

Optimizing Square Matrix Symmetry Verification and Transposition Using OpenMP and MPI

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Abstract—This comparative study examines various approaches to square matrix operations - specifically transposition and symmetry verification - implemented sequentially and in parallel using both OpenMP and MPI frameworks. The research evaluates performance enhancements through parallelization, measuring acceleration and efficiency improvements versus the sequential approach. Additionally, it evaluates the constraints and capabilities of OpenMP and MPI across different implementation strategies and hardware solutions.

I. INTRODUCTION

Matrix computations represent key components in scientific computing, underpinning everything from image analysis to simulation models. The speed and efficiency of these essential operations significantly influence overall computational performance. [1]

The primary goal of this project is to compare four distinct implementations of square matrix operations:

- Sequential implementation
- Parallel implementation using OpenMP
- Parallel implementation using MPI
- Parallel implementation using MPI dividing matrix into Blocks

The comparison focuses on execution time to determine the effectiveness of each optimization approach.

II. STATE OF THE ART

Matrix transposition optimization has been largely studied in literature [17] [15] [2] [3] [23] [24]. While extensive research exists on matrix transposition optimization, several gaps remain:

- Lack of systematic comparison between basic, OMP and MPI implementations
- Need for practical guidelines based on matrix size and hardware capabilities for MPI
- Study of the impact of thread and also process numbers in addition to matrix size
- Detailed comparison of various techniques on distributed systems using MPI

The objective of our research is to determine which techniques, when combined, yield the fastest performance for matrix transposition and symmetry calculations.

III. CONTRIBUTION AND METHODOLOGY

The project contributes to existing knowledge by delivering comprehensive performance comparisons, analyzing how different optimizations work together, and sharing practical insights for implementation.

For the sequential version we reproduce the code in the previous Assignment [22] that consists of two simple for loops that traverse all matrix values. The parallel version on a single system uses combined OMP techniques [10] and memory access optimizations as in the previous Assignment [22]. The parallel version on distributed systems uses combined MPI techniques [4] [5] for data exchange. All versions were studied with float data type. Matrix dimensions: $n \in 2^4, 2^5, \dots, 2^{12}$. Maximum number of processors: 96; Maximum number of threads: 96; The study was conducted on a single node to avoid network latency issues (which would be limited to 10 G/s and would introduced a delay), thus improving data locality and performance for moderately-sized matrices. The study was carried out on a system with 64-byte aligned memory [6]. An iterative approach was taken, testing different implementations and comparing results to identify the best version.

IV. EXPERIMENTS AND SYSTEM DESCRIPTION

A. Hardware

UniTn Cluster [21] with: Ram: 32k DDR SRAM; [13] Processors: Intel® Xeon® Gold 6252N Processor 35.75M cache, 2.30 GHz; [12] [?] Number of cores: 96; Name of the processor: hpc-c11-node07.unitn.it

B. Software

Compiler: GCC 9.1; Libraries: stdio.h, stdlib.h, time.h, immintrin.h, sys/time.h, omp.h, math.h, getTimeOfDay [14]; OpenMP version 3.1; File PBS; File CSV; Python 3.7.2 with pandas, matplotlib, pyplot, sys, os; Mpich version 3.2.1

C. Sequential Version

The pragma option `override(checkSym, "opt(level, 0)")` was used to remove all possible compiler optimizations. The implementation consists of simple nested loops that traverse the entire matrix to make the results independent of the matrix data. [22] Fig. 1 shows its time performance (SEQ lines).

D. OpenMP

It consists of using cache blocking and pragma to optimize and improve data access in memory and parallelize among threads. [22] In Fig. 1 we can see its time performance (OMP lines).

E. MPI

A version has been implemented that shares the entire matrix with all processors; each processor transposes its own rows and then sends them back to processor 0 to create the transposed matrix. Simple MPI_Recv and MPI_Send were used. (MPI base) Another version that uses Alltoall and AllGather for transposition, which requires some checks because the use of Alltoall requires each processor to work with exactly one row and no more. (MPI AlltoAll) [7] A final version using MPI datatypes and simple communicators like gather and scatter, which improve performance. (MPI DT) [20] [8] [25] We can see in Table I, for check symmetry, and in Table II, for the transposition, the comparison between all of it.

| Processors | Dim | MPI base | MPI AlltoAll | MPI DT |
|------------|------|-----------|--------------|-----------|
| 2 | 16 | 0.0000196 | - | 0.000106 |
| 16 | 16 | 0.0003756 | 0.0002184 | 0.0006662 |
| 32 | 32 | 0.0004772 | 0.0003604 | 0.0004302 |
| 64 | 64 | 0.0009314 | 0.0009056 | 0.000746 |
| 26 | 128 | 0.0005418 | - | 0.0004648 |
| 53 | 256 | 0.0018184 | - | 0.0017326 |
| 87 | 512 | 0.0179904 | - | 0.0178608 |
| 44 | 1024 | 0.0096436 | - | 0.0087542 |
| 72 | 2048 | 0.037802 | - | 0.0371126 |
| 95 | 4096 | 0.2196158 | - | 0.2102584 |

TABLE I
COMPARISON TIME[S] FOR CHECK SYMMETRY TIME FOR VERSION AND PROCESSORS

| Processors | Dim | MPI base | MPI AlltoAll | MPI DT |
|------------|------|-----------|--------------|-----------|
| 2 | 16 | 0.0005334 | - | 0.000106 |
| 16 | 16 | 0.0003886 | 0.000176 | 0.0002614 |
| 32 | 32 | 0.0012018 | 0.0003638 | 0.0023944 |
| 64 | 64 | 0.0007288 | 0.0007936 | 0.0007432 |
| 24 | 128 | 0.0010518 | - | 0.0003068 |
| 55 | 256 | 0.0030182 | - | 0.0015578 |
| 81 | 512 | 0.0130306 | - | 0.010048 |
| 43 | 1024 | 0.03303 | - | 0.012872 |
| 78 | 2048 | 0.1464398 | - | 0.0546082 |
| 92 | 4096 | 0.7141268 | - | 0.214745 |

TABLE II
COMPARISON TIME[S] FOR TRANSPOSITION TIME FOR VERSION AND PROCESSORS

In table I and II, note how the DT, version performs worse in cases of well-distributed work among processors (first rows), but performs better when the work is not evenly distributed. This is because MPI datatypes [8] provide a more efficient way to handle communications with irregular and non-contiguous workloads, reducing overhead and allowing optimization at the implementation level. Furthermore, notice how with DT, when the workload increases, the performance improves significantly.

Finally, a last version was implemented by dividing the matrix into blocks [16], sharing and transposing only those

blocks. Multiple experiments were conducted with this version: base version (MPI BB) using simple send and receive; using datatypes (MPI BOD); adding scatter, gather and collective communicators (MPI BNVD) [18]; using "variable" versions of collective communicators like gather and scatterv (MPI BDV) [19]. This last implementation only works with specific dimensions and number of processors, since dividing the matrix into blocks and sharing it requires the matrix to be exactly divisible by the number of processors. Table III contains some data about the comparison of these last versions.

| Processors | Dim | MPI BB | MPI BDV | MPI BOD | MPI BNVD |
|------------|------|-----------|-----------|-----------|-----------|
| 4 | 16 | 0.0005008 | 0.000597 | 0.000351 | 0.0003992 |
| 16 | 16 | 0.000614 | 0.0006654 | 0.0003196 | 0.000313 |
| 16 | 32 | 0.000788 | 0.0009246 | 0.0006452 | 0.0002608 |
| 64 | 64 | 0.002114 | 0.0013482 | 0.0013552 | 0.0011696 |
| 16 | 128 | 0.0016578 | 0.0008668 | 0.0003506 | 0.0007334 |
| 4 | 256 | 0.0015676 | 0.0006844 | 0.0007632 | 0.0011232 |
| 64 | 512 | 0.0117464 | 0.0028946 | 0.0024816 | 0.0053942 |
| 64 | 1024 | 0.0274762 | 0.0085702 | 0.0114406 | 0.017472 |
| 16 | 2048 | 0.0844384 | 0.02403 | 0.0242252 | 0.060321 |
| 64 | 4096 | 1.2823244 | 0.08869 | 0.0954242 | 0.2753908 |

TABLE III
COMPARISON TIME[S] BETWEEN DIFFERENT BLOCK DIVIDING IMPLEMENTATIONS

As can be noted in Table III, for small-sized matrices BOD performs better, while when the workload increases BDV becomes better.

V. RESULTS AND DISCUSSION

The best version (MPI DT) was compared with the sequential and OpenMP implementations to analyze their execution times; In the Fig.1 and Fig.2 there are the trends of it.

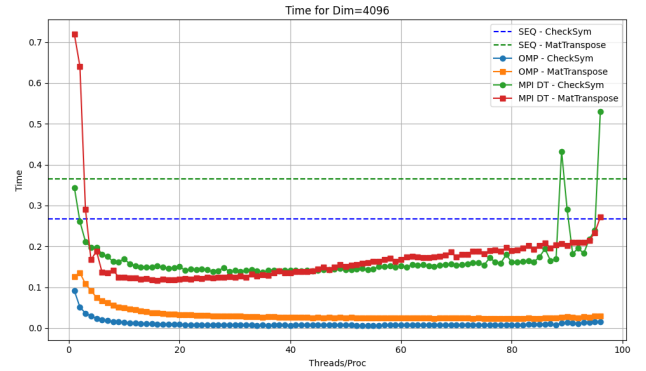


Fig. 1. time[s] performances for Dim = 4096

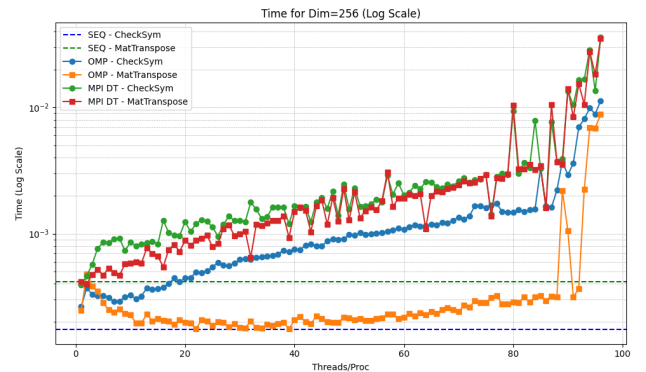


Fig. 2. time[s] performances for Dim = 256 (log scale)

As we can notice in Fig 2, the best MPI version, turns out to be very slow, even worse than the sequential version (this is true up to the matrix dimension of 2048) due to several reasons like significant communication overhead: as processors need to communicate by sending and receiving messages, overhead associated with process creation and management and the cost for data distribution; this is no longer true in the version that divides the matrix into blocks addressing some mentioned problems improving the performances. Let's now analyze speedup (1), efficiency (2), and scaling (3) for a better understanding of the results.

$$\frac{\text{Time On Sequential Version}}{\text{Time On N processors}} = \text{speedup} \quad (1)$$

$$\left(\frac{\text{speedup}}{\text{number Of Processors}} \right) \cdot 100 = \text{efficiency} \quad (2)$$

$$\left(\frac{\text{Single processor time for size: } (N)}{P \text{ processors time for size: } (p \cdot N)} \right) = \text{scalability} \quad (3)$$

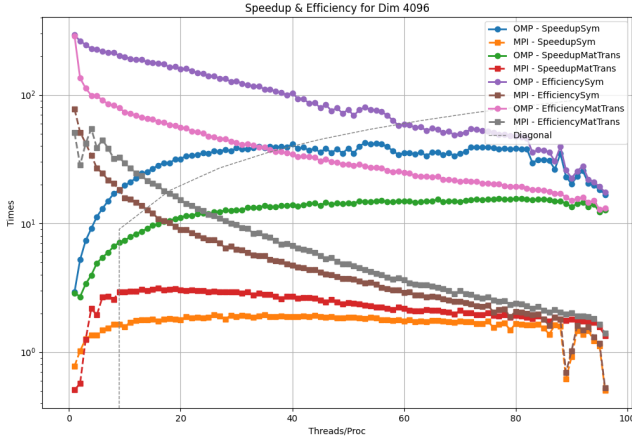


Fig. 3. efficiency and speedup for Dim = 4096 (log scale)

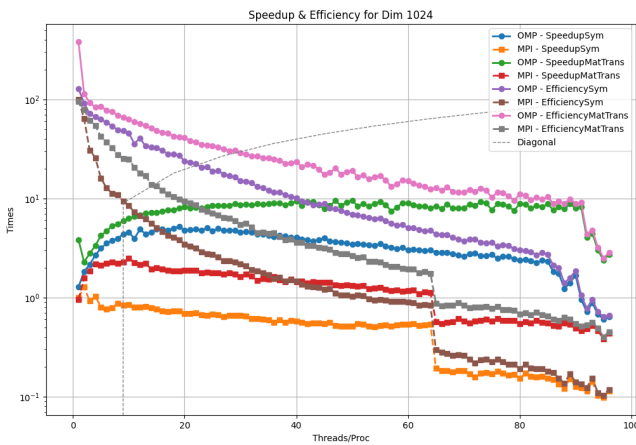


Fig. 4. speedup and efficiency for Dim = 1024 (log scale)

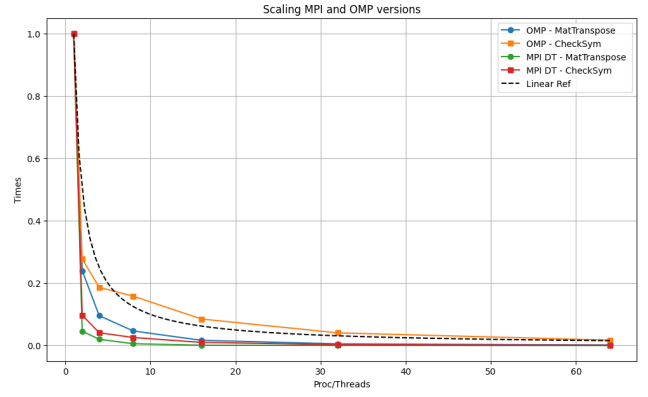


Fig. 5. scaling

As can be seen in Fig. 3 and Fig. 4, the version using OpenMP performs better due to the lack of need to share information and data condivision. Despite the elimination of network latency when using a single node, due to inefficiencies related to internal management and sharing the entire matrix with all processors, the MPI version achieves significantly lower results compared to the OpenMP version. Note how MPI however scales better Fig. 5.

A. Bandwidth

We computed the bandwidth [22], only for the Dim 4096, the most relevant one, and we have the data in the table IV. We have the best bandwidth with OMP

| SEQ | OMP | MPI | SystemPeak |
|---------------------|----------------------|----------------------|----------------------|
| 368*10 ⁶ | 5785*10 ⁶ | 2358*10 ⁶ | 2820*10 ⁷ |

TABLE IV
SISTEM BANDWIDTH ON DIFFERENT VERSIONS

B. Block vs No-Block

A comparison was then made between the best version that shares the entire matrix (MPI DT) and the best one that shares and works only on a single block (MPI BDV). As expected the performances improves and the effcieny remains better respect to Non-Blocking version seen in Fig. 6 and Fig.7 Demonstrating that sharing the entire matrix with all processors represents an unnecessary bottleneck that worsens performance.

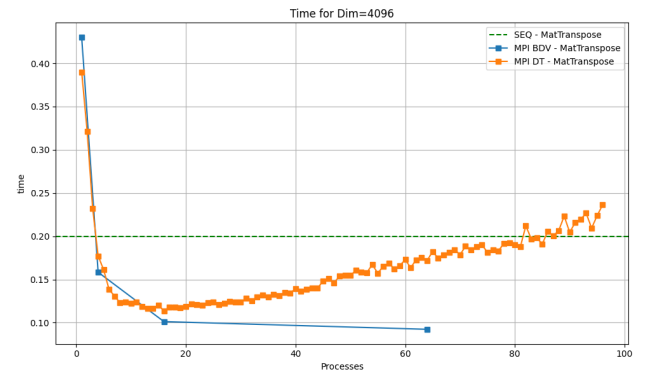


Fig. 6. time[s] performances for Dim = 4096 (log scale)

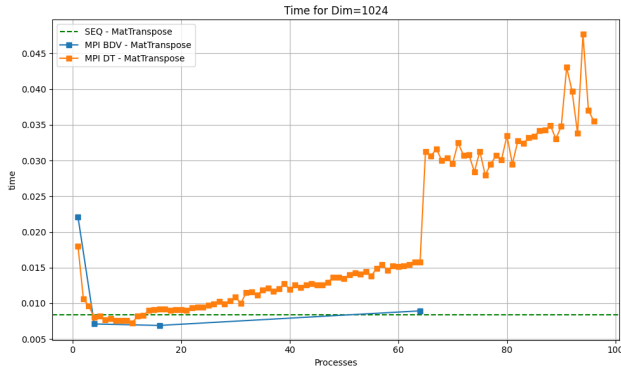


Fig. 7. time[s] performances for Dim = 1024 (log scale)

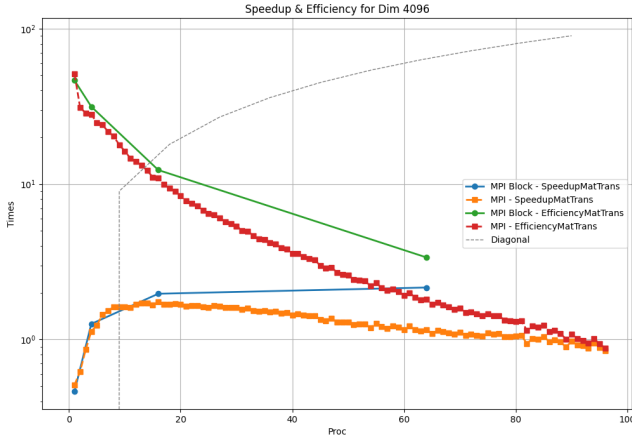


Fig. 8. speedup and efficiency for Dim = 4096 (log scale)

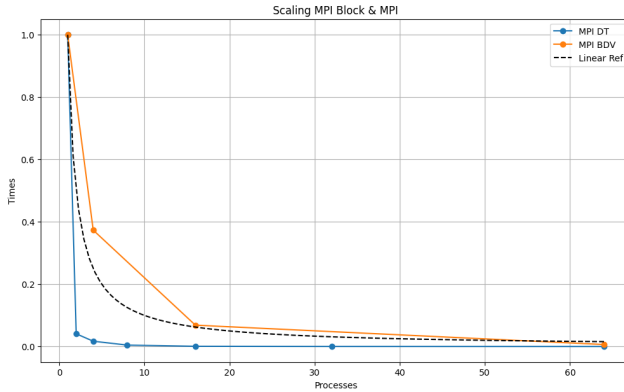


Fig. 9. scaling

However, as seen in Fig. 8 and Fig. 9 the speedups still deviate significantly from the ideal, and the version that divides the matrix into blocks scales slightly worse principally due to the specific constraint on the data shared and processed.

C. Problems Encountered

The synchronization of communication between processors required careful coordination, and debugging proved complex in a distributed environment. It was also necessary to

implement checks on dimensions and number of processors, given the particular functioning of some implementations that only work if the rows or matrix dimensions are divisible by the number of processors; Initially, we tried to abort superfluous processors, for example, by dividing processors into sets and subsets with global communicators [11], which proved to be a poor choice due to its implementation difficulty and leak of performances; therefore, we opted to abort the entire program execution. It was also necessary to divide the workload as uniformly as possible among processors while avoiding sharing the entire matrix with all processors.

VI. CONCLUSIONS

We have demonstrated various versions for performing matrix transposition operations and symmetry checking, showing different optimization methods through both OpenMP and MPI parallelization. We have shown how a multithreaded approach brings undisputable benefits both when working in monolithic environments with OpenMP that is better than MPI in the same environment. The two methods cannot be directly compared given their strengths on completely different physical systems, and our data shows that, using a single node, OpenMP is undoubtedly more efficient. Our experiments also confirm that avoiding sharing the entire matrix among processors in MPI is highly recommended as it introduces a significant bottleneck. Furthermore, the choice to divide the matrix into blocks, share it, and then receive back the transposed blocks proved better in terms of performance but worse in terms of scalability. We registered the better system usage with the OMP version as the higher Bandwidth still far from system peak of 2.82E+10 Gbps. Finally, for very small matrices, a sequential approach is preferable even to OpenMP.

VII. FURTHER WORKS

An interesting additional analysis would be to compare the MPI "Blocked Matrix" versions with OpenMP and using a large distributed hardware environment to show the true potential of MPI.

GIT AND INSTRUCTIONS FOR REPRODUCIBILITY

You can find all complete data and codes here, with the instructions for reproducibility <https://github.com/mosearc/ParallelProgramming.git>

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