Recent HPC developments for Multidimensional Scaling (MDS)

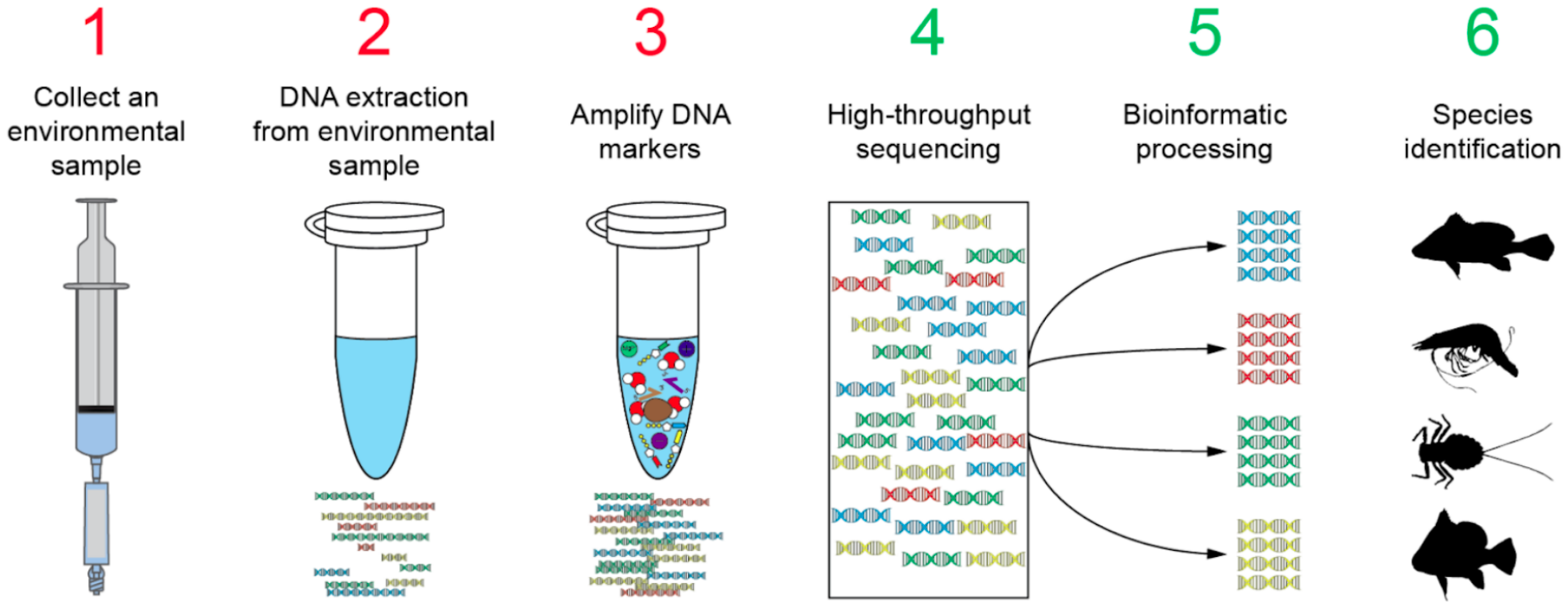
HPC Scalable ecosystem plenary meeting

Romain Peressoni

Centre Inria de l'Université de Bordeaux

31/03/2023

Metabarcoding



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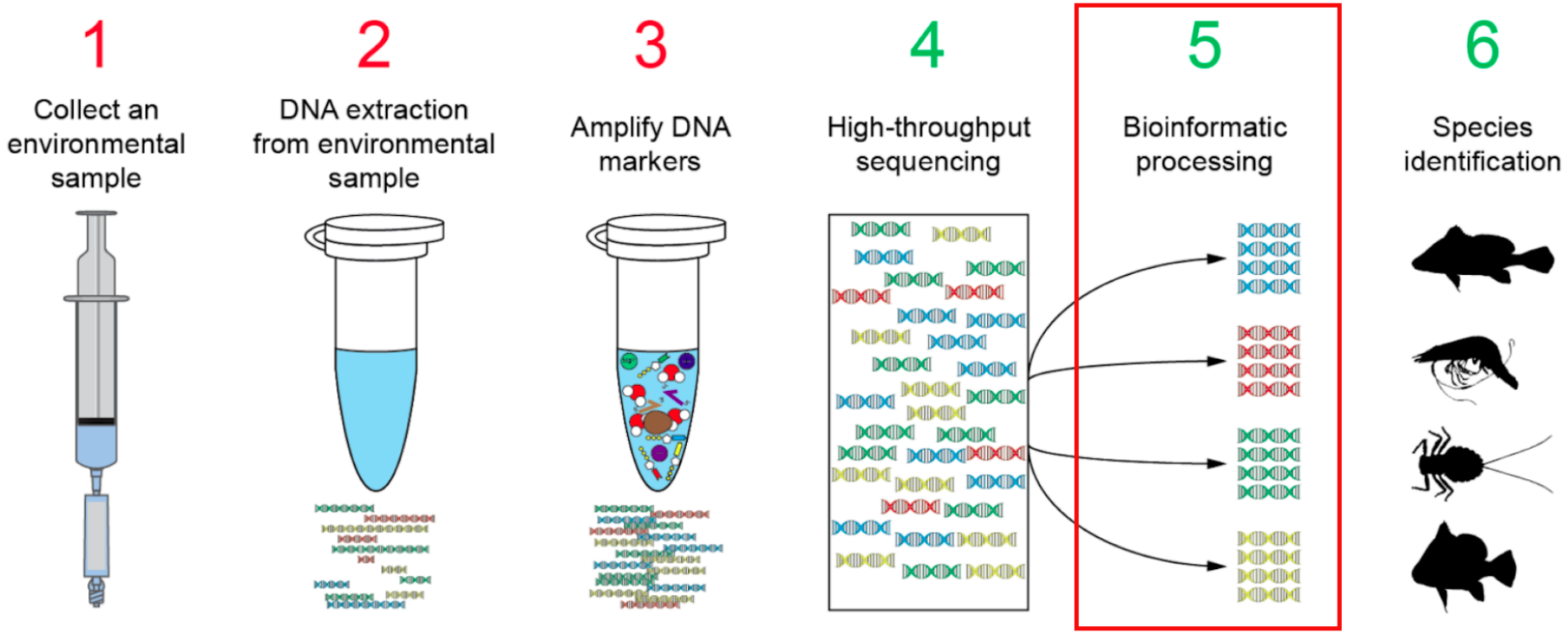

MDS (Euclidean distance matrix case)

MDS is a dimension reduction algorithm

Concept

Based on the link between

- Input: Distance (D)
- Inner Products (G)
- Output: Position (X)

Computation

- $G \leftarrow$ double centering of D
- // G $= XX^T$ by definition
- $Q, \Lambda, Q^T \leftarrow sEVD(G)$
- $X \leftarrow Q\Lambda^{\frac{1}{2}}$

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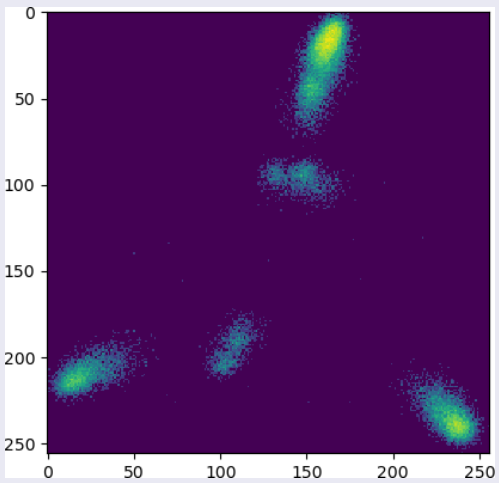
Output : Point Cloud



Limiting Factor

Cost of the sEVD

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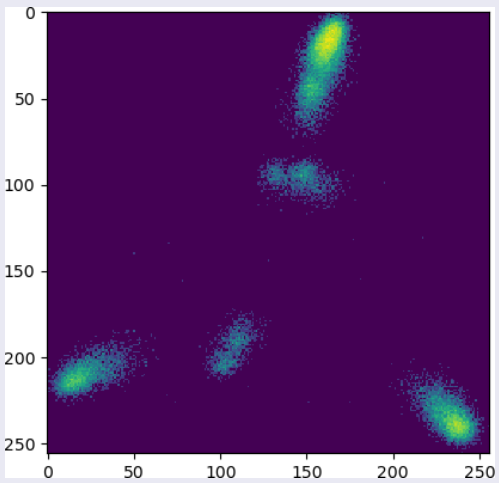
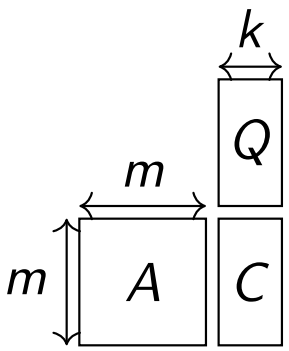


Limiting Factor

Cost of the sEVD or SVD

Solution : randomized algorithms

- Approximate $A \approx AQQ^T$ (Halko et al., 2011; Martinsson, 2016)
- Define $C = AQ$
- Compute $SVD(C) = U_C \Sigma V_C^T$



Implementation

- Random projection based MDS (Blanchard et al., 2018; Blanchard, 2017; Franc et al., 2020; Paradis, 2018)
- Task based HPC implementation of RSVD in the context of the Gordon Project (Agullo et al., 2022)

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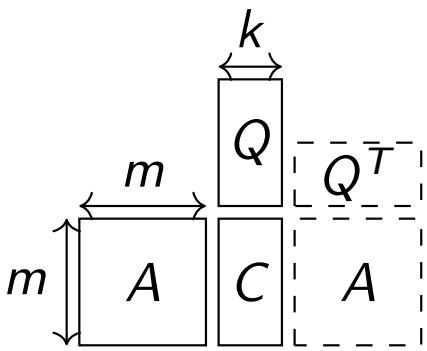
- Multiply by Q^T on the right to get $RSVD(A)$



Implementation

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Random Projection based SVD

Algorithm: Random projection SVD algorithm: $(U, \Sigma, V) \simeq \text{RSVD(A)}$

Input: A: $m \times m$, k prescribed rank
Output: $A \simeq U\Sigma V^T$

1. Ω: $m \times k$ random matrix // RAND
2. $Y = A\Omega$ // MM1
3. Y: $QR = Y$ // QR
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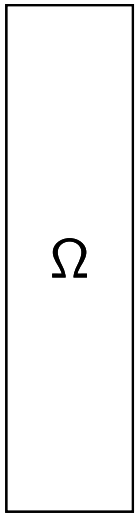
5. C: $U_C \Sigma V_C^T = C$ // QR-SVD
6. $U = U_C$ and $V = QV_C$ // MM3
7. **return** U, Σ, V

Random Projection based SVD

RAND



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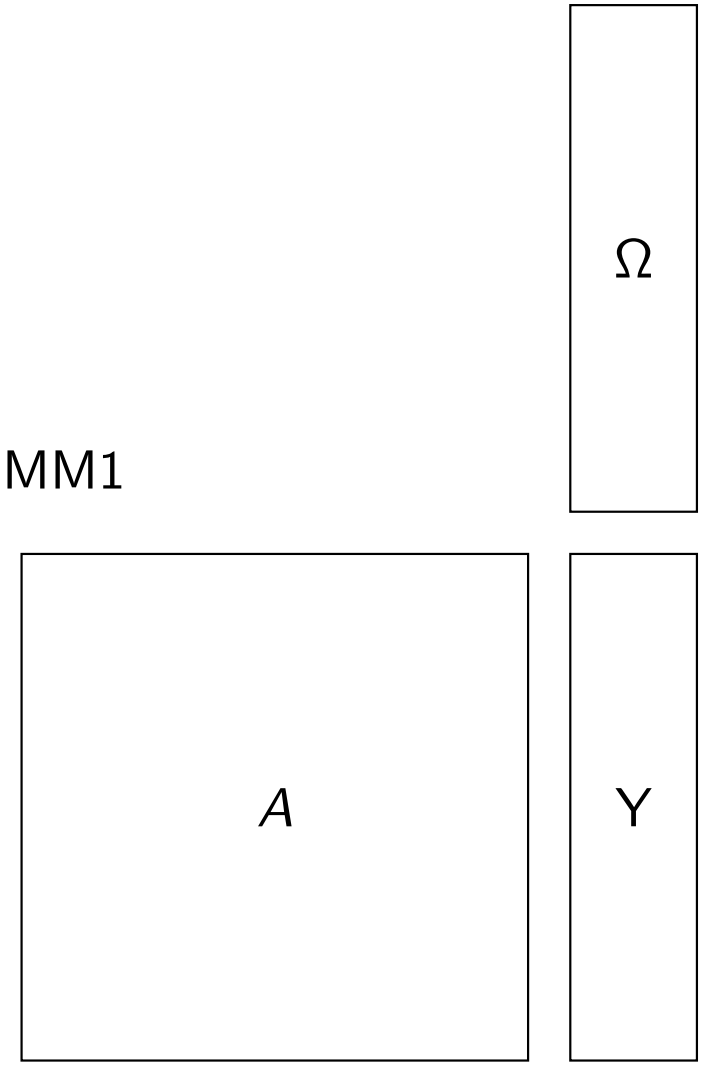

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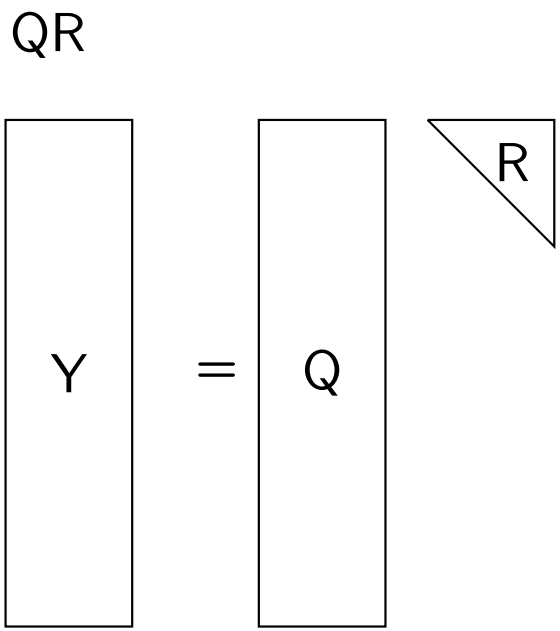

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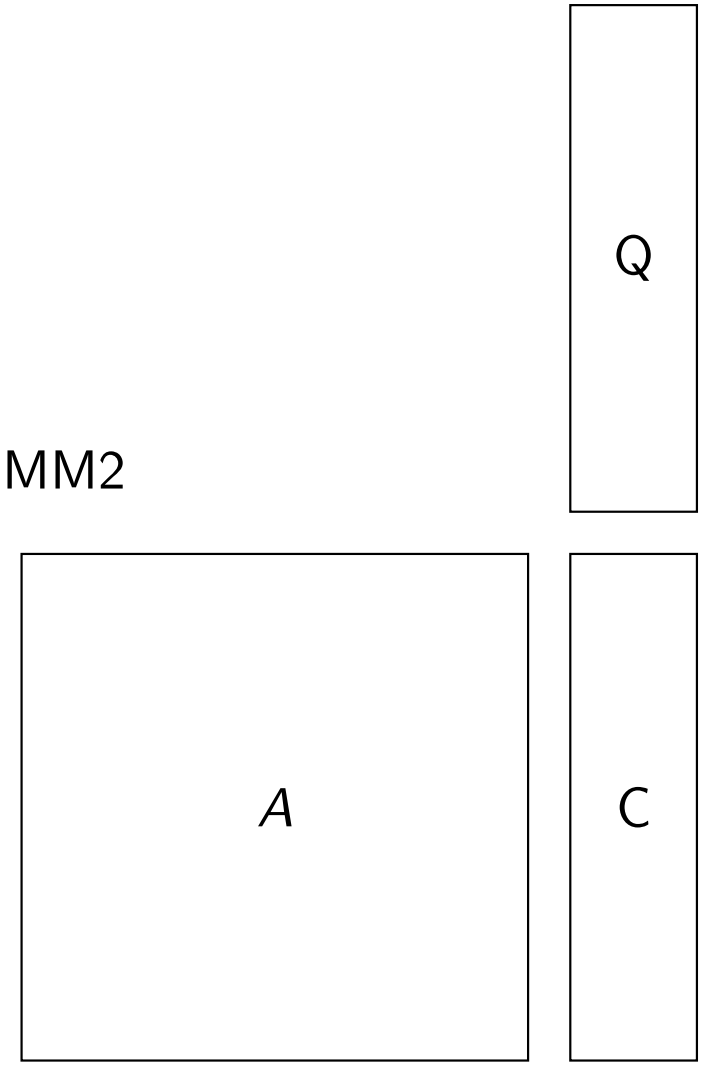

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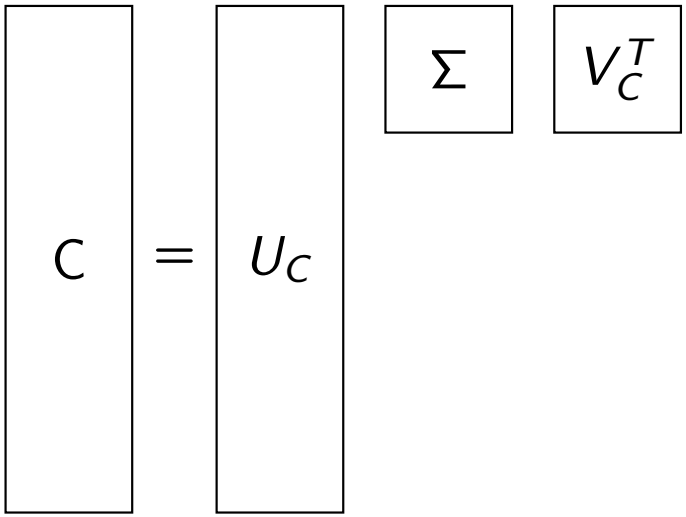
SVD



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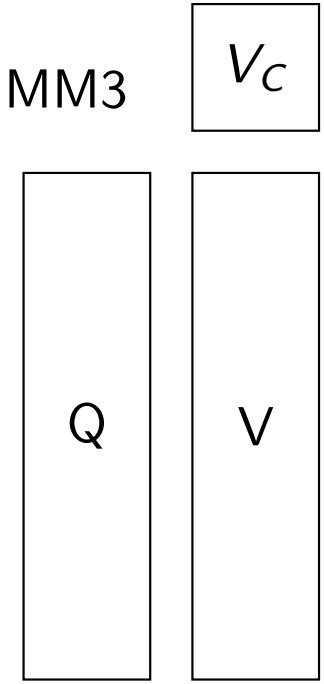

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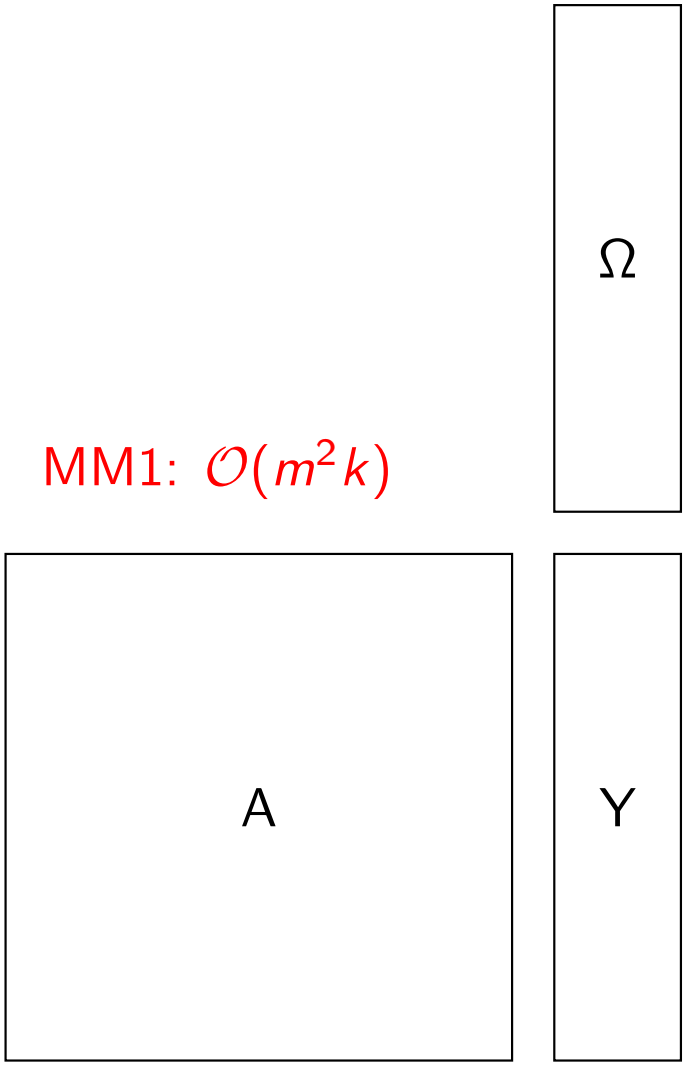

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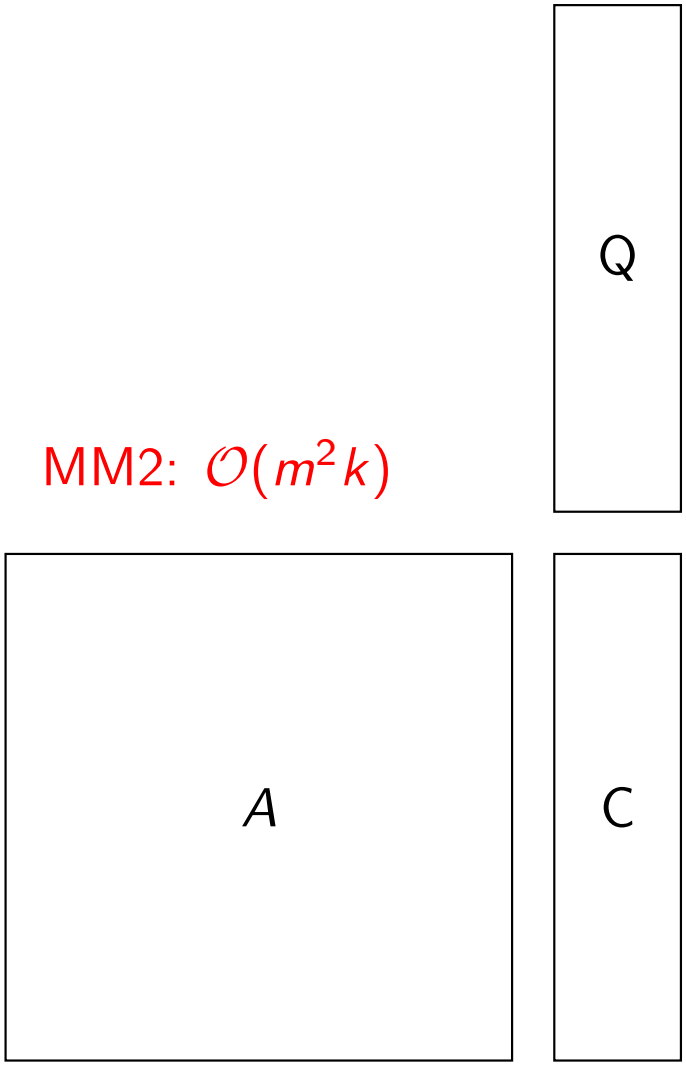

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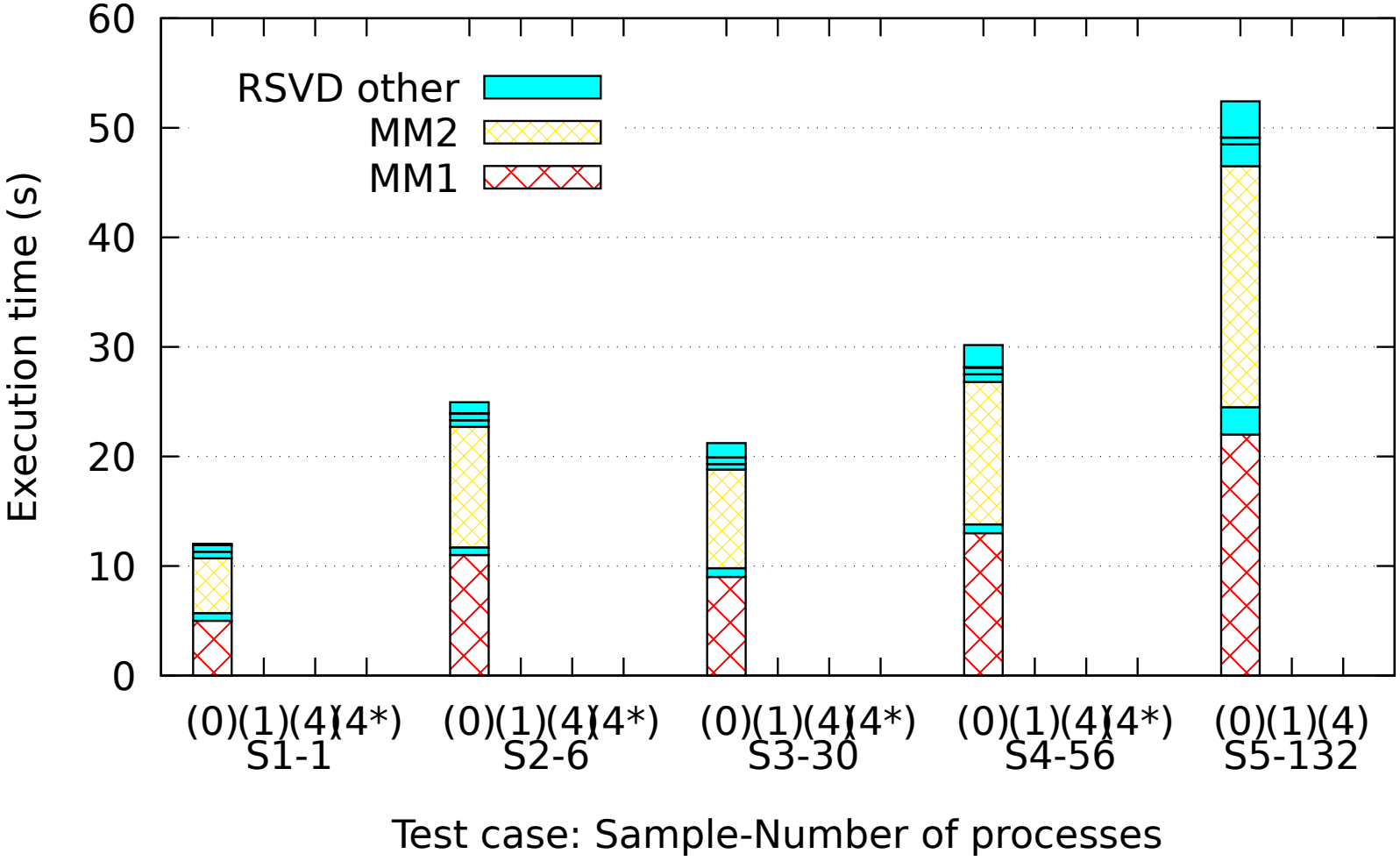
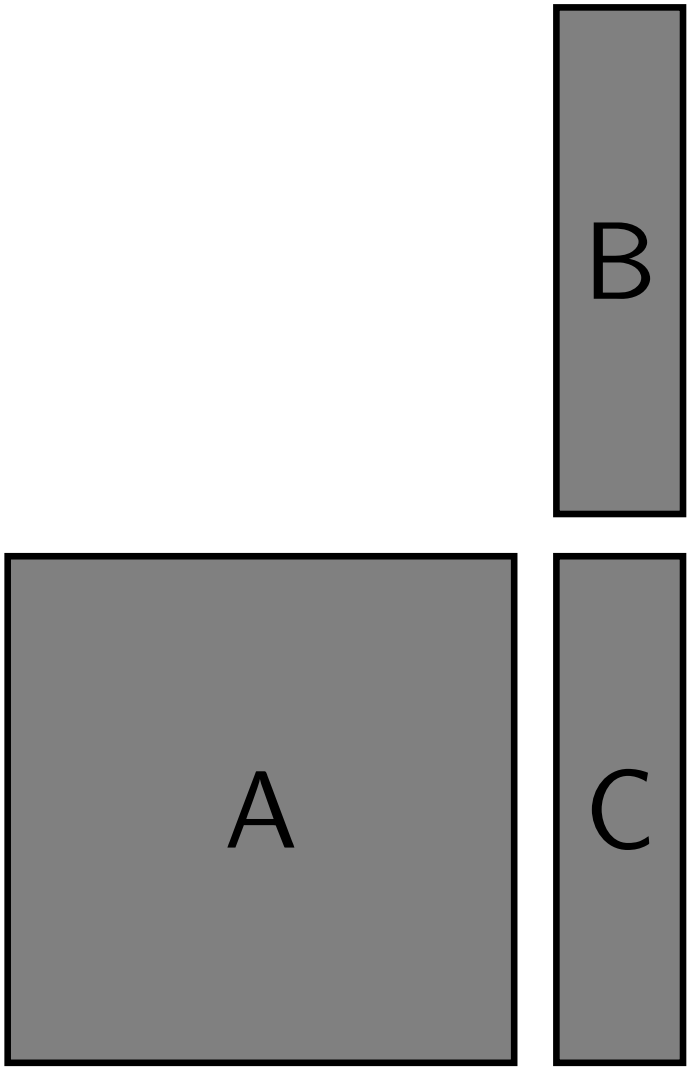
RSVD-MDS

Execution time for each step of the RSVD-MDS (Agullo et al., 2022)



GEMM (GEneral Matrix-Matrix multiplication)



- Computing $C = AB$

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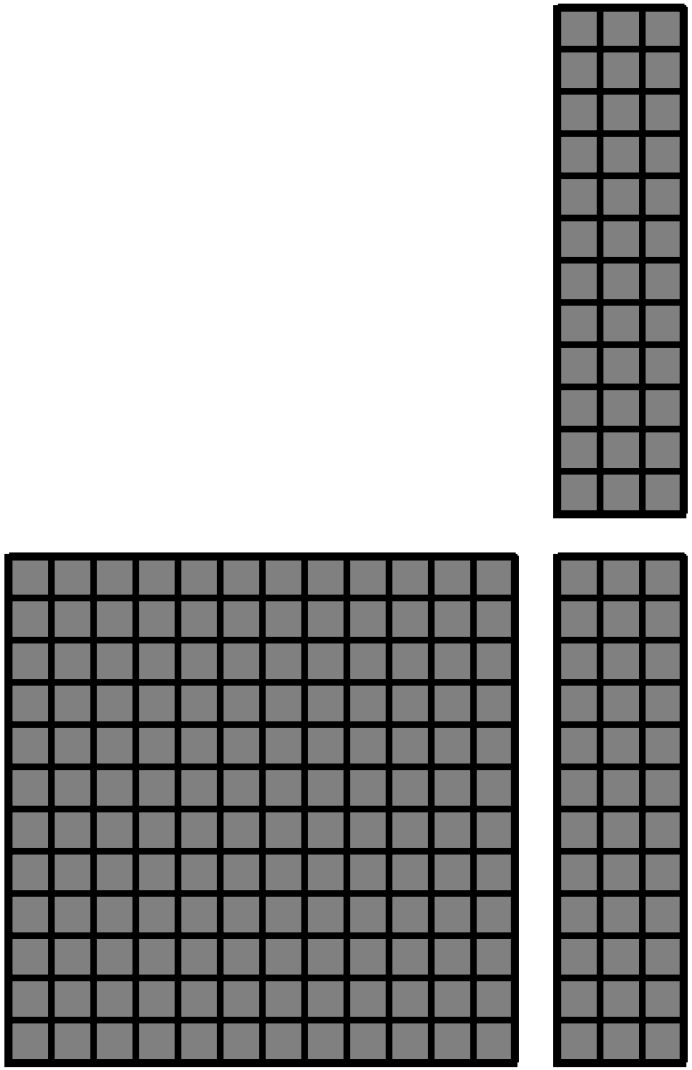

- Computing $C = AB$
- $C_{i,j} = \sum_{\ell=1}^{m} A_{i,\ell} B_{\ell,j}$

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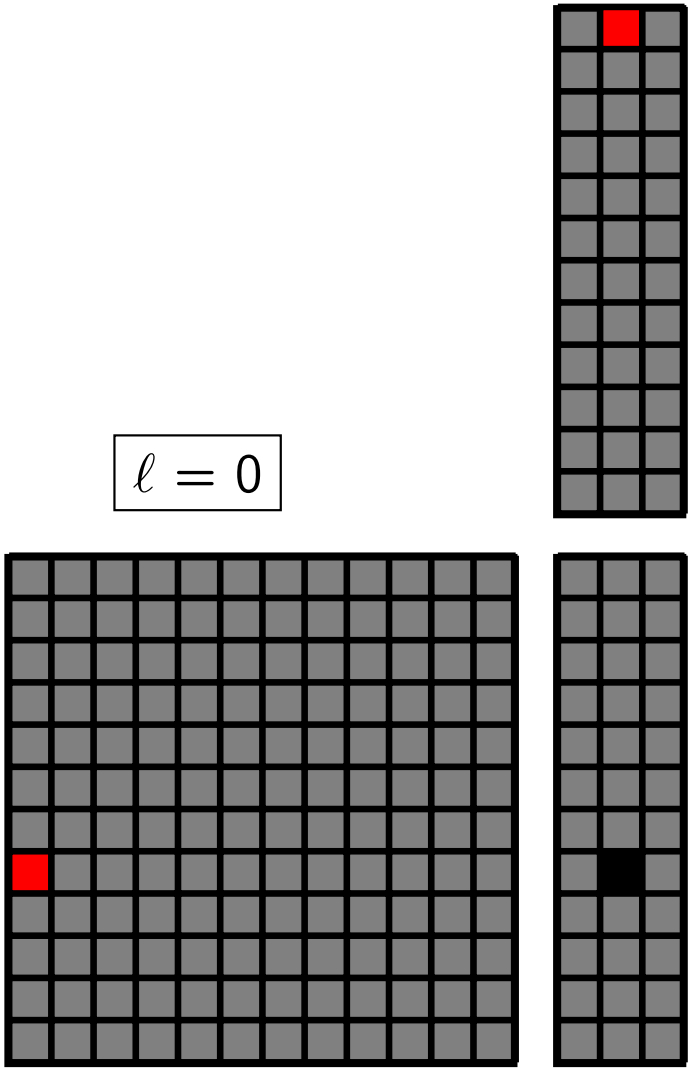

- Computing $C = AB$
- $C_{7,1} = \qquad A_{7,0}B_{0,1} + \dots$

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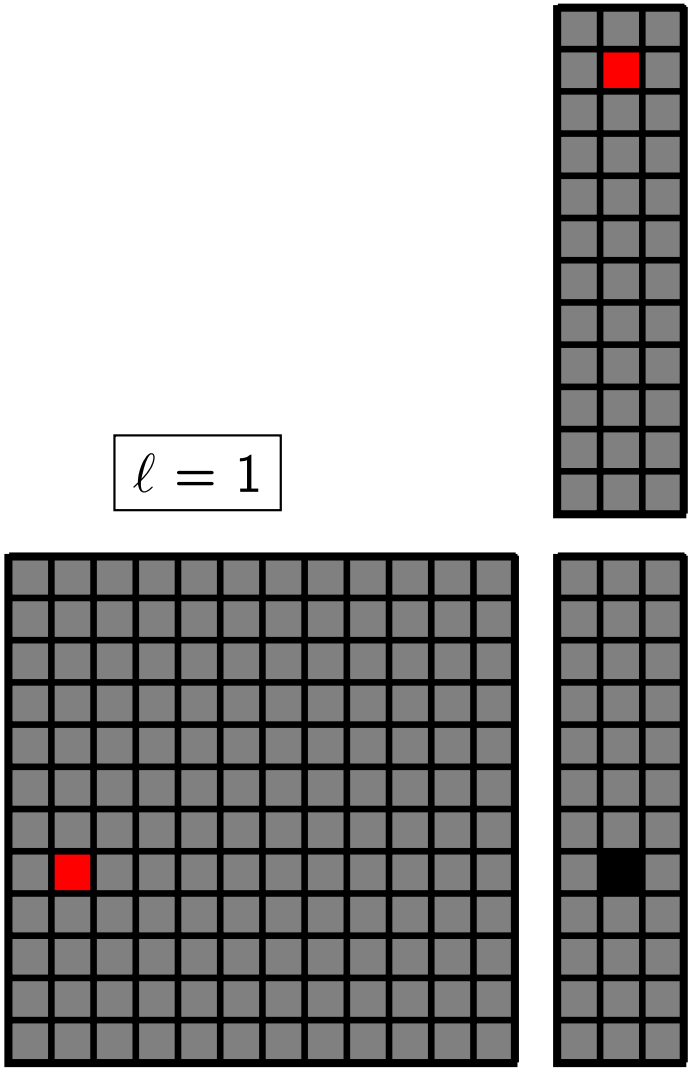

- Computing $C = AB$
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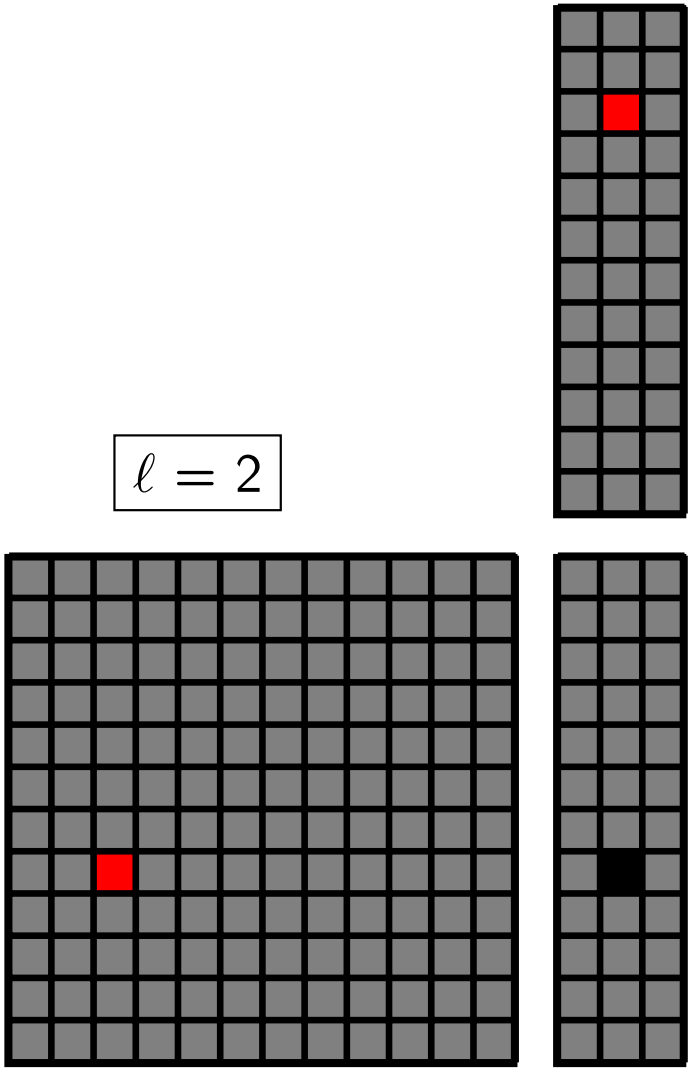

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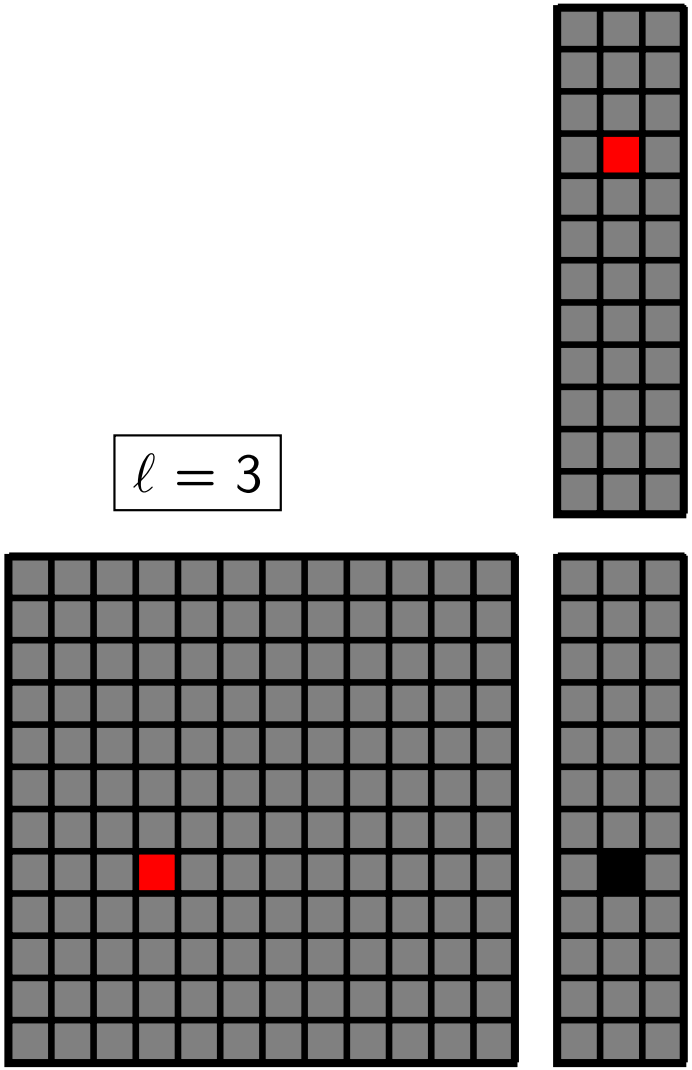

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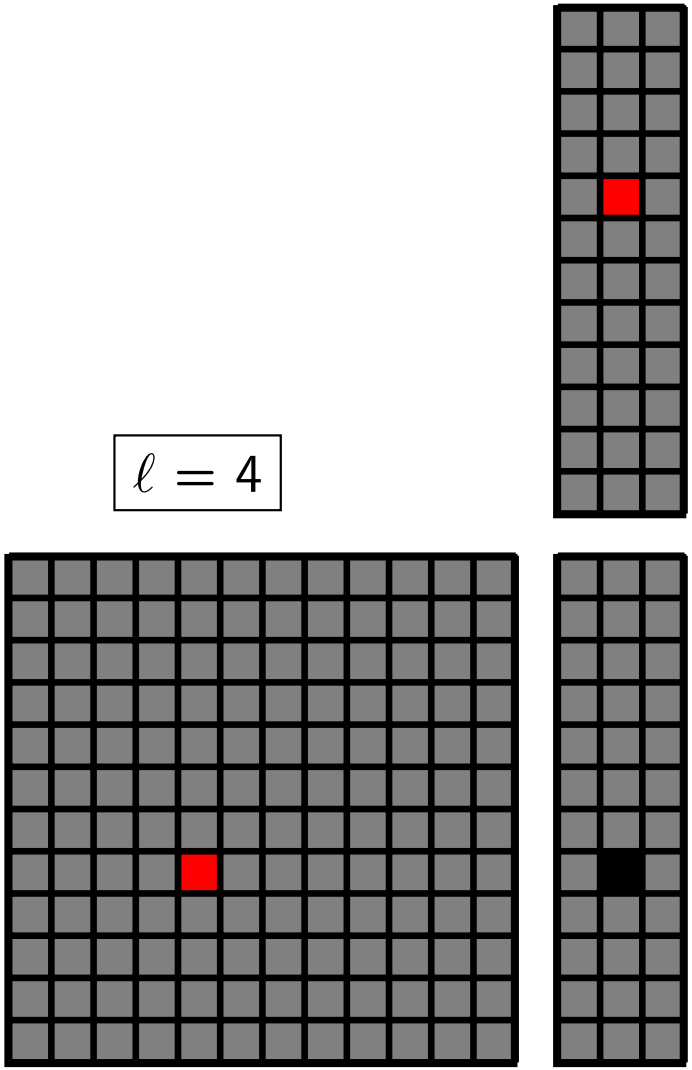

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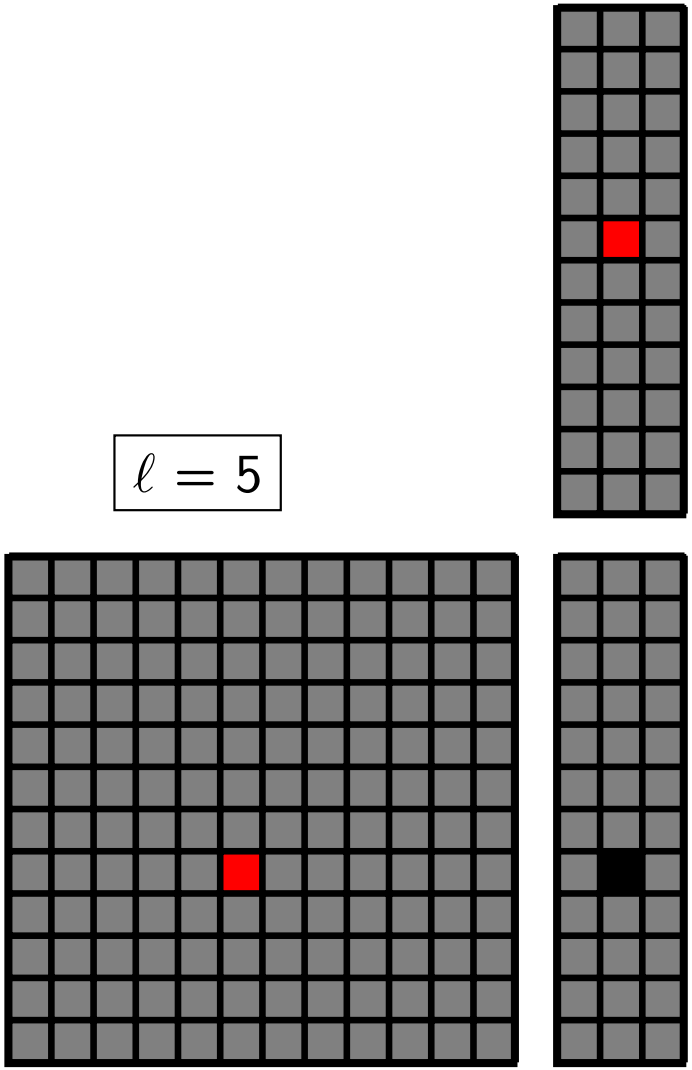

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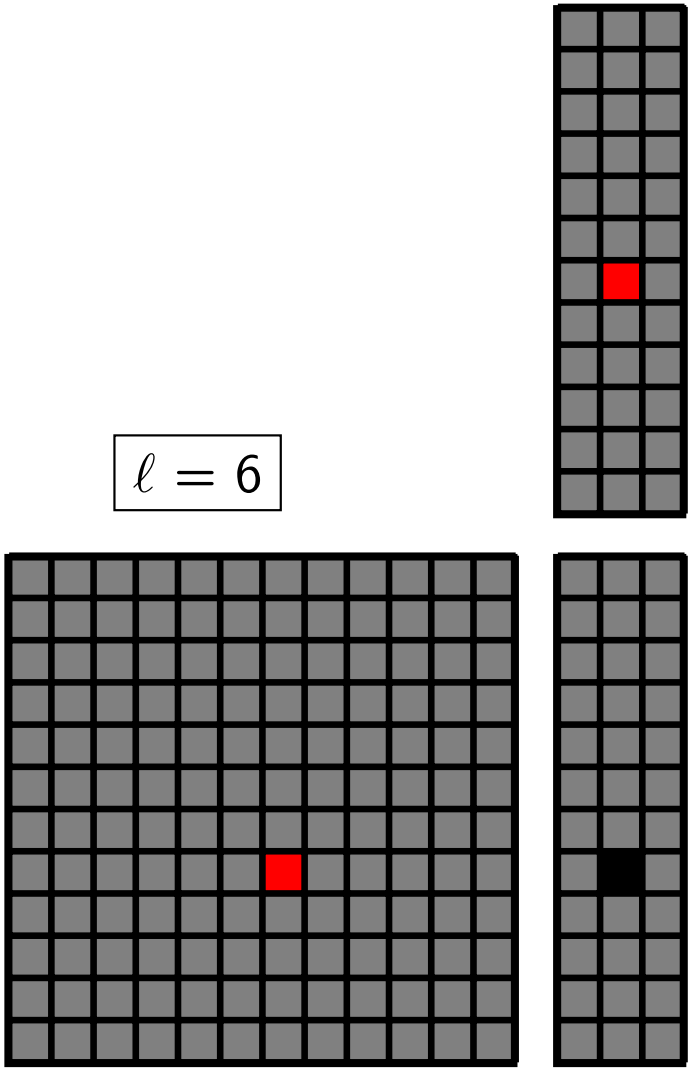

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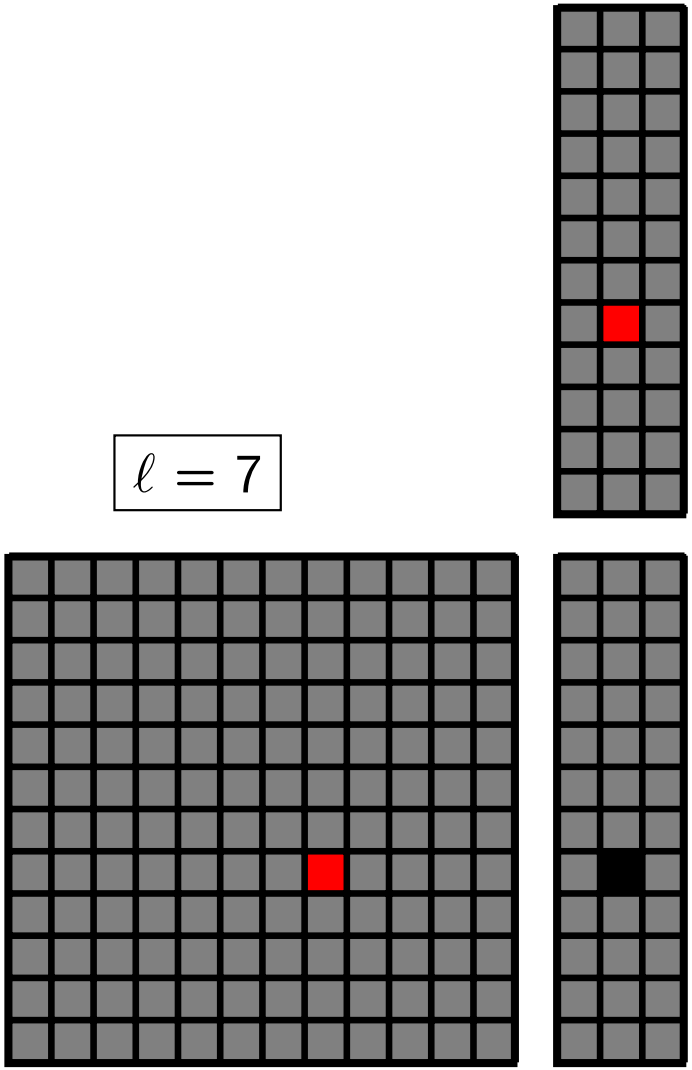

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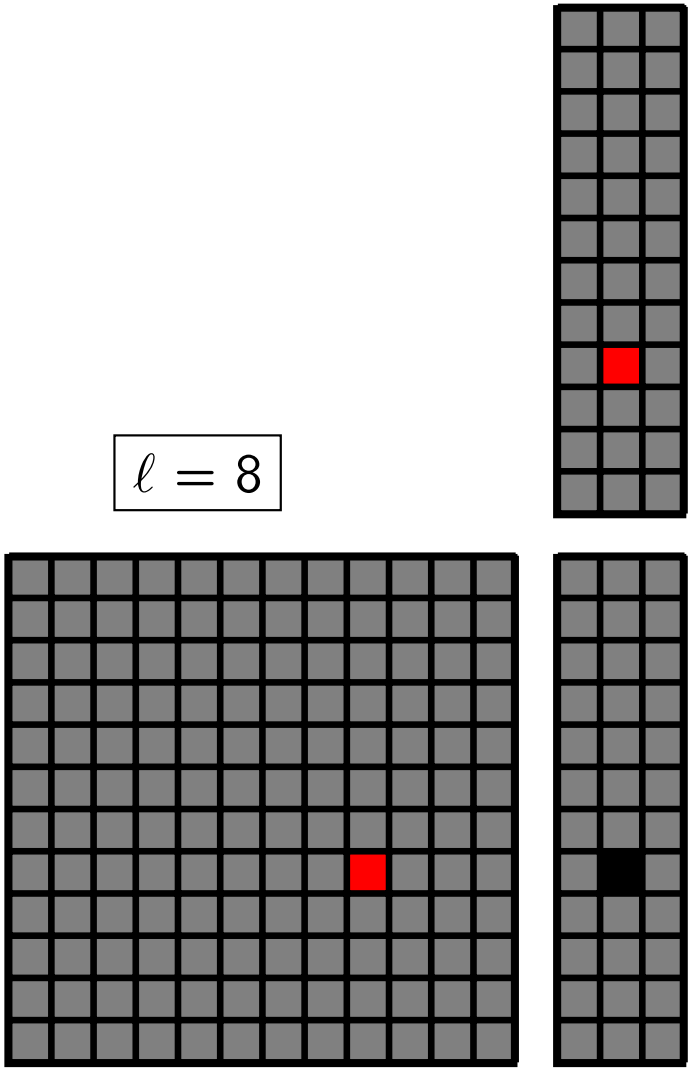

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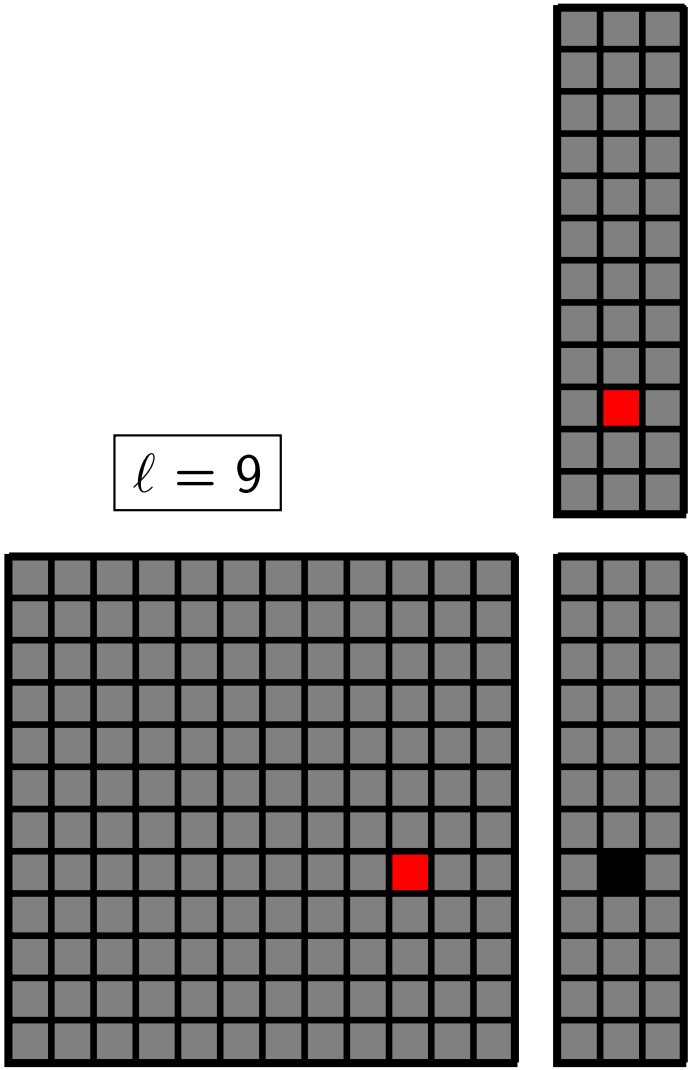

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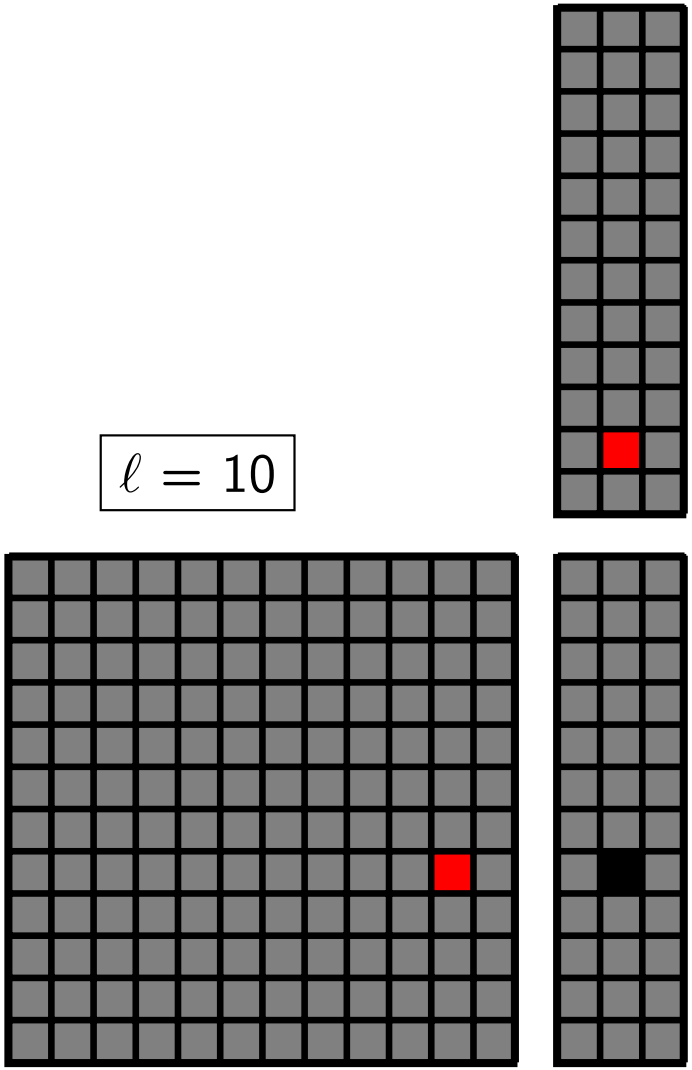

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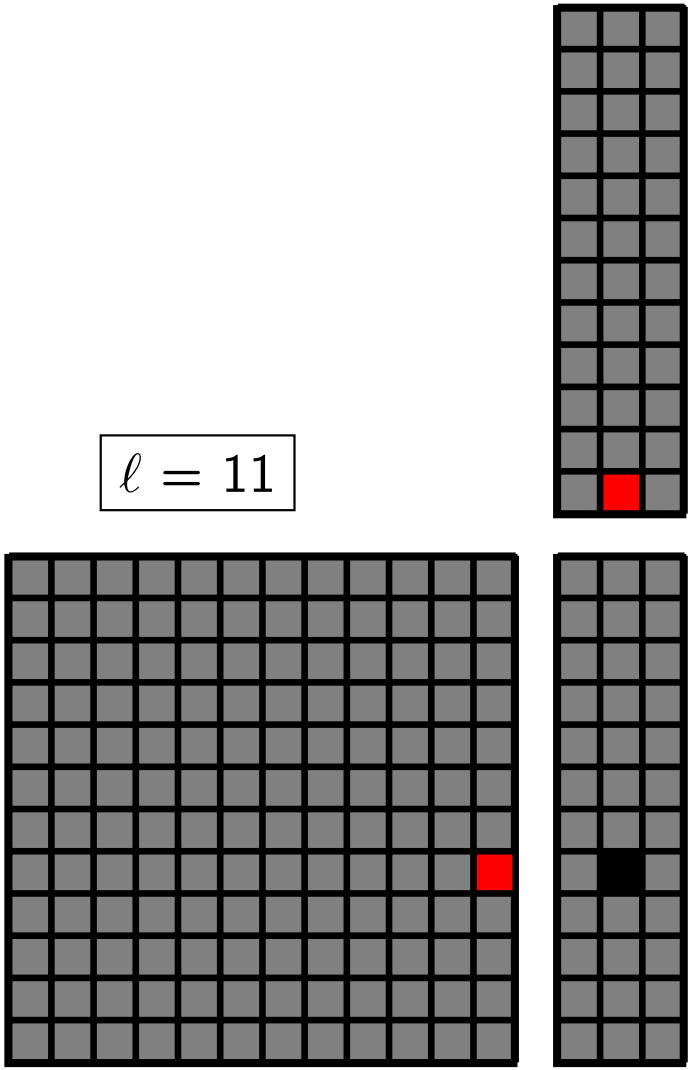

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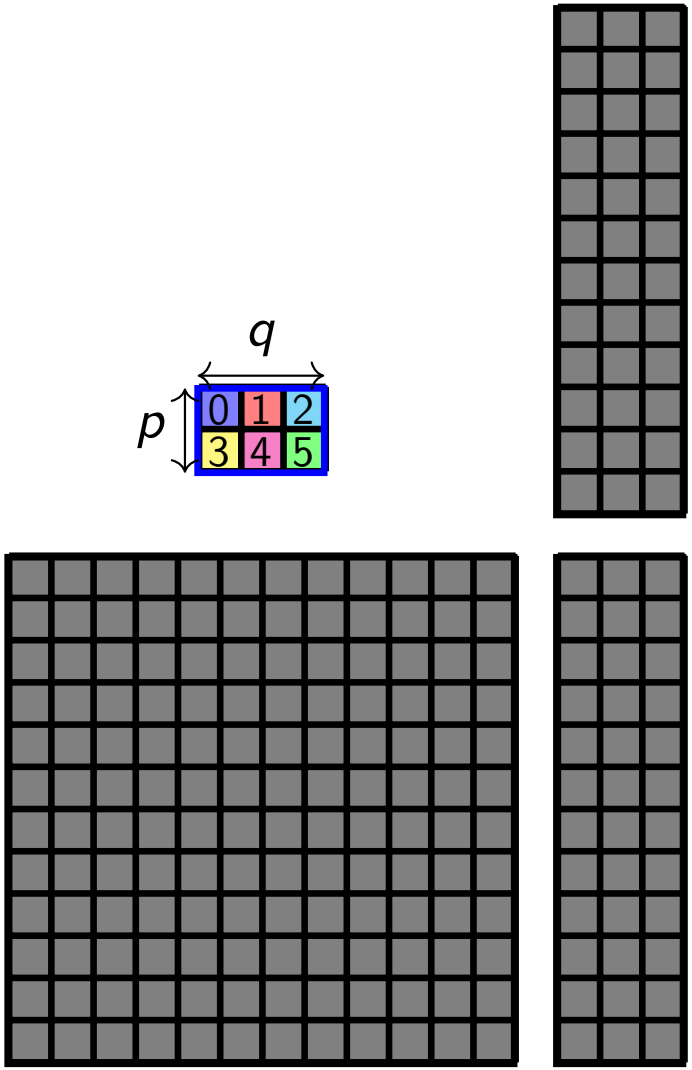

- Computing $C = AB$
- With P nodes : 2D Block-Cyclic scheme Blackford et al., 1997; van de Geijn and Watts, 1997

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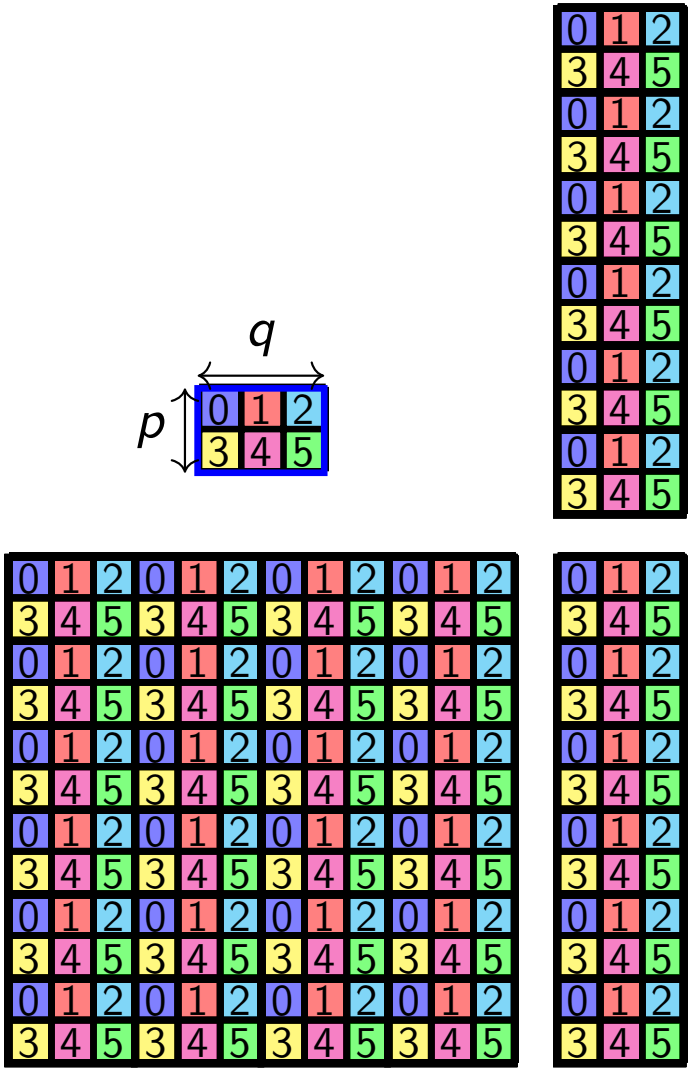

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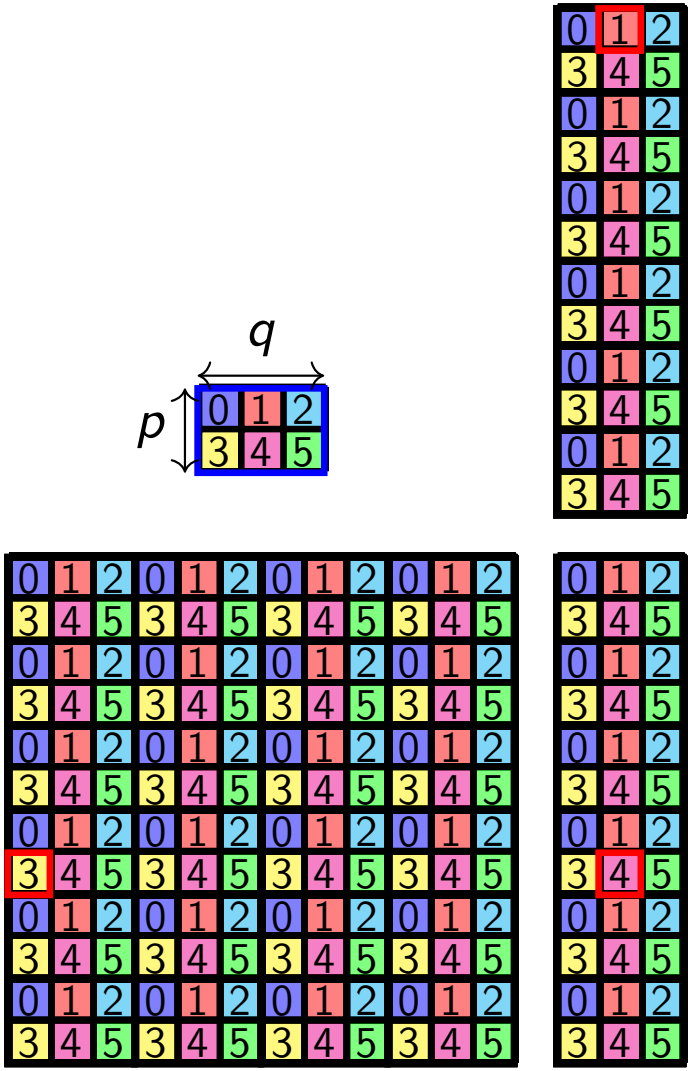
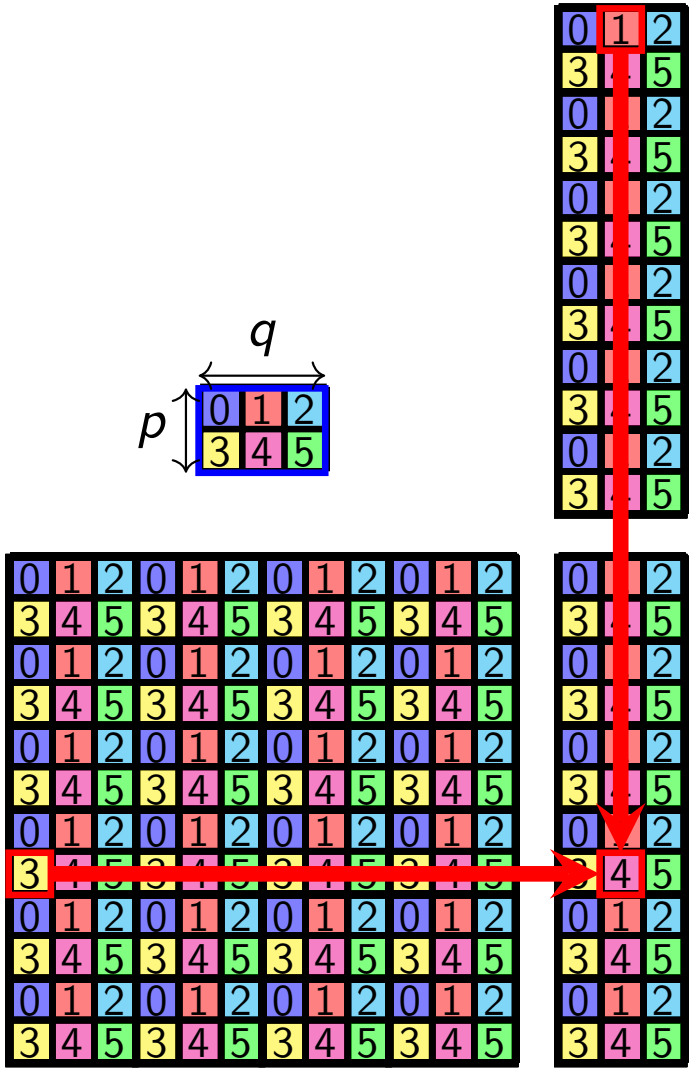


- Computing $C = AB$
- To compute one tile we need to transfer all the data to the corresponding node

GEMM (GEneral Matrix-Matrix multiplication)



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- Moving the data to the node that posseses the tile of C is called a C-Stationary scheme

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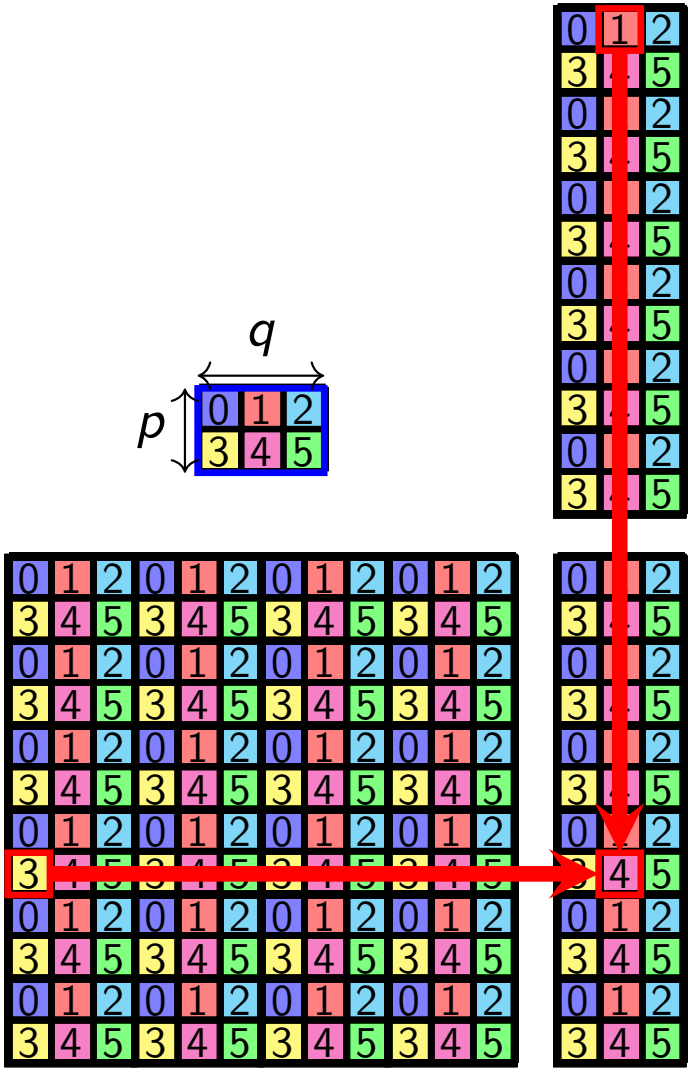

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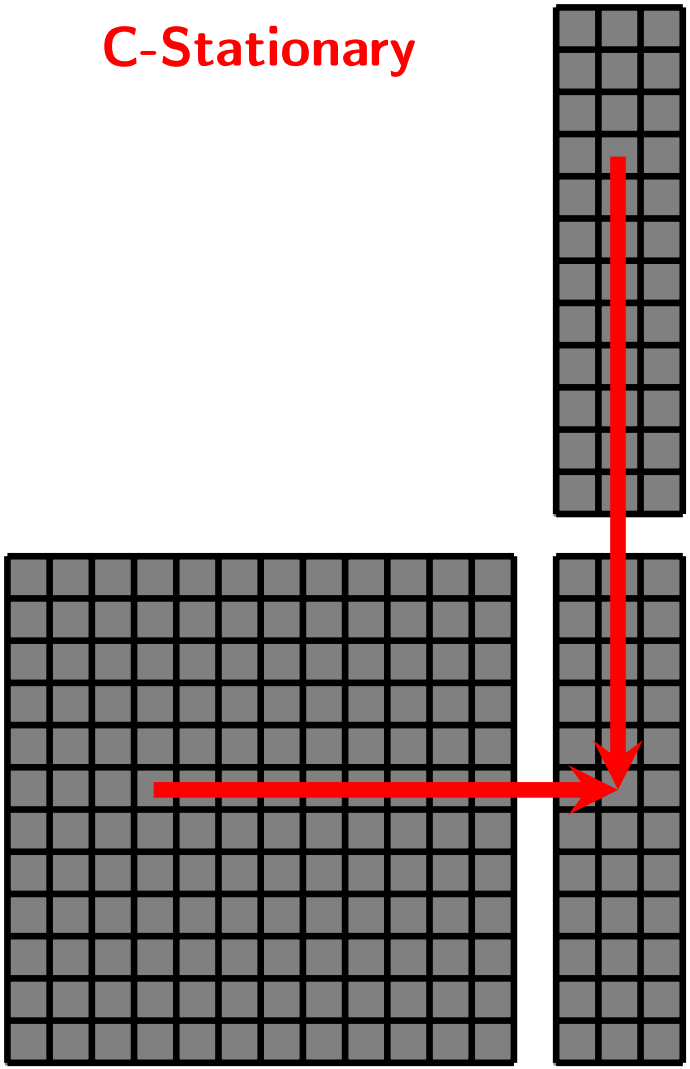
GEMM C-Stat	$qm^2 + pmk$

A-stationary GEMM



Standard : C-Stationary

We move the blocks of A and B to be computed on C

Aim : A-Stationary

We move the blocks of B and C to be computed on A (Agullo et al., 2023)

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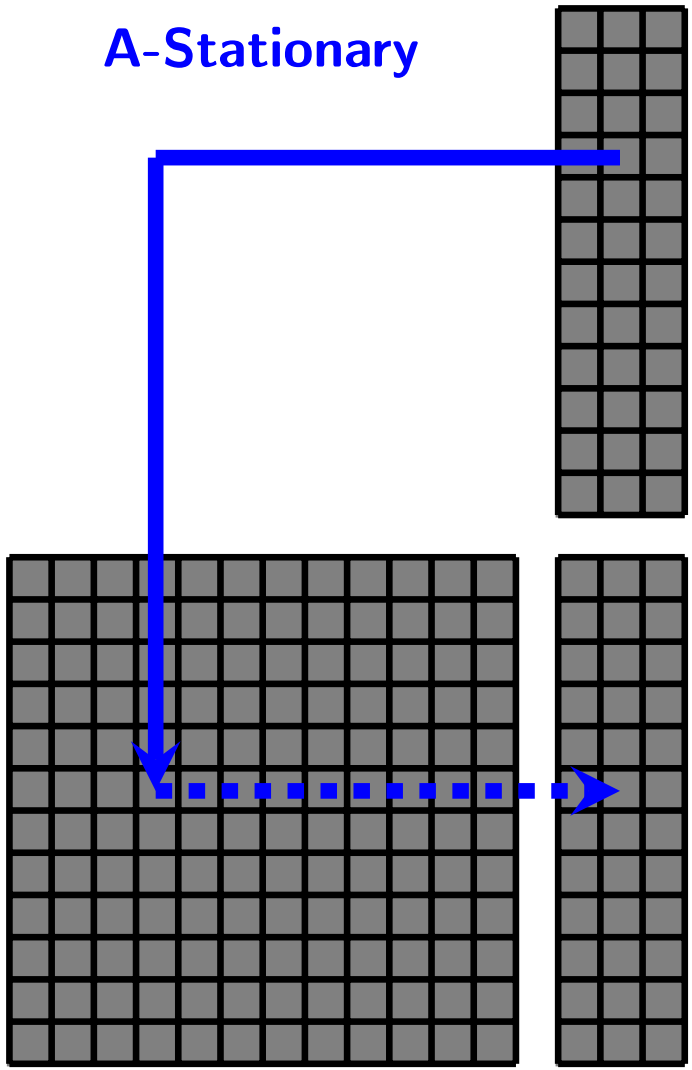
A-stationary GEMM



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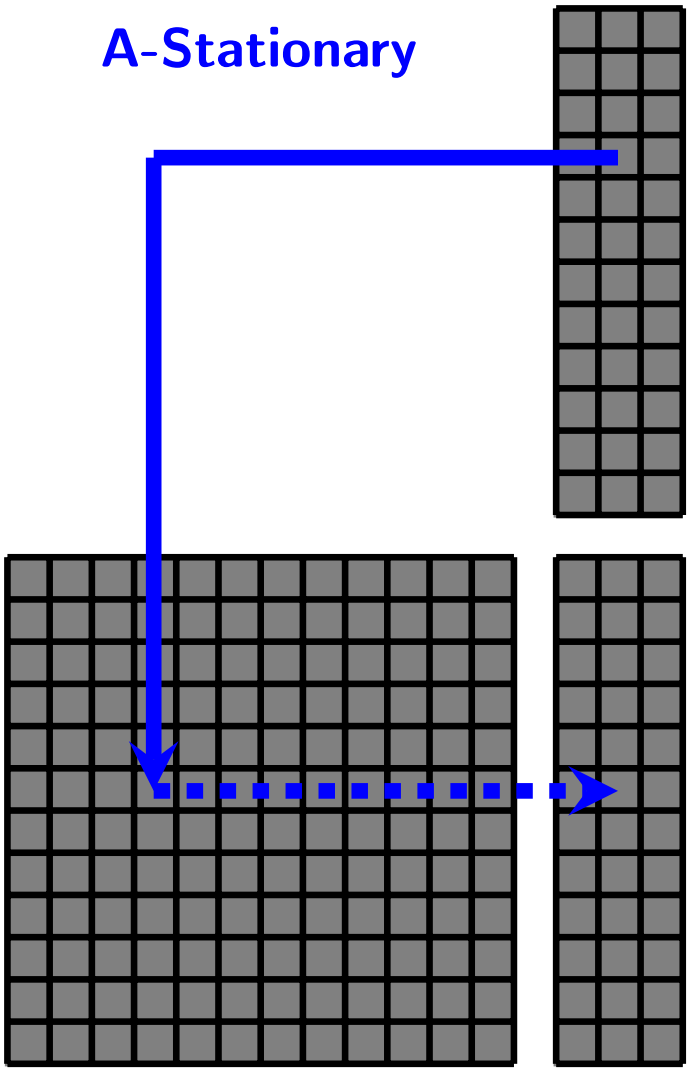
Aim : A-Stationary

We move the blocks of B and C to be computed on A (Agullo et al., 2023)

Method	Comm. Volume
GEMM C-Stat	$qm^2 + pmk$

A-stationary GEMM



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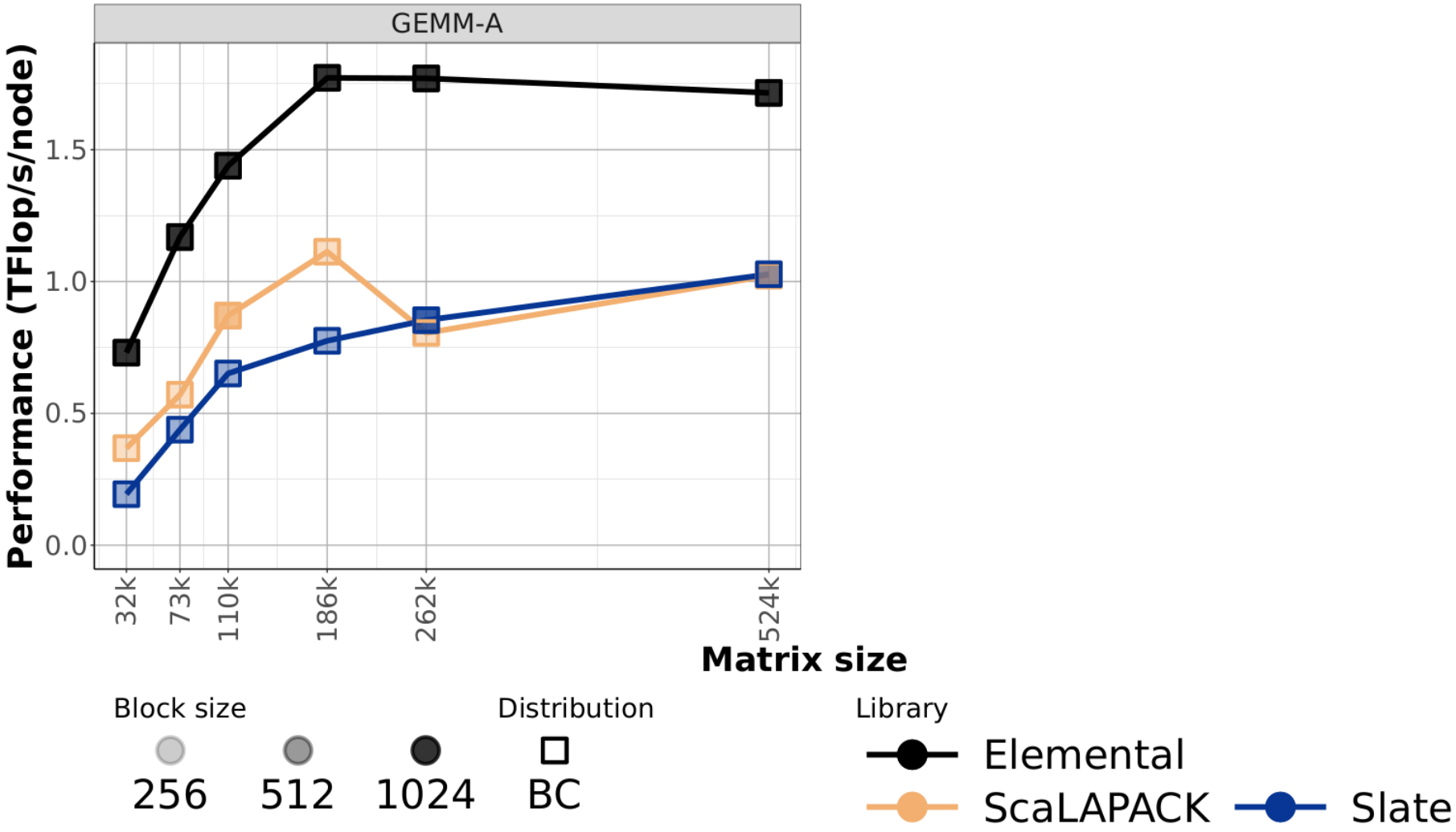
Performance of A-Stationary GEMM



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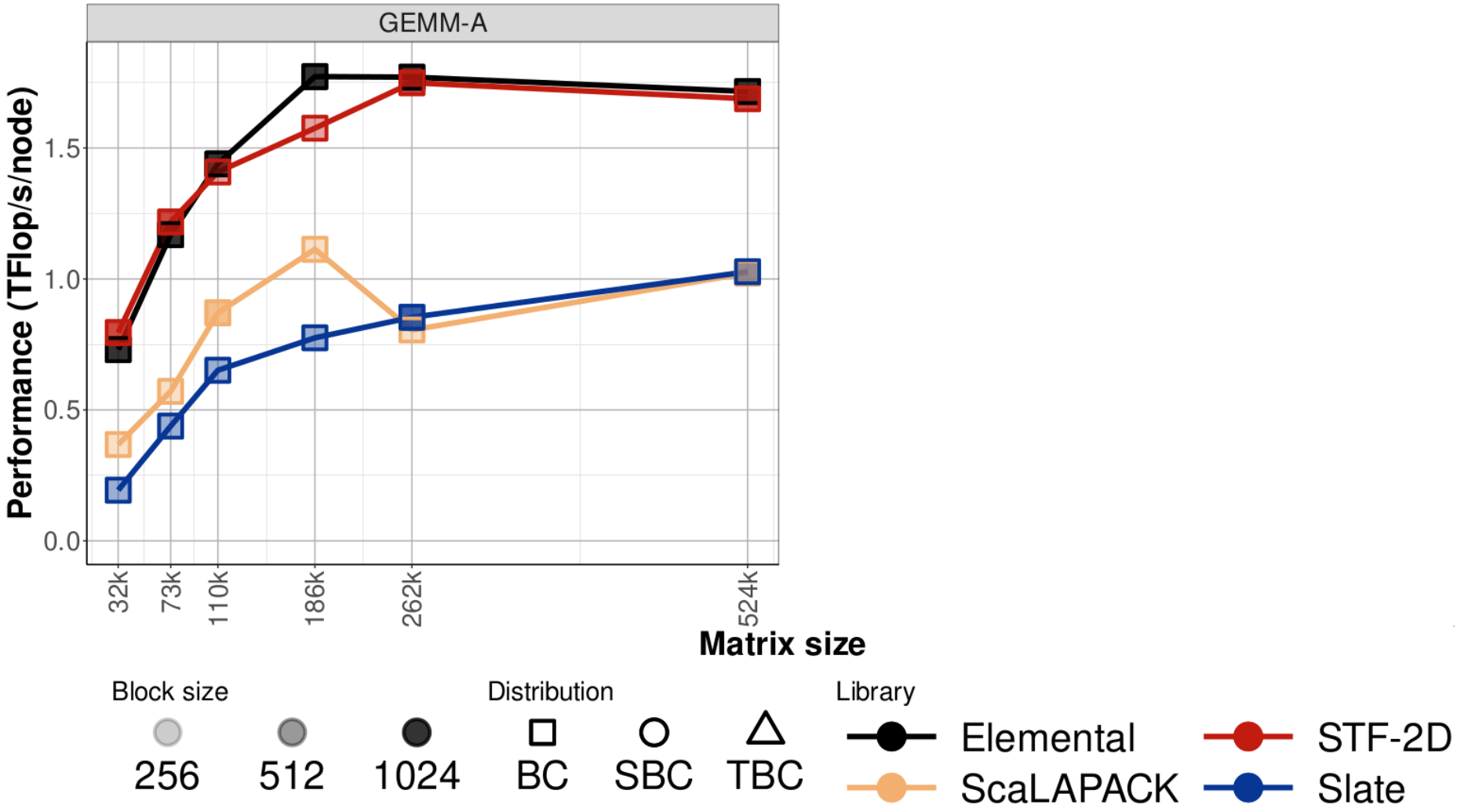
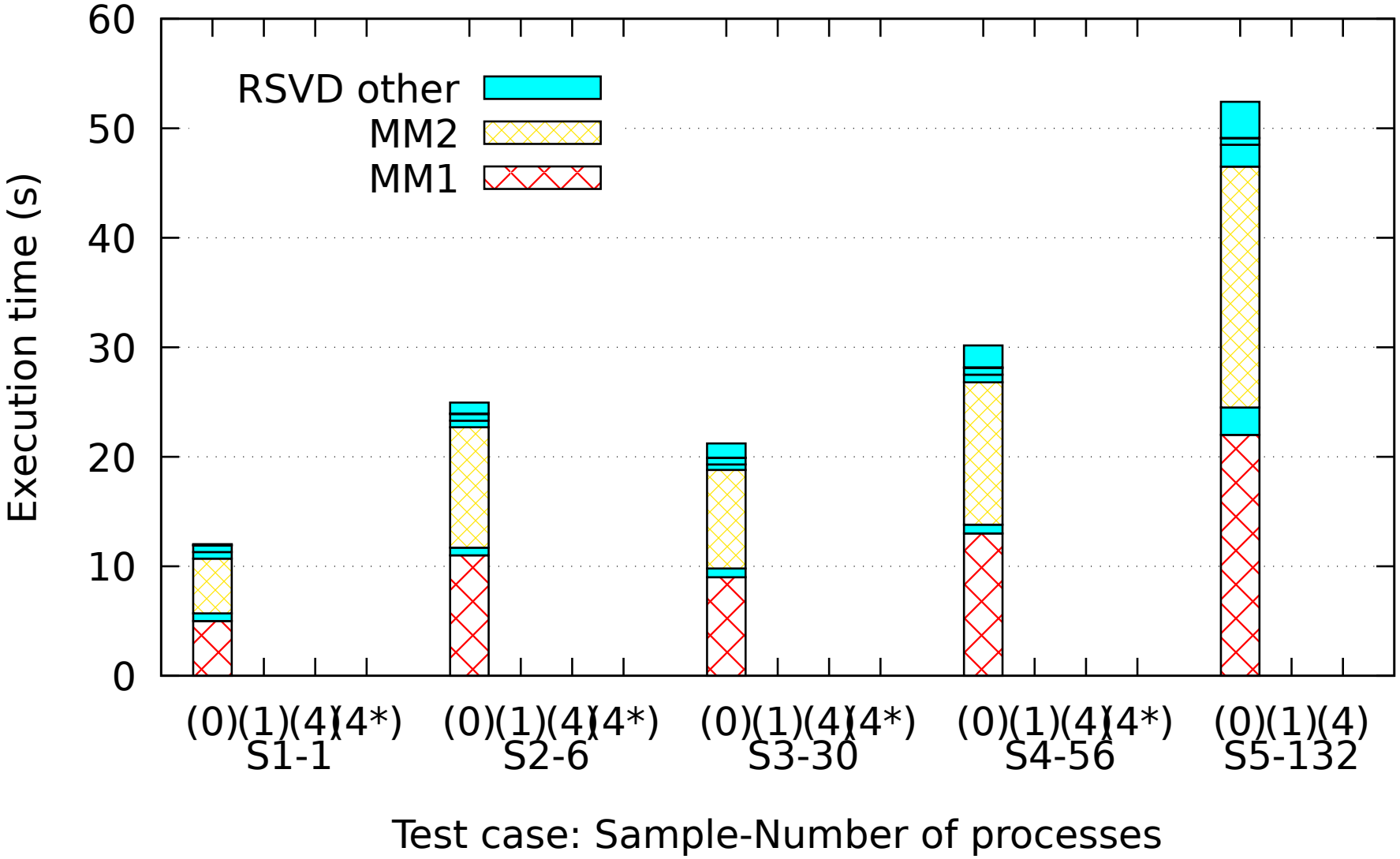
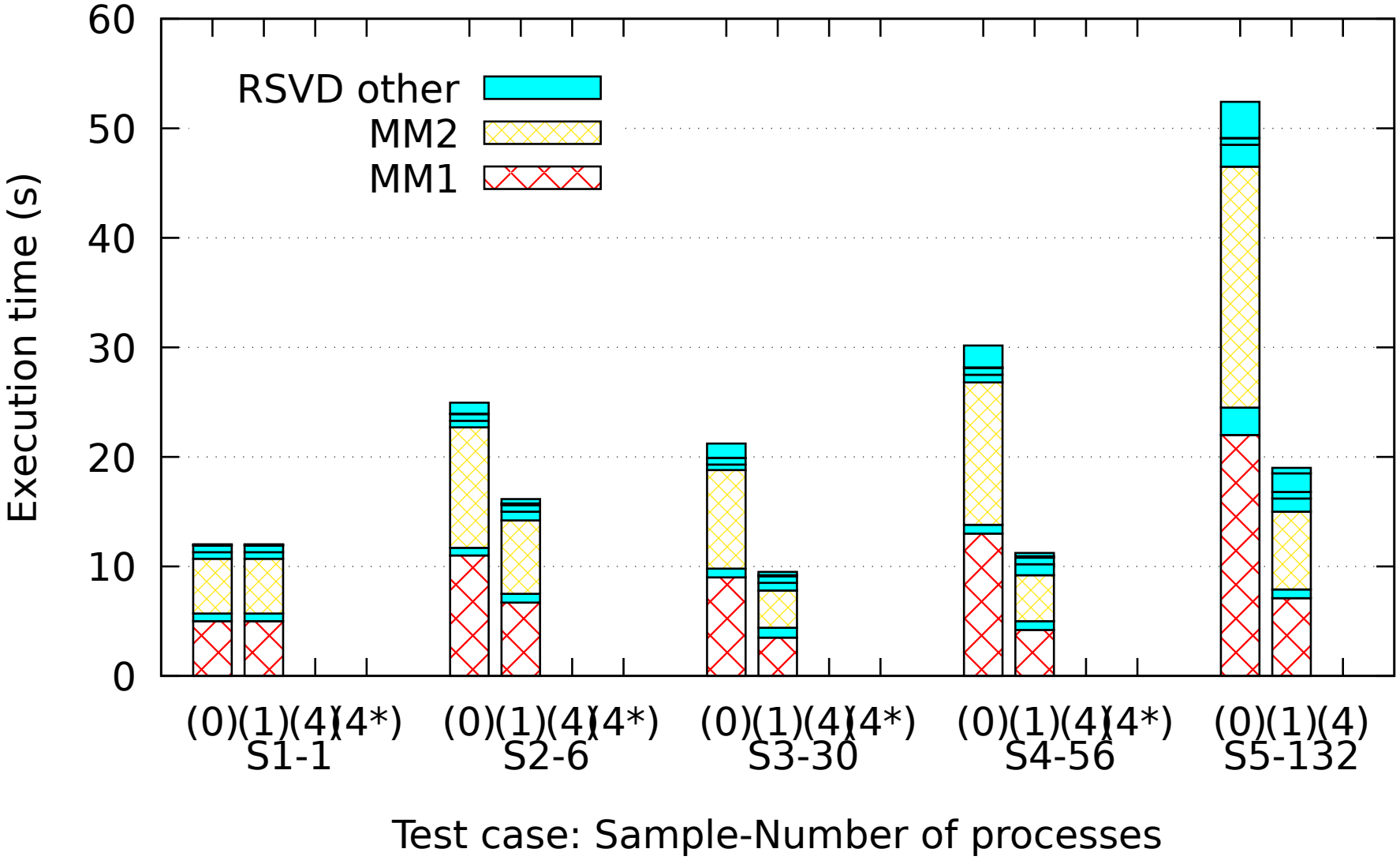


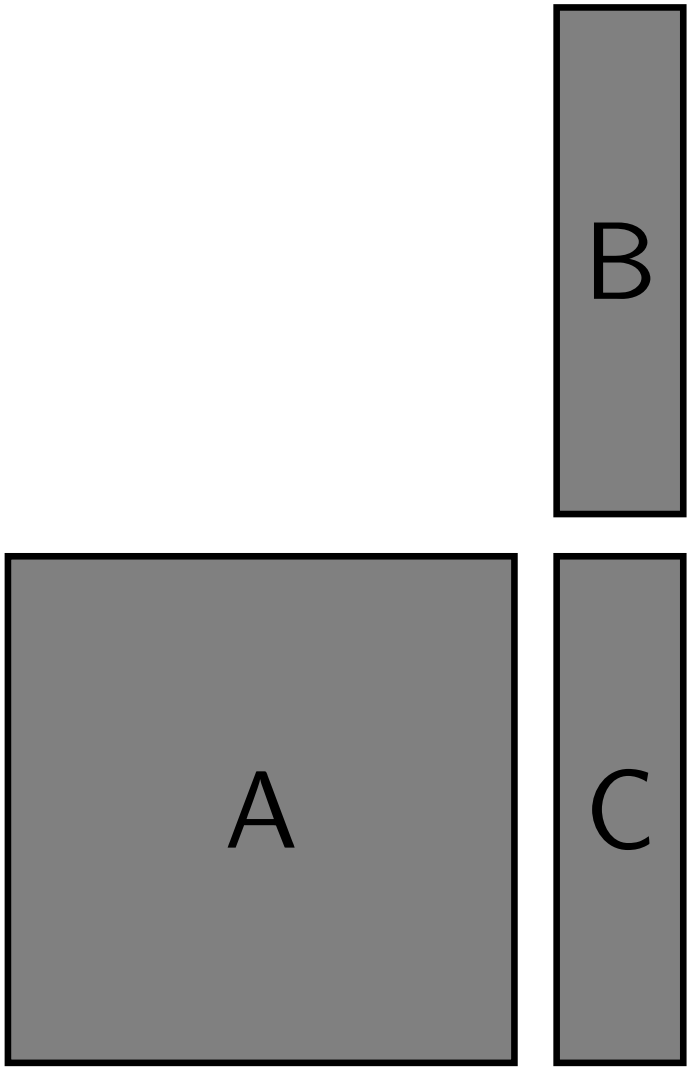
Impact of A-Stationary GEMM for RSVD-MDS



Impact of A-Stationary GEMM for RSVD-MDS

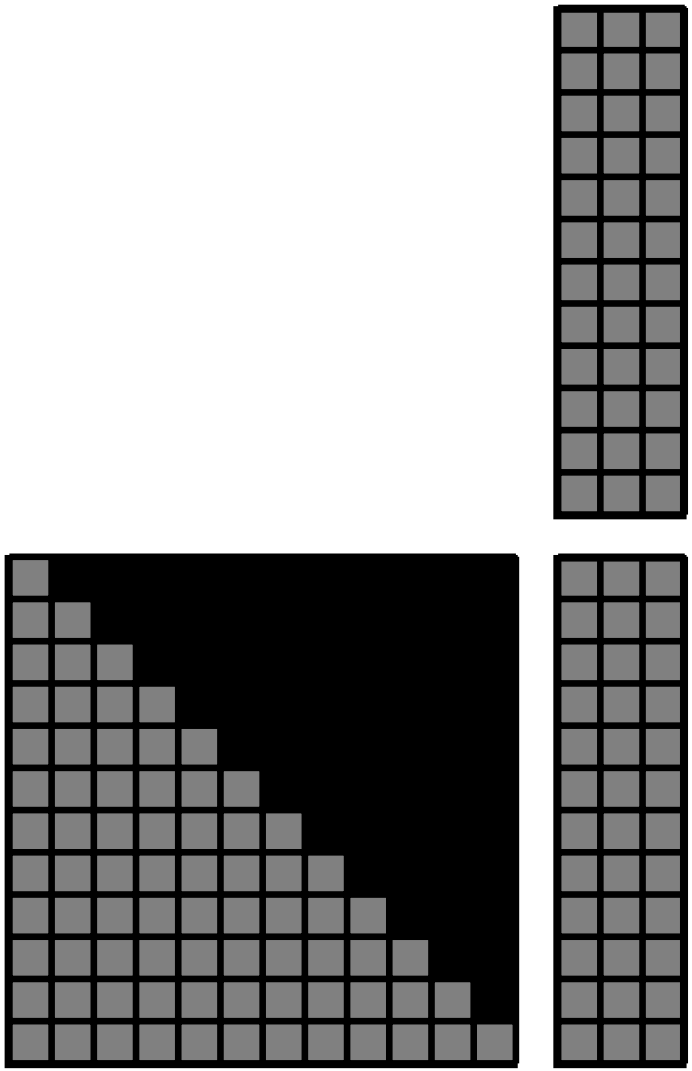


SYMM (SYmmetric Matrix-Matrix multiplication)



- Computing $C = AB$

SYMM (SYmmetric Matrix-Matrix multiplication)



- Computing $C = AB$
- $C_{i,j} = \sum_{\ell=1}^{i} A_{i,\ell} B_{\ell,j} + \sum_{\ell=i+1}^{m} A_{\ell,i}^{T} B_{\ell,j}$

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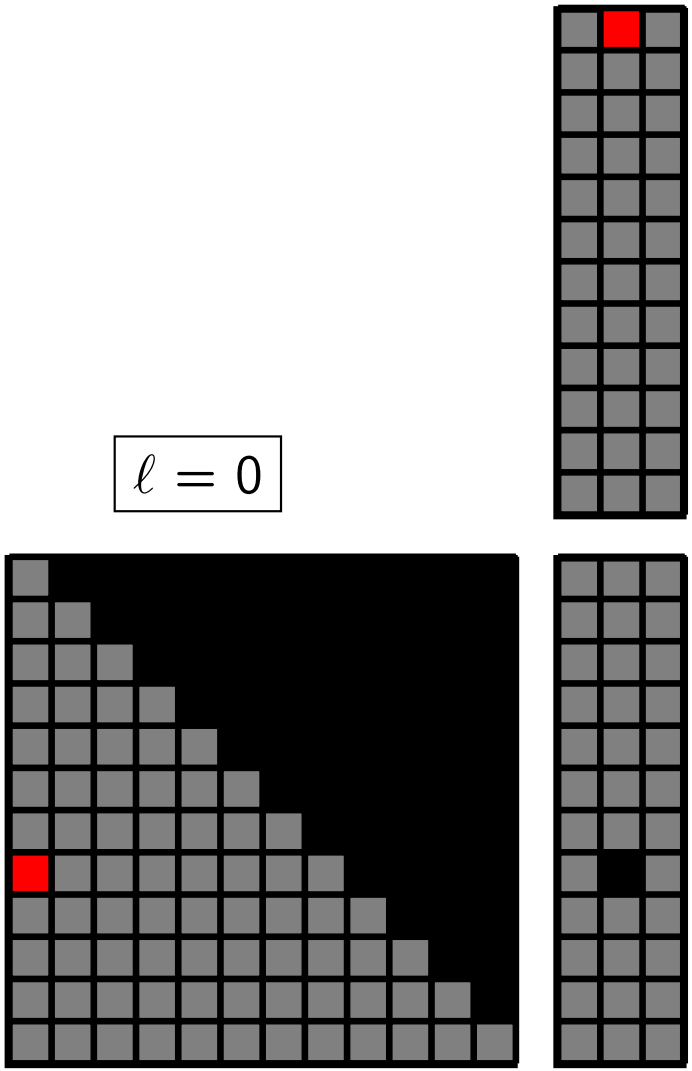

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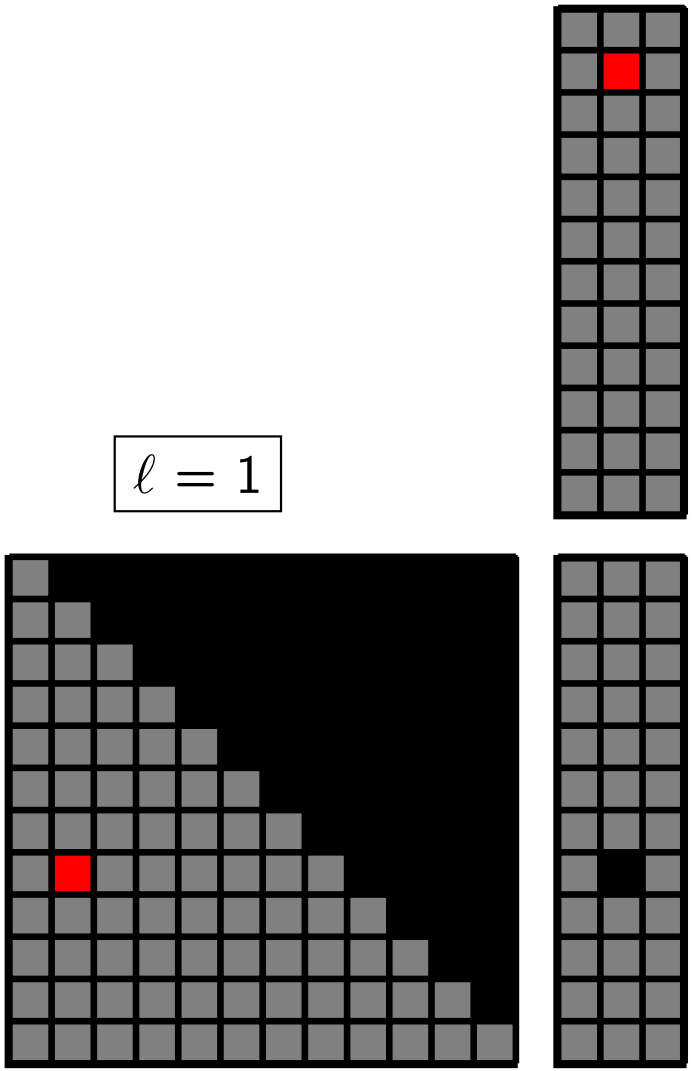

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- $C_{7,1} = \ldots + A_{7,1} B_{1,1} + \ldots$

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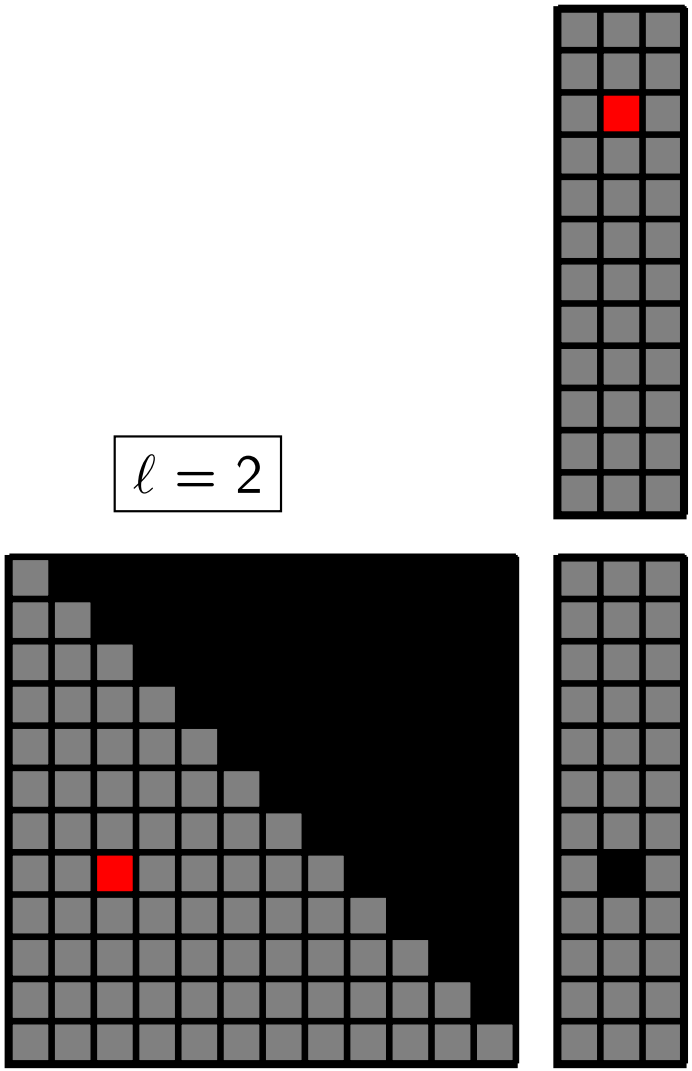

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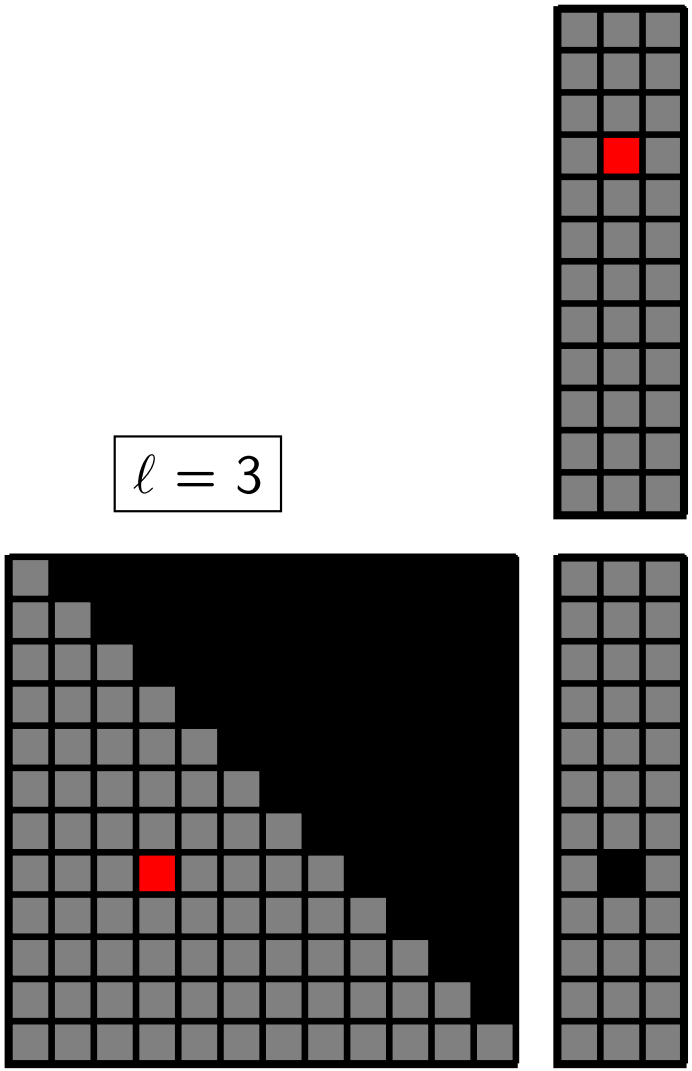
SYMM (SYmmetric Matrix-Matrix multiplication)



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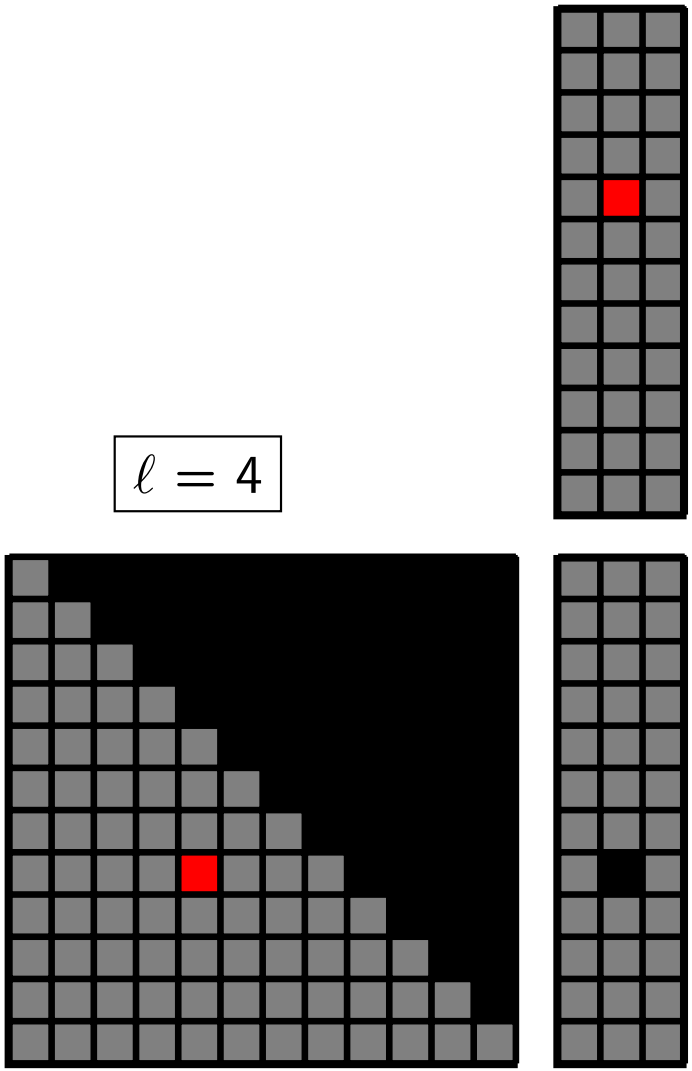

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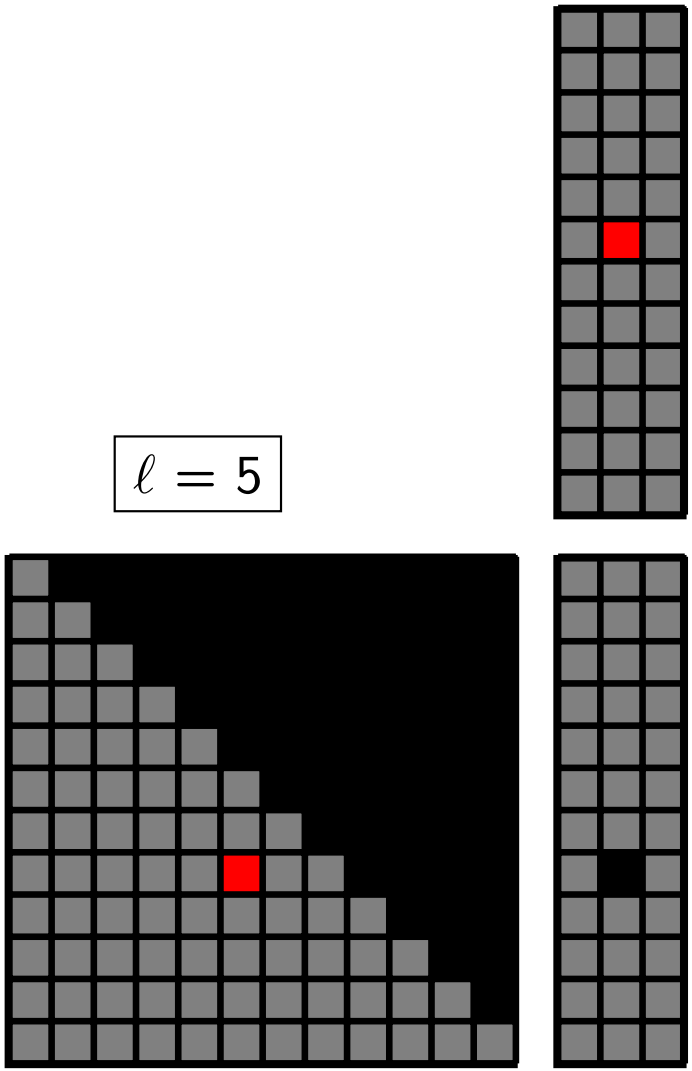

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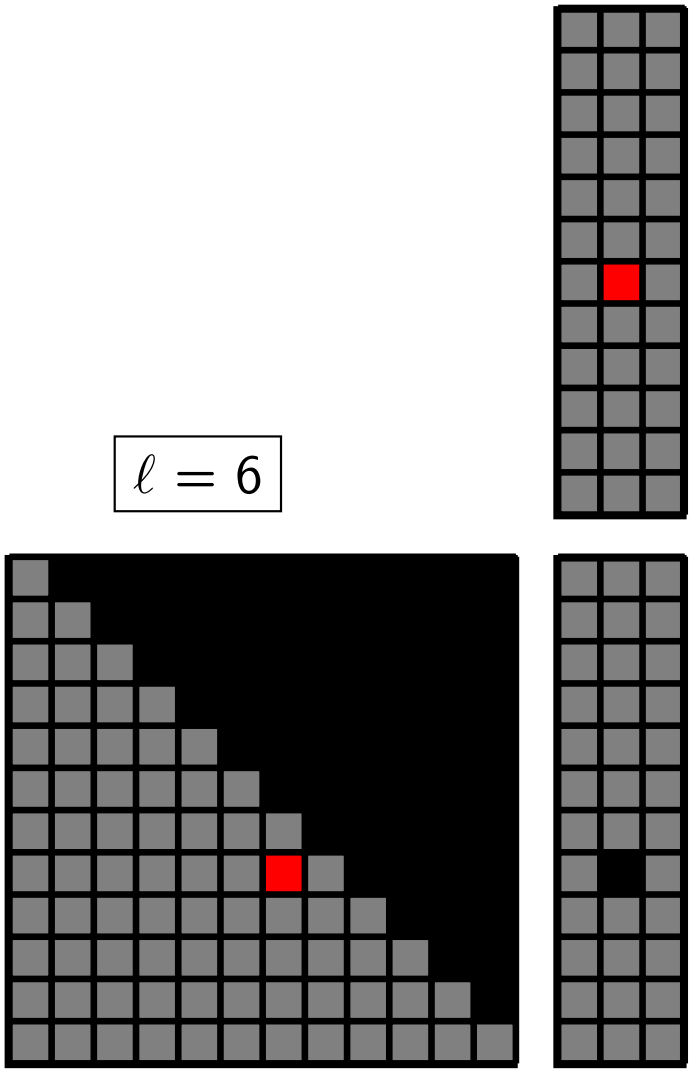

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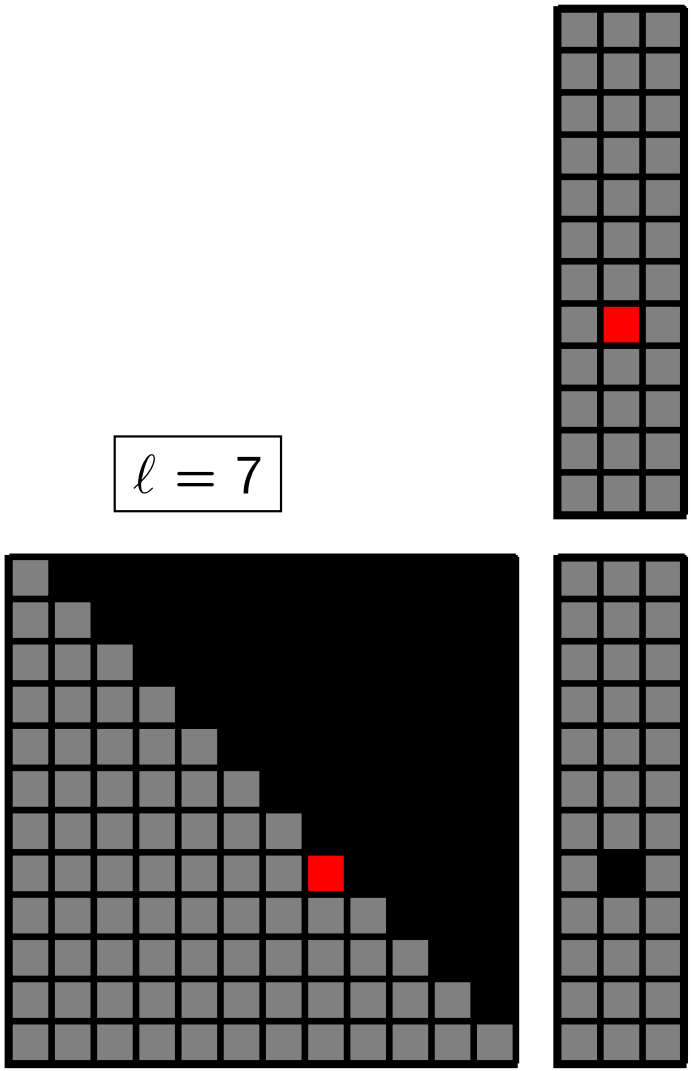

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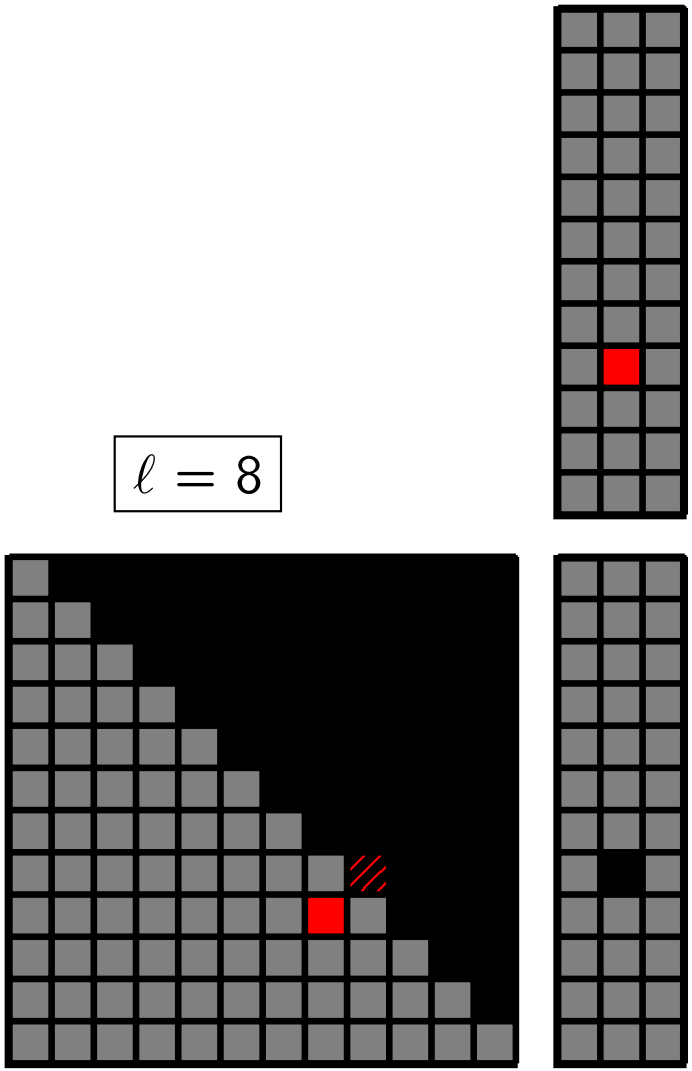

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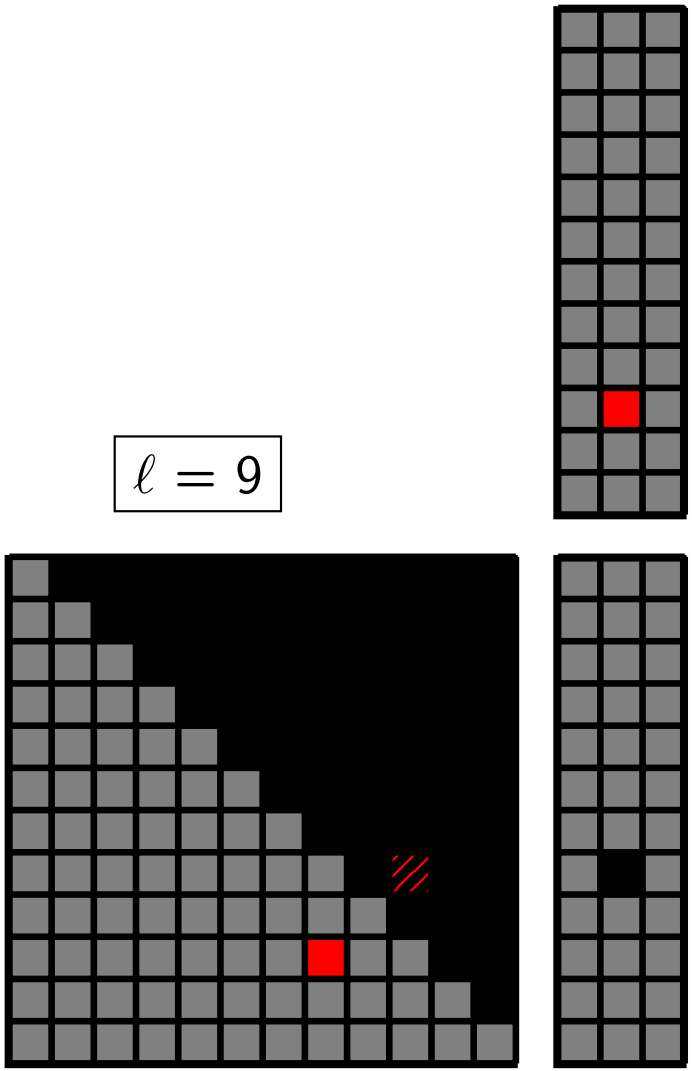

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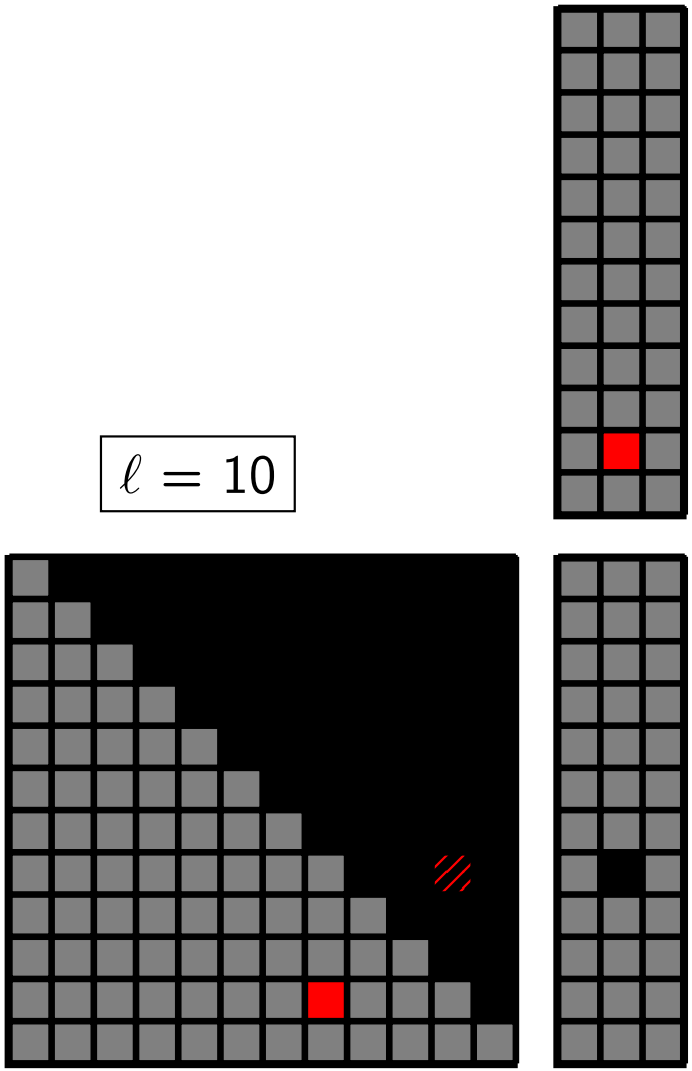

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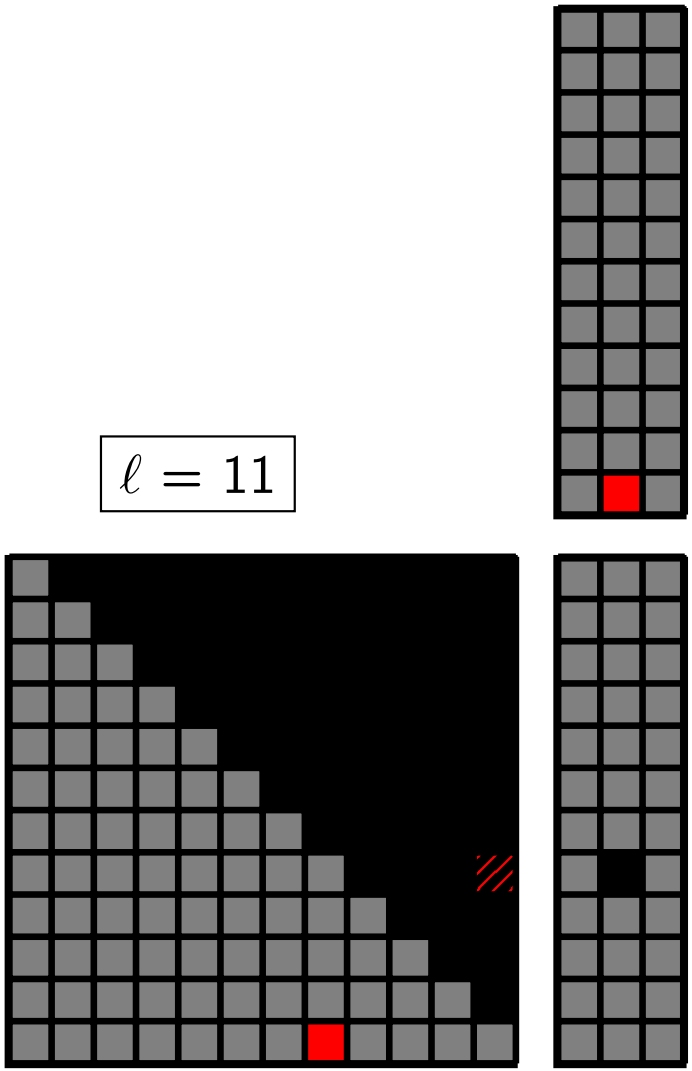

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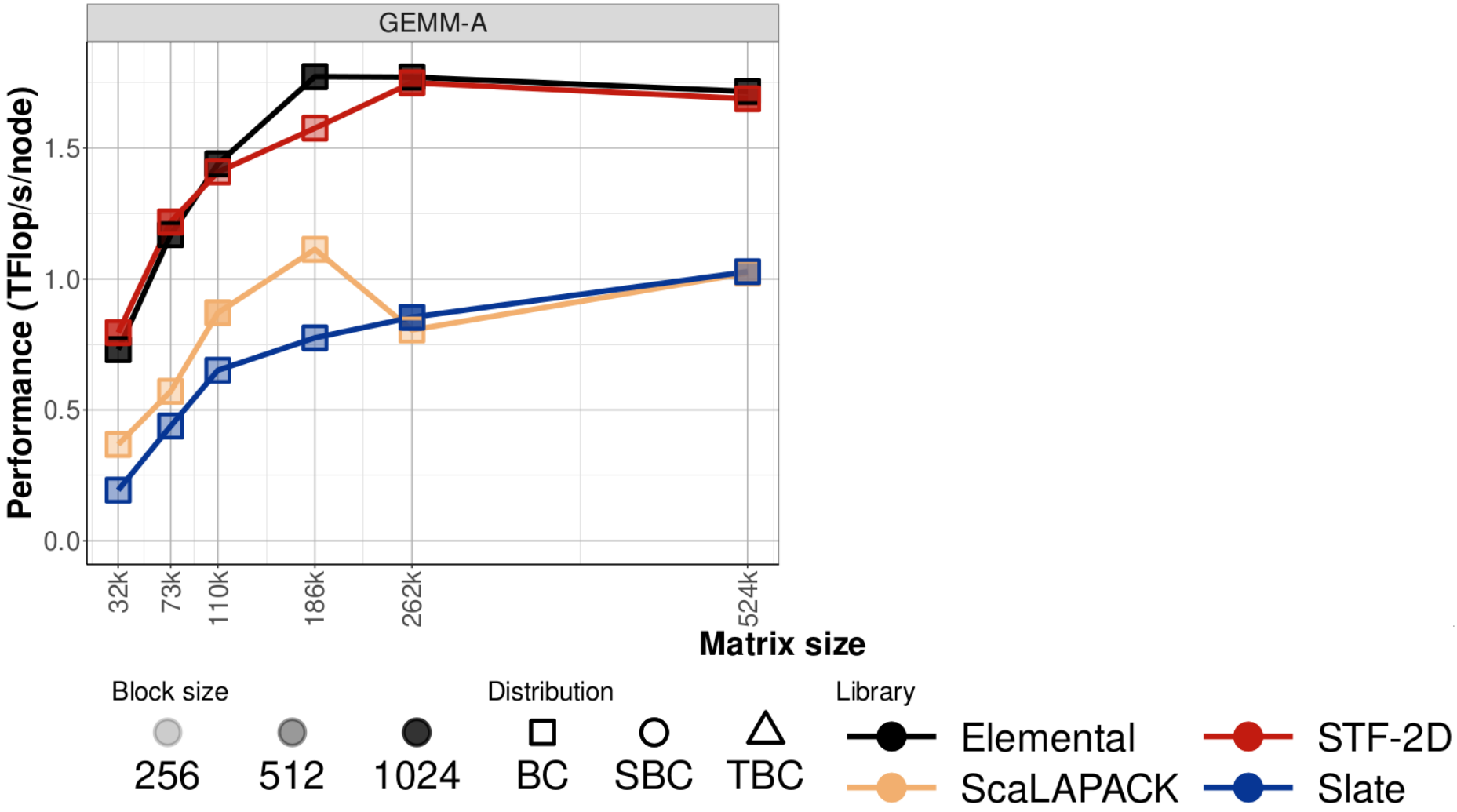
Baseline performance of SYMM



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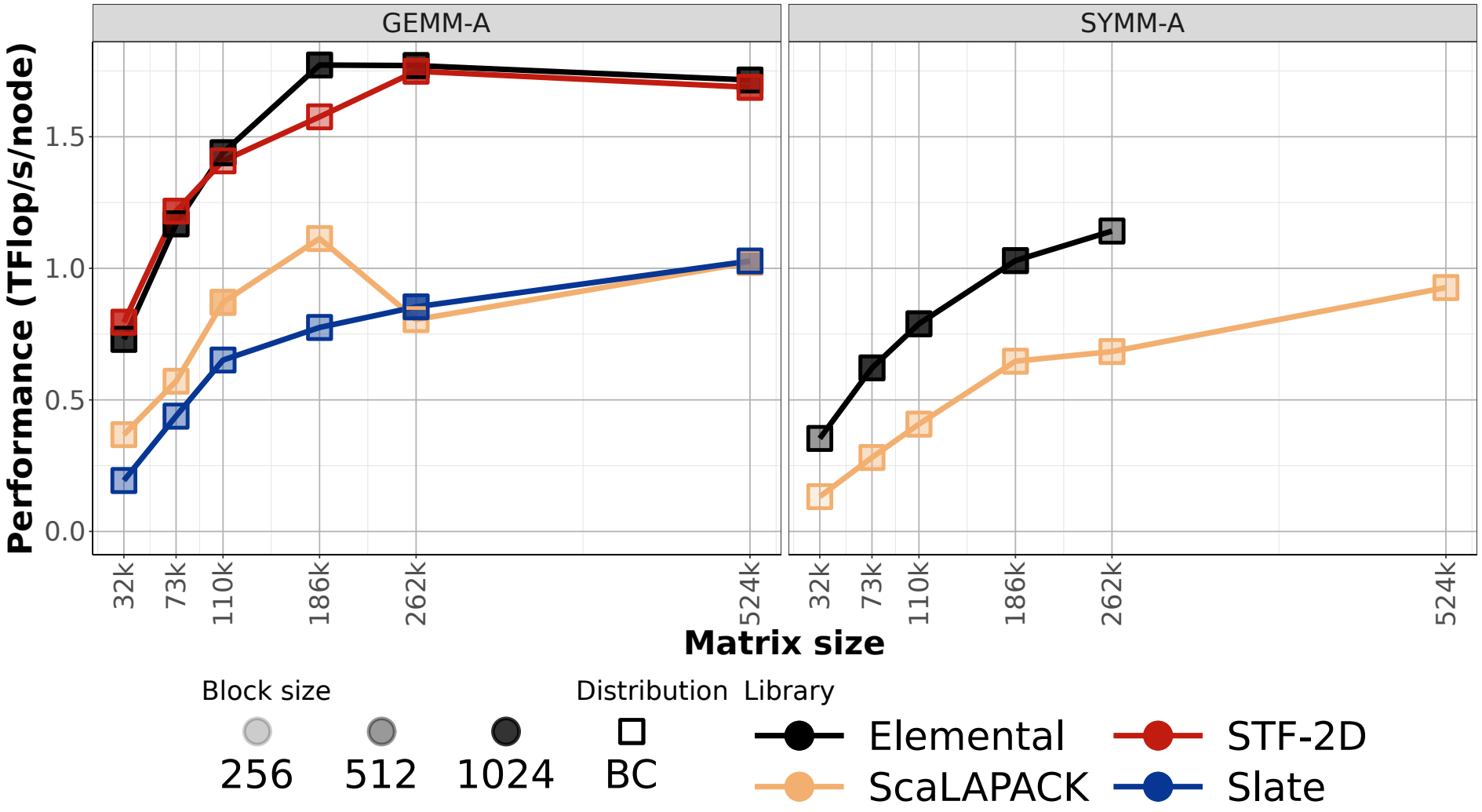

Question

	Arithmetic Intensity ($\frac{Computation}{Communication}$)	Memory footprint
GEMM	☺	☹
SYMM	☹	☺

Joint Work

Emmanuel Agullo, Alfredo Buttari, Olivier Coulaud, Lionel Eyraud-Dubois, Mathieu Faverge, Alain Franc, Abdou Guermouche, Antoine Jego, Romain Peressoni and Florent Pruvost

Question

	Arithmetic Intensity ($\frac{Computation}{Communication}$)	Memory footprint
GEMM-2DBC	☺	☹
SYMM-2DBC	☹	☺

Joint Work

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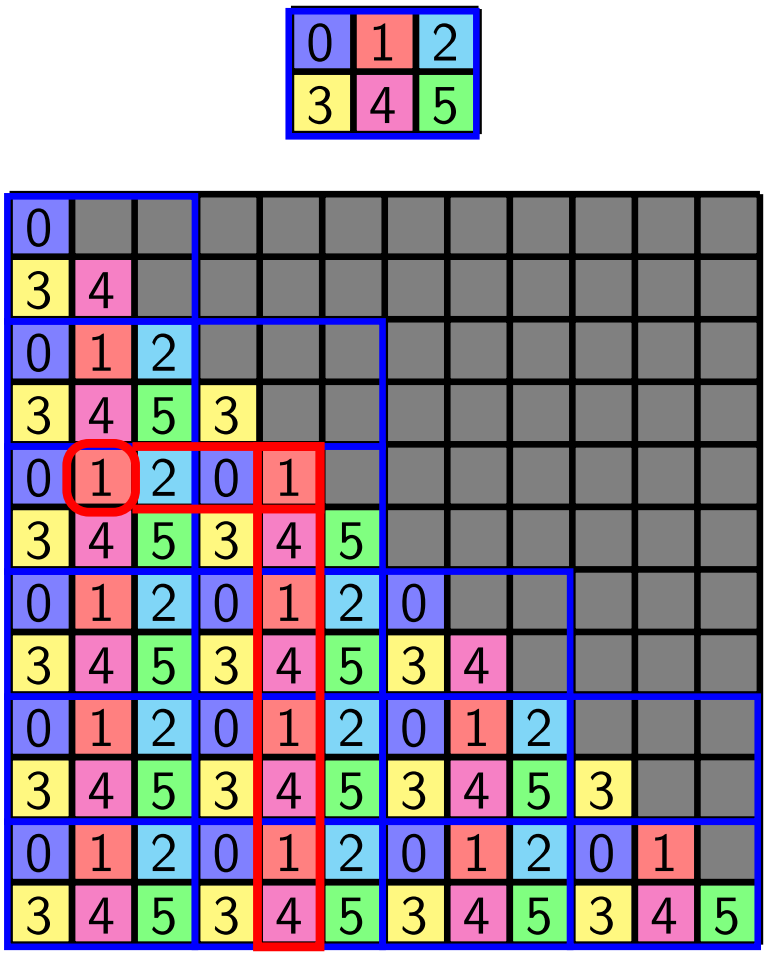
2D Block-Cyclic Distribution



- For a **symmetric** matrix each line is present on both a line and a column.
- In a $p \times q$ distribution, each line is distributed among $p + q - 1$ nodes.

$(p \approx q \approx \sqrt{P})$

Method	Comm. Volume
GEMM C-Stat	$qm^2 + pmk$
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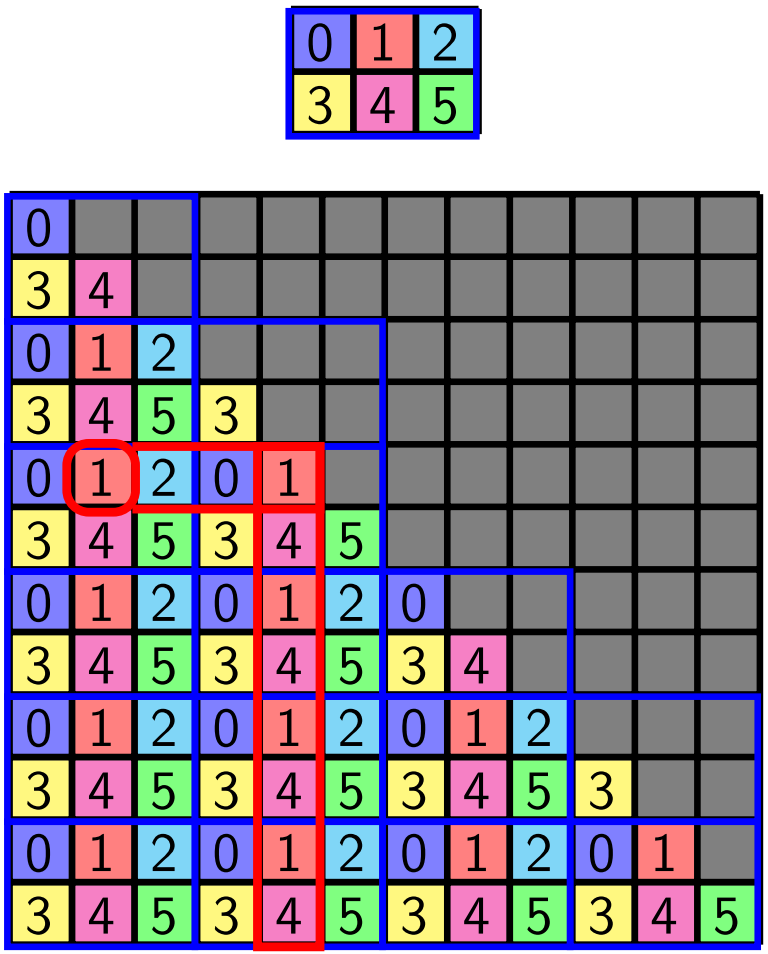

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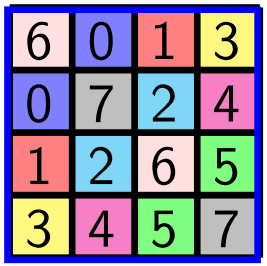
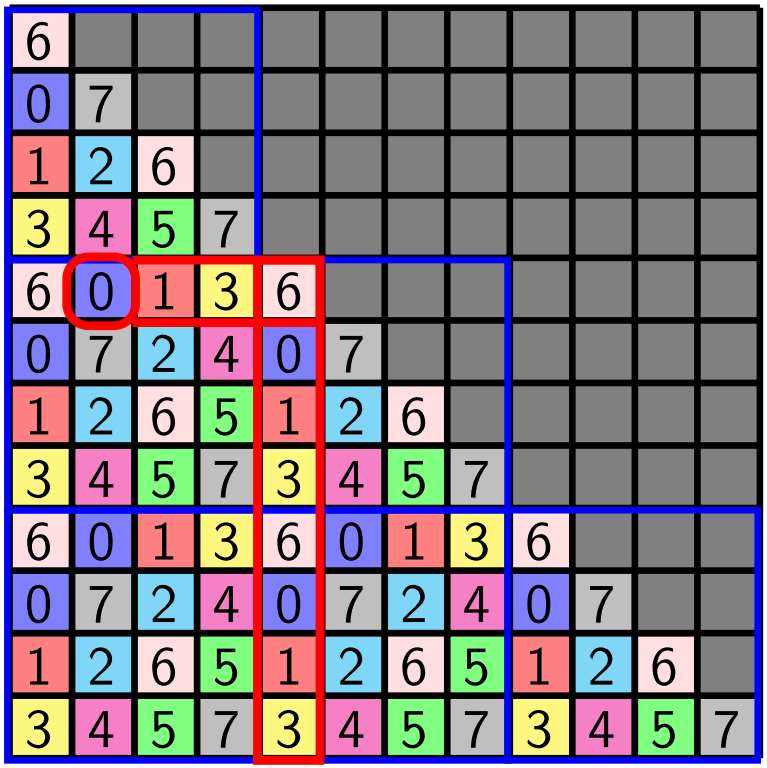
SYMM 2DBC	$\approx 4\sqrt{P}mk$

Symmetric Block-Cyclic Distribution





- Blocks of size $r \times r$ with $P = \frac{r^2}{2}$ Beaumont, Duchon, et al., 2022
- Optimises the number of nodes on which lines are distributed

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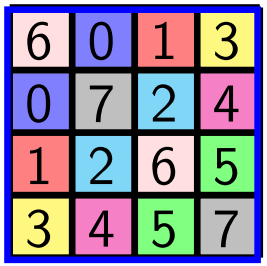
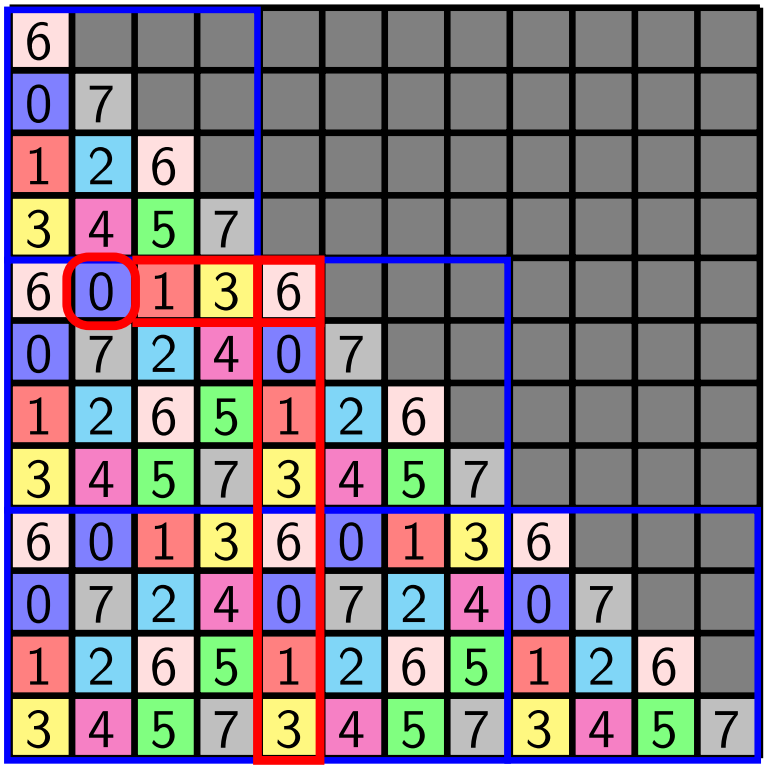
Symmetric Block-Cyclic Distribution





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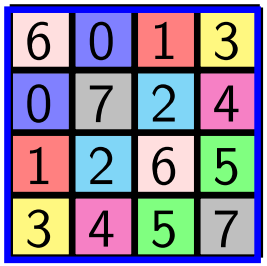
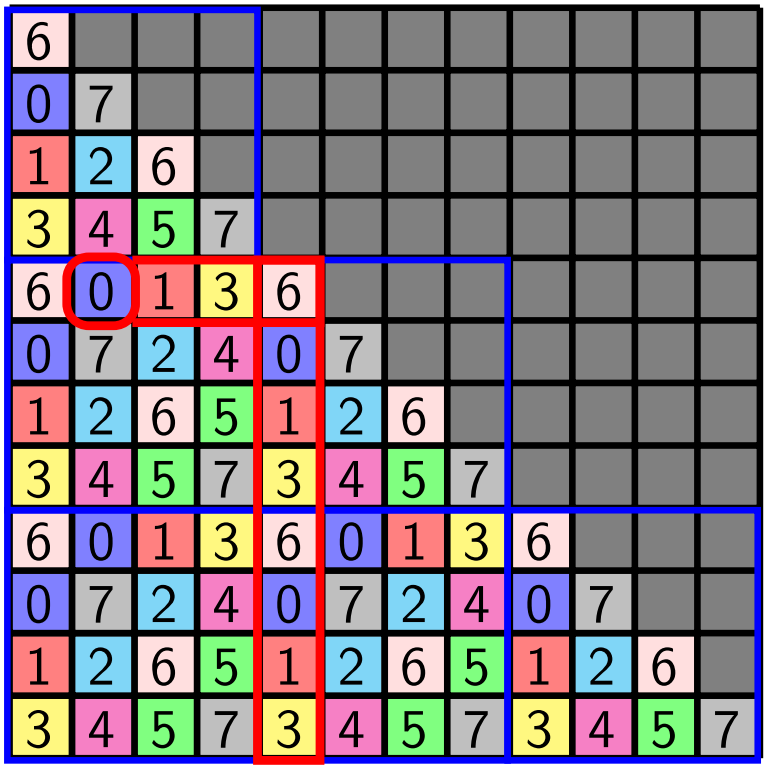
Symmetric Block-Cyclic Distribution





- Blocks of size $r \times r$ with $P = \frac{r^2}{2}$ Beaumont, Duchon, et al., 2022
- Optimises the number of nodes on which lines are distributed
- It is possible to reach an even lower communication volume using a TBC distribution Beaumont, Eyraud-Dubois, et al., 2022

Method	Comm. Volume
GEMM C-Stat.	$qm^2 + pmk$
GEMM A-Stat.	$\approx 2\sqrt{P}mk$
SYMM 2DBC	$\approx 4\sqrt{P}mk$
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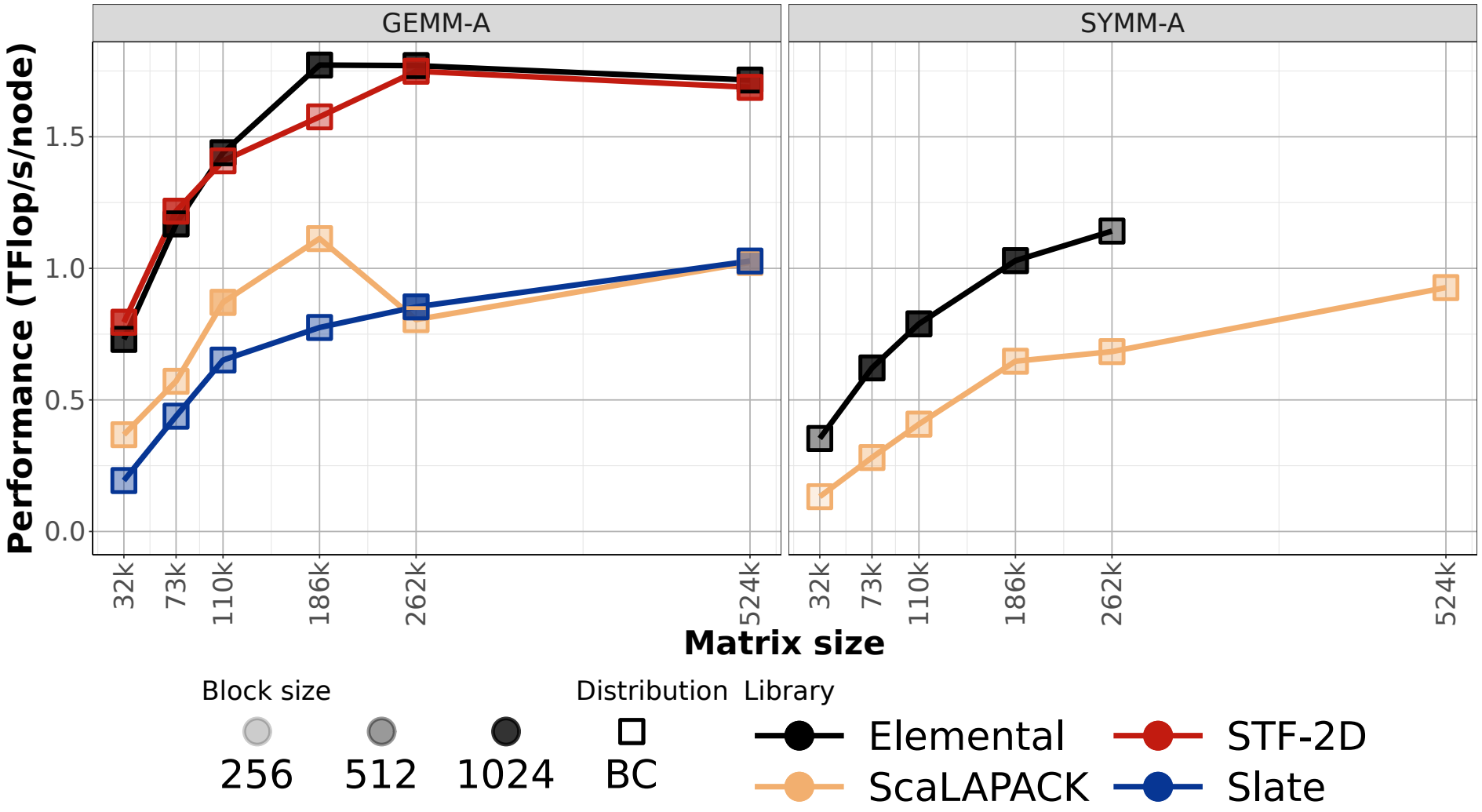
SYMM TBC	$\approx 2\sqrt{P}mk$

Performance of new A-Stationary SYMM



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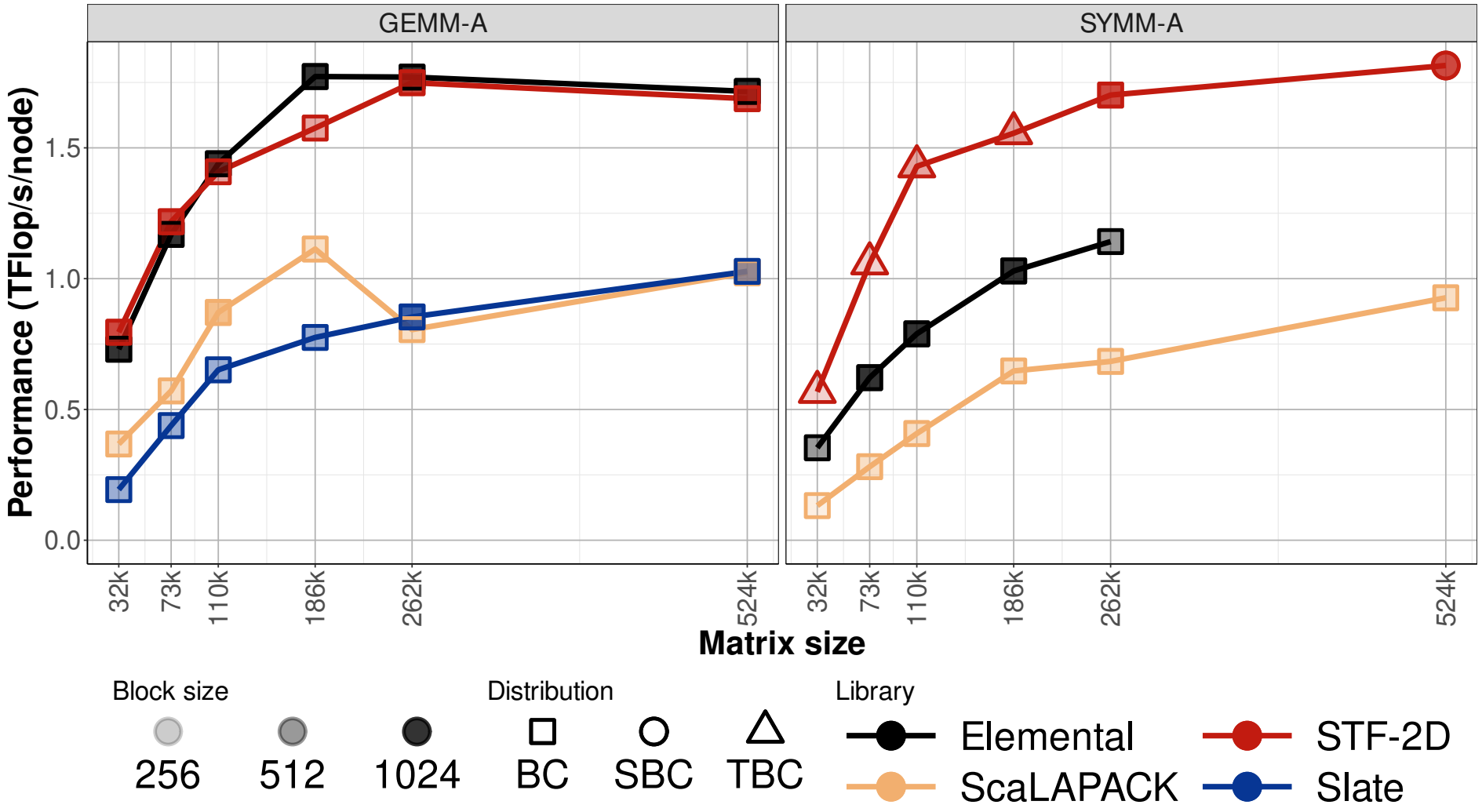
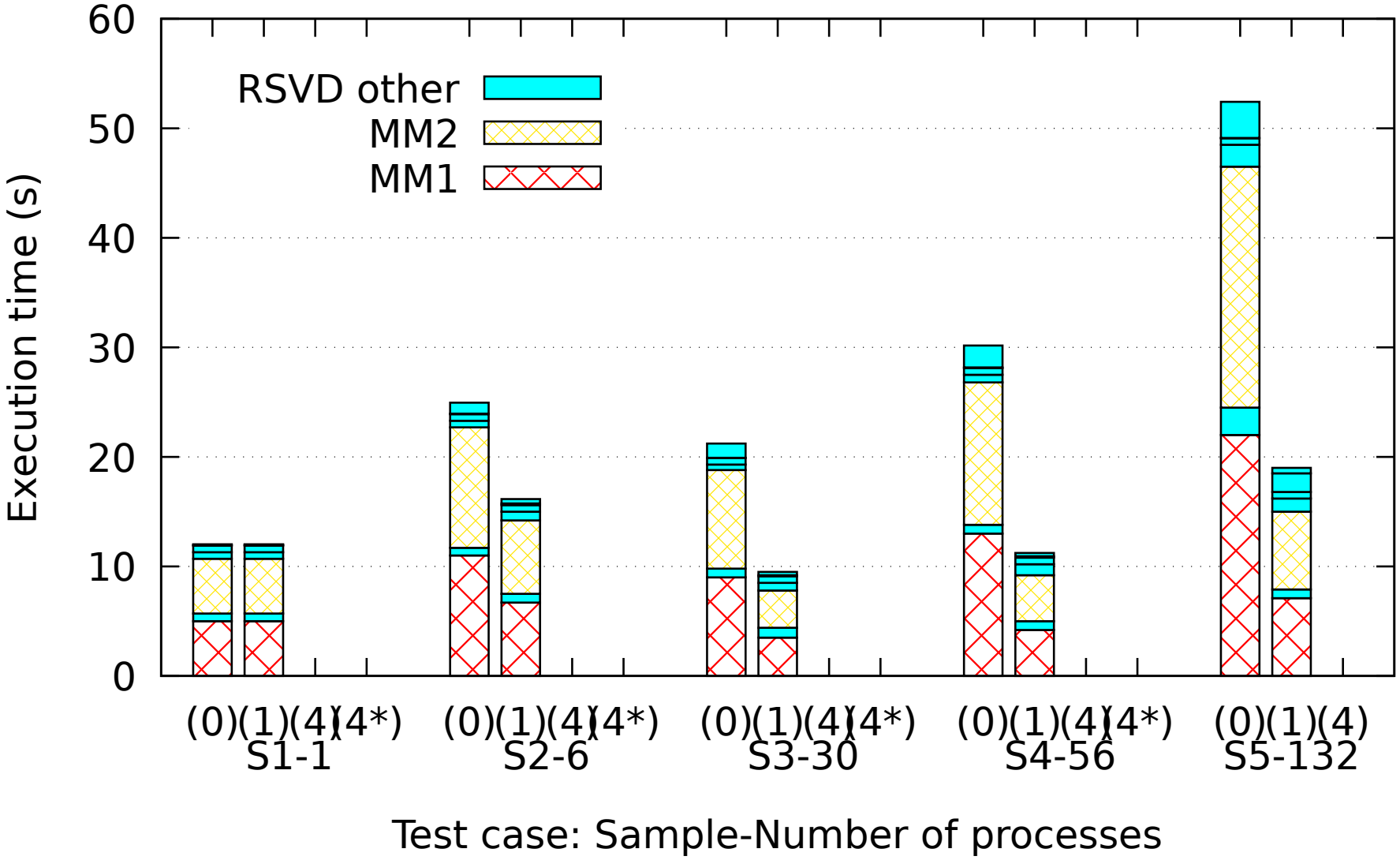


Performance of RSVD-MDS using our improved SYMM



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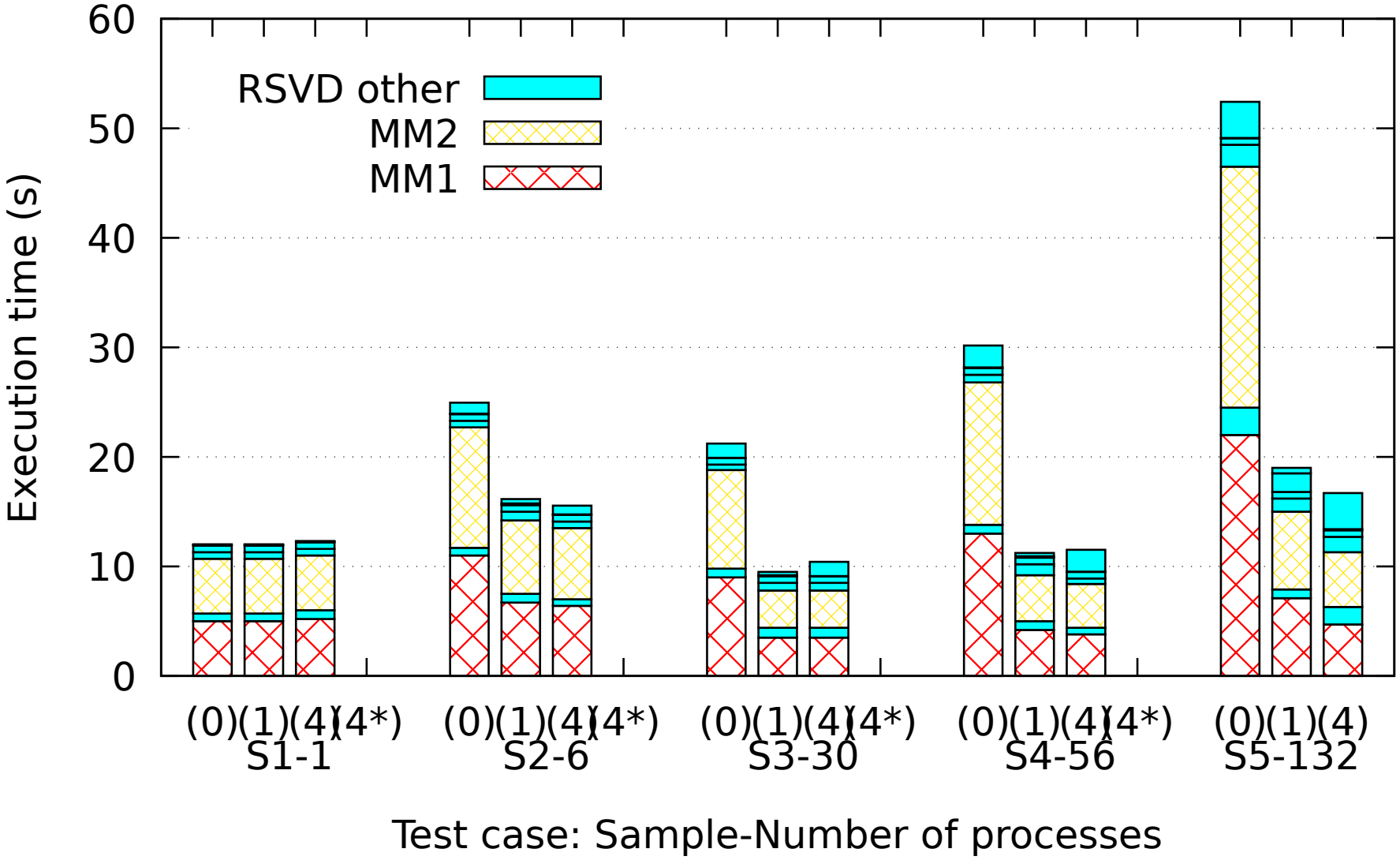

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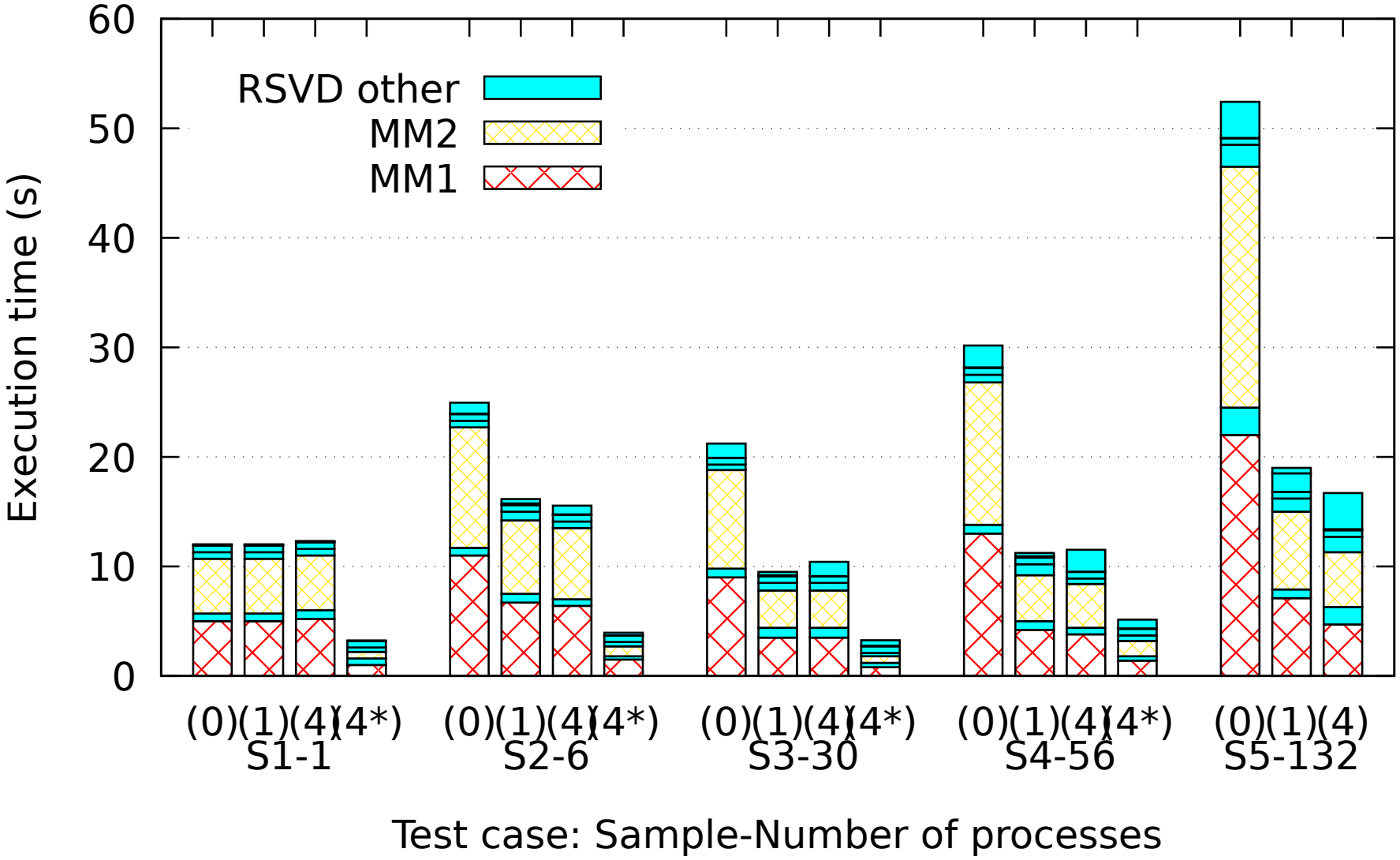
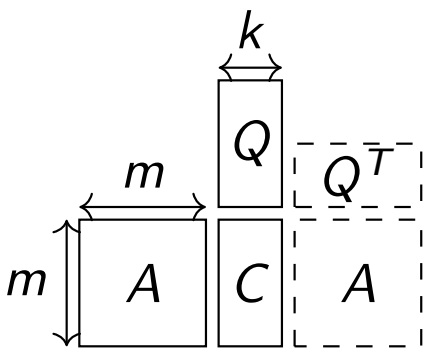


Summary of matrix multiplication improvements

- We implemented an A-Stationary GEMM implementation into Chameleon
- Using Abstract programming models we implemented a SYMM competitive with GEMM
- This work was accepted in IPDPS 2023

Reminder on random projection

- Approximate $A \approx AQQ^T$ (Halko et al., 2011; Martinsson, 2016)
- Define $C = AQ$
- Compute $SVD(C) = U_C \Sigma V_C^T$
- Multiply by Q^T on the right to get $RSVD(A)$



Evaluation of the symmetry of AQQ^T

A: symmetric
AQQ^T: ?

$$\begin{aligned} A &= A_{sym} + A_{skew} \\ A_{sym} &= \frac{A + A^T}{2} \\ A_{skew} &= \frac{A - A^T}{2} \end{aligned}$$

Evaluation of the symmetry of AQQ^T

A: symmetric
AQQ^T: ?

$$A = A_{sym} + A_{skew}$$

$$A_{sym} = \frac{A + A^T}{2}$$

$$A_{skew} = \frac{A - A^T}{2}$$

$$\chi = \frac{||A_{skew}||}{||A||}$$

Evaluation of the symmetry of AQQ^T

Skew-symmetry induced by the projection

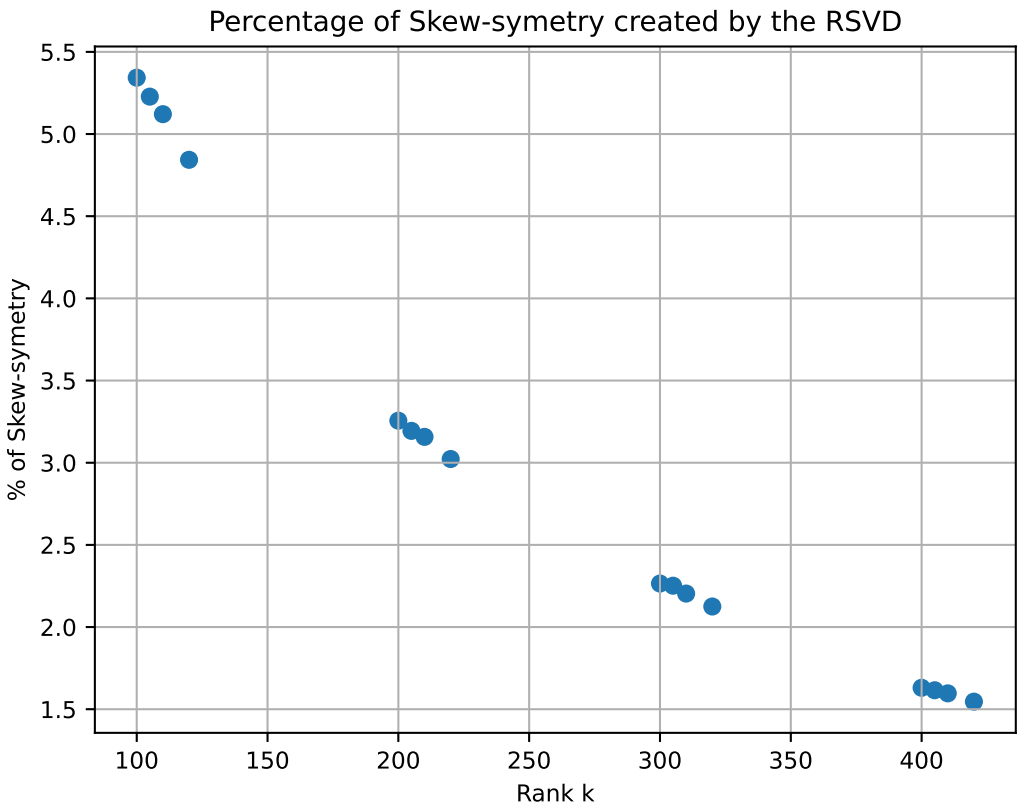
A: symmetric
AQQ^T: ?

$$A = A_{sym} + A_{skew}$$

$$A_{sym} = \frac{A + A^T}{2}$$

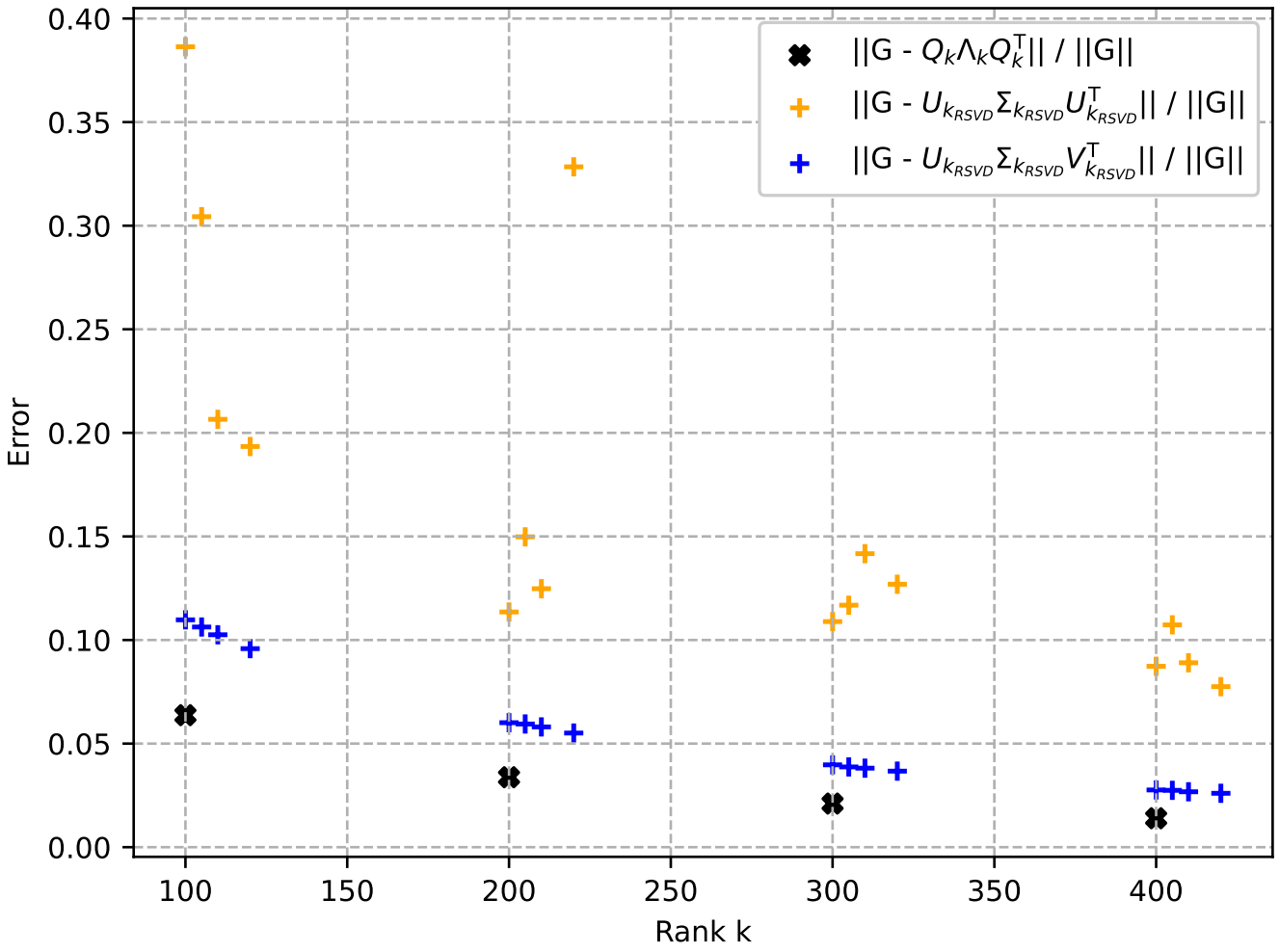
$$A_{skew} = \frac{A - A^T}{2}$$

$$\chi = \frac{||A_{skew}||}{||A||}$$



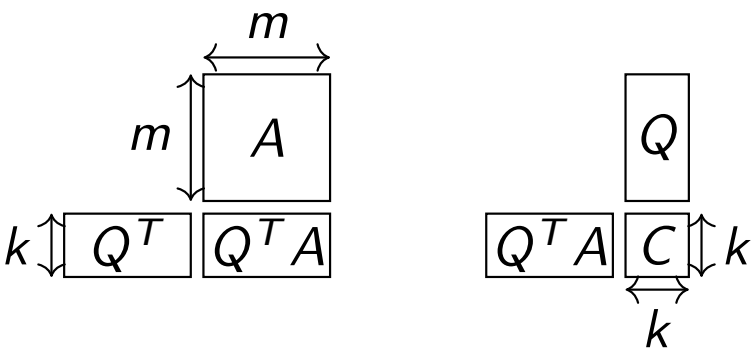
Impact on MDS

Impact of the loss of symmetry on MDS.



Proposed solution : double projection

- Approximate $A \approx QQ^T AQQ^T$ (Halko et al., 2011; Martinsson, 2016)
- Define $C = Q^T AQ$
- Compute $sEVD(C) = Q_C \Lambda Q_C^T$
- Multiply by Q on both sides to get RsEVD(A)



Summary

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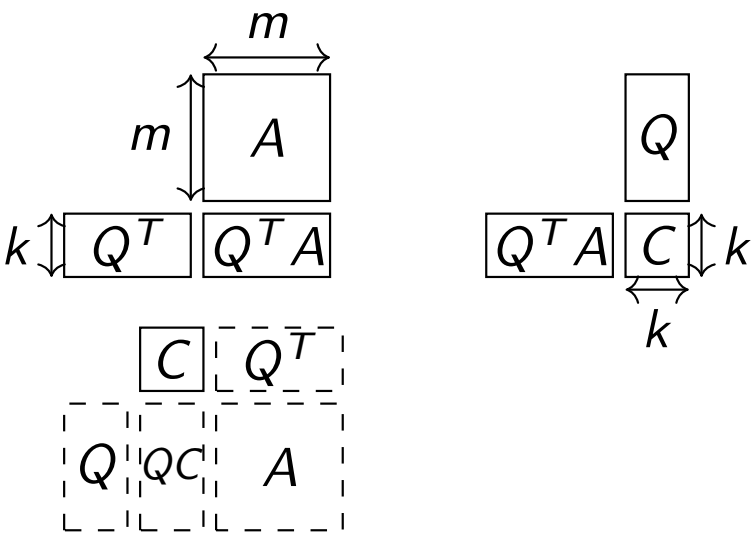
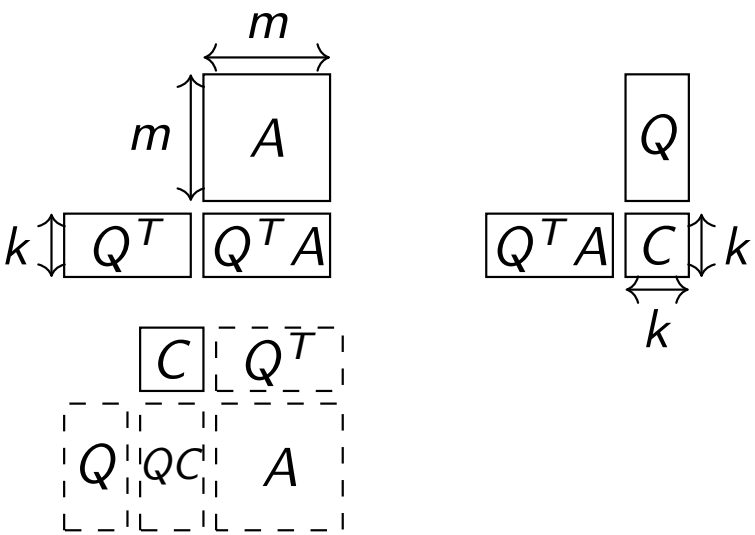
- Define $C = Q^T AQ$
- Compute $sEVD(C) = Q_C \Lambda Q_C^T$
- Multiply by Q on both sides to get RsEVD(A)



Summary

Proposed solution : double projection

- Approximate $A \approx QQ^T AQQ^T$ (Halko et al., 2011; Martinsson, 2016)
- Define $C = Q^T AQ$
- Compute $sEVD(C) = Q_C \Lambda Q_C^T$
- Multiply by Q on both sides to get RsEVD(A)



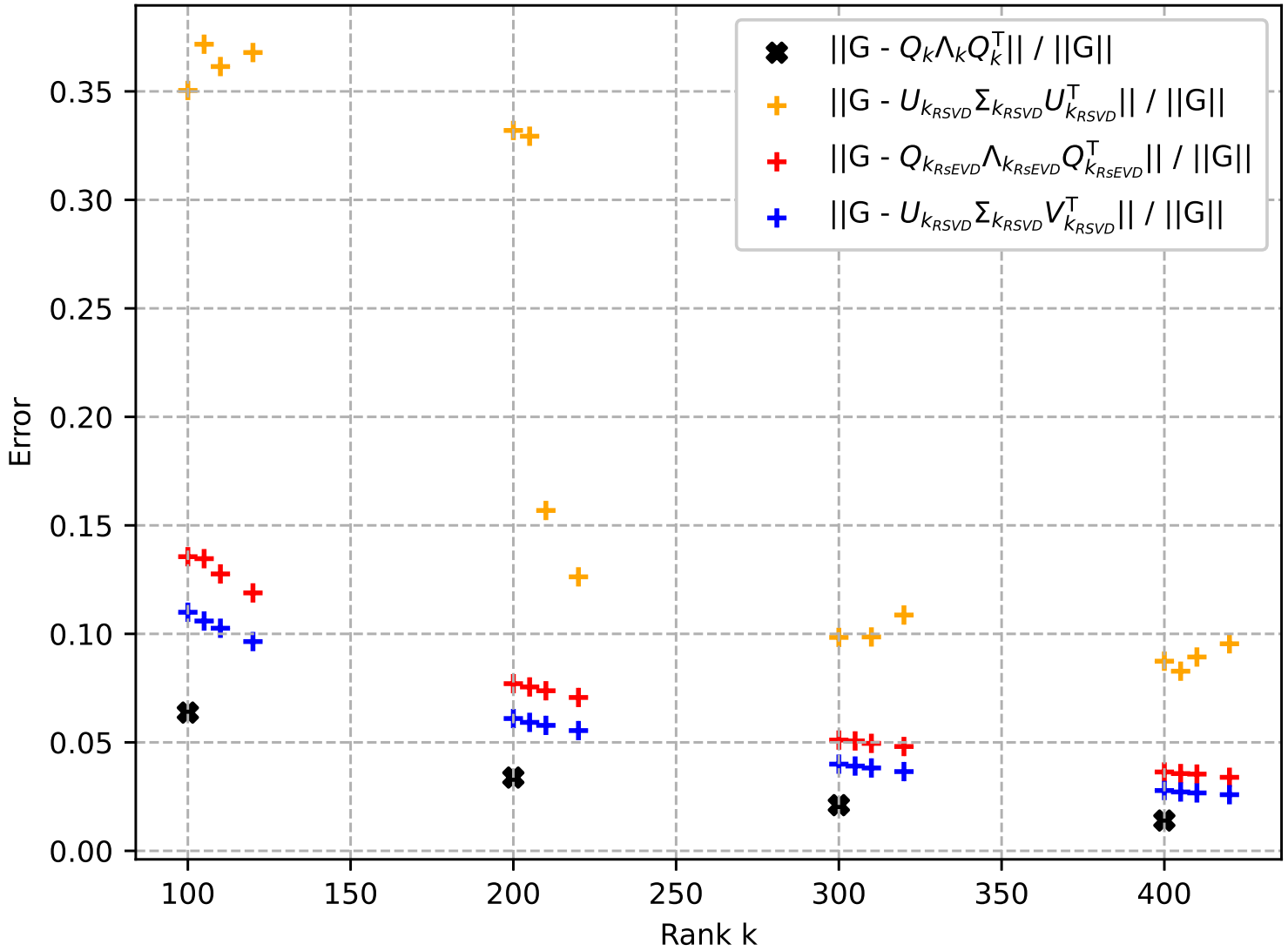
Summary

	Error	Symmetry preserving
RSVD	ϵ	?
REVD	2ϵ	✓

(Halko et al., 2011; Martinsson, 2016)

Evaluation of the error

Comparison of the different random projection error in the context of MDS



Experimental setup

About the test

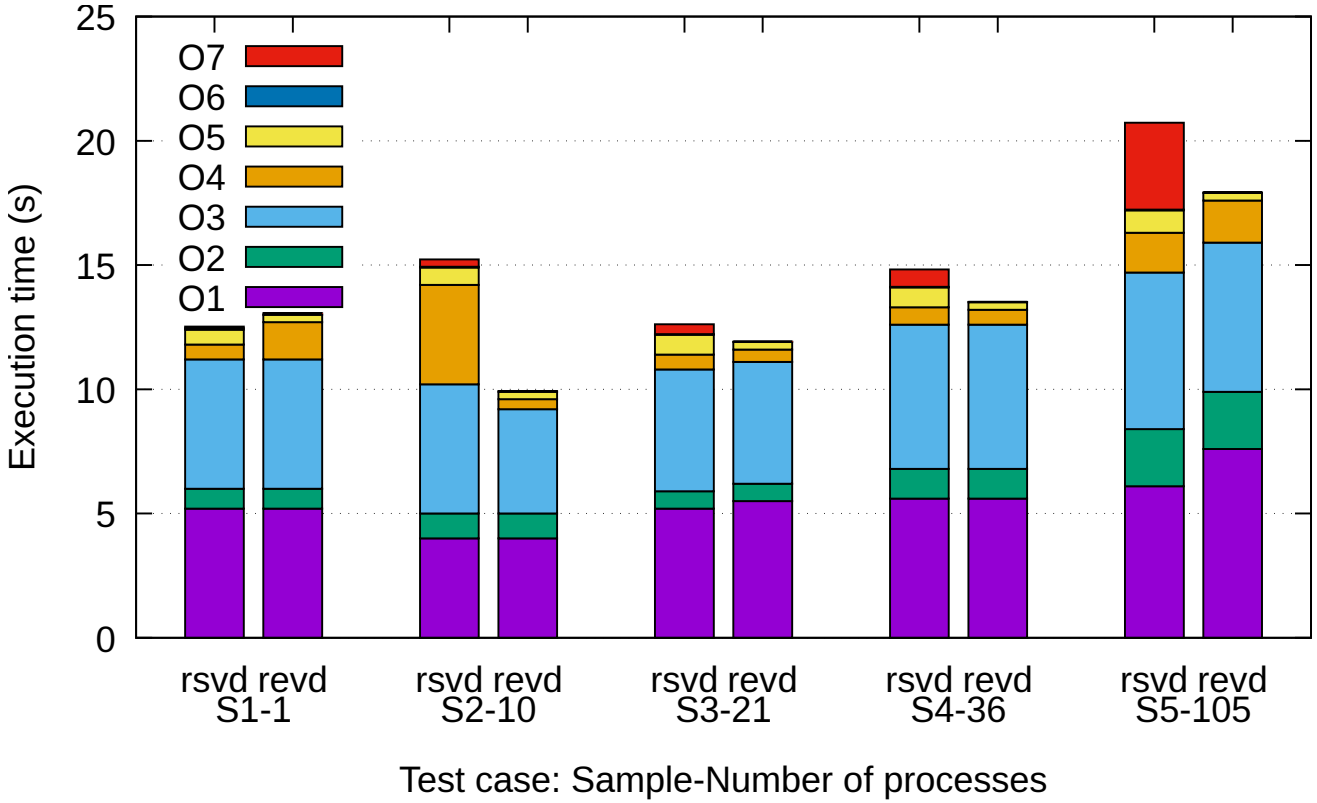
- Sample size ranges from 99, 954 (S1) to 1,043,192 (S5).
- MM1 and MM2 are presented as O1 and O3 respectively.

Machine used

- Results obtained on the Jean Zay supercomputer.
- Each node has 192 GB of memory
- Each node has two 20 cores Cascade Lake 6248 @ 2.5 GHz processors (40 cores per node)
- Used between 1 and 105 nodes

Work done in collaboration with Florent Pruvost

Performance results



Contributions

Improving the Matrix-Matrix multiplication step (Accepted into IPDPS 2023)

- Implementation of an A-Stationary GEMM into Chameleon
- Design and implementation of a A-Stationary SYMM with performance similar to GEMM

Task-based RsEVD for MDS

- Numerical study of RSVD and RsEVD
- HPC implementation of RsEVD and performance analysis

Conclusion

On matrix-Matrix Multiplication

- We showed that we can reduce the communication volume of SYMM to the same amount as the communication volume of GEMM.
- Using abstract programming models, we can seamlessly implement the different data distributions presented.
- We showed that our approach allowed us to reach performance for SYMM roughly matching those of GEMM, while only having to use half the amount of memory.
- We implemented our code in the context of an RSVD-MDS application and showed significant performance improvements.

On RsEVD for MDS

- We showed RSVD in the context of MDS may lead to error in the projection
- We presented an HPC RsEVD-MDS code and showed that it achieves similar performance than the RSVD-MDS approach.

Thank you for listening

Any questions ?

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"HPC scalable ecosystem"

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