High Performance Computing Project

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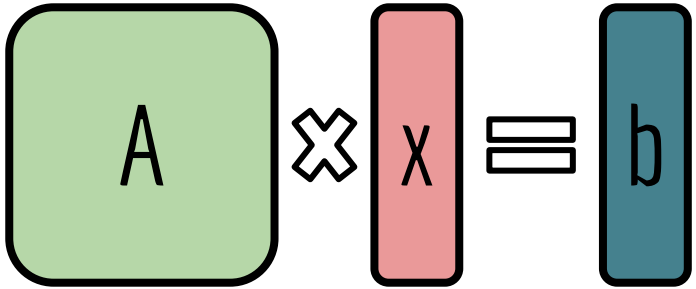
Context

Goal: Solve



GEMM (GEneral Matrix Multiplication)

$$C = \alpha A \times B + \beta C$$

C has size of $M \times N$ A has size of $M \times K$ B has size of $K \times N$

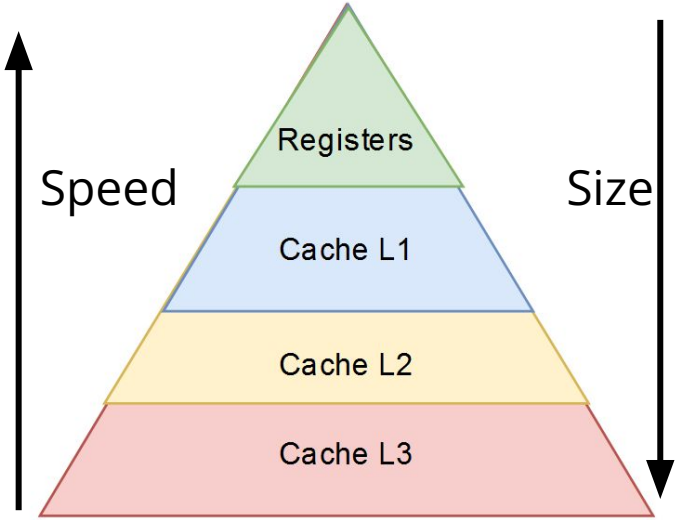
GEMM : Kernels

The goal of a kernel is to be do an operation very efficiently on a small subset of the problem.

We just have to divide our big problem into multiple smaller ones and apply the kernel on them.

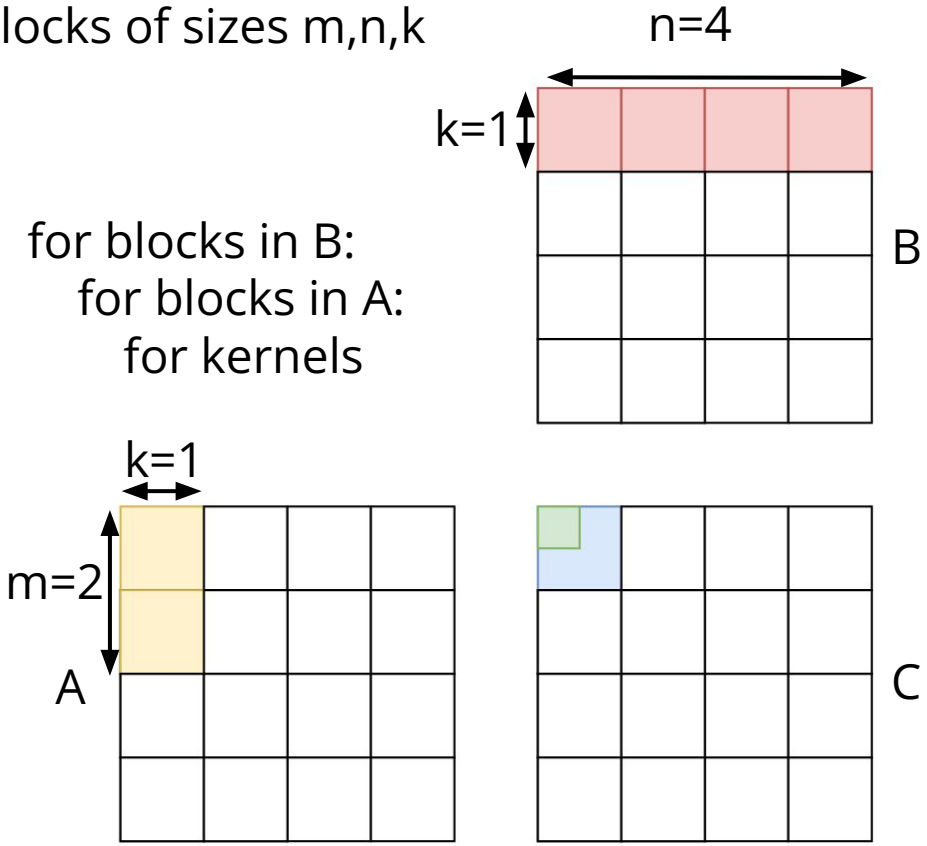
GEMM : Blocks

Goal : Maximize cache utilization



Blocks of sizes m,n,k

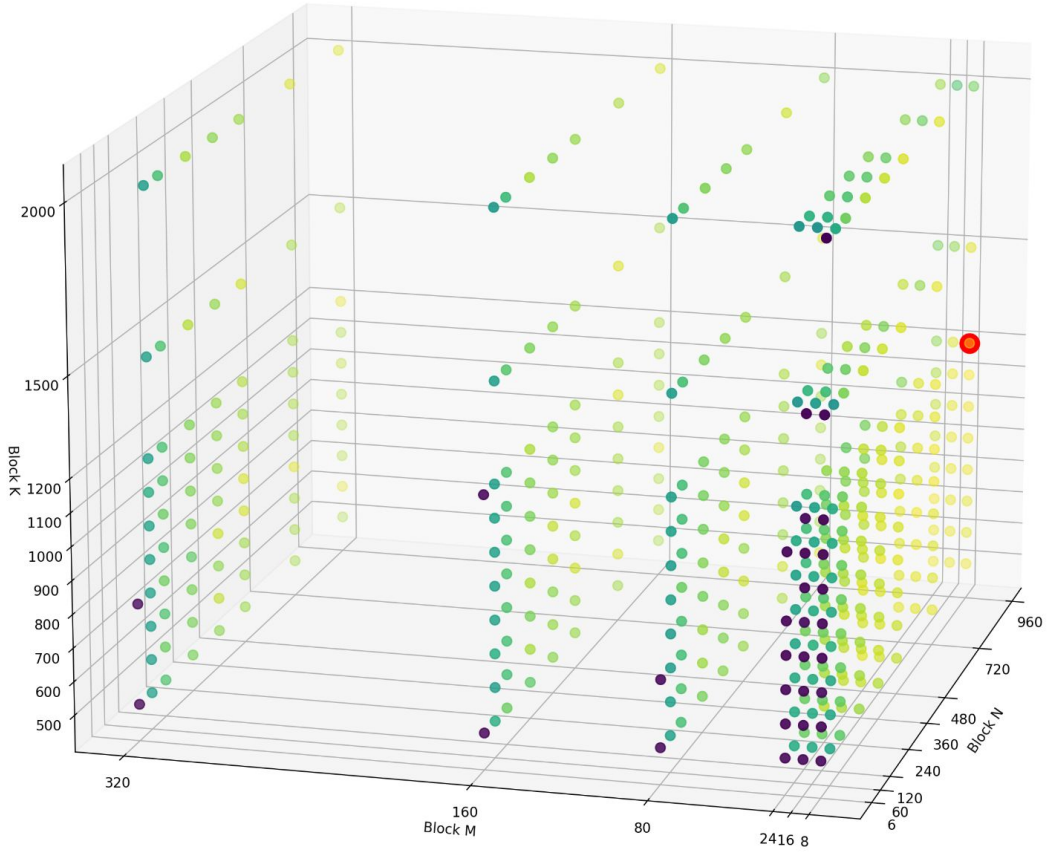
```
for blocks in B:
    for blocks in A:
        for kernels
```



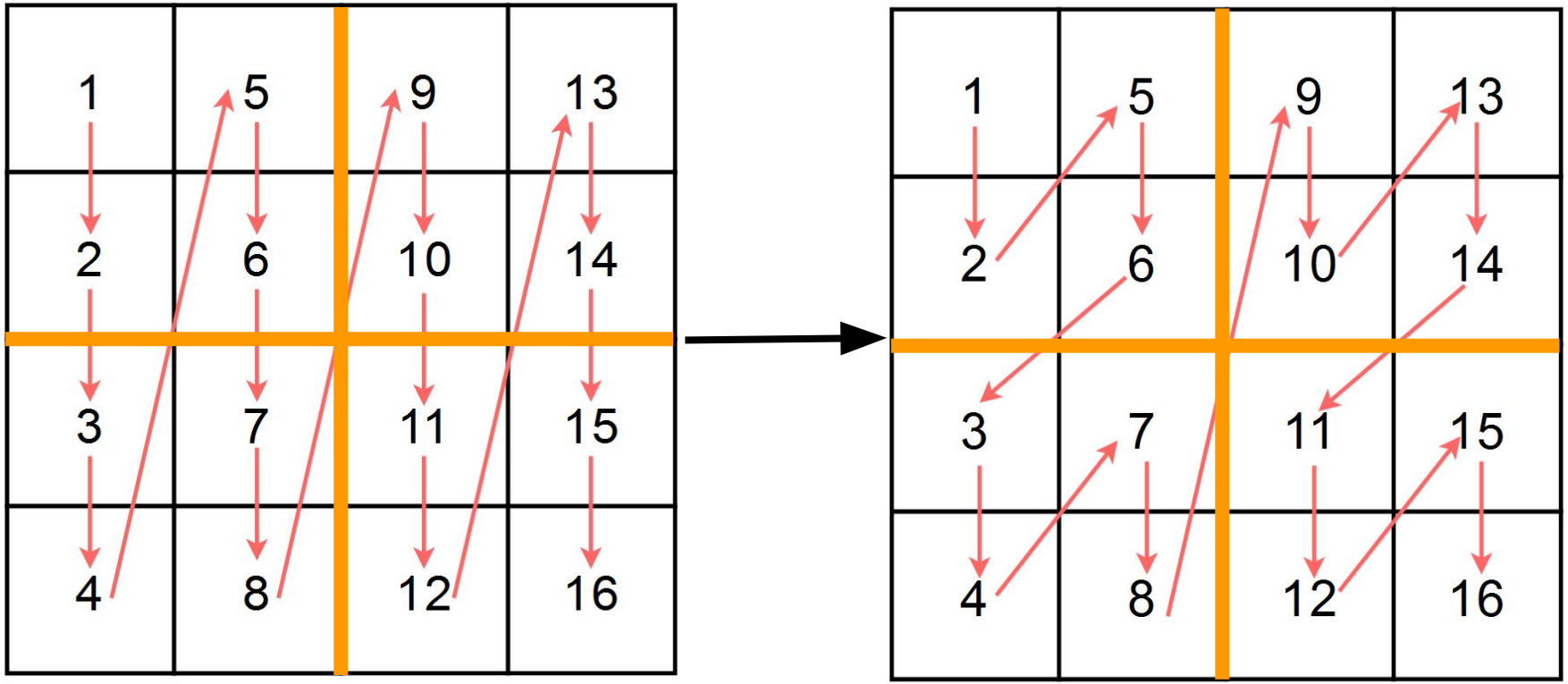
GEMM : Blocks

In practice slightly tweaked block sizes gives better performances

M=8, K=1200, N=960

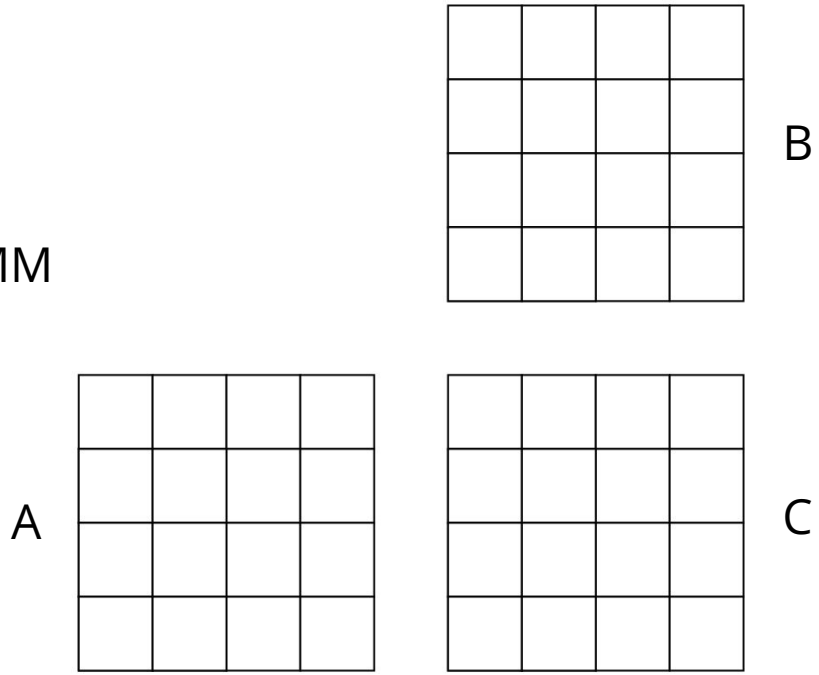


GEMM : Packing to optimize the memory layout



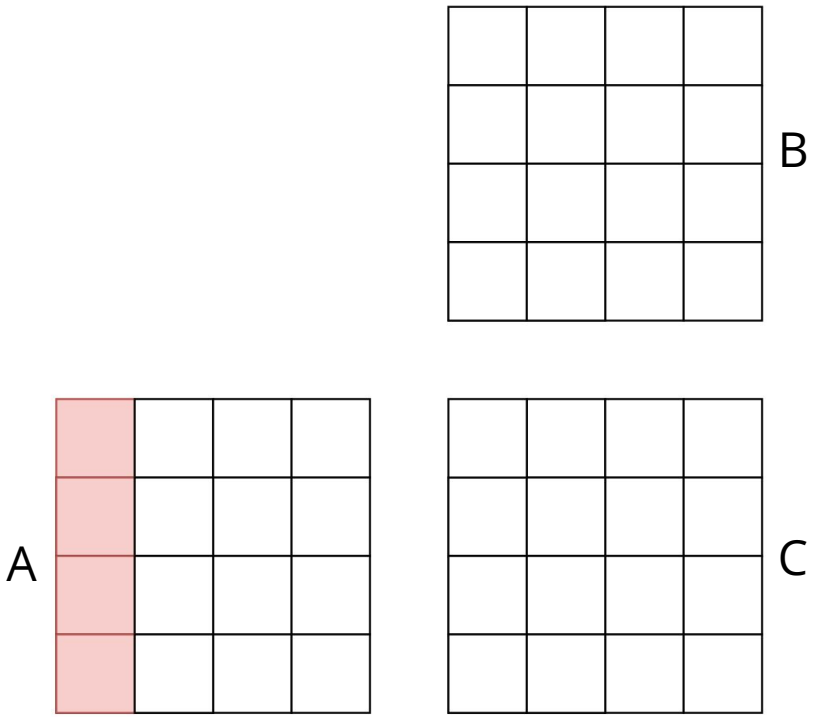
GEMM : Kernels

4*4 kernel for GEMM

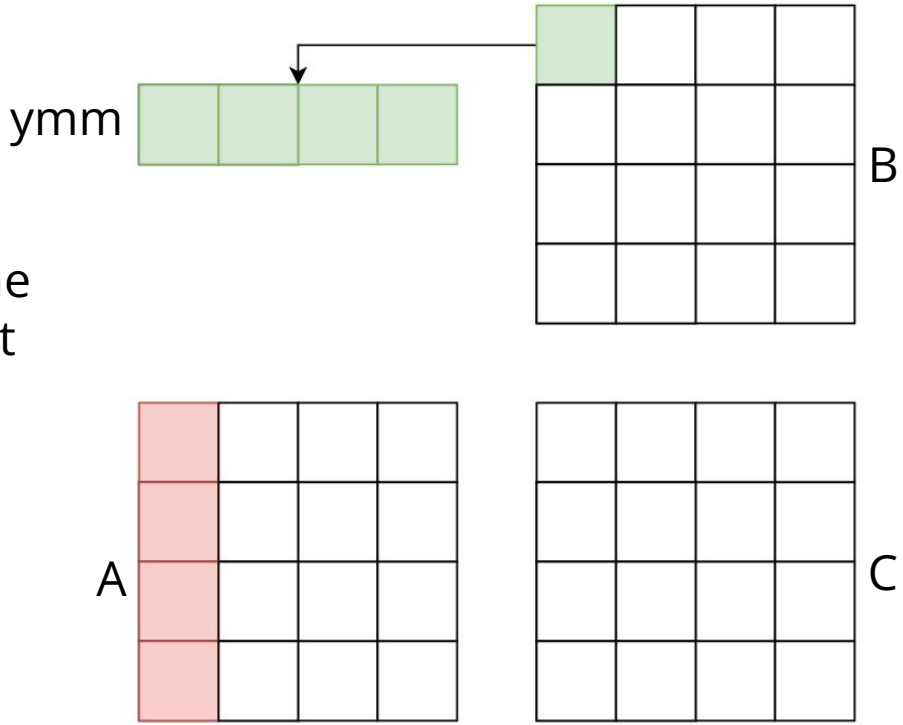


GEMM : Kernels

Load first column of A



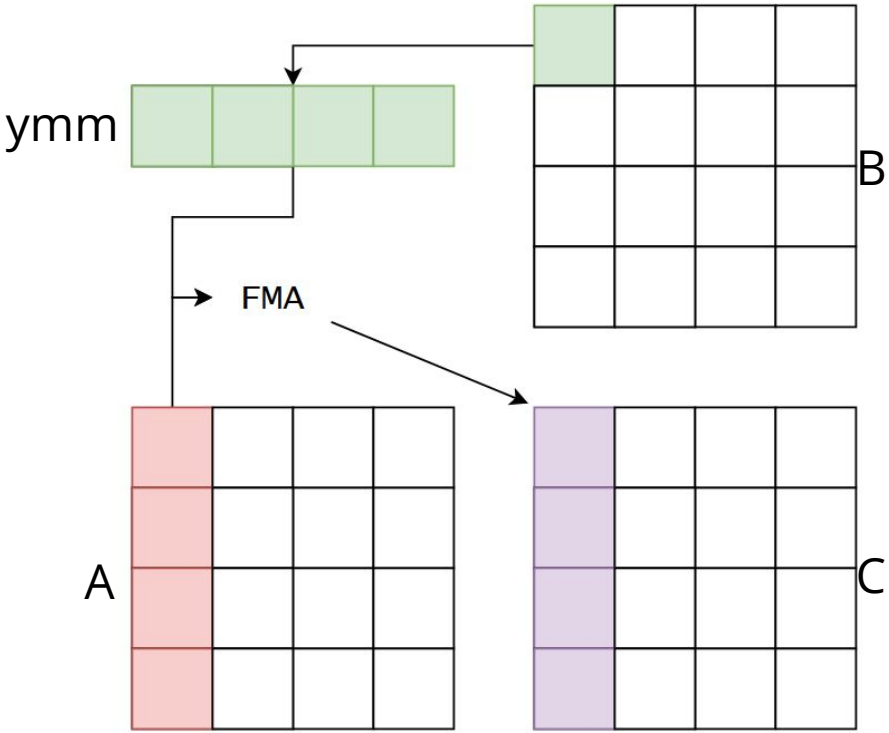
GEMM : Kernels



Fill a register with the first value of the first row of B

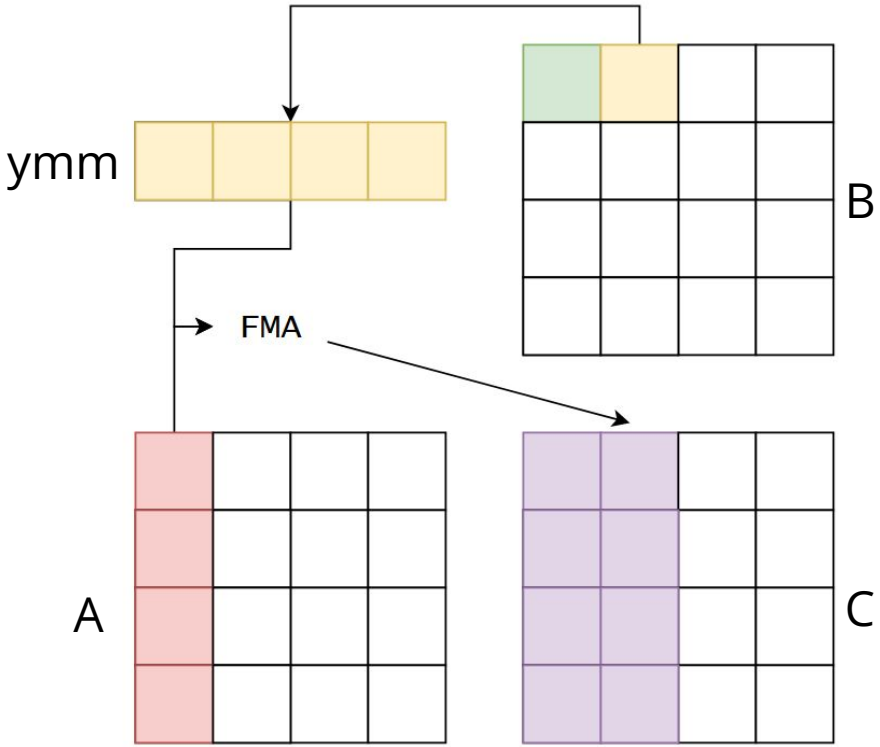
GEMM : Kernels

FMA the 2 registers into C



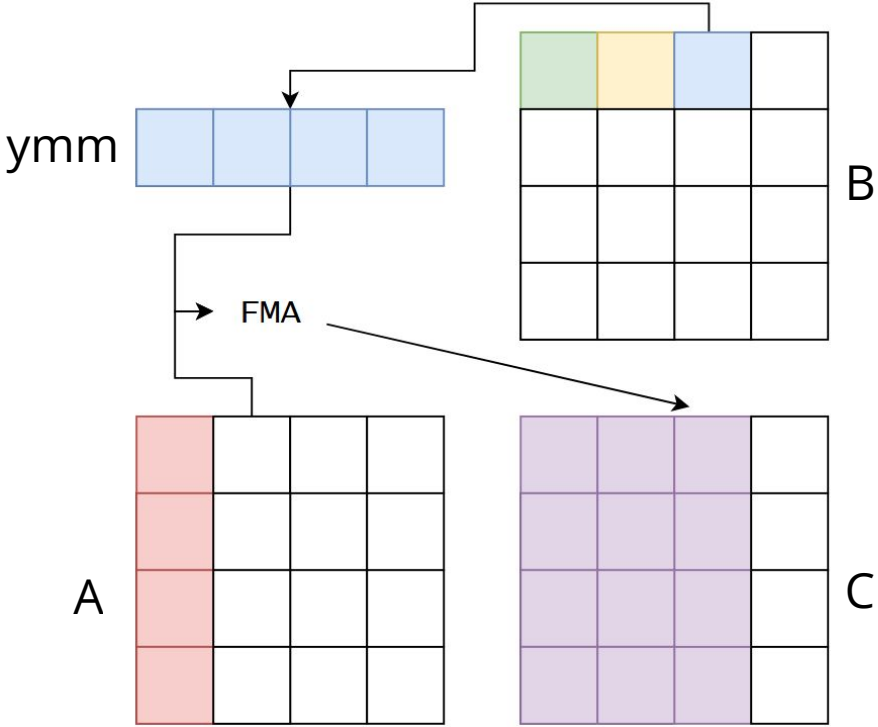
GEMM : Kernels

Get the next value in the row of B



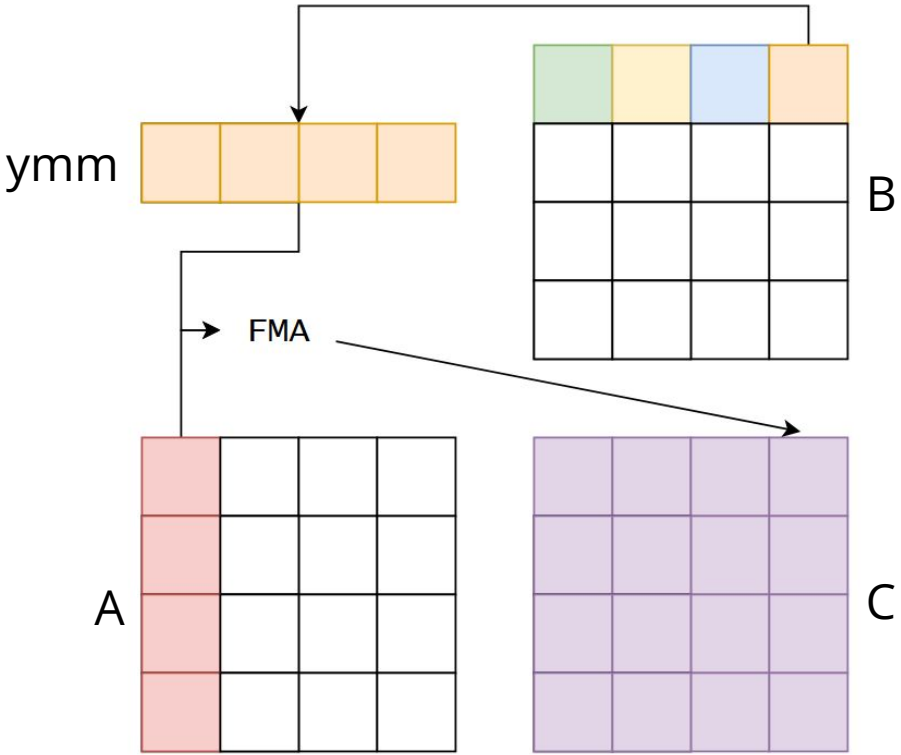
GEMM : Kernels

Again



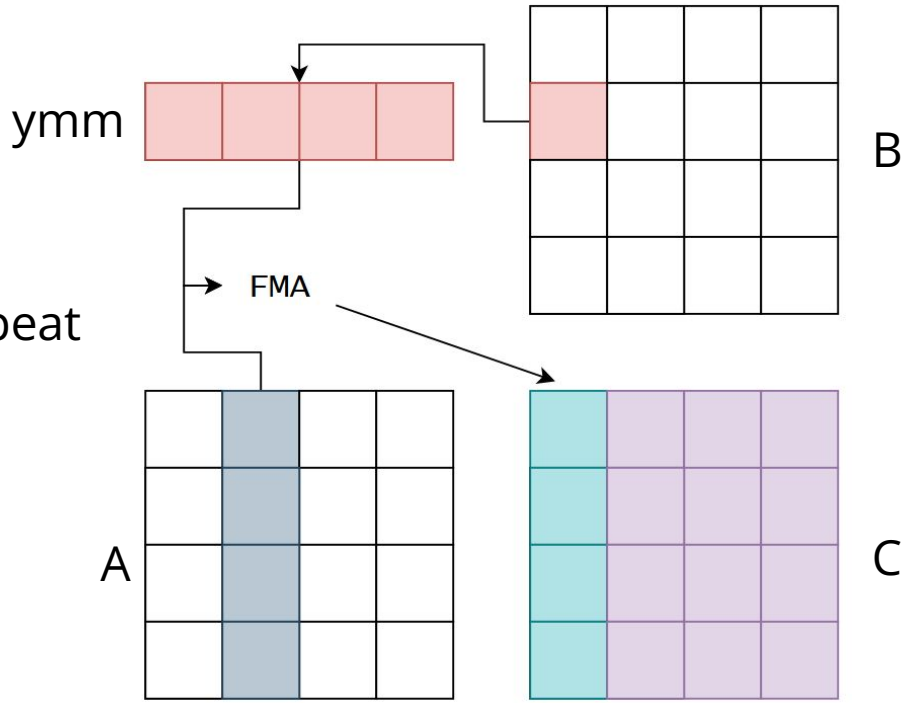
GEMM : Kernels

And again



GEMM : Kernels

Then load the next column of A and repeat



GEMM : Kernels

The kernel should maximise the amount of registers used.
Haswell processors have 16 ymm registers.
We chose a kernel m*n of size 8*6 :

- 1 register for the B value
- 2 registers for the column of A (8 elements)
- 12 registers to load C (48 elements)
    - 15 out of 16 register used

GEMM : Kernels

"We don't care about implementation details"

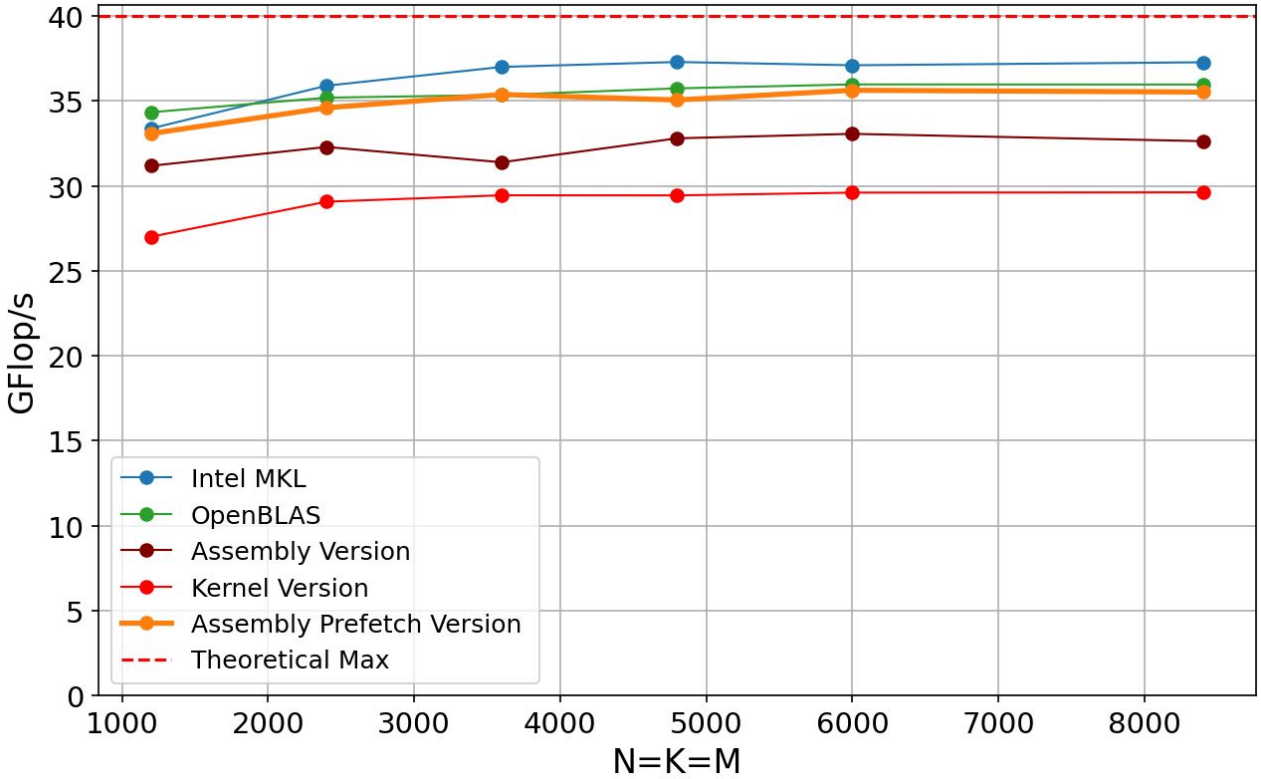
In this case, we **DO** care : that's what makes the difference

Not shown :
Unroll x4

```
kernel8x6_asm:
.LOOP_K:
    # Load A matrix
    vmovapd (%rdi), %ymm12  # Load A[0:3]
    vmovapd 32(%rdi), %ymm13 # Load A[4:7]
    prefetcht0 512(%rdi) # Prefetch 2 4-unroll iterations ahead for A
    prefetcht0 576(%rdi)
    prefetcht0 640(%rdi)
    prefetcht0 704(%rdi)

    prefetcht0 384(%rsi) # Prefetch 2 4-unroll iterations ahead for B
    prefetcht0 432(%rsi)
    prefetcht0 480(%rsi)
    prefetcht0 528(%rsi)

    # Broadcast B matrix elements and multiply
    vbroadcastsd (%rsi), %ymm14              # Broadcast B[0]
    vbroadcastsd 8(%rsi), %ymm15             # Broadcast B[1]
    vfmadd231pd %ymm12, %ymm14, %ymm0        # C += A * B[0]
    vfmadd231pd %ymm13, %ymm14, %ymm1
    vfmadd231pd %ymm12, %ymm15, %ymm2
    vfmadd231pd %ymm13, %ymm15, %ymm3

    vbroadcastsd 16(%rsi), %ymm14            # Broadcast B[2]
    vbroadcastsd 24(%rsi), %ymm15            # Broadcast B[3]
    vfmadd231pd %ymm12, %ymm14, %ymm4
    vfmadd231pd %ymm13, %ymm14, %ymm5
    vfmadd231pd %ymm12, %ymm15, %ymm6
    vfmadd231pd %ymm13, %ymm15, %ymm7
    # Repeat for the other columns ...
```

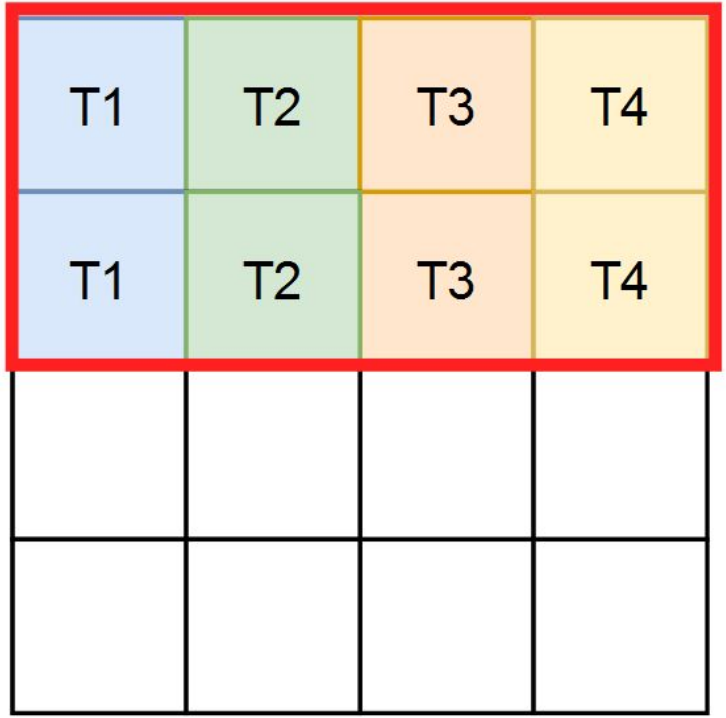
GEMM : Performances

- Reaches **performance equivalent to OpenBLAS** and 95% of IntelMKL
- Using assembly allow explicit control over register spilling
- Works for every kind of matrices
- A and/or B transposed doesn't affect performances



GEMM : Multithreading

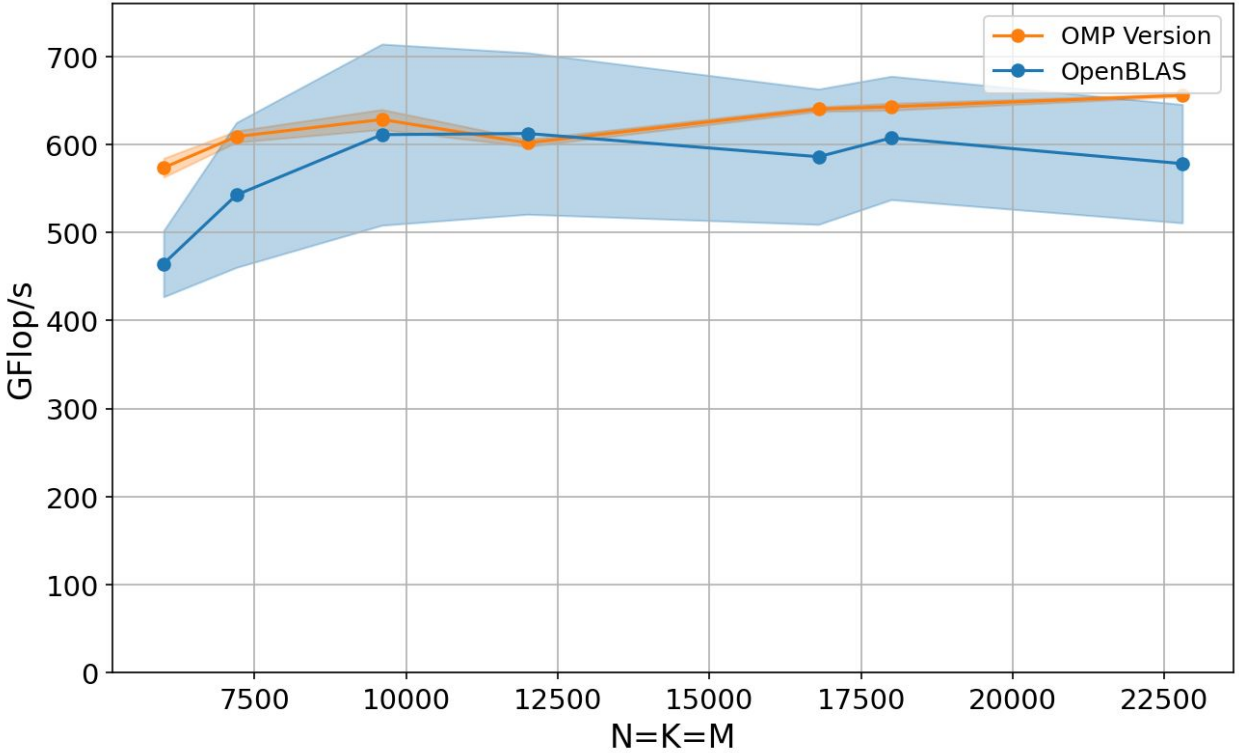
- Multithreading using OpenMP
- Dispatch threads to each compute a group of kernels inside a block
- Each thread have the same amount of work



GEMM : Multithreading

Our implementation :

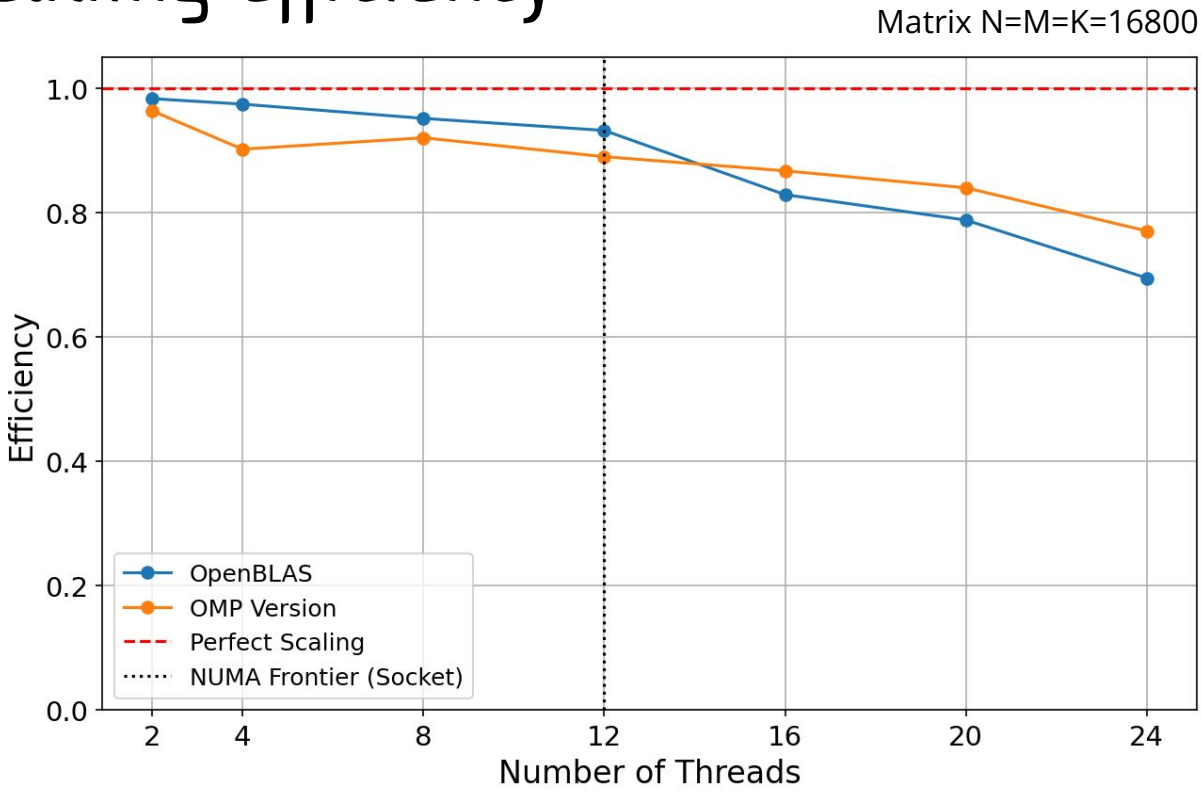
- Beats OpenBLAS with 650 GFlop/s
- Achieves a small standard deviation (8 GFlop/s vs 75 GFlop/s)



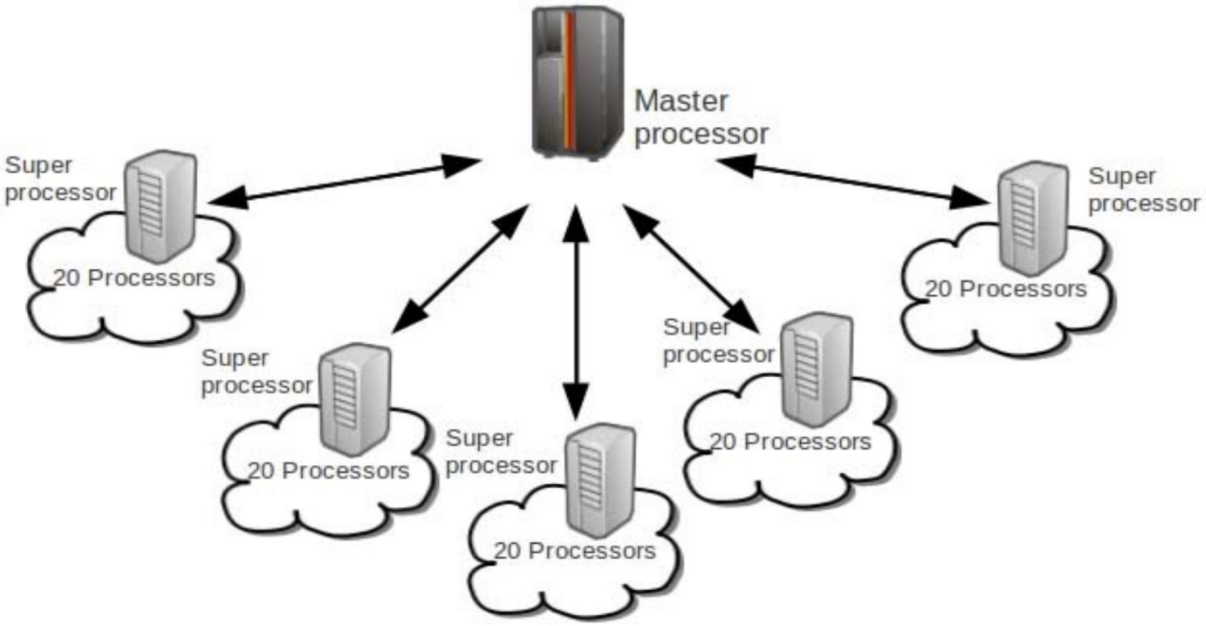
Block sizes : M=768,K=900,N=11520

GEMM : Multithreading efficiency

- Better efficiency than OpenBLAS for threads >= 16
- OpenBLAS impacted by NUMA
- Could achieve better efficiency



GEMM : Distributed version



GEMM : Giving data to each node

1	2	1	2
3	4	3	4
1	2	1	2
3	4	3	4

1	2	1	2
3	4	3	4
1	2	1	2
3	4	3	4

1	2	1	2
3	4	3	4
1	2	1	2
3	4	3	4

GEMM : Giving data to each node

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3	4	3	4
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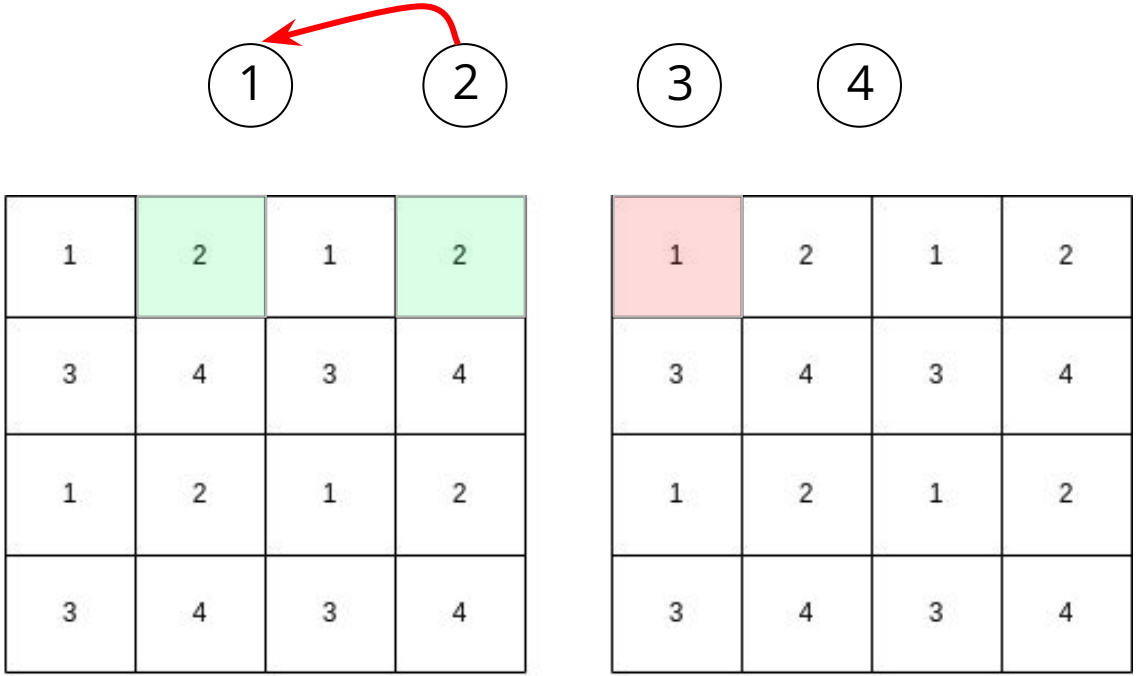
3	4	3	4
1	2	1	2
3	4	3	4

GEMM : Giving data to each node



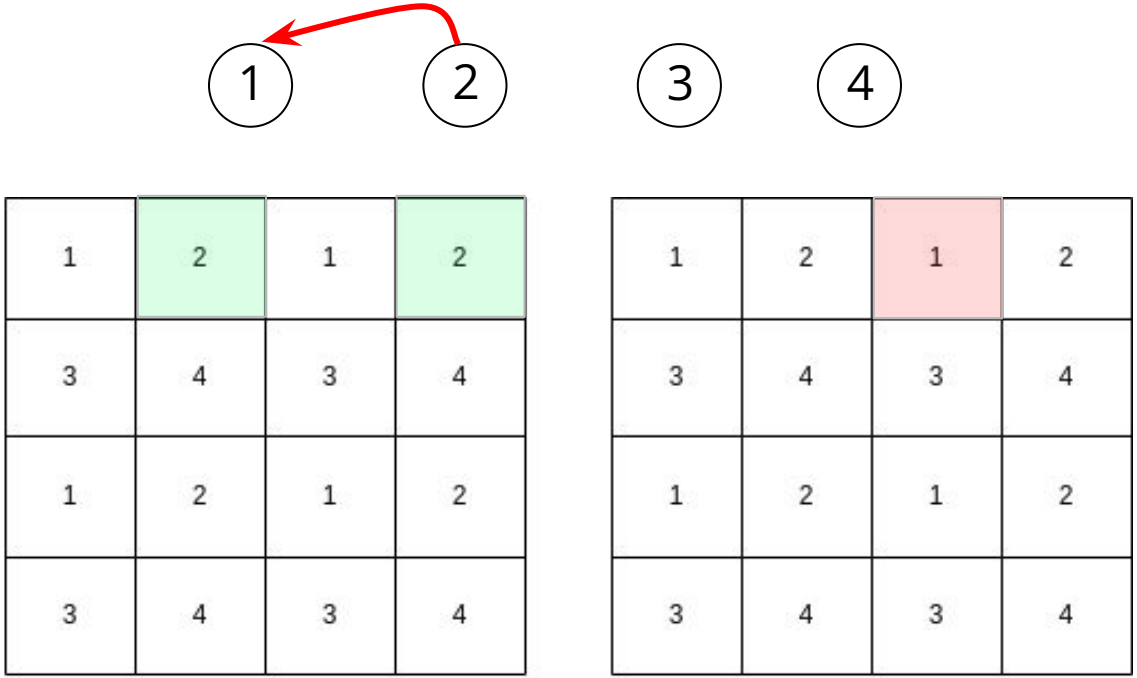
GEMM : Giving data to each node

1	2	1	2
3	4	3	4
1	2	1	2
3	4	3	4

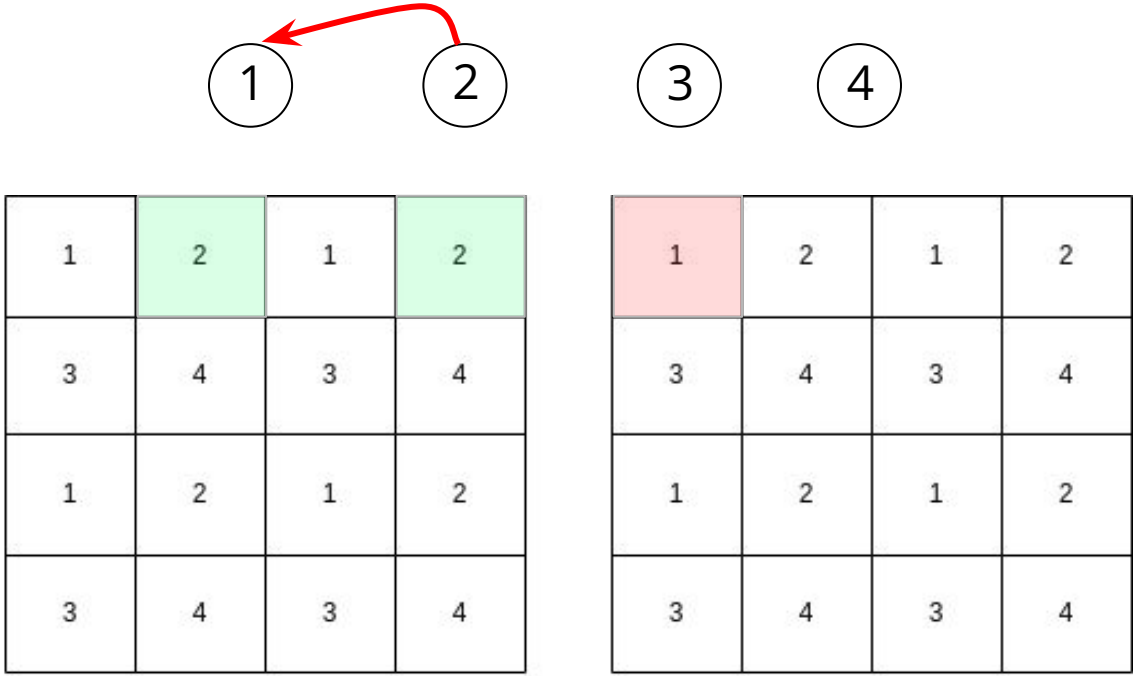
1	2	1	2
3	4	3	4
1	2	1	2
3	4	3	4

1	2	1	2
3	4	3	4
1	2	1	2
3	4	3	4

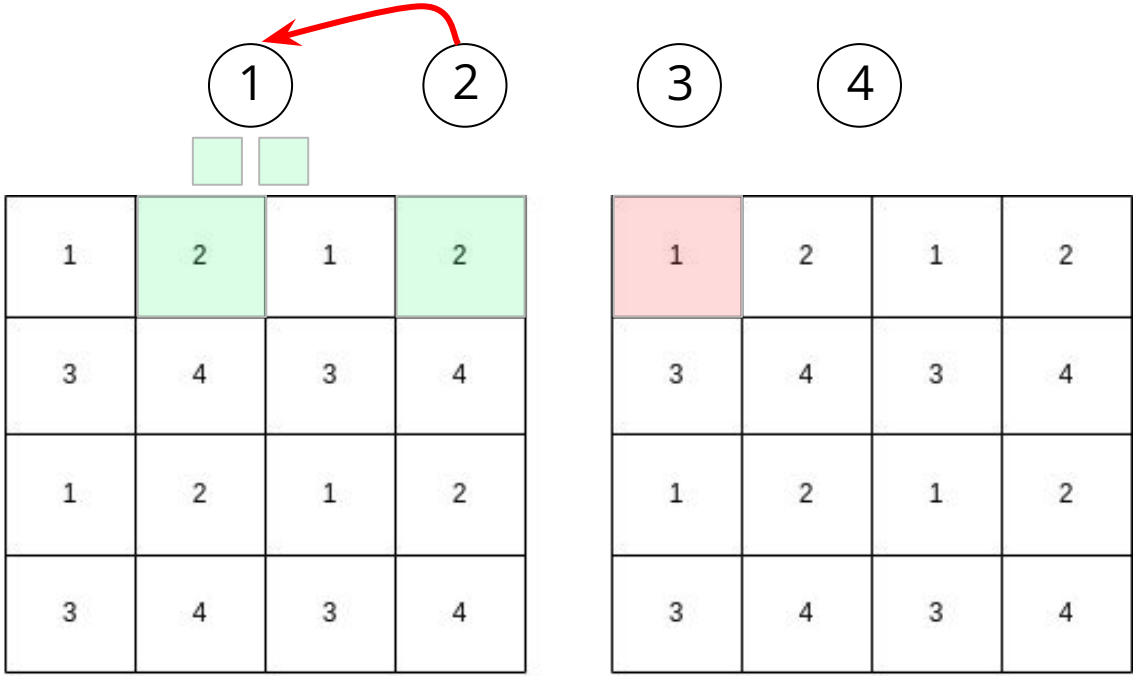
GEMM : Giving data to each node



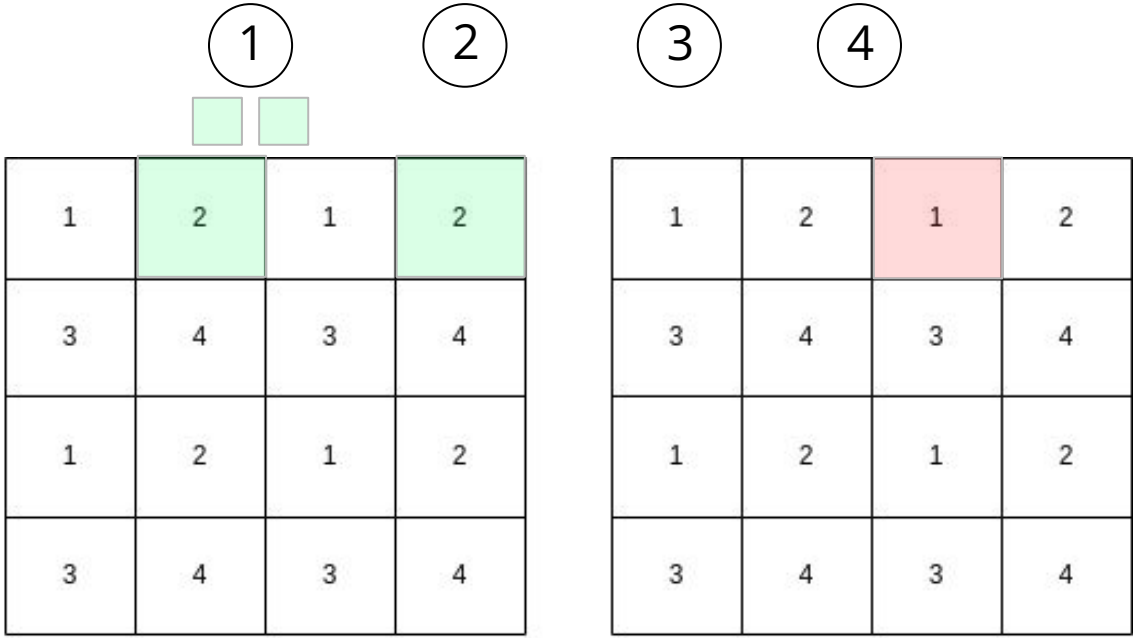
GEMM : Giving data to each node



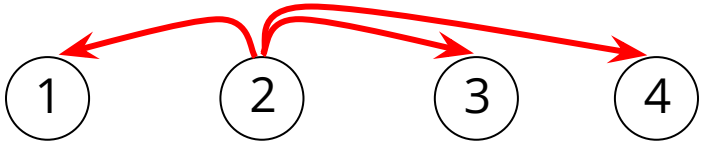
GEMM : Giving data to each node



GEMM : Giving data to each node



GEMM : Giving data to each node



1	2	1	2
3	4	3	4
1	2	1	2
3	4	3	4

1	2	1	2
3	4	3	4
1	2	1	2
3	4	3	4

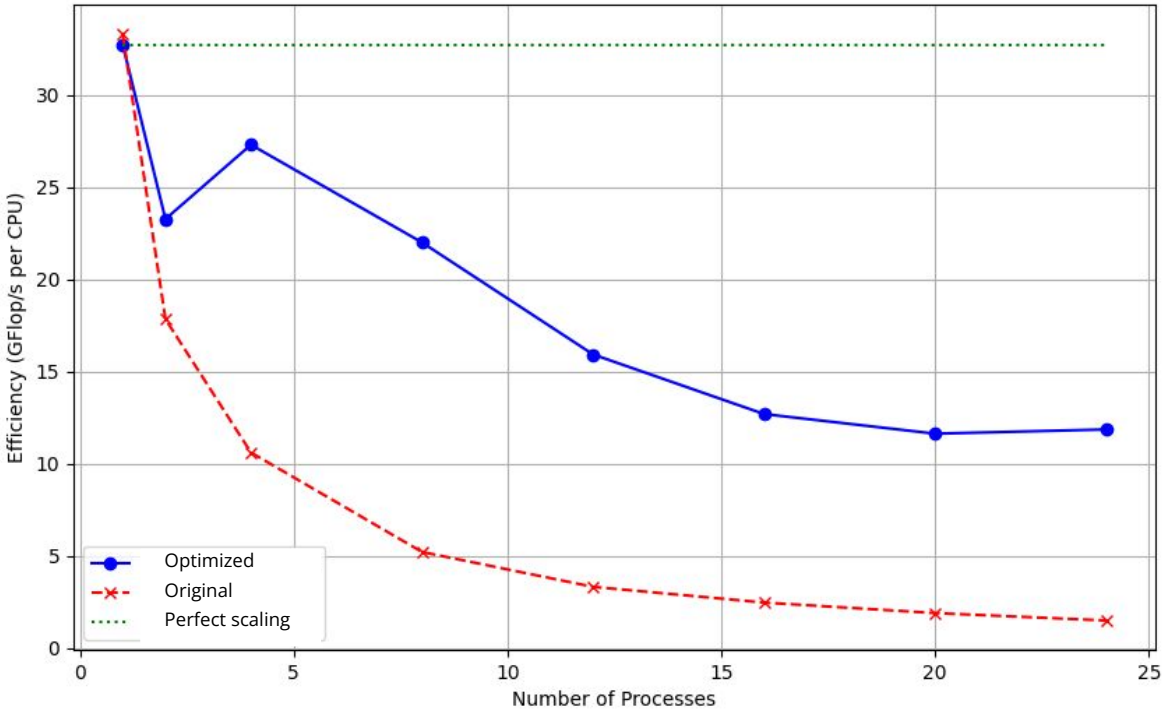
GEMM : Giving data to each node

1	2	1	2
3	4	3	4
1	2	1	2
3	4	3	4

1	2	1	2	(1,2)
3	4	3	4	(3,4)
1	2	1	2	(1,2)
3	4	3	4	(3,4)

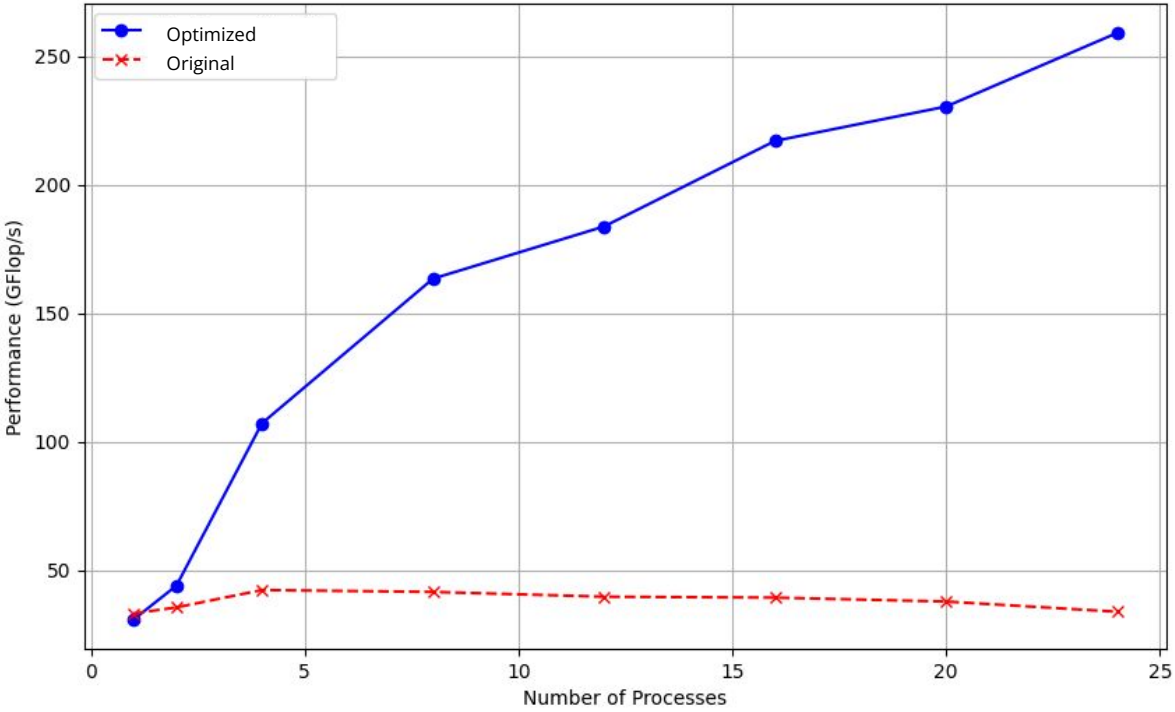
GEMM : MPI Results

Weak scalability, with each process computing 5000^3 flops



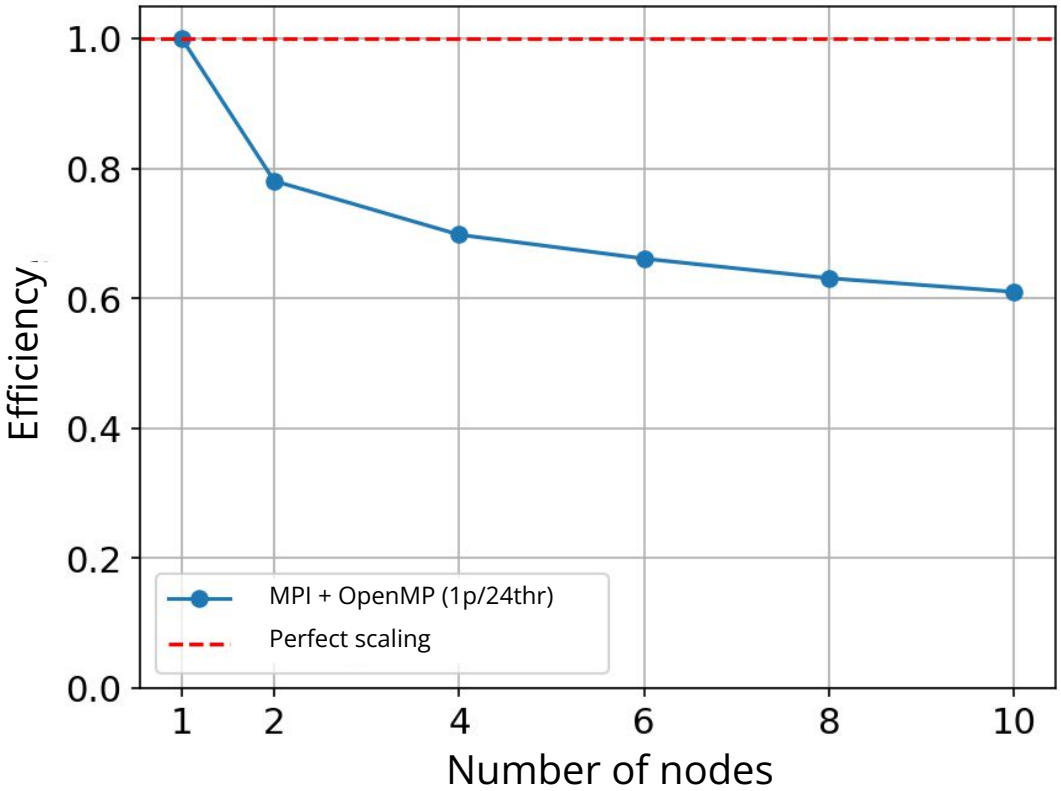
GEMM : MPI Results

Strong scalability for N = M = K = 13440 and b = 13440/n



GEMM : MPI + X weak scaling

MPI + OpenMP with 1 process per node with 24 threads each



GEMM : MPI + X

Peak performance on 10 nodes :
4 TFlop/s !!!

(Do not take this seriously, this is a joke)

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JUNE 2000

TOP 10 Sites for June 2000

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LIST STATISTICS

TREE MAPS

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TOP500 LIST (EXCEL)

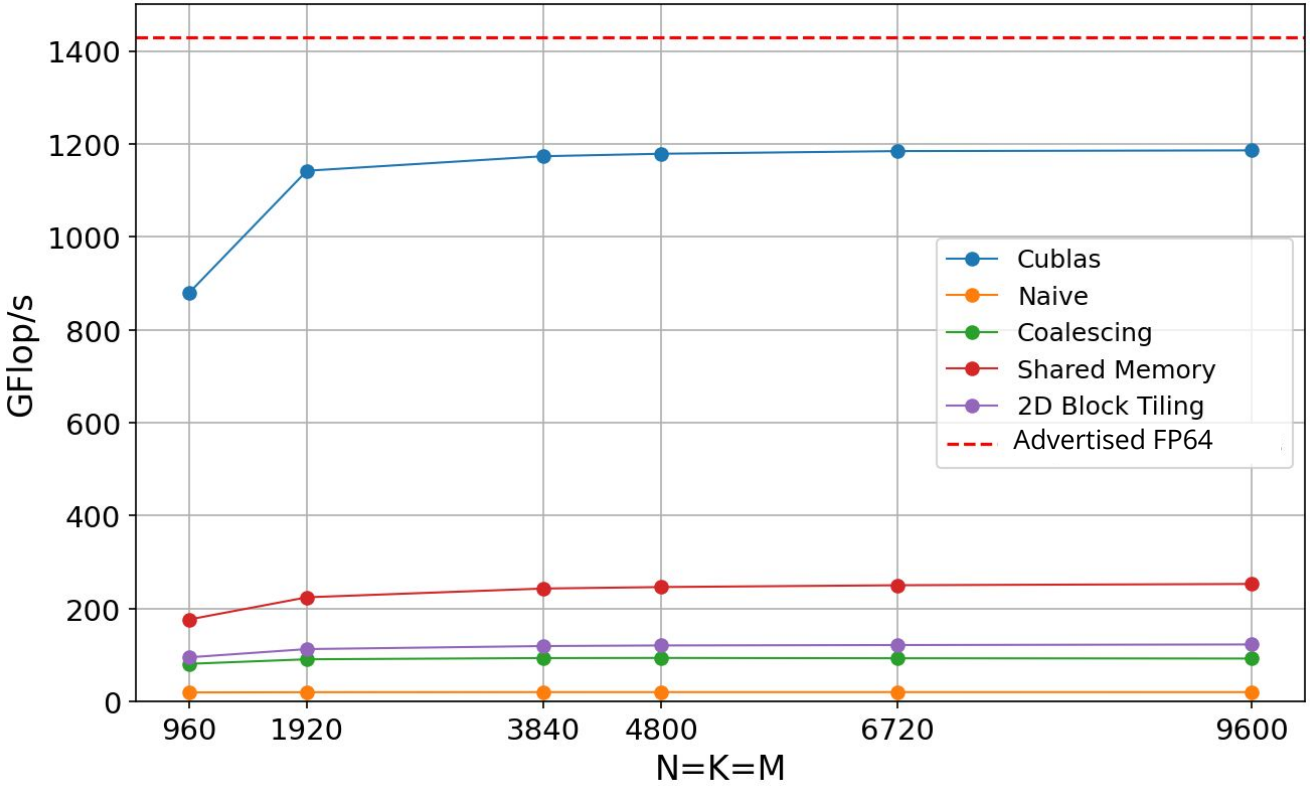
TOP500 POSTER

POSTER IN PDF

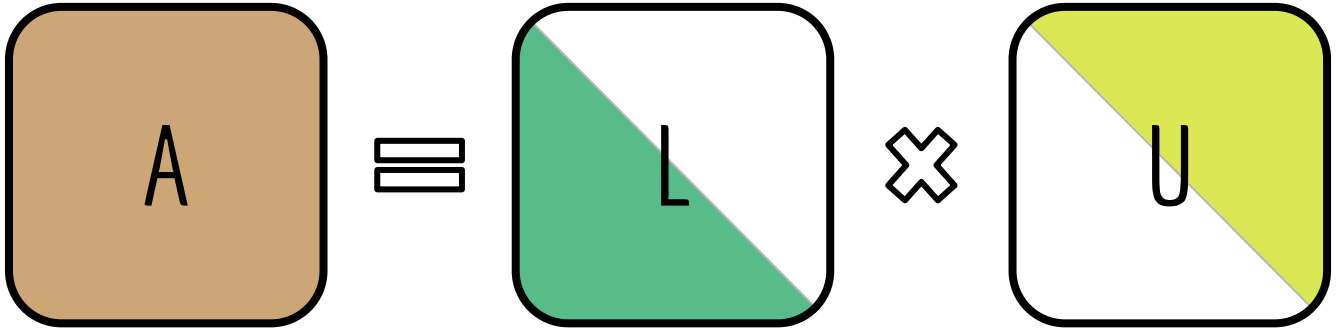
Rank	System	Cores	Rmax (GFlop/s)	Rpeak (GFlop/s)	Power (kW)
1	Plafrim, LAKA ENSEIRB-MATMECA France	240	4000.00	4000.00	
2	ASCI Blue-Pacific SST, IBM SP 604e, IBM Lawrence Livermore National Laboratory United States	5,808	2,144.00	3,856.50	
3	ASCI Blue Mountain, HPE Los Alamos National Laboratory United States	6,144	1,608.00	3,072.00	
4	SP Power3 375 MHz, IBM	1,336	1,417.00	2,004.00	

GEMM : CUDA

- Best version is shared memory with 250 GFlop/s
- 2D Block Tiling needs more work (each thread computes a sub-block of C)



GETRF (GEneral TRiangular Factorization)



A has size of M × N

Lower triangular

Upper triangular

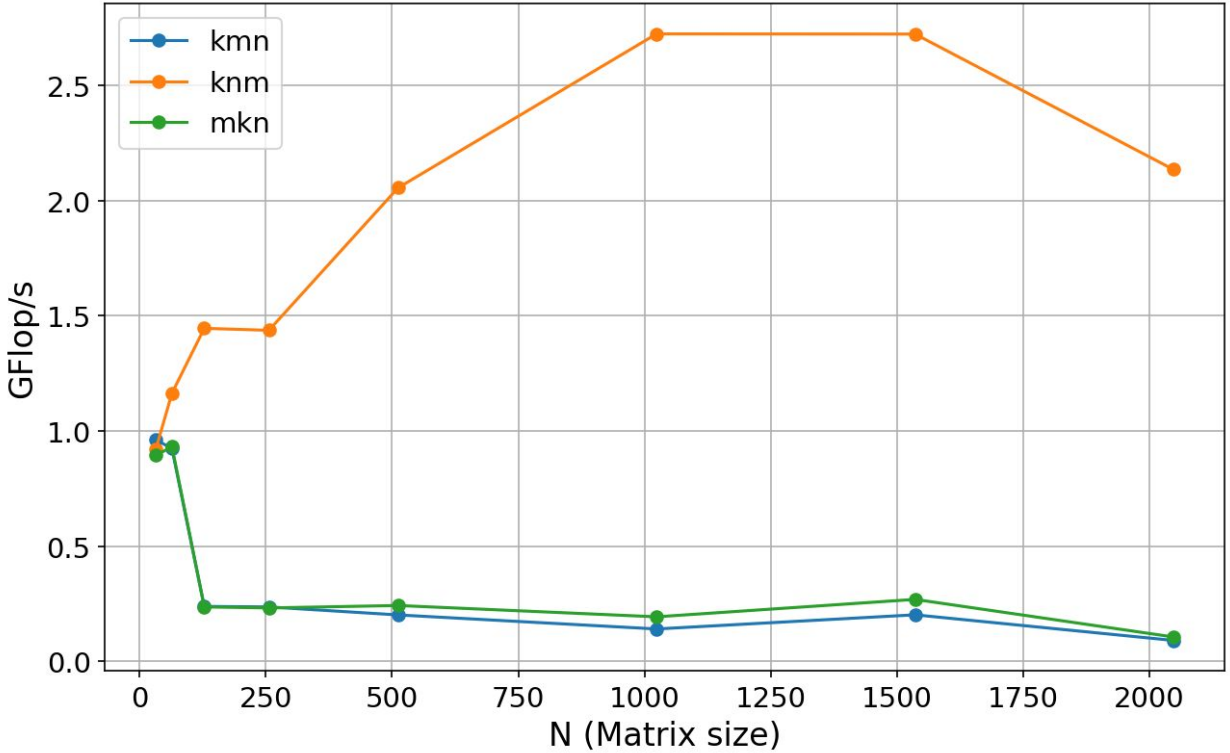
GETRF : Sequential Version

```
int dgetrf_seq(int M, int N, double *A)
{
    int m, n, k;

    for( k=0; k<K; k++ ) {
        for( m=k+1; m<M; m++ ) {
            A[m, k] = A[m, k]/A[k, k];
            for( n=k+1; n<N; n++ ) {
                A[m, n] = A[m, n] - A[m, k]*A[k, n];
            }
        }
    }
    return ALGONUM_SUCCESS; /* Success */
}
```

$$\begin{pmatrix} 1 & 7 & 3 & 4 & 9 \\ 2 & 3 & 5 & 2 & 2 \\ 4 & 6 & 8 & 6 & 6 \\ 9 & 3 & 4 & 7 & 1 \\ 1 & 8 & 0 & 6 & 3 \end{pmatrix}$$

GETRF : Sequential Version (Loop Orders)

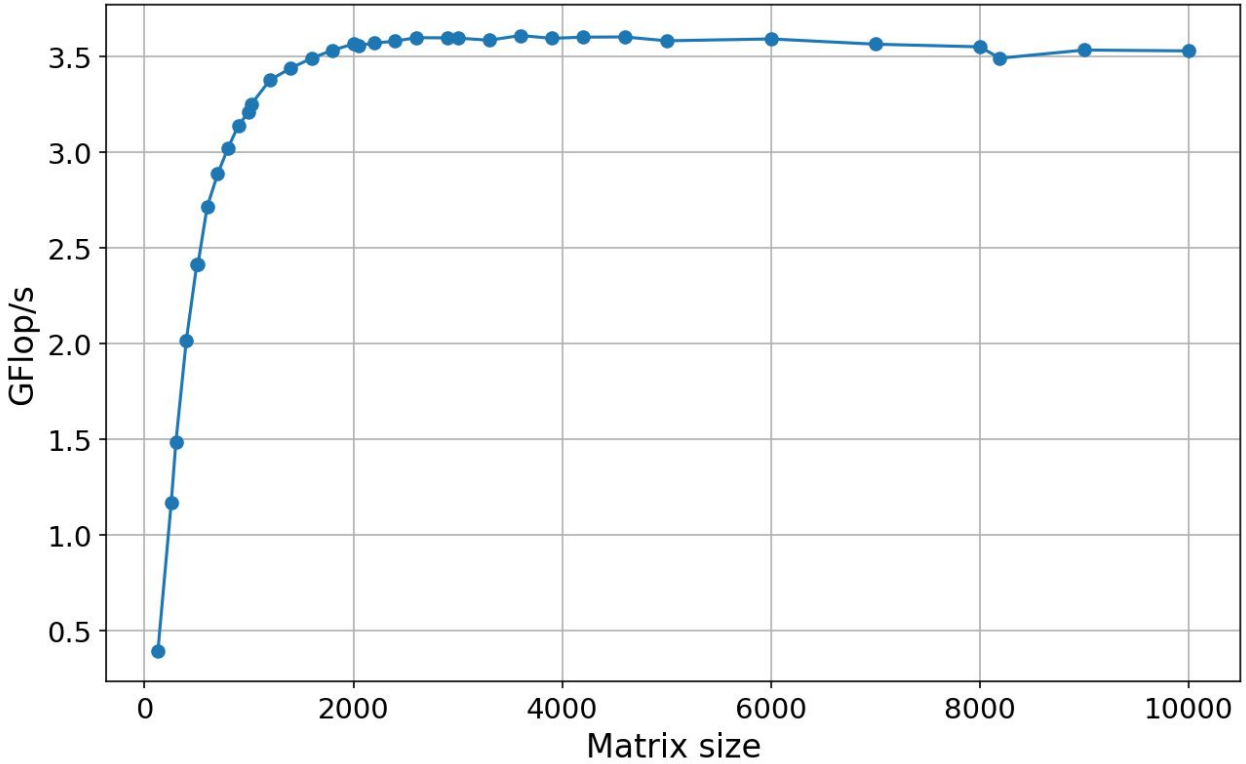


GETRF : Vectorization

$$\begin{pmatrix} 1 & 7 & 3 & 4 & 9 \\ 2 & 3 & 5 & 2 & 2 \\ 4 & 6 & 8 & 6 & 6 \\ 9 & 3 & 4 & 7 & 1 \\ 1 & 8 & 0 & 6 & 3 \end{pmatrix}$$

Speedup of 1.5 by vectorizing

GETRF : Cuda


GFlop/s
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
2000
4000
6000
8000
10000
Matrix size

GETRF : Block-ing

1 - Compute L/U_{00} using GETRF

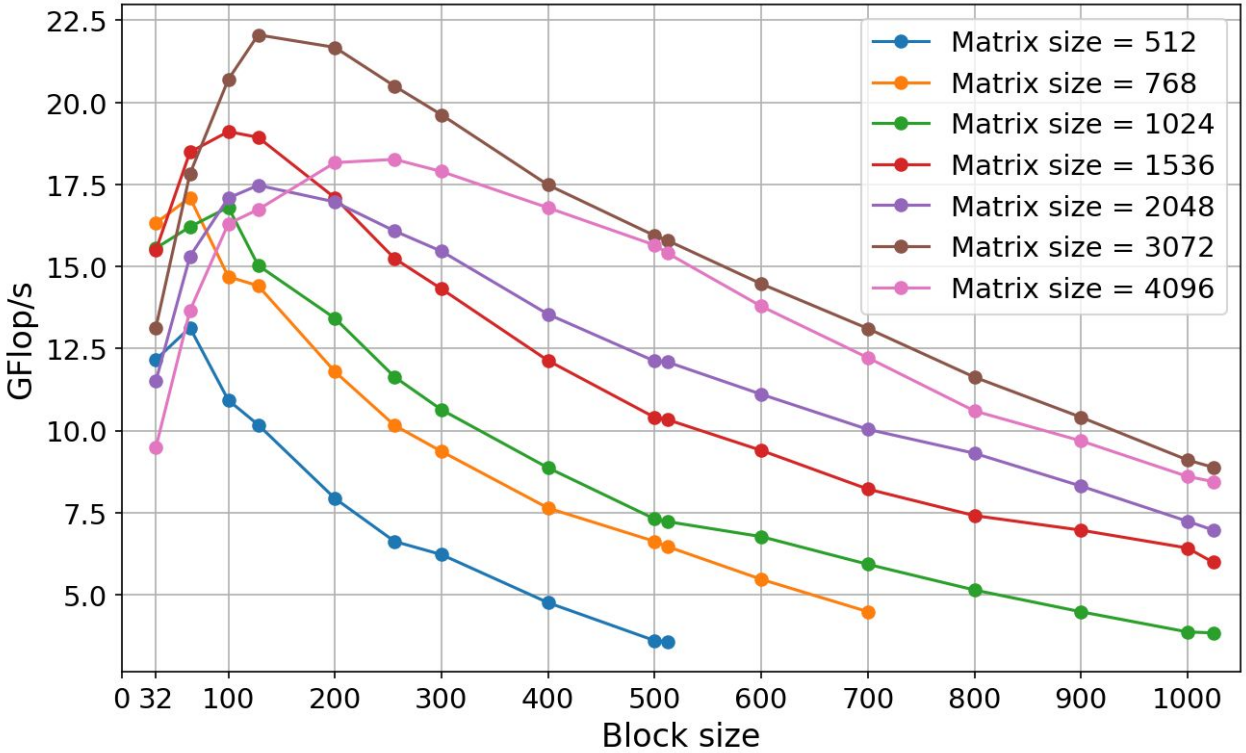
2 - Compute L_{10} and U_{01} using TRSM

3 - Compute A'_{11} using GEMM

4 - Apply the process on A'_{11}

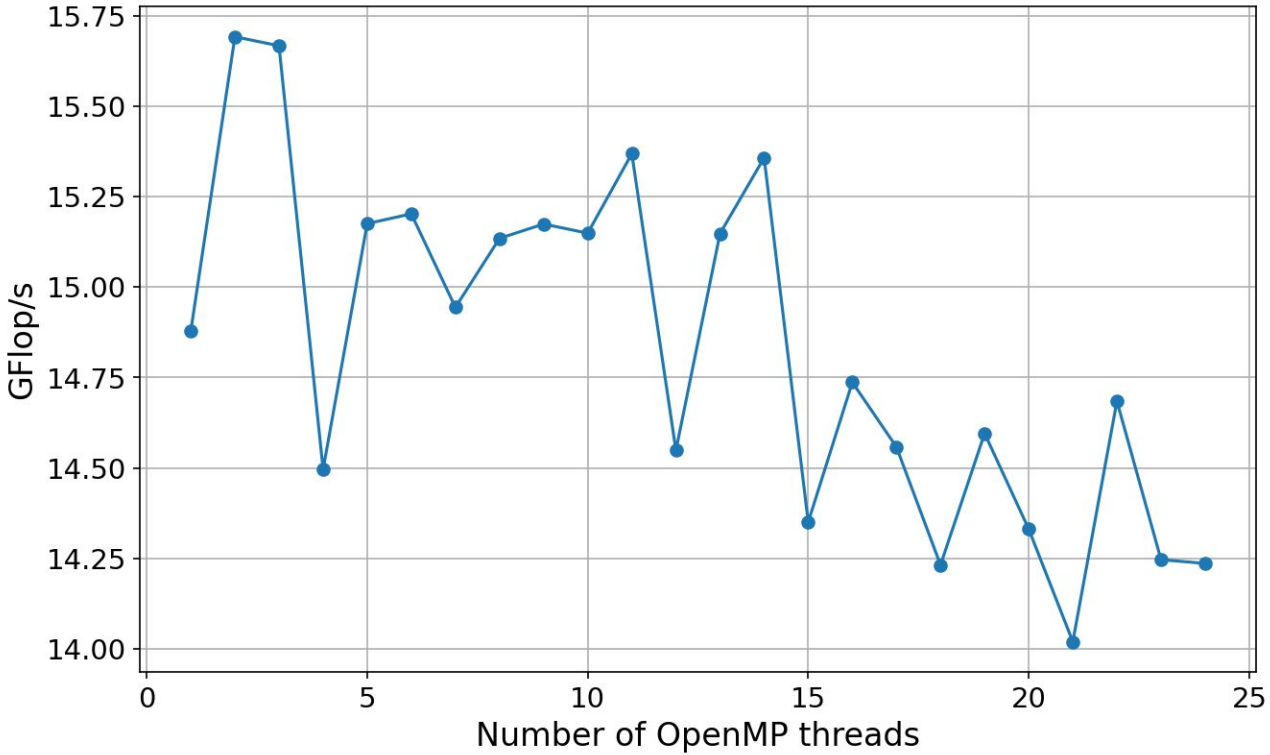
GETRF	TRSM	TRSM	TRSM	TRSM
TRSM	GEMM	GEMM	GEMM	GEMM
TRSM	GEMM	GEMM	GEMM	GEMM
TRSM	GEMM	GEMM	GEMM	GEMM
TRSM	GEMM	GEMM	GEMM	GEMM

GETRF : Sequential Version (Block-ed)



GETRF : OpenMP

Matrix size: 2048
Block size: 64



GETRF : MPI (1)

1 - GETRF ⟶ broadcast result

2 - Broadcast TRSM results of the first line
Send TRSM results of the second line to processes computing GEMM

3 - Receive TRSM results if needed and compute GEMM

4 - Apply the process on A'_{11}

Block-cyclic distribution

0	2	0	2	0	2
1	3	1	3	1	3
0	2	0	2	0	2
1	3	1	3	1	3
0	2	0	2	0	2
1	3	1	3	1	3

GETRF : MPI (2)

1 - GETRF ⟶ broadcast result

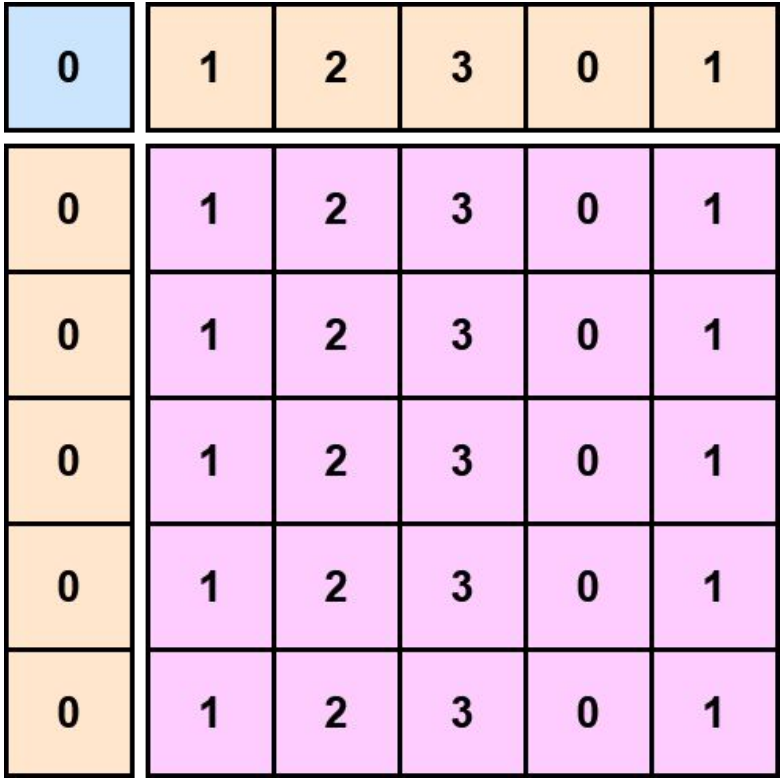
2 - Each process compute its TRSM in the first line / Process 0 computes the TRSM in the second line and broadcast the result.

3 - Compute GEMM of the second line

4 - Repeat 2 and 3 on remaining lines

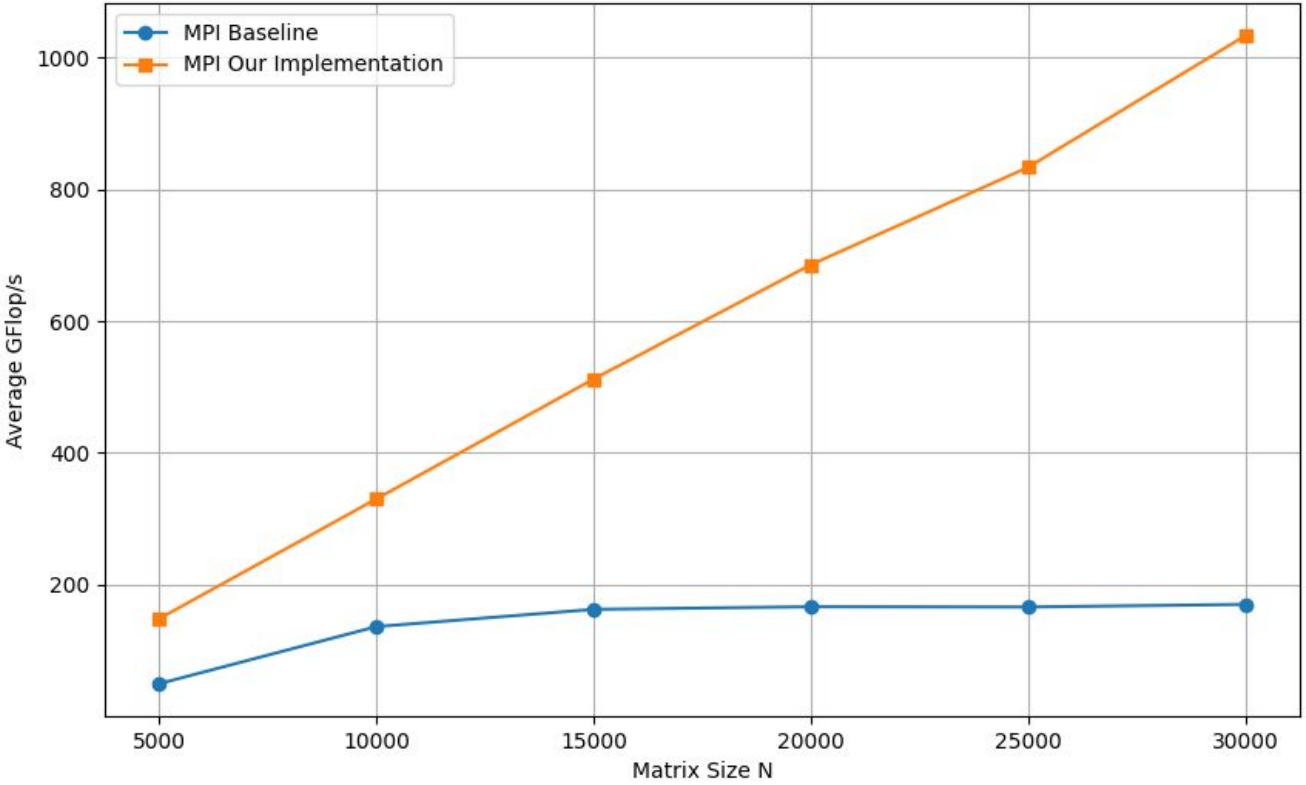
5 - Apply the process on A'_{11}

Column distribution



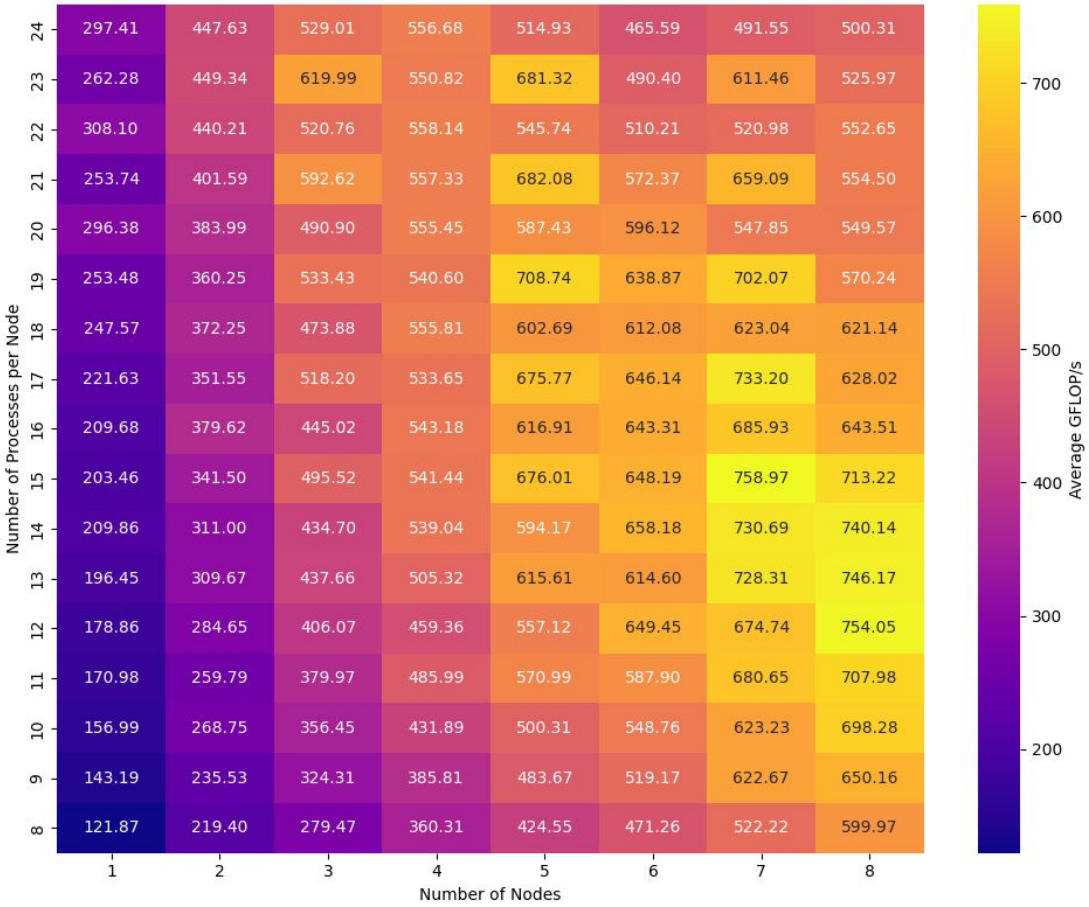
GETRF : MPI (4)

blocks size = 320
8 nodes
12 processes per node



GETRF : MPI (5)

M = N = 30000
blocks = 150

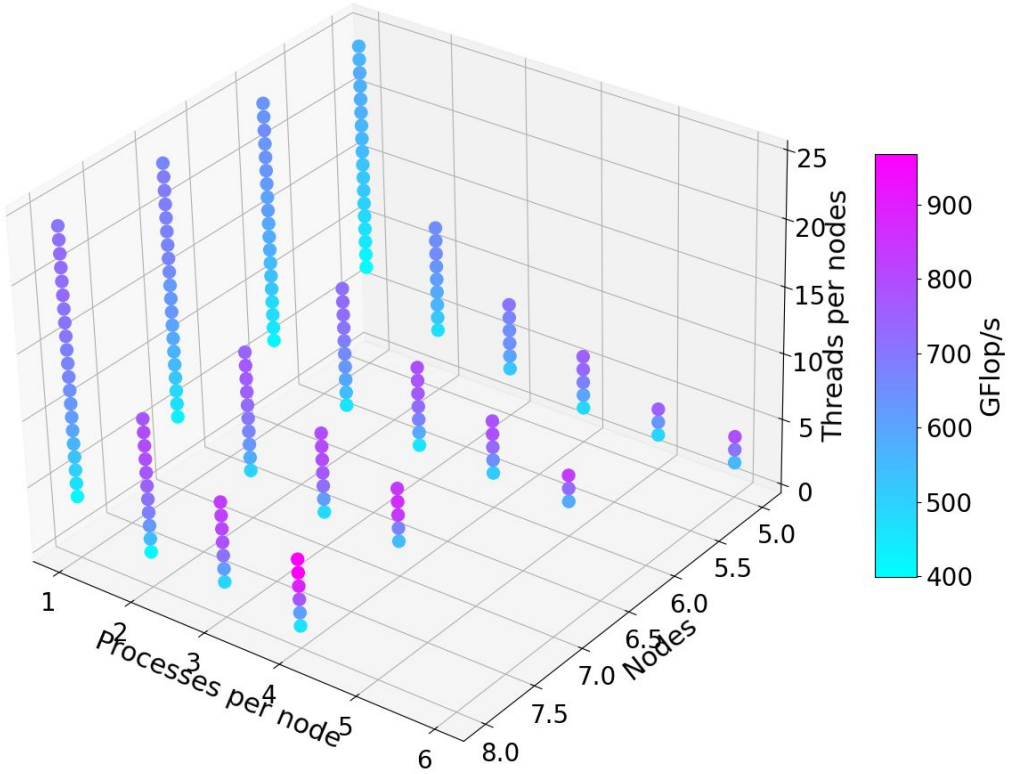


GETRF : MPI + OpenMP

M = N = 35000

MPI blocks size = 1024

OMP blocks size = 100



Experimentation

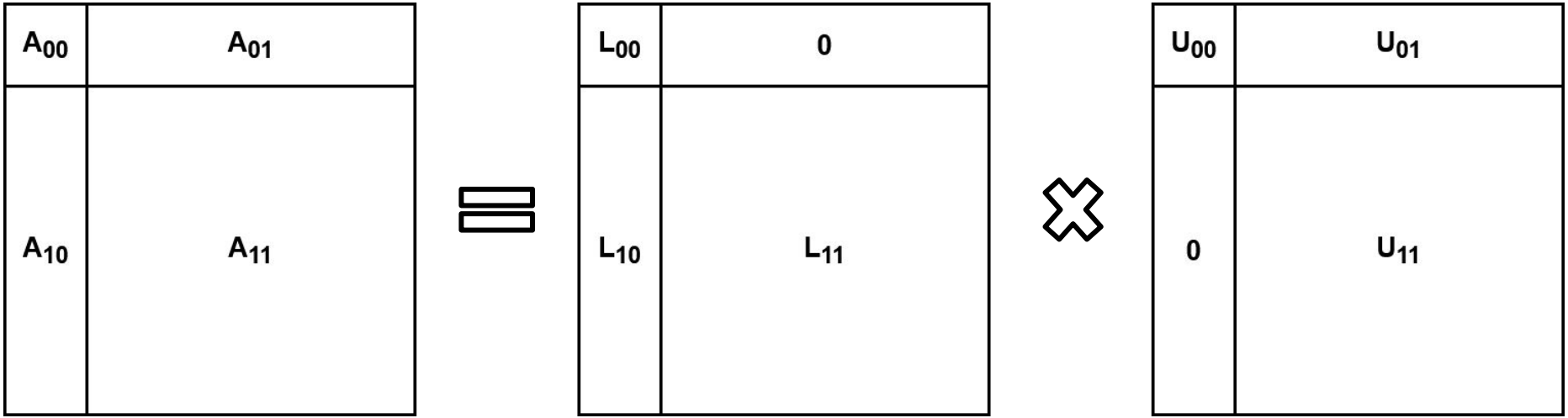
- Turbo boost enabled on miriel039 and miriel040;
- Cluster-On-Die BIOS option is disabled on miriel023;
  - We noticed those misconfigurations during the analysis of our results and benchmarks.

Conclusion

- **Great performance** for **GEMM**, and works on any matrix size and transposition;
- **Relatively good results** for **GETRF**, and works on any matrix size;
- Many **parameters left to be tested** such as:
  - Optimize MPI + OpenMP block sizes
  - Process binding for MPI
- **Improvements** to be done:
  - GEMM MPI algorithm (Cannon's algorithm, 2.5D algorithms)
  - Cuda (GETRF especially)
- **Other solutions/implementations** to test:
  - GETRF OpenMP with for (instead of tasks)

Questions ?

GETRF : Blocking (1)



$$(1) \quad L_{00}U_{00} = A_{00}$$

$$(2) \quad L_{10}U_{00} = A_{10}$$

$$(3) \quad L_{00}U_{01} = A_{01}$$

$$(4) \quad L_{10}U_{01} + L_{11}U_{11} = A_{11}$$

GETRF : Blocking (2)

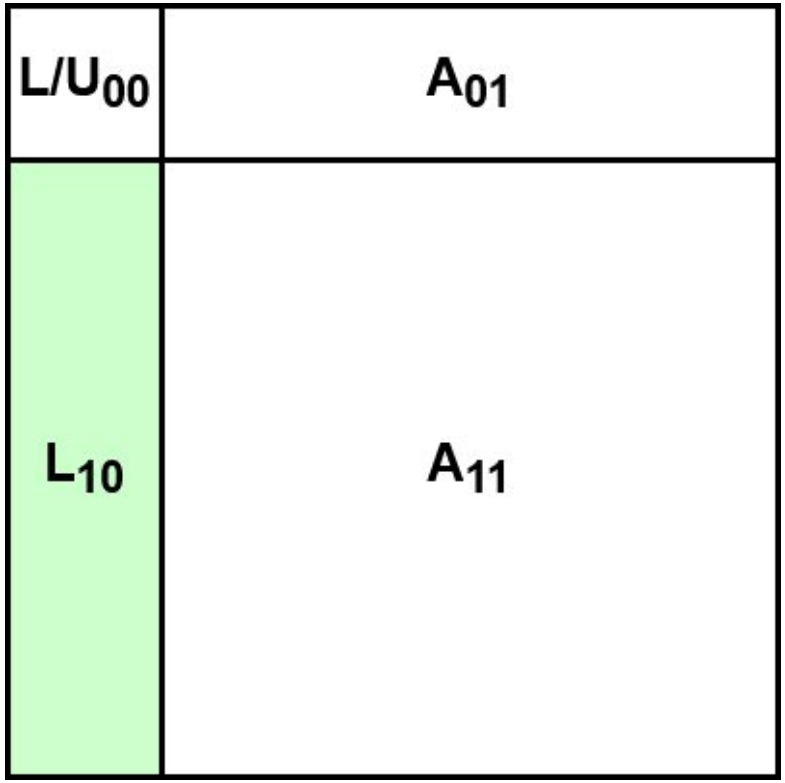
$$(1) \quad L_{00}U_{00} = A_{00}$$

$$GETRF(A_{00}) = (L_{00}, U_{00})$$

GETRF : Blocking (3)

$$(2) \quad L_{10}U_{00} = A_{10}$$

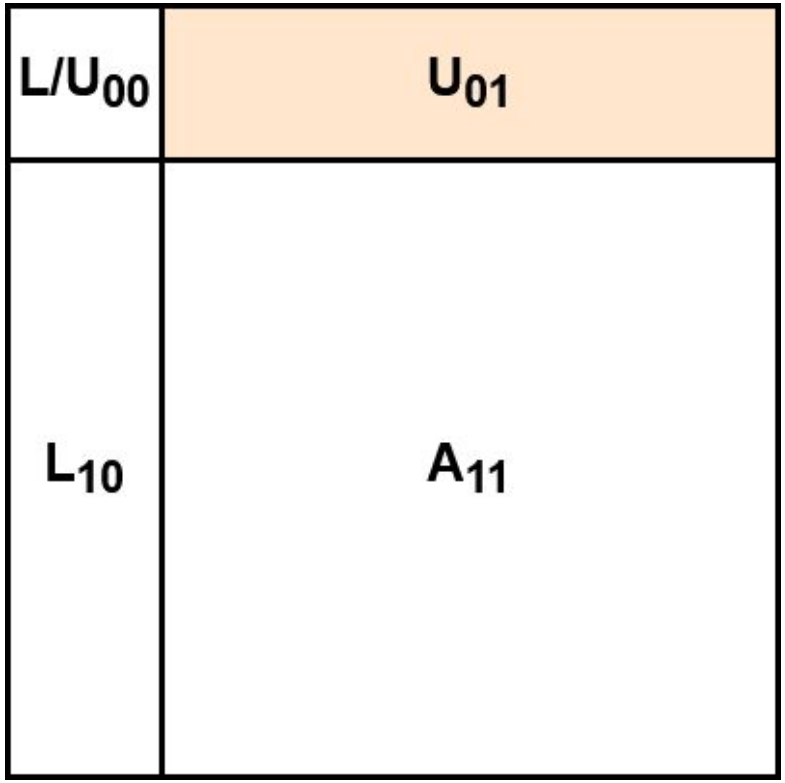
$$TRSM(A_{10}, U_{00}) = L_{10}$$



GETRF : Blocking (4)

$$(3) \quad L_{00}U_{01} = A_{01}$$

$$TRSM(A_{01}, L_{00}) = U_{01}$$

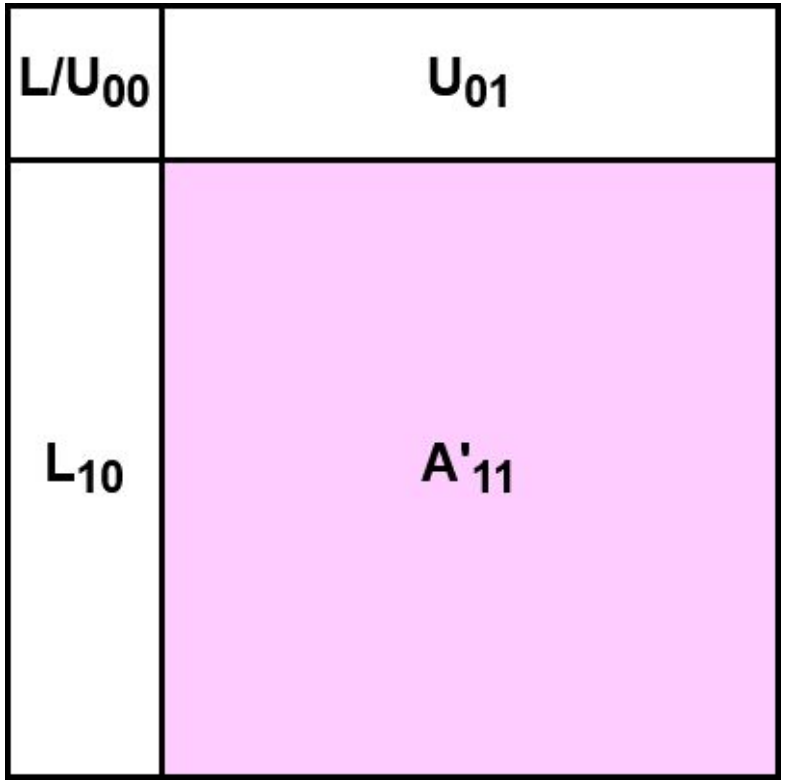


GETRF : Blocking (5)

$$(4) \quad L_{10}U_{01} + L_{11}U_{11} = A_{11}$$

$$(4) \quad A'_{11} = \underbrace{A_{11} - L_{10}U_{01}}_{\text{GEMM}} = L_{11}U_{11}$$

Apply the process on A'_{11} to compute L_{11} and U_{11}



GETRF : Blocking (6)

1 - Compute L/U_{00} using GETRF

2 - Compute L_{10} and U_{01} using TRSM

3 - Compute A'_{11} using GEMM

4 - Apply the process on A'_{11}

GETRF	TRSM	TRSM	TRSM	TRSM
TRSM	GEMM	GEMM	GEMM	GEMM
TRSM	GEMM	GEMM	GEMM	GEMM
TRSM	GEMM	GEMM	GEMM	GEMM
TRSM	GEMM	GEMM	GEMM	GEMM

GEMM : Theoretical performances

$$\text{GFlop/s} = \text{CPU Freq} \times \frac{\text{SIMD Width}}{\text{Type size}} \times \text{FMA} \times \text{FMA Throughput}$$

GEMM : Theoretical performances

model name : Intel(R) Xeon(R)
CPU E5-2680 v3 @ 2.50GHz

AVX2

FMA (a += b*c)

$$\text{GFlop/s} = 2.5\,\text{GHz} \times \frac{256}{64} \times 2 \times 2 = 40\,\text{GFlop/s}$$

sizeof(double)

Latency and Throughput

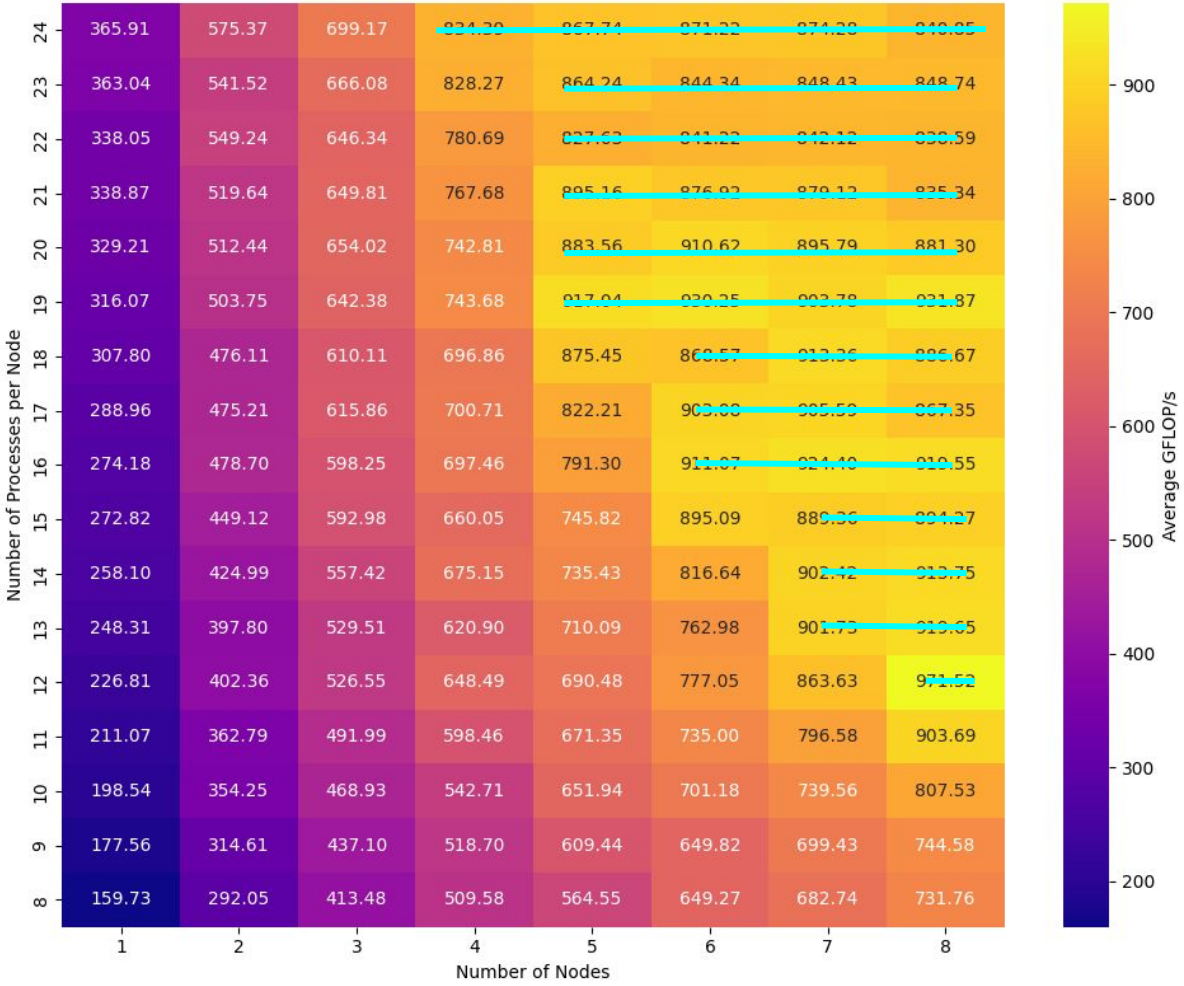
Architecture	Latency	Throughput (CPI)
Alderlake	4	0.5
Icelake Intel Core	4	0.5
Icelake Xeon	4	0.5
Sapphire Rapids	4	0.5
Skylake	4	0.5

$$\text{GFlop/s} = \text{CPU Freq} \times \frac{\text{SIMD Width}}{\text{Type size}} \times \text{FMA} \times \text{FMA Throughput}$$

https://www.intel.com/content/www/us/en/docs/intrinsics-guide/index.html#techs=AVX_ALL&text=_mm256_fmadd_pd

M = N = 30000

blocks = 320



M = N = 30000
blocks = 320