Fast Hierarchical QR Factorization of Sparse Matrices

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Goal

We want to develop a fast, sparse QR factorization of A and use it to solve:

- Sparse linear systems

$$Ax = b$$

  where A is of size $N \times N$, sparse and unsymmetric

- Sparse linear least squares systems

$$\min_x \|Ax - b\|^2$$

  where A is $M \times N$, $M \geq N$, full column rank and sparse

Direct vs Iterative methods for sparse matrices

Direct methods	**Iterative methods**
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Robust	Need domain knowledge
Accurate	No convergence guarantees
Generic	Specific
Expensive	Cheap

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Incomplete factorizations provide a compromise between the two

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Incomplete LU, Incomplete QR, Hierarchical methods

Tunable accuracy

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Use as direct method or preconditioner

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spaQR is an example of this kind and produces a fast, sparse, approximate QR factorization of a given matrix.

- Fast: $\mathcal{O}(M \log N)$ time to factorize and $\mathcal{O}(M)$ to apply/solve with a vector
- Accuracy: Controllable with parameter ϵ defined by the user

Motivation

Row/Column reordering

- Matrix is typically reordered to minimize fill-in entries

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  - If $A = QR$, then R^T is also the Cholesky factor of $A^T A$

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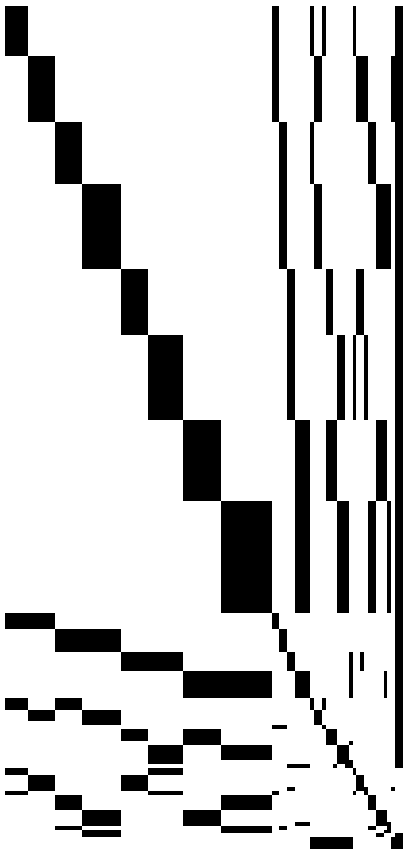
- Row ordering: Done such that the diagonal blocks in the reordered matrix has a small condition number (based on heuristics)

Multifrontal sparse QR: Challenges



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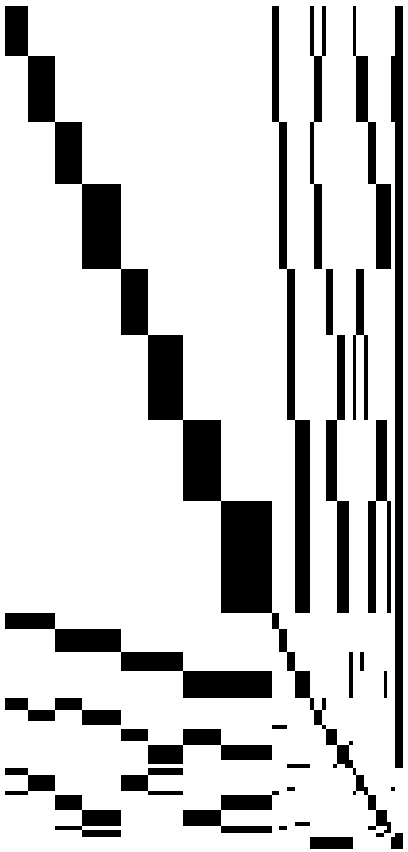

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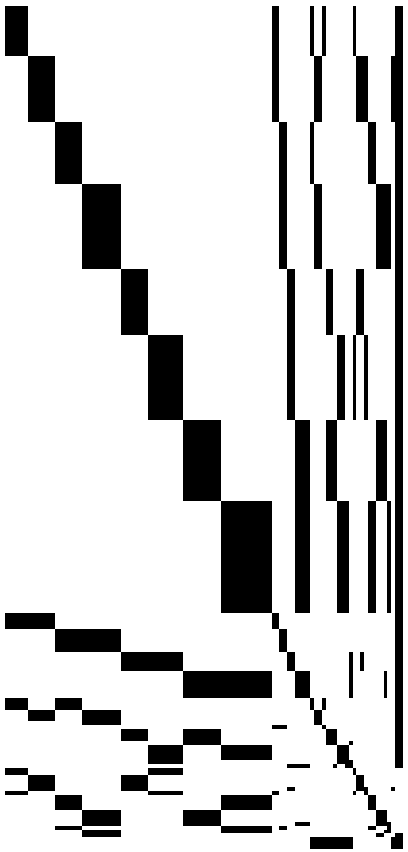

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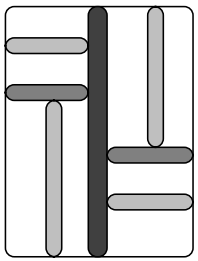

(a) separators

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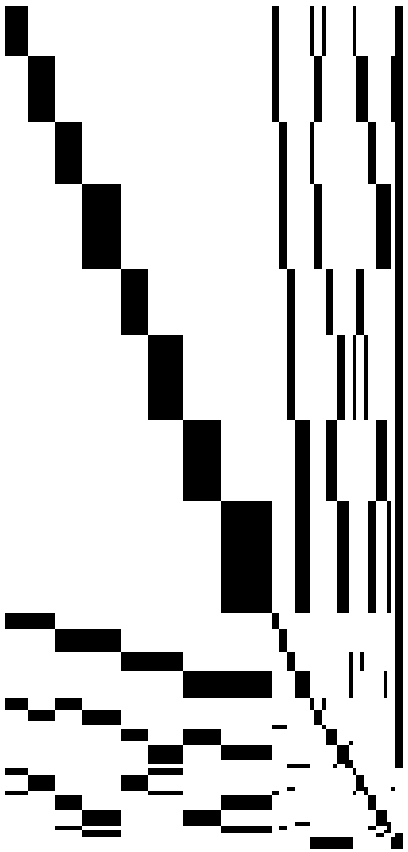

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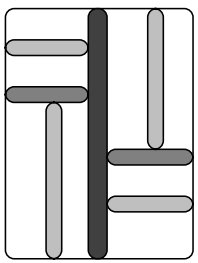

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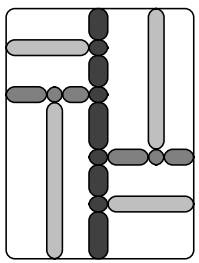

(b) interfaces

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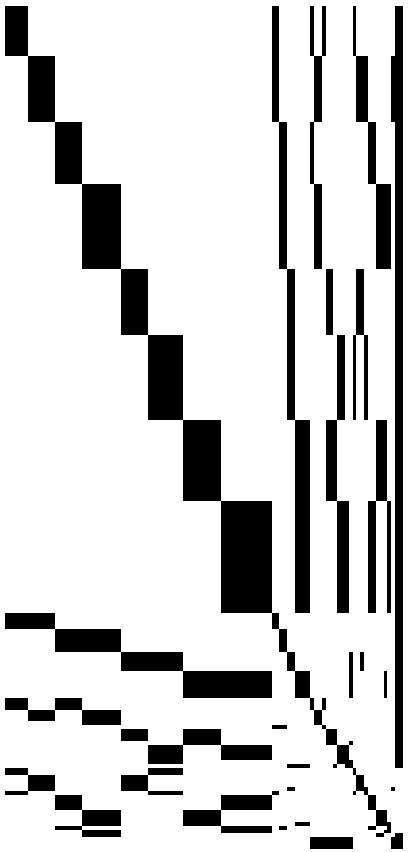

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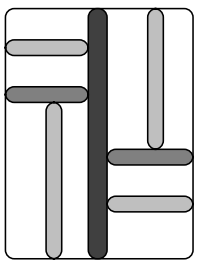

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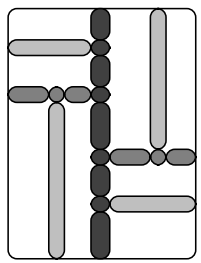

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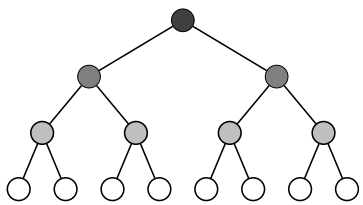

(c) elimination tree

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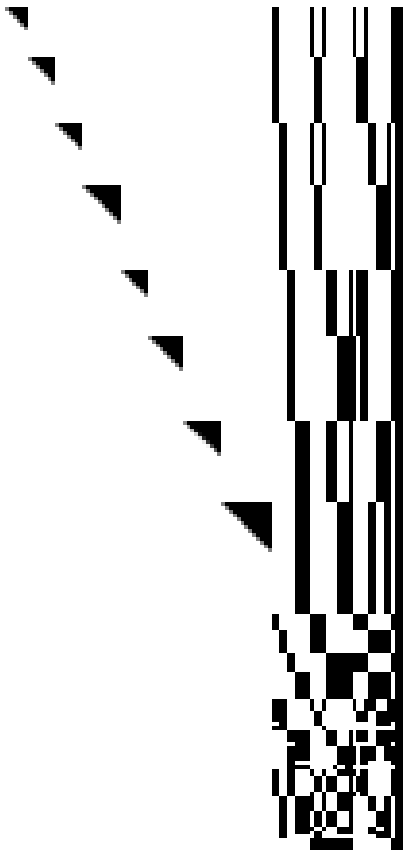

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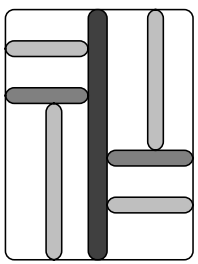

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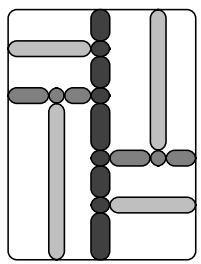

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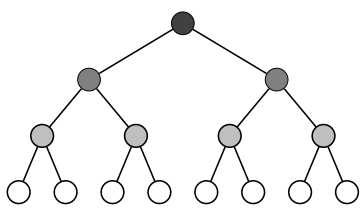

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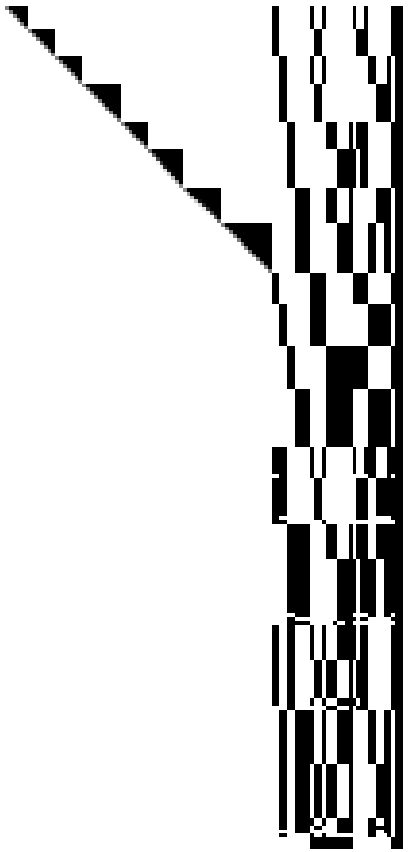

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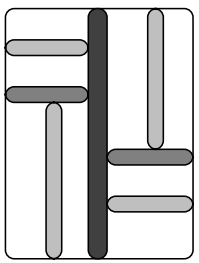

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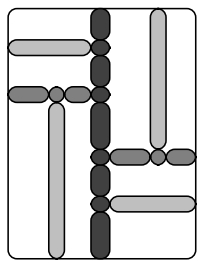

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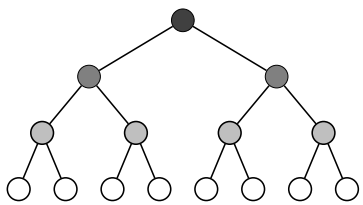

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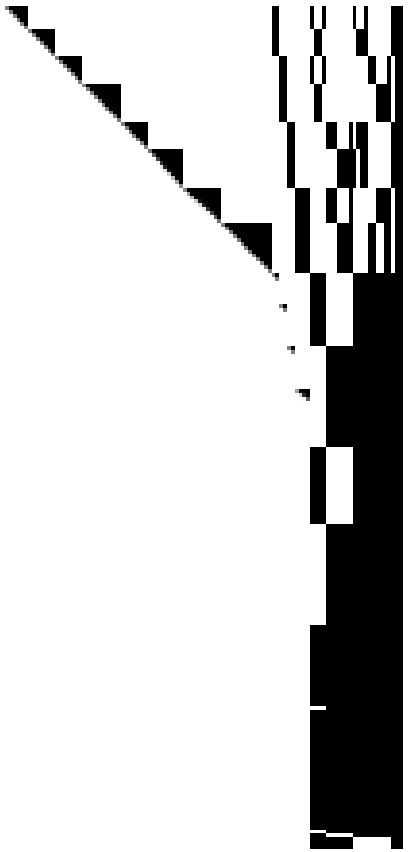

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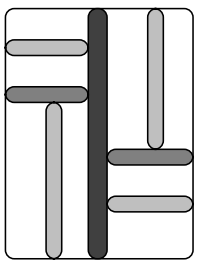

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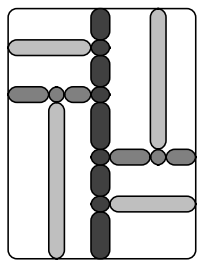

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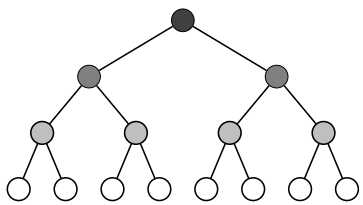

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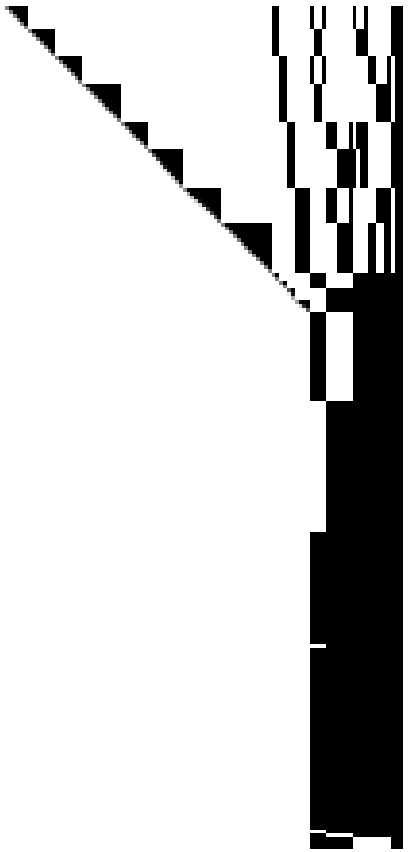

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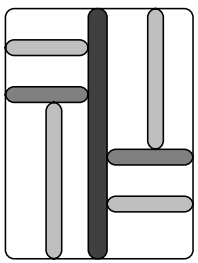

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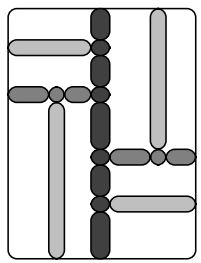

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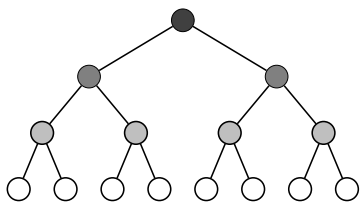

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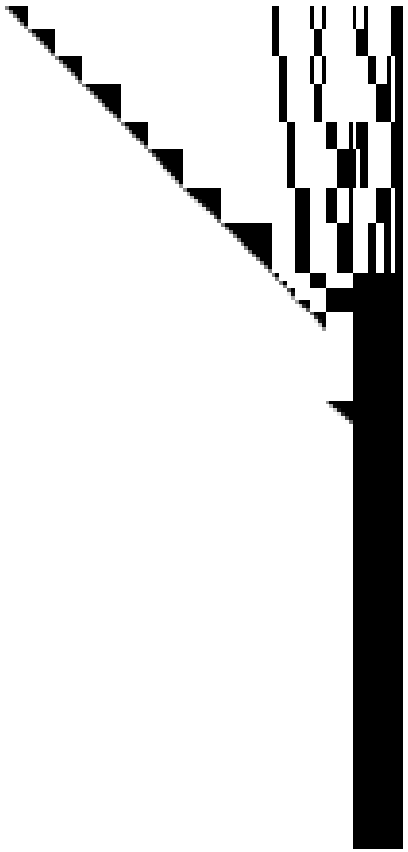

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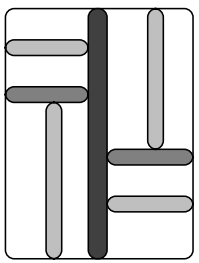

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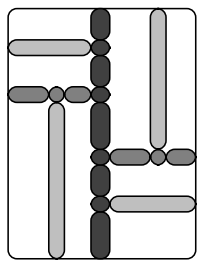

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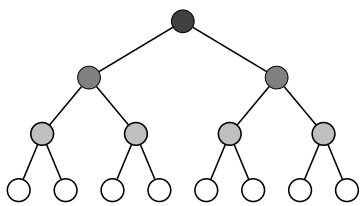

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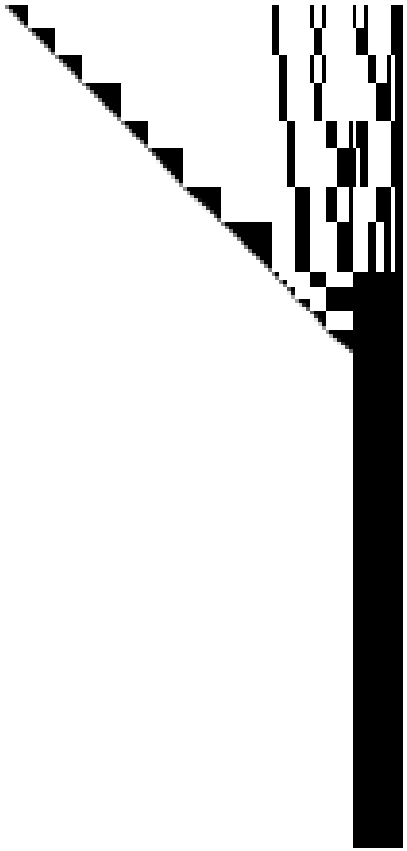

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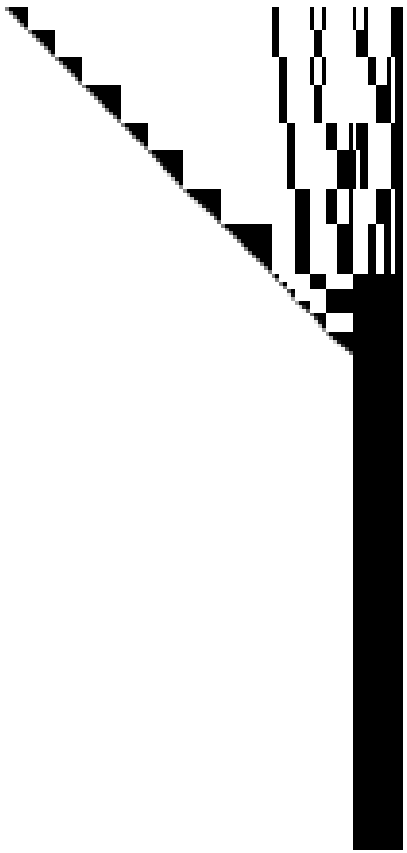

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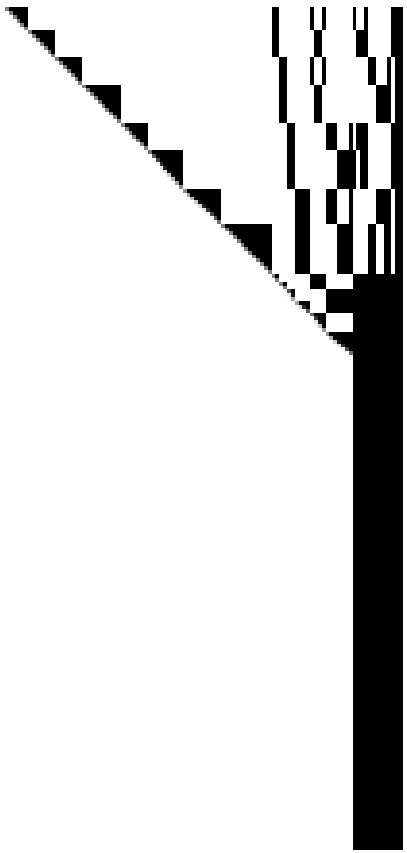

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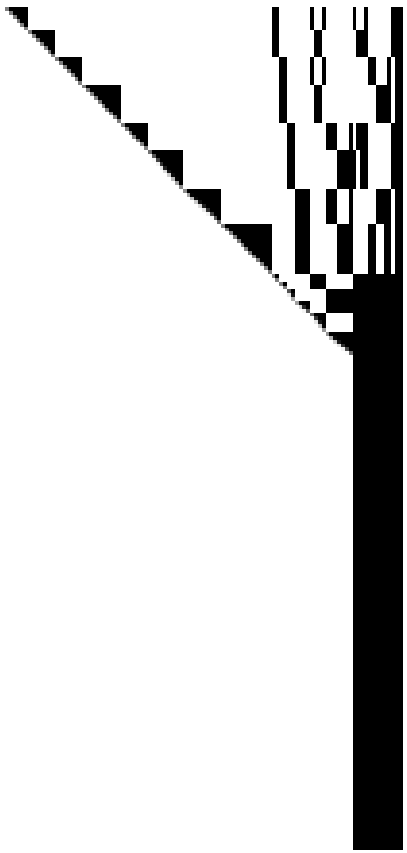

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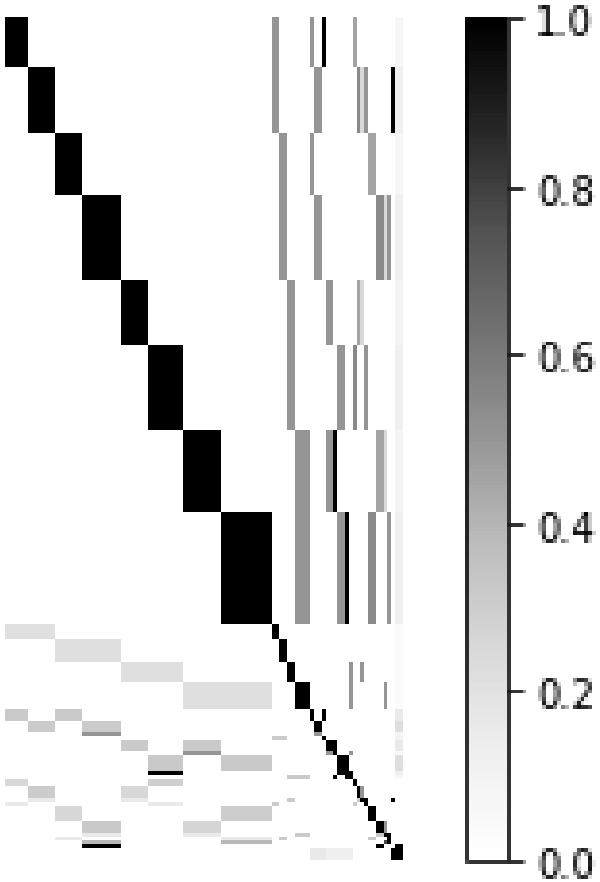
- Costs $\mathcal{O}\left((M-N)N^{4/3}\right)$ to factorize just this block! Expensive!

Ranks of off-diagonal blocks

How can we improve?



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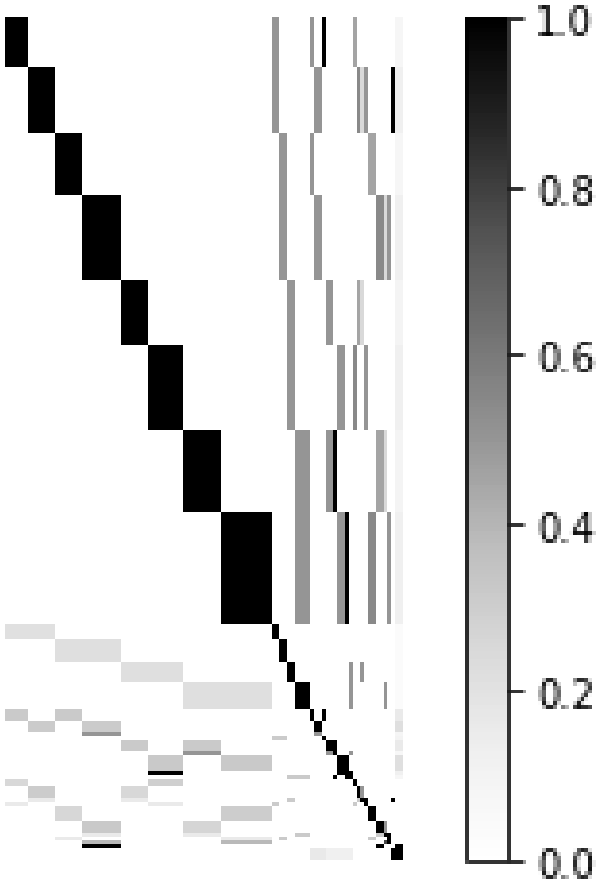

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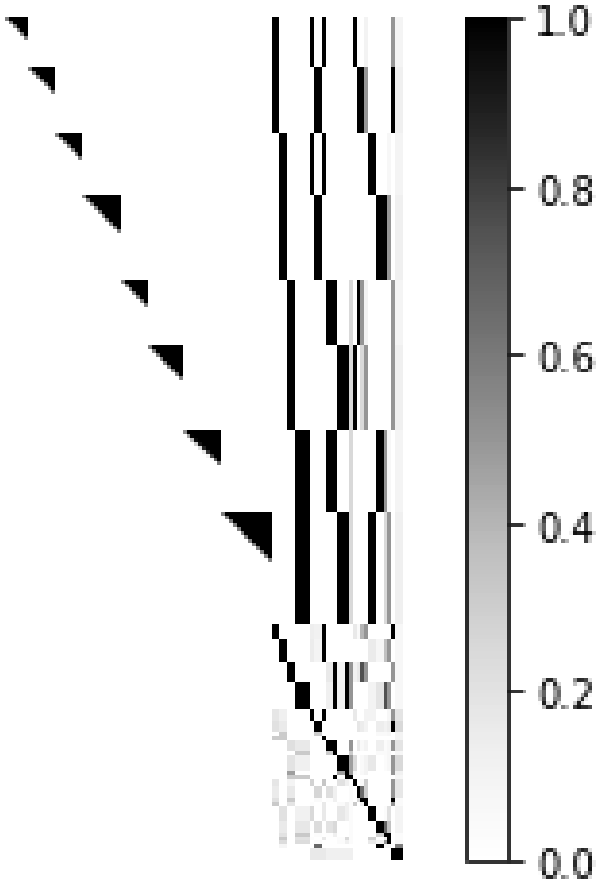

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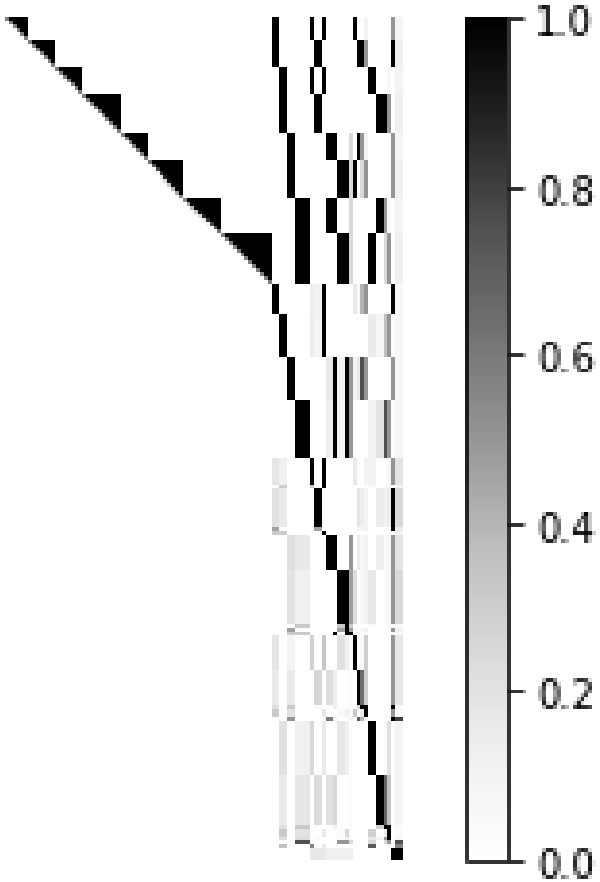

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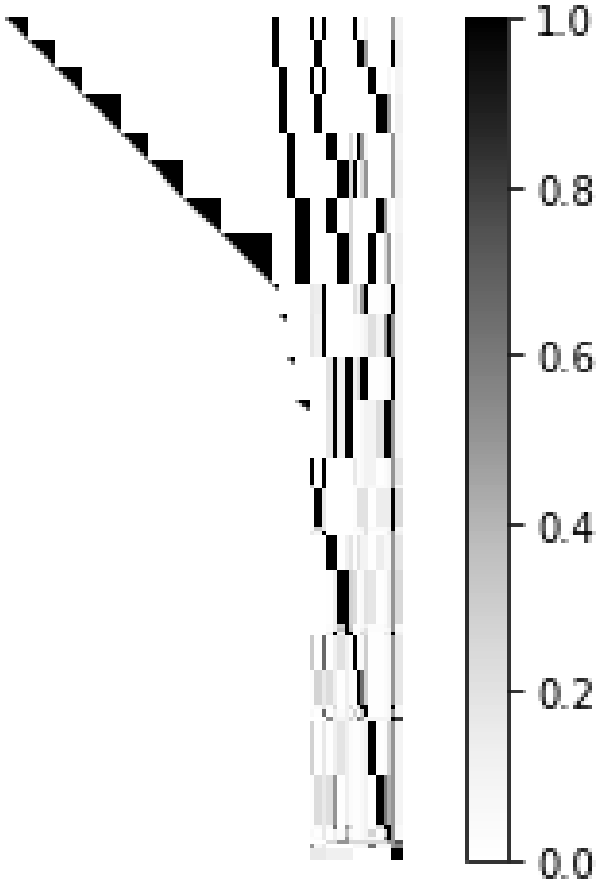

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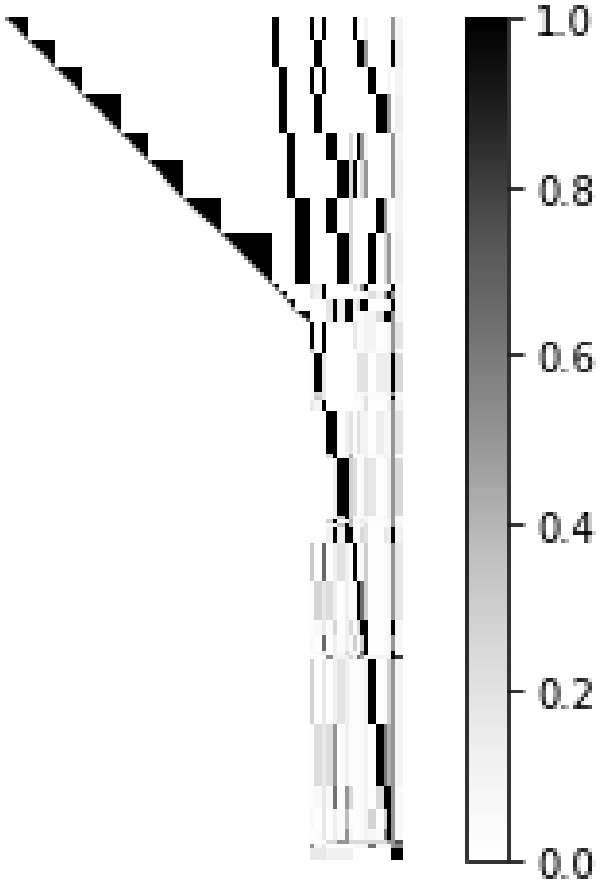

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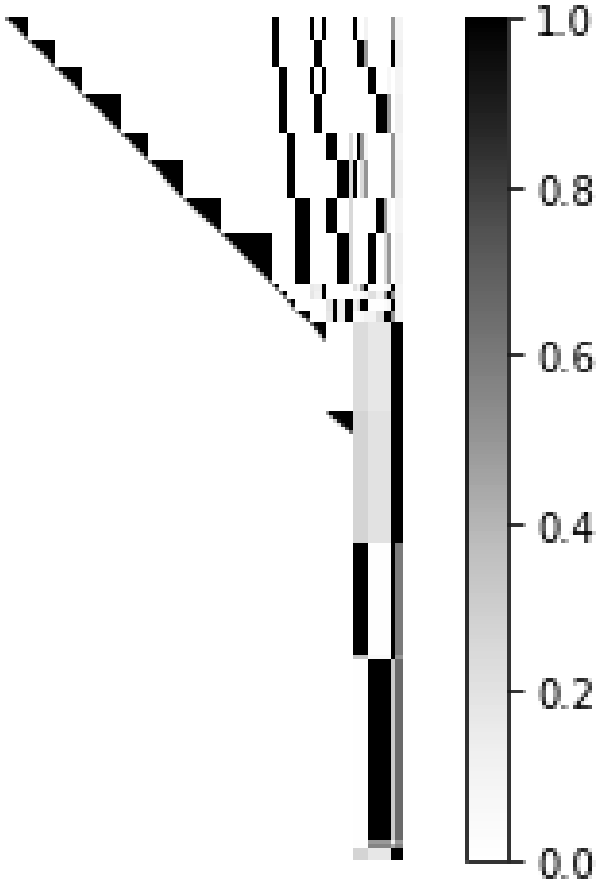

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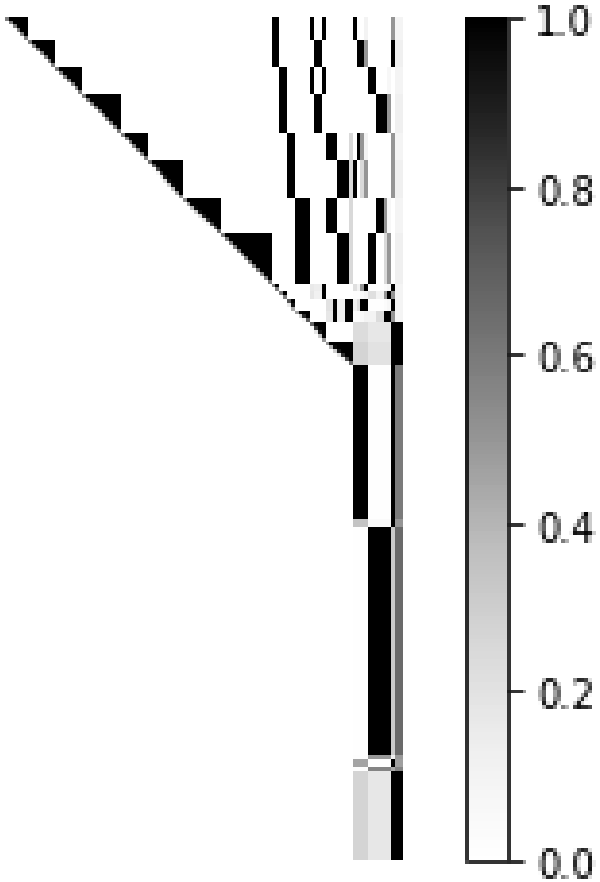

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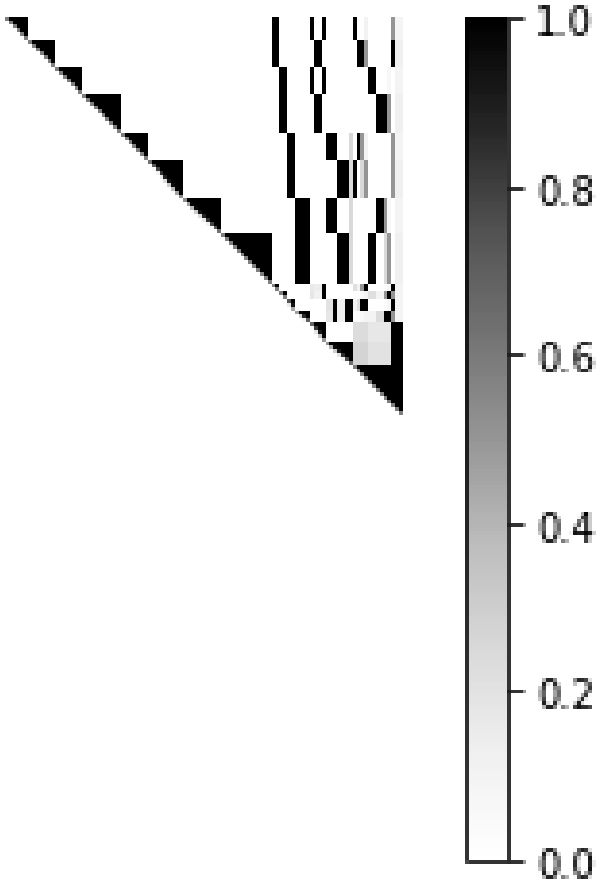

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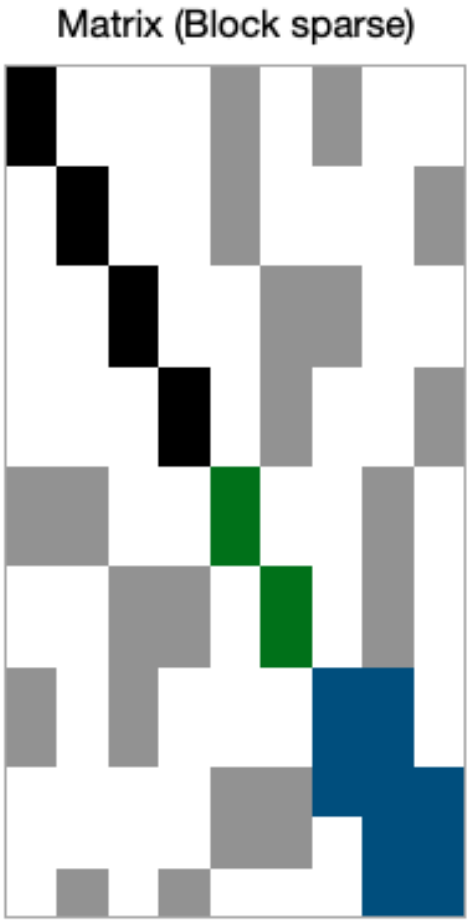
Overview: spaQR algorithm

spaQR algorithm



Require: Matrix $A \in \mathbb{R}^{M \times N}$, $M \geq N$

Require: Tolerance ϵ

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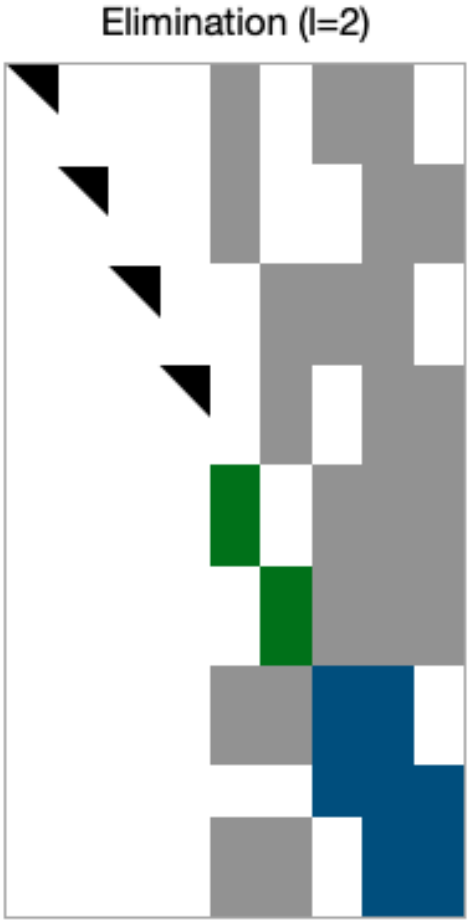

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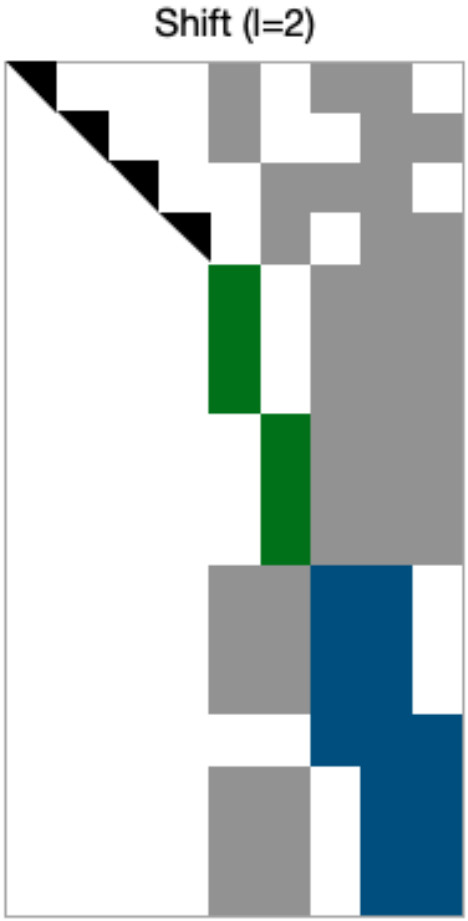
for all $l = L-1, L-2, \ldots 0$ **do**

1. Factorize interiors at level l

spaQR algorithm



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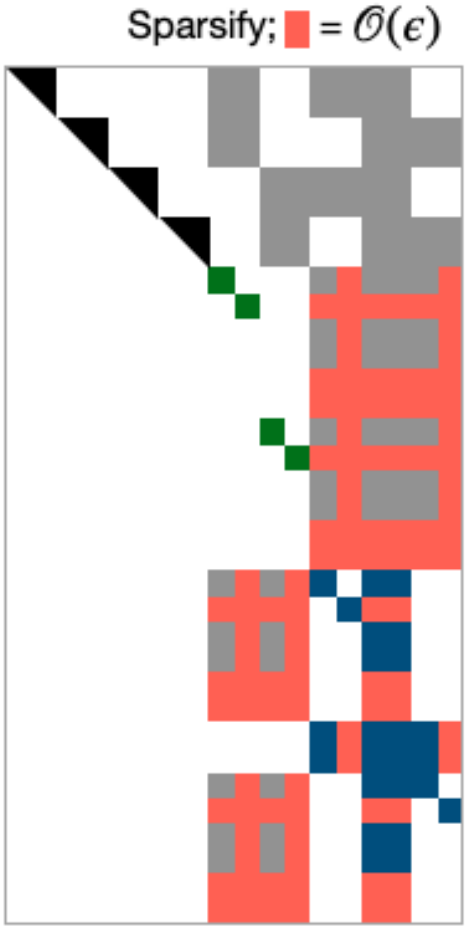
1. Factorize interiors at level l
2. Shift rows below diagonal of eliminated interiors

spaQR algorithm



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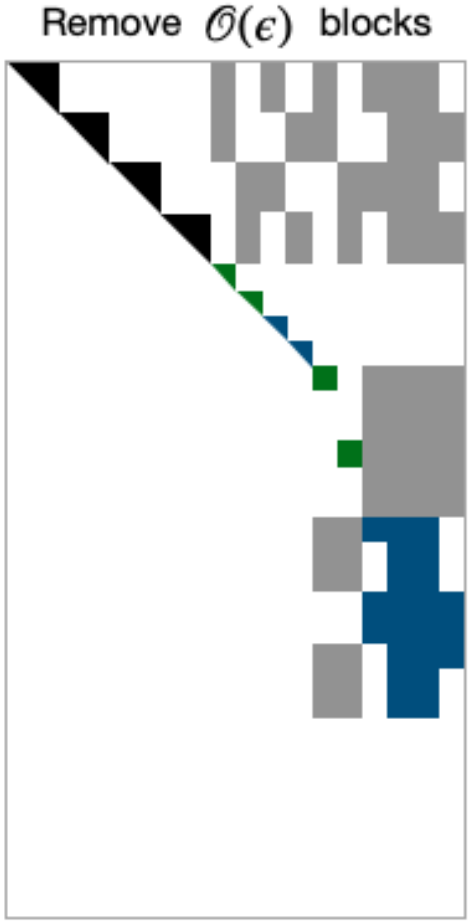

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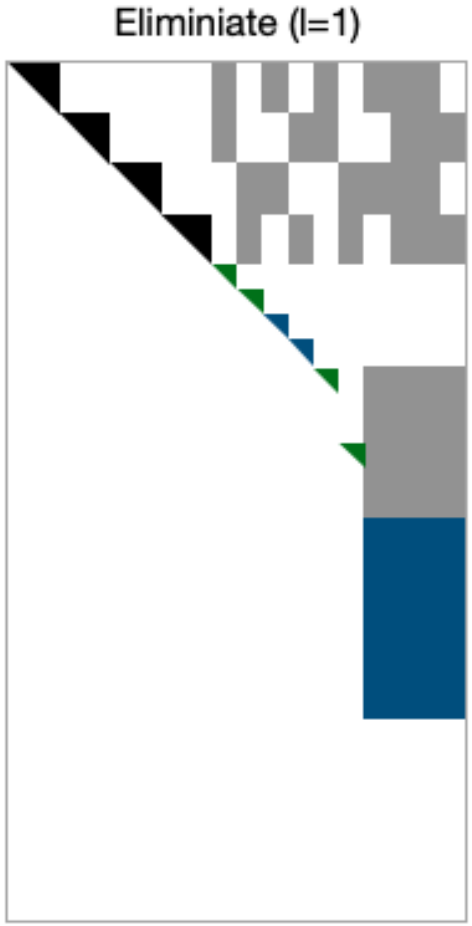

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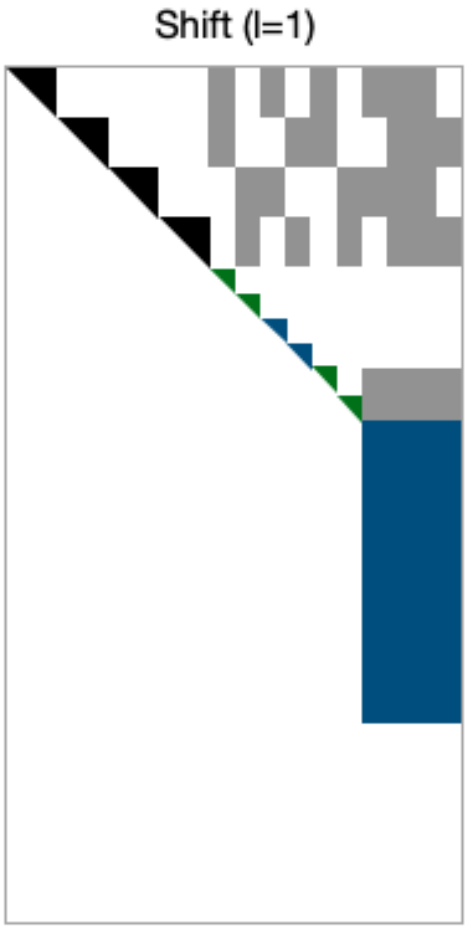

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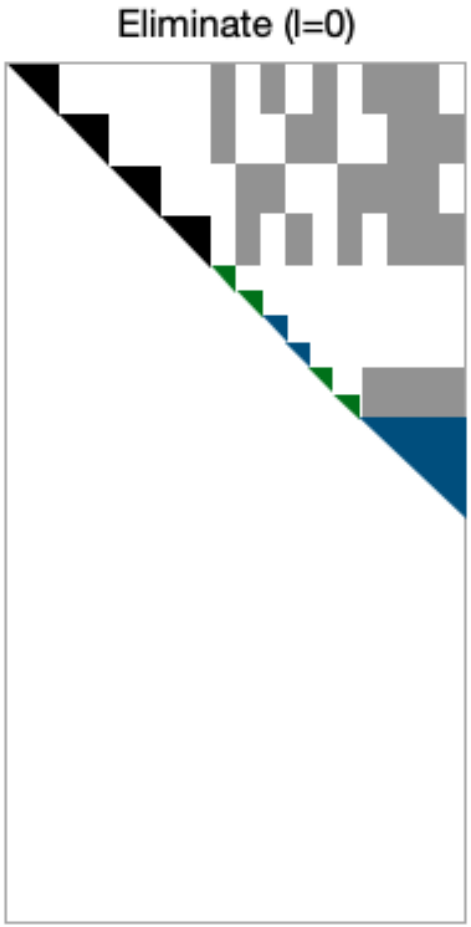

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Sparsification

Sparsification in spaQR

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- Consider an interface p, the nodes n connected to p in the graph of $A^T A$
- Consider a small piece of the matrix, focusing on the non-zero blocks for p and n,

$$A_p = \begin{bmatrix} A_{pp} & A_{pn} \\ A_{np} & A_{nn} \end{bmatrix} =$$

Step 1: Scaling

We first scale the diagonal blocks of each interface. For interface p, using the QR decomposition of $A_{pp} = U_{pp} \begin{bmatrix} R_{pp} \\ 0 \end{bmatrix}$

$$\bar{A}_p = \begin{bmatrix} U_{pp} & \\ & I \end{bmatrix}^T A_p \begin{bmatrix} R_{pp} & \\ & I \end{bmatrix}^{-1} = \begin{bmatrix} I & \bar{A}_{p_1 n} \\ & \bar{A}_{p_2 n} \\ \bar{A}_{np} & A_{nn} \end{bmatrix} =$$

Step 2: Compress rows $\bar{A}_{p_2 n}$

Consider a low rank approximation of $A_{p_2 n}$,

$$A_{p_2 n} = Q'_{pp} W'_{pn} = \begin{bmatrix} Q'_{pc} & Q'_{pf} \end{bmatrix} \begin{bmatrix} W'_{cn} \\ W'_{fn} \end{bmatrix} \quad \text{with} \quad \|W'_{fn}\|_2 = \mathcal{O}(\epsilon)$$

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Define, $Q'_p = \begin{bmatrix} I & & \\ & Q'_{pp} & \\ & & I \end{bmatrix}^T$

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$\|W'_{fn}\| = \mathcal{O}(\epsilon)$ and the corresponding rows are removed

Step 2: Compress block $\begin{bmatrix} A_{np}^T & A_{p_1 n} \end{bmatrix}$

$$\begin{bmatrix} A_{np}^T & A_{p_1 n} \end{bmatrix} = Q_{pp} W_{pn} = \begin{bmatrix} Q_{pf} & Q_{pc} \end{bmatrix} \begin{bmatrix} W_{fn}^{(1)} & W_{fn}^{(2)} \\ W_{cn}^{(1)} & W_{cn}^{(2)} \end{bmatrix}$$

where $\| W_{fn}^{(1)} \|_2 \approx \| W_{fn}^{(2)} \|_2 = \mathcal{O}(\epsilon)$. Define, $Q_p = \begin{bmatrix} Q_{pp} & & \\ & I & \\ & & I \end{bmatrix}$

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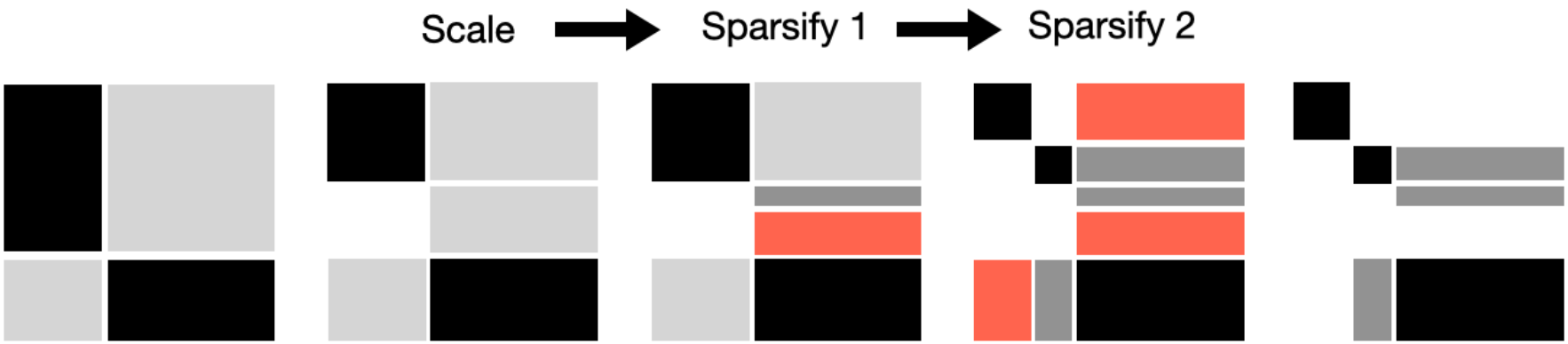
Ignore the $\mathcal{O}(\epsilon)$ blocks

Summary



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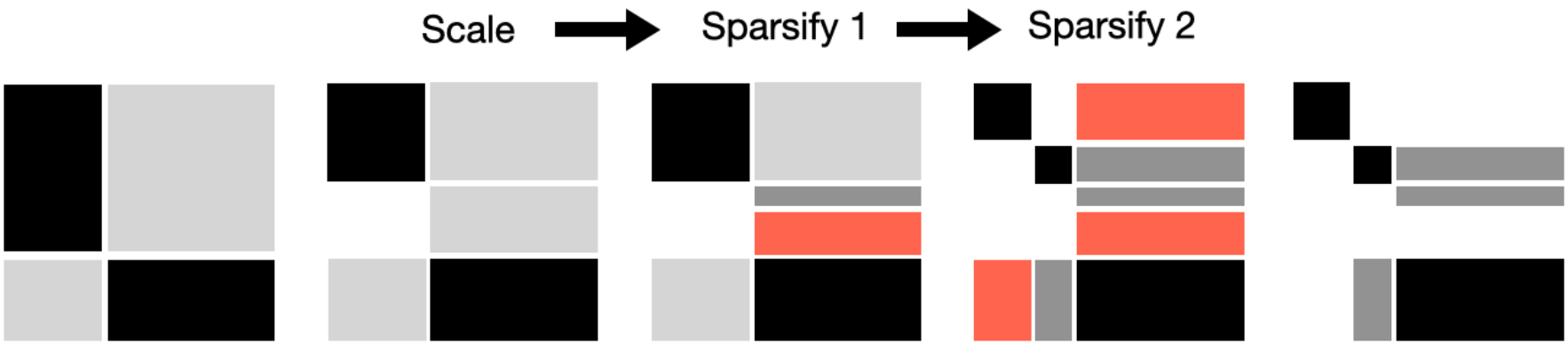

Sparsification,

- Reduces the size of the interfaces

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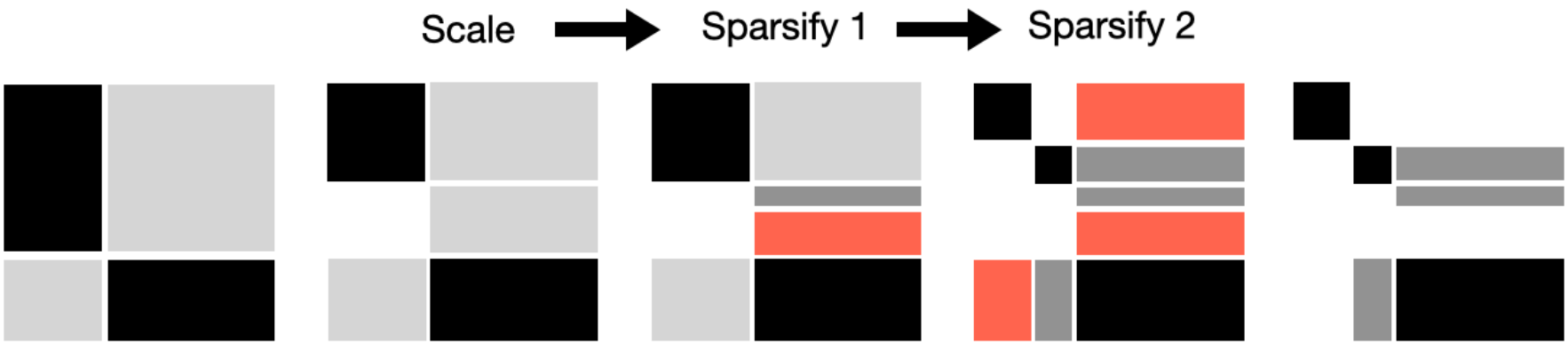

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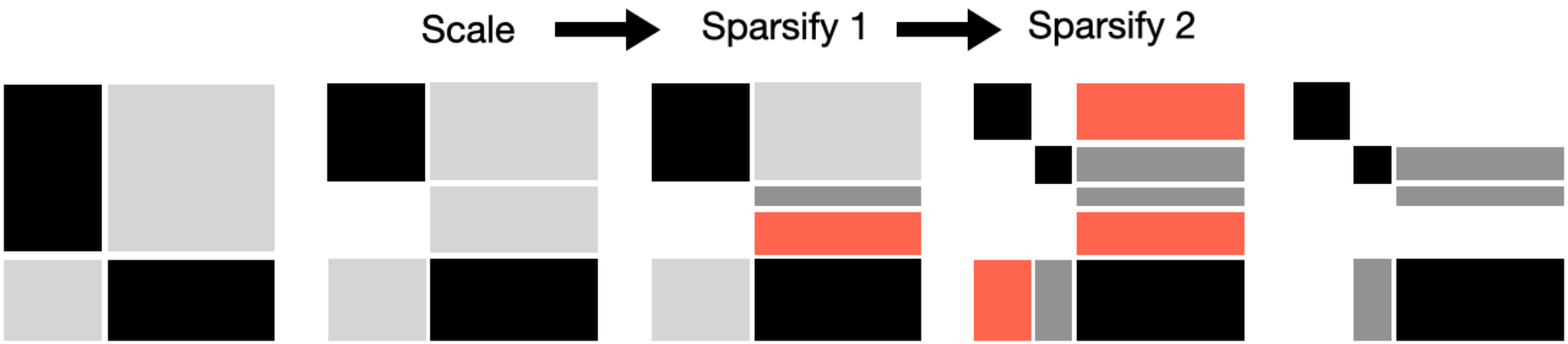

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- Reduces the size of the interfaces
- Does not introduce additional fill-in
- **(Important)** Does not affect the elimination tree of $A^T A$, i.e., any two disjoint subtrees of the etree remain disjoint after sparsification of any interface.

Complexity

Complexity: Square matrices

3D PDE discretizations

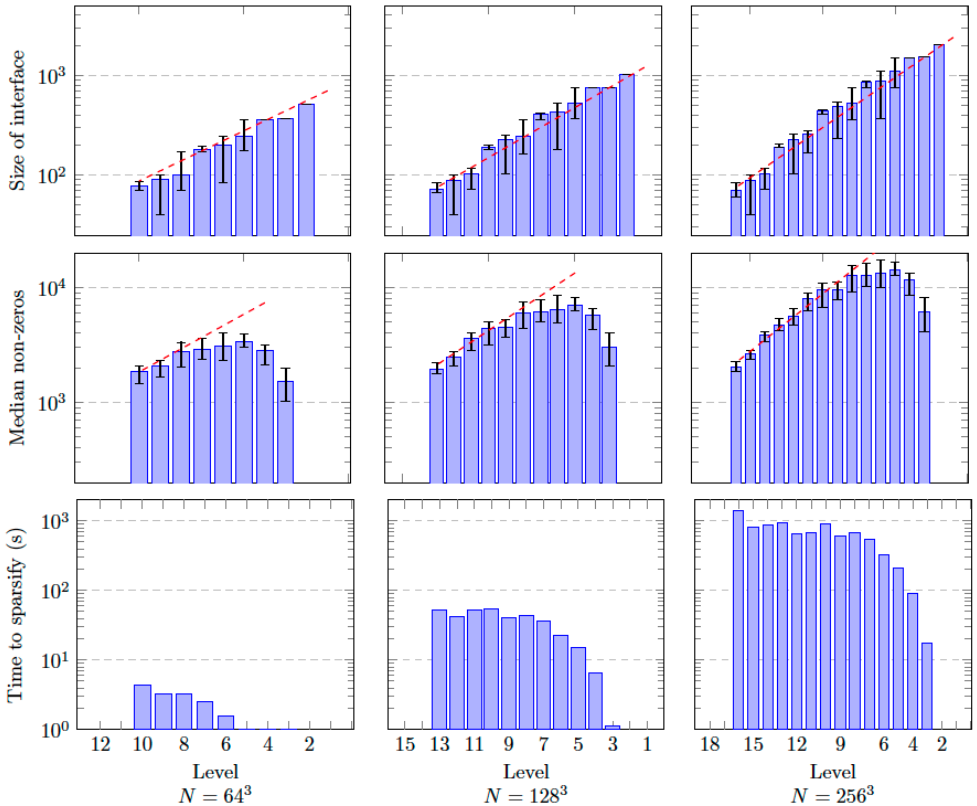

Figure: 3D Advection-Diffusion problem. Red dashed line indicates $2^{-l/3}$ scaling.

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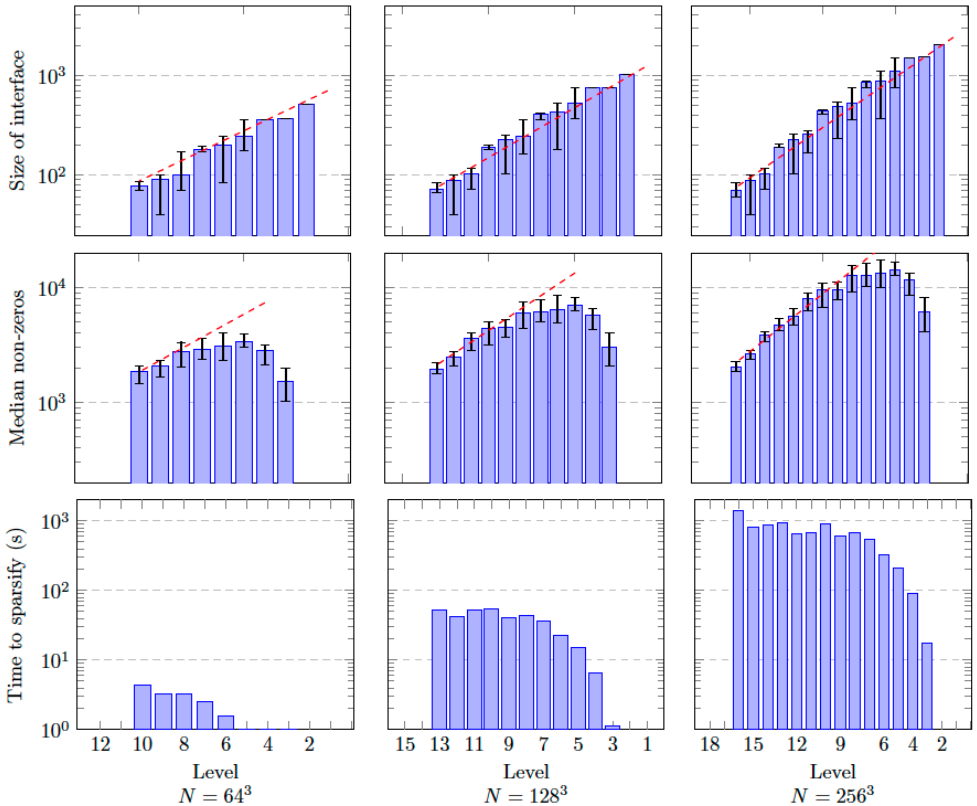

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$$c_l \in \mathcal{O}(2^{-l/3} N^{1/3})$$

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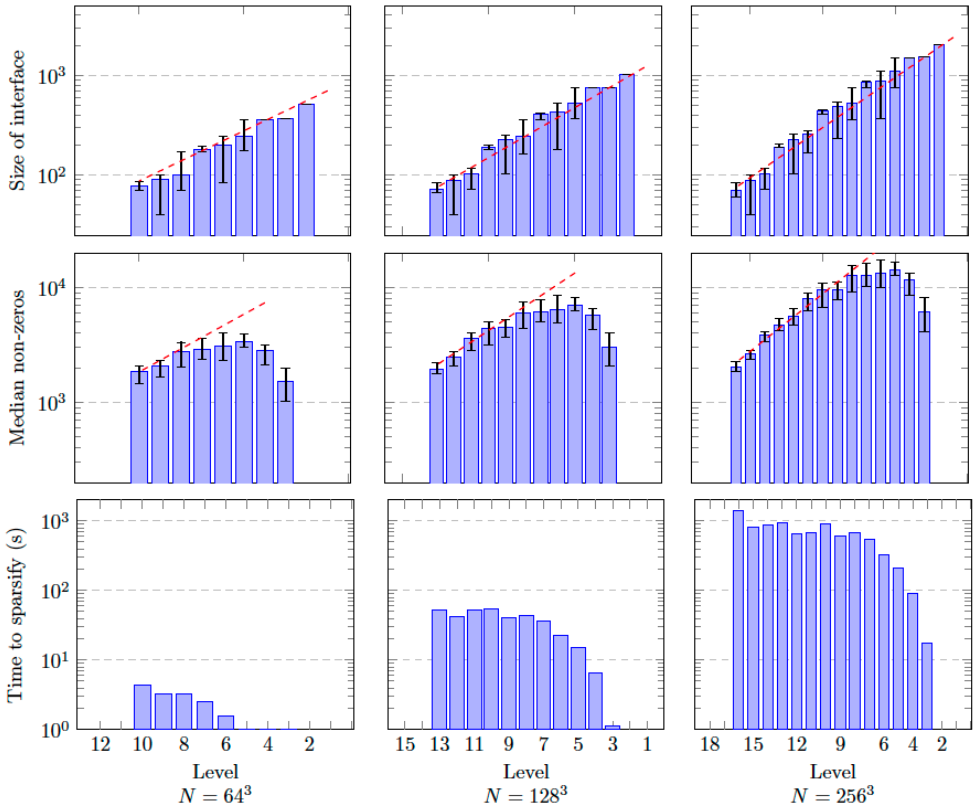

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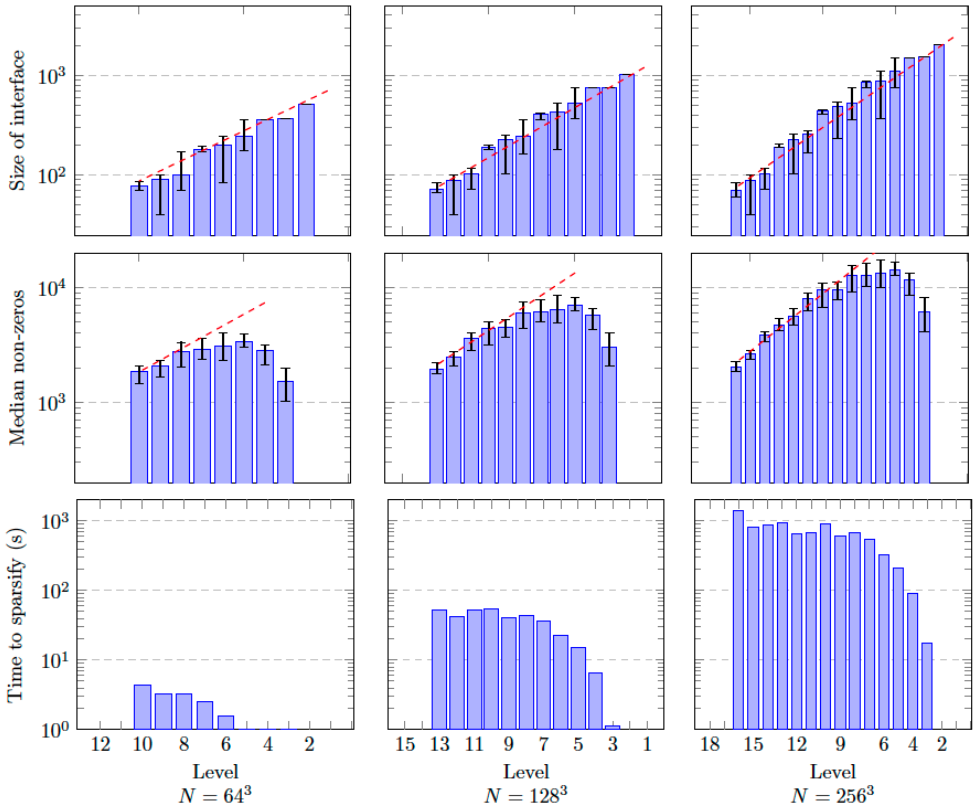

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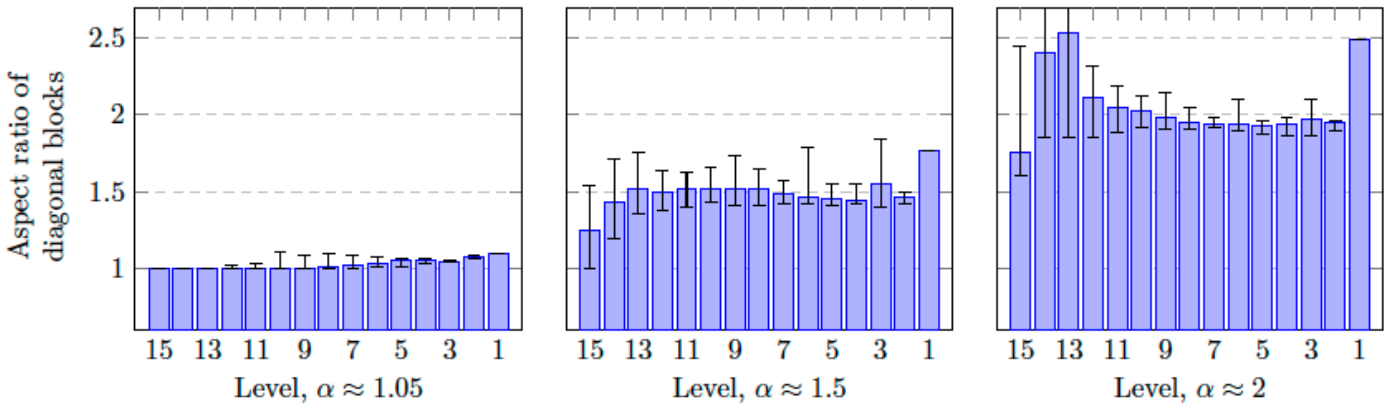
Complexity: Rectangular matrices



- Aspect ratio (# rows/ # cols) of each interface block is bounded, $\theta(\alpha)$, where $\alpha = M/N$

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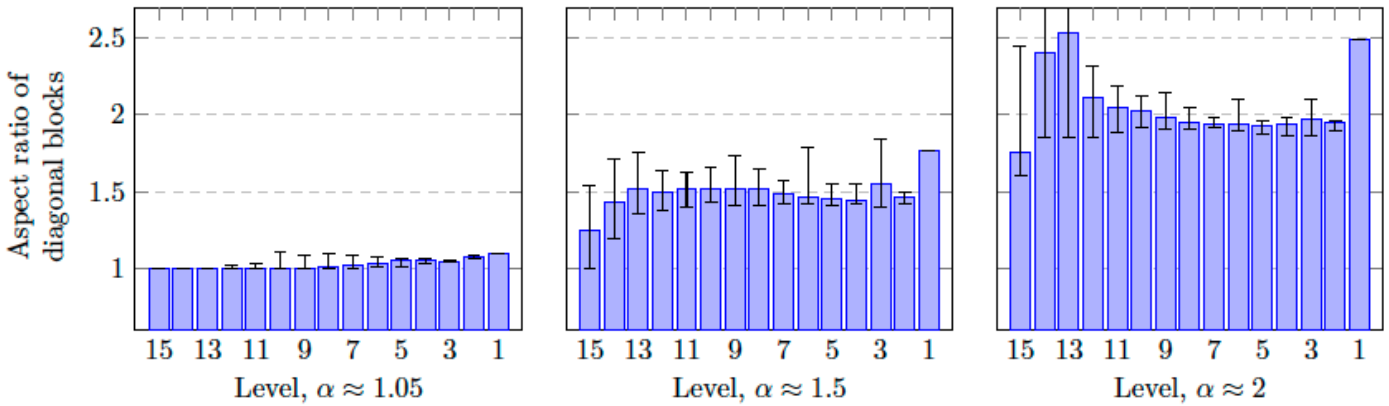

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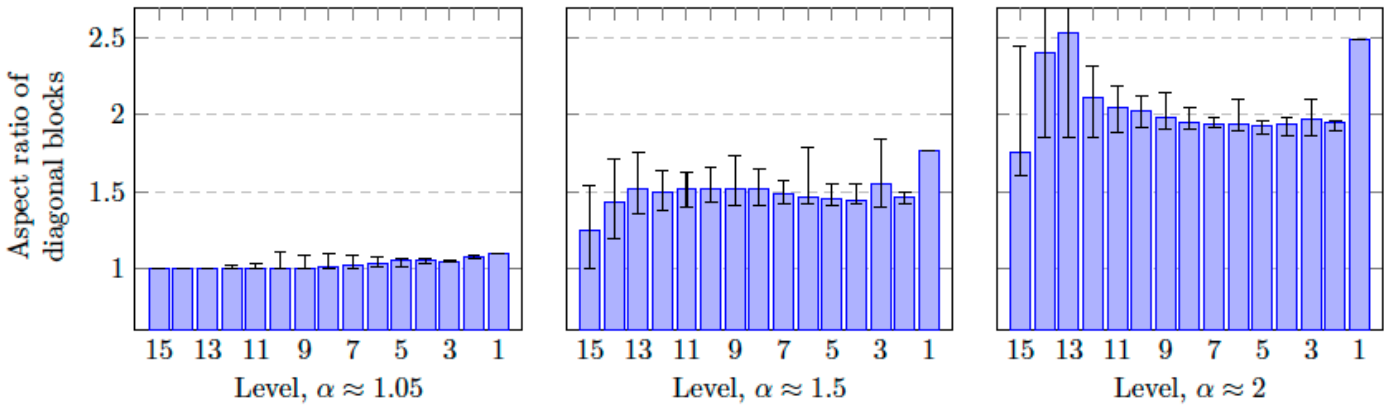

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- We have $L = \log N$ levels, so total cost of $\mathcal{O}(M \log N)$

Numerical results

Results: Unsymmetric matrices

Advection-Diffusion Equation discretized using finite difference on a regular 3D grid

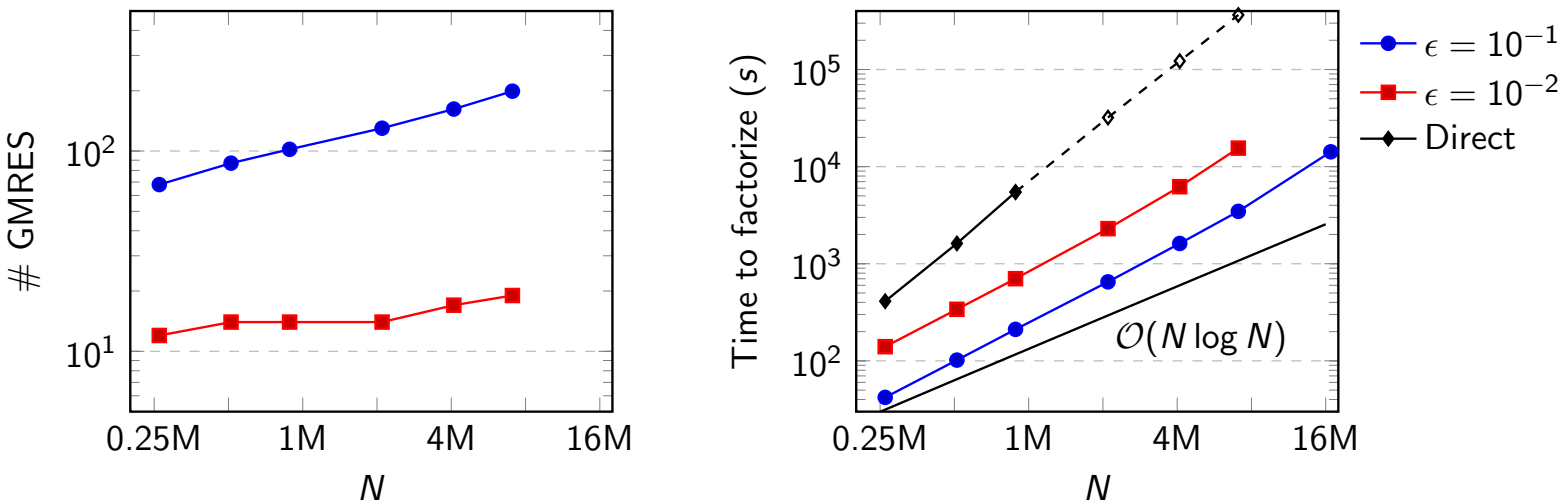

Figure: Variation in the number of GMRES iterations and time to factorize.

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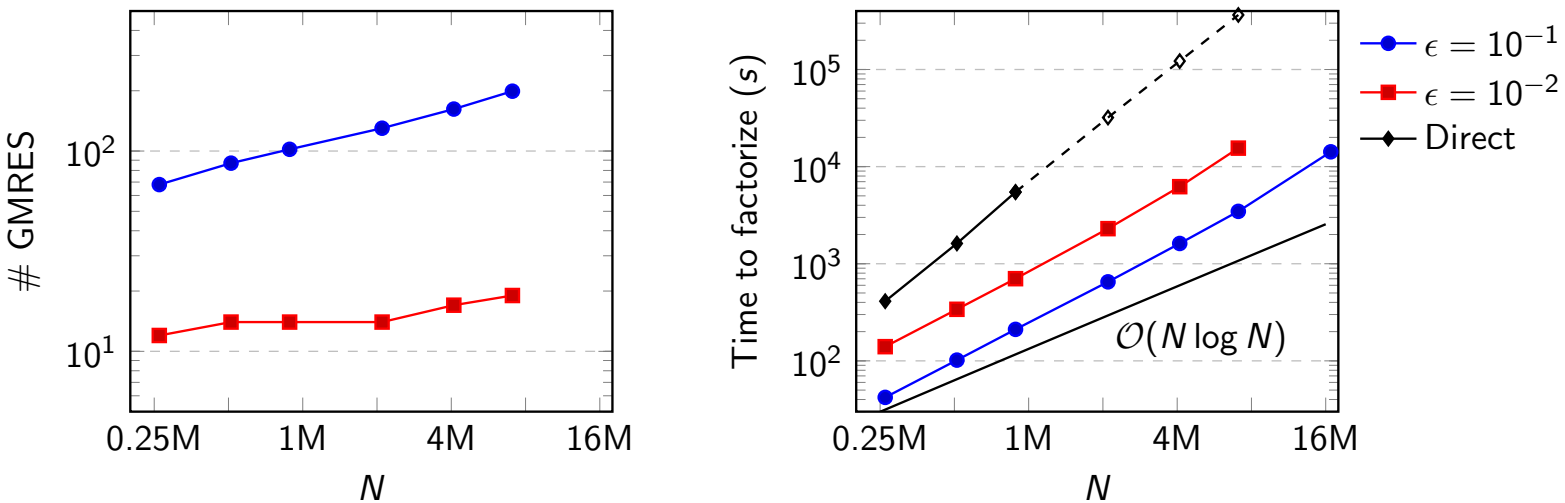


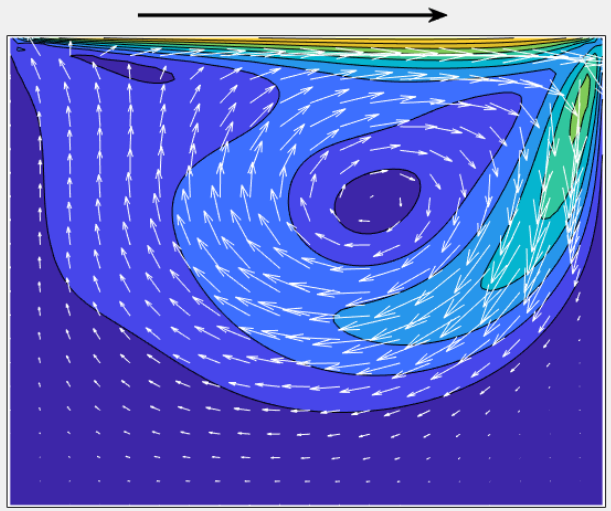
Figure: Variation in the number of GMRES iterations and time to factorize.

- Theoretical complexity is $\mathcal{O}(N \log N)$
- Empirically, the factorization time scales as $\mathcal{O}(N^{1.4})$ likely due to non-asymptotic effects

Results: Lid driven flow in a 2D square cavity

- Unsymmetric matrices
- Preconditioners based on LU factorization fail to converge

		# GMRES, $\epsilon = 10^{-5}$	
Matrix[1]	Re	# GMRES	Residual
E40R0000	0	6	1.9×10^{-14}
E40R0100	100	7	1.5×10^{-13}
E40R0500	500	6	4.1×10^{-13}
E40R1000	1000	11	3.3×10^{-14}
E40R2000	2000	23	7.9×10^{-14}
E40R3000	3000	19	1.5×10^{-13}
E40R4000	4000	36	1.6×10^{-12}
E40R5000	5000	21	5.9×10^{-13}



- spaQR stable and converges in less than 50 iterations for a wide range of Reynolds number

[1] Matrices taken from the SPARSKIT collection

PDE constrained optimization

$$\begin{aligned} \min_{u,z} \quad & \frac{1}{2}\int_\Omega (u-u_d)^2 dx + \frac{1}{2}\lambda \int_\Omega z^2 dx \\ \text{subject to} \quad & -\nabla \cdot (z\nabla u) = h \text{ in } \Omega \\ & u = 0 \text{ in } d\Omega \end{aligned}$$

- Recover u, z at every grid point, using available states u_d

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- Recover u, z at every grid point, using available states u_d
- One approach involves solving the least squares problem

$$J^T x = b$$

where J is the Jacobian of the discretized equations

Results: 2D Inverse Poisson

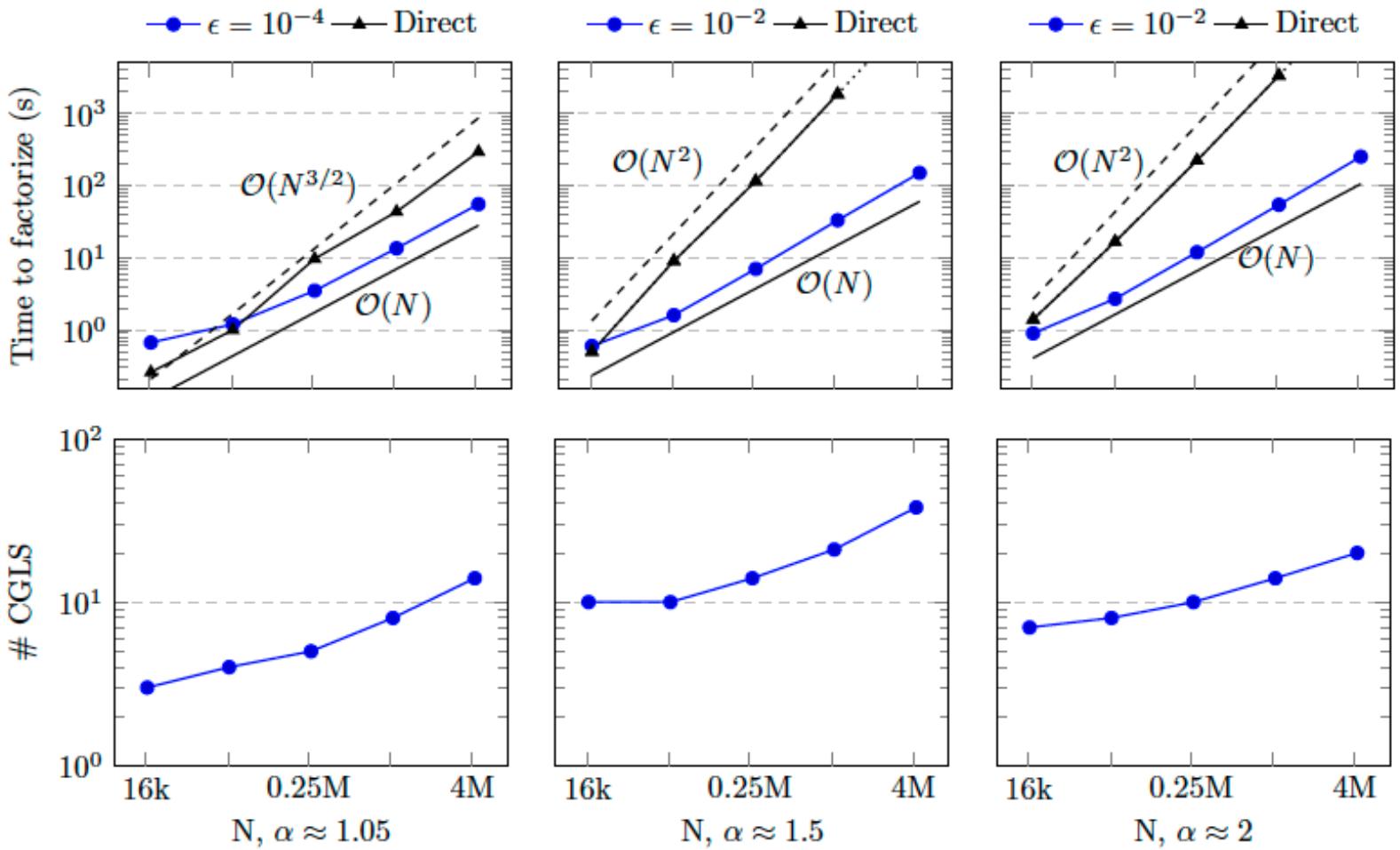

Figure: Results of 2D Inverse Poisson least squares problem for different values of aspect ratio $\alpha = M/N$

Results: 3D Inverse Poisson

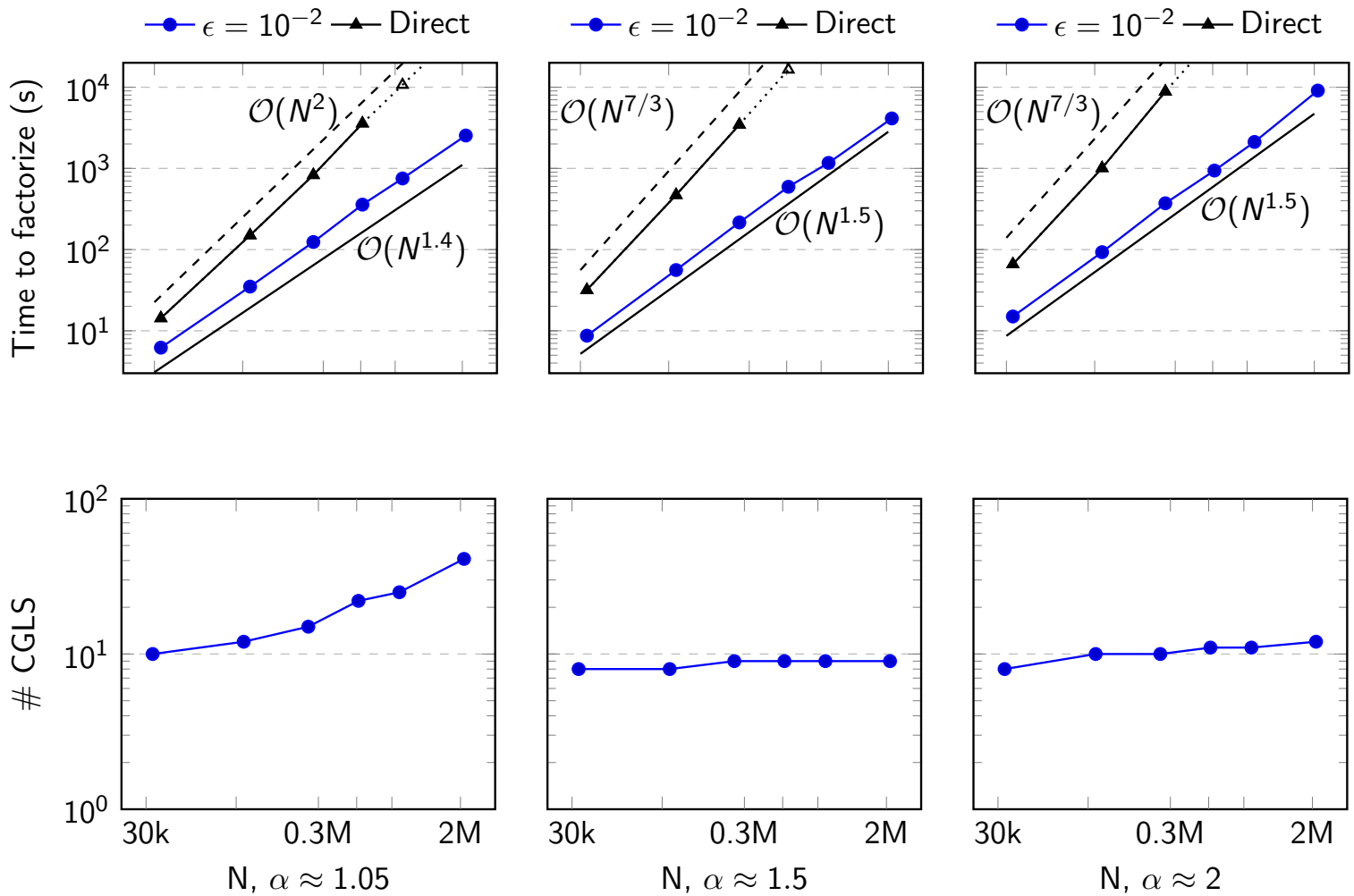

Figure: Results of 3D Inverse Poisson least squares problem for different values of aspect ratio, $\alpha = M/N$.

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- spaQR is a hierarchical factorization that produces a fast, sparse, approximate QR factorization of large sparse matrices
- Cost vs Accuracy compromise achieved with the parameter ϵ
- Structure of the spaQR algorithm naturally exhibits parallelism
- Useful for various applications in CFD, PDE constrained optimization and applications in computer graphics and vision

References & Funding

- References:
  - A. Gnanasekaran and E. Darve, Hierarchical orthogonal factorization: Sparse Square Matrices, 2020, `https://arxiv.org/abs/2010.06807`
  - A. Gnanasekaran and E. Darve, Hierarchical orthogonal factorization: Sparse Least Squares Problems, 2021, `https://arxiv.org/abs/2102.09878`
- spaQR code:
  - `https://github.com/Abeynaya/spaQR_public`
- Funding:
  - LDRD Research Grant from Sandia National Laboratories
  - NASA grant #80NSSC18M0152