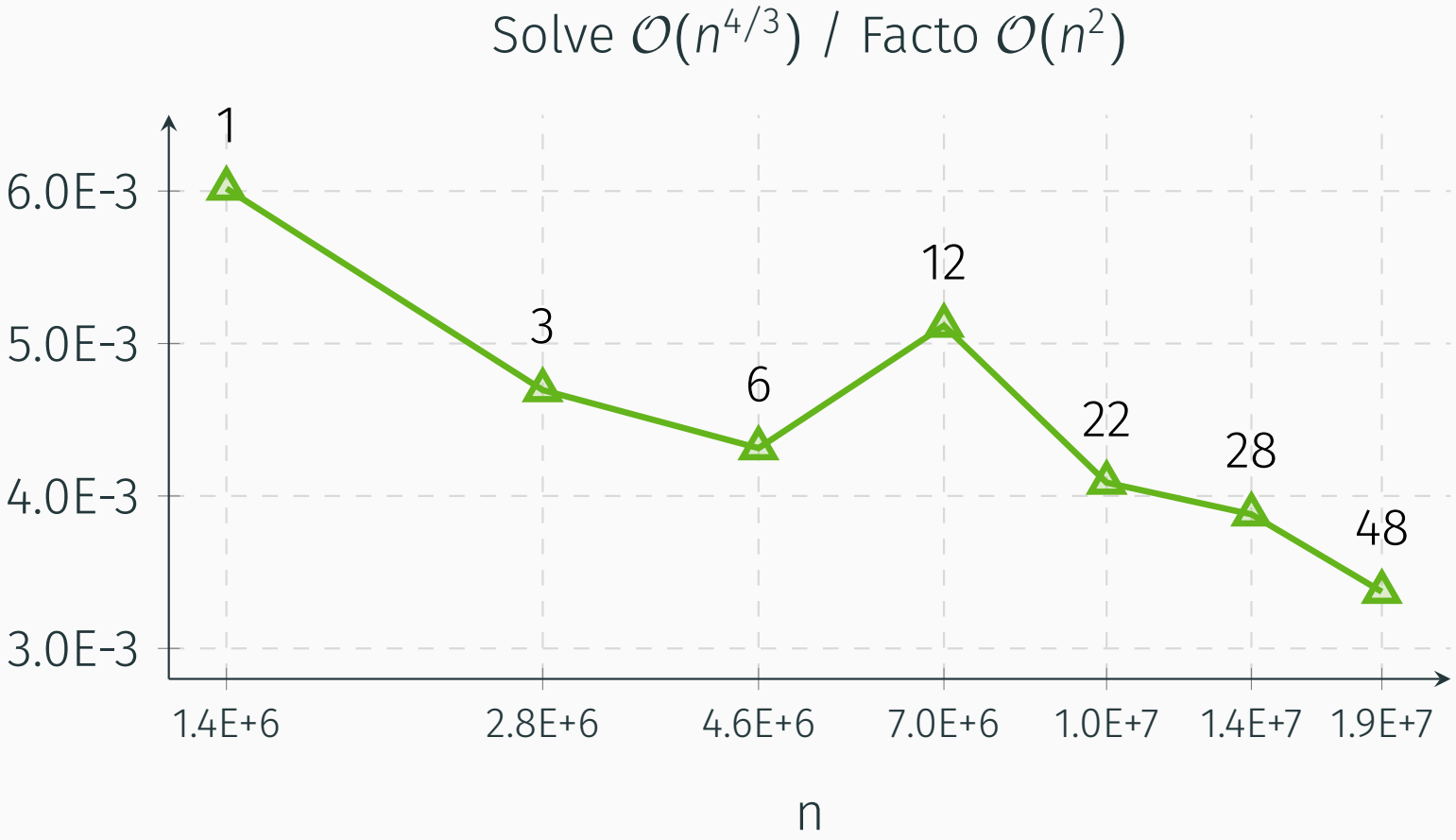
$\Rightarrow$ Up to 5.6$\times$ faster and 4.4$\times$ less memory with the same accuracy on the solution than DMUMPS!

Strong scaling (6OMP/MPI) : Time and mem w.r.t. DMUMPS



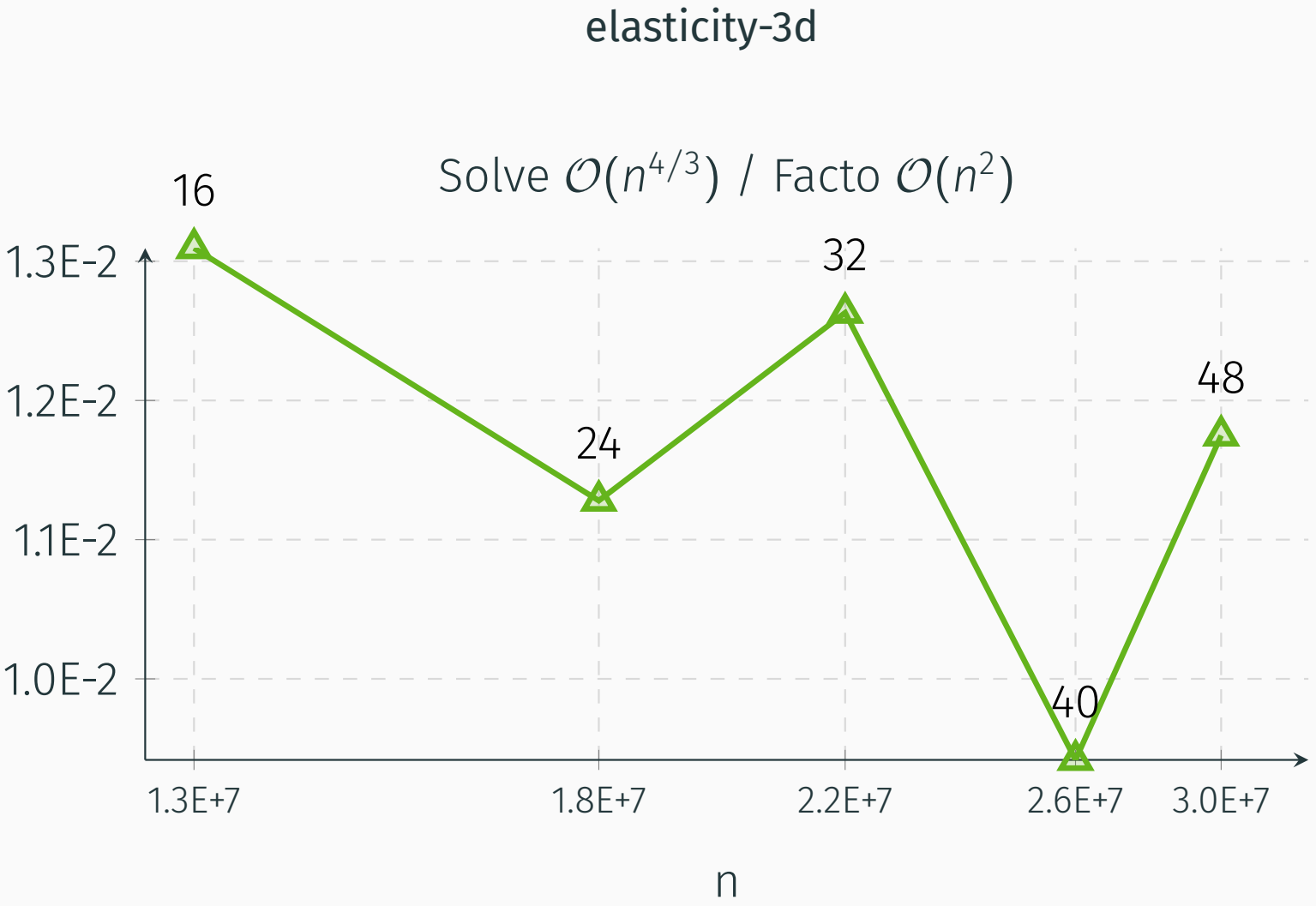
Weak scaling (18OMP/MPI) : Memory/#MPI = cst

Helmholtz



$\Rightarrow$ Less costly refinement steps as n increases.

Weak scaling (18OMP/MPI) : Memory/#MPI = cst



$\Rightarrow$ Constant cost of the refinement steps as n increases.

Conclusion

Summary

Goal : Solve $Ax = b$ with a sparse direct solver ideally with the least memory and computational time.

Nowadays solutions : Combination of numerical approximations and low precisions.

Drawback : Loss of accuracy on the solution.

Proposal : Use iterative refinement to provide an accurate solution for sparse direct solver at low cost [3].

We wish to thank our Industrial partners and the EoCoE project for providing access to their matrices.

3. Amestoy, Buttari, Higham, L'Excellent, Mary, and Vieublé, *Combining sparse approximate factorizations with mixed precision iterative refinement*, 2022