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Abstract

Replace with your abstract text of not more than 300 words.

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Chapter 1

Introduction

Chapter 2

Methodology

2.1 Sequential Algorithm

The algorithm for multiplying a sparse matrix by a dense vector can be efficiently implemented using the Compressed Sparse Row (CSR) format. The CSR format represents a sparse matrix using three arrays: `values`, `col_indices`, and `row_pointers`. Given a sparse matrix M in CSR format and a dense vector v , the product $M \times v$ is computed as follows:

Algorithm 1 Sequential algorithm

Require: M is an $m \times n$ sparse matrix

Require: v is an $n \times k$ dense vector

Ensure: $Result$ is an $m \times k$ matrix

$Result \leftarrow$ zero matrix of size $m \times k$

for $i \leftarrow 0$ **to** $m - 1$ **do**

for each non-zero element (j, value) in row i of M **do**

for $l \leftarrow 0$ **to** $k - 1$ **do**

$Result[i][l] \leftarrow Result[i][l] + (\text{value} \times v[j][l])$

end for

end for

end for

return $Result$

2.1.1 Complexity Analysis

The complexity analysis of the algorithm for multiplying a sparse matrix by a dense vector focuses on two main aspects: temporal complexity and spatial complexity.

2.1.1.1 Temporal Complexity

The temporal complexity of the algorithm depends on how the sparse matrix is stored and the number of non-zero elements in the matrix.

- **Traversing Rows:** The algorithm traverses each row of the matrix. If the matrix has m rows, this step has a complexity of $O(m)$.

- **Traversing Non-Zero Elements:** Inside each row, the algorithm traverses the non-zero elements. If the total number of non-zero elements in the matrix is n_{nz} , the traversal of all these elements has a complexity of $O(n_{nz})$.

The total temporal complexity is therefore $O(m + n_{nz})$. However, in practice, this complexity is often considered as $O(n_{nz})$, as the number of non-zero elements is usually the dominating factor, especially in very sparse matrices.

2.1.1.2 Spatial Complexity

The spatial complexity is related to the amount of memory required by the algorithm.

- **Storing the Sparse Matrix:** The way the sparse matrix is stored affects the spatial complexity. Generally, storage formats like CSR or COO allow storing a sparse matrix with a complexity of $O(n_{nz})$, where n_{nz} is the number of non-zero elements.
- **Dense Vector:** The dense vector has a spatial complexity of $O(n)$, where n is the size of the vector.
- **Result Vector:** The result vector also has a size of $O(m)$, where m is the number of rows in the matrix.

The total spatial complexity is therefore $O(n_{nz} + m + n)$, but in practice, the focus is mainly on the $O(n_{nz})$ term as it is generally the most significant.

2.1.2 Example

Dans le format CSR, la matrice est représentée par trois vecteurs : values, rows, et cols. Pour notre exemple, ces vecteurs sont définis comme suit:

- values = {1, 2, 3, 4}
- rows = {0, 2, 3, 3, 4}
- cols = {0, 2, 1, 3}

La matrice creuse correspondante peut être visualisée comme:

$$\begin{bmatrix} 1 & 0 & 2 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix}$$

Le vecteur dense est simplementq:

$$\begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}$$

La multiplication de la matrice creuse par le vecteur dense est effectuée ligne par ligne. Le résultat peut être visualisé comme :

$$\begin{bmatrix} 1 & 0 & 2 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix} \times \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix} = \begin{bmatrix} 1 \times 1 + 0 \times 2 + 2 \times 3 + 0 \times 4 \\ 0 \times 1 + 0 \times 2 + 3 \times 3 + 0 \times 4 \\ 0 \times 1 + 0 \times 2 + 0 \times 3 + 0 \times 4 \\ 0 \times 1 + 0 \times 2 + 0 \times 3 + 4 \times 4 \end{bmatrix} = \begin{bmatrix} 7 \\ 9 \\ 0 \\ 16 \end{bmatrix}$$

2.2 Line-Based Parallelism

This algorithm partitions a sparse matrix into row chunks and distributes these chunks across multiple processes for parallel computation in a line-based manner.

Algorithm 2 Line-based parallel sparse matrix-vector multiplication

Require: M is an $m \times n$ sparse matrix

Require: v is an $n \times k$ vector

Require: $numProcs$ is the number of processes

Require: $rank$ is the rank of the current process

Ensure: $Result$ is a part of the $m \times k$ matrix computed by this process

$rowsPerProc \leftarrow m / numProcs$

$startRow \leftarrow rank \times rowsPerProc$

$endRow \leftarrow startRow + rowsPerProc$

$Result \leftarrow$ zero matrix of size $rowsPerProc \times k$

for $i \leftarrow startRow$ **to** $endRow - 1$ **do**

for each non-zero element $(j, value)$ in row i of M **do**

for $l \leftarrow 0$ **to** $k - 1$ **do**

$Result[i - startRow][l] \leftarrow Result[i - startRow][l] + (value \times v[j][l])$

end for

end for

end for

if $rank \neq 0$ **then**

 Send $Result$ to process 0

else

$FinalResult \leftarrow$ zero matrix of size $m \times k$

 Copy $Result$ into $FinalResult$

for $p \leftarrow 1$ **to** $numProcs - 1$ **do**

 Receive partial $Result$ from process p

 Copy received $Result$ into appropriate position in $FinalResult$

end for

end if

if $rank = 0$ **then return** $FinalResult$

2.2.1 Complexity Analysis

2.2.1.1 Temporal Complexity

- **MPI Initialisation and Rank and Size Determination:** This step is generally fast, with a complexity close to $O(1)$, as it mainly involves setup operations.
- **Calculation of the Number of Rows per Process:** This operation also has a complexity of $O(1)$ as it requires only simple arithmetic based on the total size of the matrix and the number of processes.
- **Calculation of Start and End Indices for Each Process:** Again, this step has a complexity of $O(1)$ as it involves simple arithmetic calculations.

- **Scatter of Rows of M and Vector v :** The complexity of this step depends on the MPI implementation and data distribution. In general, it can be considered as $O(\frac{n_{nz}}{p})$, where n_{nz} is the total number of non-zero elements in the matrix and p is the number of processes.
- **Local Computation in Each Process:** Each process performs the matrix-vector product computation for its assigned portion of the matrix. The complexity of this step is $O(\frac{n_{nz}}{p})$ in the ideal case where the non-zero elements are evenly distributed among the processes.
- **Gather of Local Results r_{local} :** The gather operation can vary in complexity, but generally, it is proportional to the total number of elements to be gathered and depends on the efficiency of communication between processes.

2.2.1.2 Spatial Complexity

- **Storage of Sparse Matrix and Dense Vector:** The storage of the matrix and vector remains $O(n_{nz} + m + n)$, where m and n are the dimensions of the matrix.
- **Local Result Vectors r_{local} :** Each process stores a local result vector of a size proportional to the portion of the matrix it processes, approximately $O(\frac{m}{p})$.

2.3 Column-Wise Parallelism

This algorithm distributes the non-zero elements of a sparse matrix among different processes, enabling parallel computation focused on each non-zero element.

Algorithm 3 Column-wise Parallelization using MPI for Sparse Matrix-Fat Vector Multiplication

Require: M is an $m \times n$ sparse matrix
Require: v is an $n \times k$ vector
Require: $numProcs$ is the number of processes
Require: $rank$ is the rank of the current process
Ensure: $PartialResult$ is a part of the $m \times k$ matrix computed by this process

```

 $colsPerProc \leftarrow k / numProcs$ 
 $startCol \leftarrow rank \times colsPerProc$ 
 $endCol \leftarrow startCol + colsPerProc$ 
 $PartialResult \leftarrow$  zero matrix of size  $m \times colsPerProc$ 
for  $i \leftarrow 0$  to  $m - 1$  do
  for each non-zero element  $(j, value)$  in row  $i$  of  $M$  do
    for  $l \leftarrow startCol$  to  $endCol - 1$  do
       $PartialResult[i][l - startCol] \leftarrow PartialResult[i][l - startCol] + (value \times$ 
 $v[j][l])$ 
    end for
  end for
end for
if  $rank \neq 0$  then
  Send  $PartialResult$  to process 0
else
   $FinalResult \leftarrow$  zero matrix of size  $m \times k$ 
  Copy  $PartialResult$  into appropriate position in  $FinalResult$ 
  for  $p \leftarrow 1$  to  $numProcs - 1$  do
    Receive partial  $PartialResult$  from process  $p$ 
    Copy received  $PartialResult$  into appropriate position in  $FinalResult$ 
  end for
end if
if  $rank = 0$  then return  $FinalResult$ 

```

2.3.1 Complexity Analysis

2.3.1.1 Temporal Complexity

- **MPI Initialisation and Rank and Size Determination:** Similar to the line-based approach, this step has a complexity of approximately $O(1)$, involving basic setup operations.
- **Distribution of Non-Zero Elements of M :** This step involves distributing the non-zero elements among the processes. The complexity depends on the distribution

mechanism but is generally proportional to the number of non-zero elements, n_{nz} , and the efficiency of the distribution algorithm used.

- **Scatter of Vector v to All Processes:** Scattering the vector v to all processes can be done efficiently in MPI and typically has a complexity proportional to the size of the vector, $O(n)$.
- **Computation of Products for Assigned Non-Zero Elements:** Each process computes the products for its assigned non-zero elements. Assuming an even distribution, the complexity for each process would be $O(\frac{n_{nz}}{p})$, where p is the number of processes.
- **MPI Atomic Operations and Reduction:** The use of atomic operations and reduction to form the final result vector can introduce additional complexity, depending on the implementation and efficiency of these operations in MPI.

2.3.1.2 Spatial Complexity

- **Storage of Sparse Matrix and Dense Vector:** The storage requirements remain the same as in the line-based approach, $O(n_{nz} + m + n)$.
- **Local Result Vectors r_{local} :** Each process maintains a local result vector, but since the computation is based on non-zero elements, the storage requirement for each r_{local} might be smaller, depending on the distribution of non-zero elements.

2.4 Non-Zero Element Parallelism

This algorithm combines line-based and non-zero element-based approaches by distributing chunks of rows to each process and then performing parallel computations on the non-zero elements within those chunks.

Algorithm 4 Non-Zero Element Parallelization using MPI for Sparse Matrix-Fat Vector Multiplication

Require: M is an $m \times n$ sparse matrix stored in a format that allows iterating over non-zero elements (e.g., COO, CSR)

Require: v is an $n \times k$ vector

Require: $numProcs$ is the number of processes

Require: $rank$ is the rank of the current process

Ensure: $PartialResult$ is a part of the $m \times k$ matrix computed by this process

$numNonZeroElements \leftarrow$ total number of non-zero elements in M

$elementsPerProc \leftarrow numNonZeroElements / numProcs$

$startIndex \leftarrow rank \times elementsPerProc$

$endIndex \leftarrow startIndex + elementsPerProc$

$PartialResult \leftarrow$ zero matrix of size $m \times k$

$NonZeroElements \leftarrow$ list of non-zero elements in M from $startIndex$ to $endIndex - 1$

for each $(i, j, value)$ in $NonZeroElements$ **do**

for $l \leftarrow 0$ **to** $k - 1$ **do**

$PartialResult[i][l] \leftarrow PartialResult[i][l] + (value \times v[j][l])$

end for

end for

if $rank \neq 0$ **then**

 Send $PartialResult$ to process 0

else

$FinalResult \leftarrow$ zero matrix of size $m \times k$

 Copy $PartialResult$ into $FinalResult$

for $p \leftarrow 1$ **to** $numProcs - 1$ **do**

 Receive partial $PartialResult$ from process p

 Add received $PartialResult$ into $FinalResult$

end for

end if

if $rank = 0$ **then return** $FinalResult$

2.4.1 Complexity Analysis

2.4.1.1 Temporal Complexity

- **MPI Initialisation and Rank and Size Determination:** As with other MPI-based algorithms, this step has a complexity of approximately $O(1)$.
- **Scattering Chunks of Rows of M to Each Process:** This step distributes parts of the matrix to different processes. Its complexity depends on the number of rows

and the distribution method, typically around $O(\frac{m}{p})$, where m is the number of rows and p is the number of processes.

- **Scatter of Vector v to All Processes:** This operation generally has a complexity of $O(n)$, where n is the size of the vector.
- **Local Computations for Non-Zero Elements:** Each process computes the products for the non-zero elements in its assigned rows. Assuming an even distribution of non-zero elements, the complexity for each process is approximately $O(\frac{n_{nz}}{p})$.
- **Gather of Local Results r_{local} into Final Result Vector r :** This step combines the partial results from all processes and typically has a complexity proportional to the total number of elements in r .

2.4.1.2 Spatial Complexity

- **Storage of Sparse Matrix and Dense Vector:** The overall storage requirements remain $O(n_{nz} + m + n)$, as in other sparse matrix-vector multiplication methods.
- **Local Result Vectors r_{local} :** Each process stores a local result vector for its chunk of rows, with the size depending on the distribution of rows and non-zero elements.

Complexity and Considerations

Each of these parallel algorithms aims to exploit different aspects of parallelism, with the primary goal of reducing the overall computation time. The actual performance gain depends on the characteristics of the sparse matrix, the number of available processing units, and the specific implementation details. Moreover, care must be taken to manage concurrency issues, such as race conditions and proper synchronization, to ensure correct and efficient execution.

Chapter 3

Conclusion

Appendix A

Documentation

Appendix A.A Project tree

```
lib /
    collecting.py
    processing.py
    storing.py
scripts /
    get_iam_credentials.sh
    start_spark_job.sh
services /
    get_iam_credentials.service
    spark_python_job.service
test /
    artillery_load_test.yml
    monitoring.py
    metrics.csv
    results.json
    visualisation_load_test.ipynb
main.py
README.md
requirements.txt
```

Appendix A.B Getting Started

To run the program, follow these steps:

1. Create a virtual environment using `python3 -m venv venv`.
2. Activate the virtual environment using `source venv/bin/activate`.
3. Install the required dependencies using `pip3 install -r requirements.txt`.
4. Run the program using `python3 main.py`.
5. Visualise the results using `visualisation.ipynb` (Jupyter Notebook).

Appendix A.C Detailed Features of Functions

`collecting.py`

- `fetch_sensors_data(sparkSession)`: Function to ingest the latest data from the sensors and returns it as a Spark DataFrame.

`processing.py`

- `get_aqi_value_p25(value)`: Function for calculating the AQI value for PM2.5.
- `get_aqi_value_p10(value)`: Function for calculating the AQI value for PM10.
- `computeAQI(df)`: Function for calculating the AQI value for each particulate matter sensor and returning the DataFrame with the AQI column.

`storing.py`

- `keepOnlyUpdatedRows(database_name, table_name, df)`: Function for keeping only the rows that have been updated in the DataFrame.
- `_print_rejected_records_exceptions(err)`: Internal function for printing the rejected records exceptions.
- `write_records(database_name, table_name, client, records)`: Internal function for writing a batch of records to the Timestream database.
- `writeToTimestream(database_name, table_name, partitioned_df)`: Function for writing the DataFrame to the Timestream database.

Appendix B

Source Codes

Appendix B.A Sequential Algorithm

B.A.1 Declaration File

```
1 #ifndef SPARSEMATRIXDENSEVECTORMULTIPLY_H
2 #define SPARSEMATRIXDENSEVECTORMULTIPLY_H
3
4 #include "MatrixDefinitions.h"
5
6 /**
7  * @brief Function to execute the sparse matrix-dense vector multiplication using
8  * sequential algorithm
9  *
10  * @param sparseMatrix Sparse matrix
11  * @param denseVector Dense vector
12  * @param vecCols Number of columns in the dense vector
13  * @return DenseVector Result of the multiplication
14  */
15 DenseVector sparseMatrixDenseVectorMultiply(const SparseMatrix &sparseMatrix,
16                                             const DenseVector &denseVector, int
17                                             vecCols);
18 #endif
```

B.A.2 Implementation File

```
1 #include "SparseMatrixDenseVectorMultiply.h"
2
3 /**
4  * @brief Function to execute the sparse matrix-dense vector multiplication using
5  * sequential algorithm
6  *
7  * @param sparseMatrix Sparse matrix
8  * @param denseVector Dense vector
9  * @param vecCols Number of columns in the dense vector
10  * @return DenseVector Result of the multiplication
11  */
12 DenseVector sparseMatrixDenseVectorMultiply(const SparseMatrix &sparseMatrix,
13                                             const DenseVector &denseVector, int
14                                             vecCols)
15 {
16     // Initialisation of the result vector
17     DenseVector result(sparseMatrix.numRows, std::vector<double>(vecCols, 0.0));
18     // Iterate over the rows of the sparse matrix
19     for (int i = 0; i < sparseMatrix.numRows; ++i)
```

```

18     {
19         // Iterate over the non-zero elements in the current row
20         for (int j = sparseMatrix.rowPtr[i]; j < sparseMatrix.rowPtr[i + 1]; ++j)
21         {
22             // Iterate over the columns of the dense vector
23             for (int k = 0; k < vecCols; ++k)
24             {
25                 result[i][k] += sparseMatrix.values[j] * denseVector[sparseMatrix.
26                     colIndices[j]][k]; // Compute the result
27             }
28         }
29         // Return the result
30         return result;
31     }

```

Appendix B.B Line-Based Parallelism

B.B.1 Declaration File

```

1  #ifndef SPARSEMATRIXDENSEVECTORMULTIPLYROWWISE_H
2  #define SPARSEMATRIXDENSEVECTORMULTIPLYROWWISE_H
3
4  #include "MatrixDefinitions.h"
5  #include <iostream> // std::cout
6
7  /**
8   * @brief Function to multiply a sparse matrix with a dense vector using row-wise
9   * distribution
10  *
11  * @param sparseMatrix The sparse matrix to be multiplied
12  * @param denseVector The dense vector to be multiplied
13  * @param vecCols Number of columns in the dense vector
14  * @return DenseVector Result of the multiplication
15  */
16  DenseVector sparseMatrixDenseVectorMultiplyRowWise(const SparseMatrix &sparseMatrix
17  ,
18  const DenseVector &denseVector,
19  int vecCols);

```

B.B.2 Implementation File

```

1  #include <mpi.h>
2  #include "SparseMatrixDenseVectorMultiplyRowWise.h"
3
4  /**
5   * @brief Function to multiply a sparse matrix with a dense vector using row-wise
6   * distribution
7   *
8   * @param sparseMatrix The sparse matrix to be multiplied
9   * @param denseVector The dense vector to be multiplied
10  * @param vecCols Number of columns in the dense vector
11  * @return DenseVector Result of the multiplication
12  */
13  DenseVector sparseMatrixDenseVectorMultiplyRowWise(const SparseMatrix &sparseMatrix
14  ,
15  const DenseVector &denseVector,
16  int vecCols)
17  {
18      // MPI Initialisation

```

```

17  int worldSize, worldRank;
18  MPI_Comm_size(MPI_COMM_WORLD, &worldSize);
19  MPI_Comm_rank(MPI_COMM_WORLD, &worldRank);
20
21  // ===== FOR DEBUGGING ONLY - START LOCAL COMPUTATION
22  // double computation_start = MPI_Wtime();
23  // ===== FOR DEBUGGING ONLY - START LOCAL COMPUTATION
24  // TIMER =====
25
26  // Distribute rows among processes
27  int rowsCountPerProcess = sparseMatrix.numRows / worldSize;
28  // Number of rows per process
29  int extraRows = sparseMatrix.numRows % worldSize;
30  // Number of extra rows to be distributed
31  among processes
32  int startRow = worldRank * rowsCountPerProcess + std::min(worldRank, extraRows)
33  ; // Starting row index for the current process
34  int endRow = startRow + rowsCountPerProcess + (worldRank < extraRows ? 1 : 0);
35  // Ending row index for the current process
36
37  // Local computation
38  int localSize = (endRow - startRow) * vecCols; // Number of elements in the
39  local result vector
40  std::vector<double> localResult(localSize); // Local result vector
41
42  // Iterate over the rows assigned to the current process
43  for (int i = startRow; i < endRow; ++i)
44  {
45      // Iterate over the non-zero elements in the current row
46      for (int j = sparseMatrix.rowPtr[i]; j < sparseMatrix.rowPtr[i + 1]; ++j)
47      {
48          int colIndex = sparseMatrix.colIndices[j]; // Column index of the non-
49          zero element
50
51          // Iterate over the columns of the dense vector
52          for (int k = 0; k < vecCols; ++k)
53          {
54              int localIndex = (i - startRow) * vecCols + k;
55              // Index of the element in the
56              local result vector
57              localResult[localIndex] += sparseMatrix.values[j] * denseVector[
58              colIndex][k]; // Compute the result
59          }
60      }
61  }
62
63  // ===== FOR DEBUGGING ONLY - STOP LOCAL COMPUTATION
64  // TIMER =====
65  // double computation_end = MPI_Wtime();
66  // double local_computation_time = computation_end - computation_start;
67  // ===== FOR DEBUGGING ONLY - STOP LOCAL COMPUTATION
68  // TIMER =====
69
70  // ===== FOR DEBUGGING ONLY - START COMMUNICATION TIMER
71  // =====
72  // Start timing for communication
73  // double communication_start = MPI_Wtime();
74  // ===== FOR DEBUGGING ONLY - START COMMUNICATION TIMER
75  // =====
76
77  // Preparation for Gather operation
78  std::vector<int> recvCounts(worldSize), displacements(worldSize);
79  if (worldRank == 0)
80  {
81      int totalSize = 0; // Total number of elements to be received
82
83      // Compute the number of elements to be received from each process
84      for (int rank = 0; rank < worldSize; ++rank)
85      {

```

```

71     int startRowThisRank = rank * rowCountPerProcess + std::min(rank,
       extraRows);           // Starting row index for the current
       process
72     int endRowThisRank = startRowThisRank + rowCountPerProcess + (rank <
       extraRows ? 1 : 0); // Ending row index for the current process
73     recvCounts[rank] = (endRowThisRank - startRowThisRank) * vecCols;
       // Number of elements to be received from
       the current process
74     displacements[rank] = totalSize;
       //
       Displacement for the current process
75     totalSize += recvCounts[rank];
       //
       Update the total number of elements to be received
76 }
77 }
78
79 // Gather all local results into the root process
80 std::vector<double> gatheredResults;
81 if (worldRank == 0)
82 {
83     gatheredResults.resize(recvCounts[0] * worldSize); // Resize the vector to
       hold all the results
84 }
85 MPI_Gatherv(localResult.data(), localSize, MPI_DOUBLE,
86             gatheredResults.data(), recvCounts.data(),
87             displacements.data(), MPI_DOUBLE, 0, MPI_COMM_WORLD); // Gather the
       local results in the root process
88
89 // ===== FOR DEBUGGING ONLY - STOP COMMUNICATION TIMER
90 // double communication_end = MPI_Wtime();
91 // double local_communication_time = communication_end - communication_start;
92 // ===== FOR DEBUGGING ONLY - STOP COMMUNICATION TIMER
93
94 // ===== FOR DEBUGGING ONLY - COLLECTING AND ANALYSING
95 // PERFORMANCE DATA =====
96 // double total_computation_time = 0.0, total_communication_time = 0.0;
97 // MPI_Reduce(&local_computation_time, &total_computation_time, 1, MPI_DOUBLE,
98 //            MPI_SUM, 0, MPI_COMM_WORLD);
99 // MPI_Reduce(&local_communication_time, &total_communication_time, 1,
100 //            MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
101 // ===== FOR DEBUGGING ONLY - COLLECTING AND ANALYSING
102 // PERFORMANCE DATA =====
103
104 // Reconstruct the final result matrix in the root process
105 DenseVector finalResult;
106 if (worldRank == 0)
107 {
108     // ===== FOR DEBUGGING ONLY - PRINTING PERFORMANCE
109     // DATA =====
110     // double avg_computation_time = total_computation_time / worldSize;
111     // double avg_communication_time = total_communication_time / worldSize;
112     // std::cout << "Row-wise Average Computation Time: " <<
113     // avg_computation_time << std::endl;
114     // std::cout << "Row-wise Average Communication Time: " <<
115     // avg_communication_time << std::endl;
116     // ===== FOR DEBUGGING ONLY - PRINTING PERFORMANCE
117     // DATA =====
118
119     finalResult.resize(sparseMatrix.numRows, std::vector<double>(vecCols, 0.0))
       ; // Resize the final result matrix
120
121     // Iterate over the rows of the final result
122     for (int i = 0, index = 0; i < sparseMatrix.numRows; ++i)
123     {
124         // Iterate over the columns of the final result
125         for (int j = 0; j < vecCols; ++j, ++index)
126         {

```



```

119         finalResult[i][j] = gatheredResults[index]; // Copy the element of
120             the final result
121     }
122 }
123
124 // Return the final result
125 return (worldRank == 0) ? finalResult : DenseVector{};
126 }

```

Appendix B.C Column-Wise Parallelism

B.C.1 Declaration File

```

1  #ifndef SPARSEMATRIXDENSEVECTORMULTIPLYCOLUMNWISE_H
2  #define SPARSEMATRIXDENSEVECTORMULTIPLYCOLUMNWISE_H
3
4  #include "MatrixDefinitions.h"
5  #include <iostream> // std::cout
6
7  /**
8   * @brief Function to execute the sparse matrix-dense vector multiplication using
9   * column-wise parallel algorithm
10  *
11  * @param sparseMatrix Sparse matrix
12  * @param denseVector Dense vector
13  * @param vecCols Number of columns in the dense vector
14  * @return DenseVector Result of the multiplication
15  */
16 DenseVector sparseMatrixDenseVectorMultiplyColumnWise(const SparseMatrix &
17     sparseMatrix, const DenseVector &denseVector, int vecCols);
18
19 #endif

```

B.C.2 Implementation File

```

1  #include <mpi.h>
2  #include "SparseMatrixDenseVectorMultiplyColumnWise.h"
3  #include <numeric> // Pour std::accumulate
4
5  /**
6   * @brief Function to execute the sparse matrix-dense vector multiplication using
7   * column-wise parallel algorithm
8   *
9   * @param sparseMatrix Sparse matrix
10  * @param denseVector Dense vector
11  * @param vecCols Number of columns in the dense vector
12  * @return DenseVector Result of the multiplication
13  */
14 DenseVector sparseMatrixDenseVectorMultiplyColumnWise(const SparseMatrix &
15     sparseMatrix, const DenseVector &denseVector, int vecCols)
16 {
17     // MPI Initialisation
18     int worldSize, worldRank;
19     MPI_Comm_size(MPI_COMM_WORLD, &worldSize);
20     MPI_Comm_rank(MPI_COMM_WORLD, &worldRank);
21
22     // ===== FOR DEBUGGING ONLY - START LOCAL COMPUTATION
23     TIMER =====
24     // double computation_start = MPI_Wtime();
25     // ===== FOR DEBUGGING ONLY - START LOCAL COMPUTATION
26     TIMER =====

```

```

23 // Distribute columns among processes
24 int colsPerProcess = vecCols / worldSize;
25 //
26 // Number of columns per process
27 int extraCols = vecCols % worldSize;
28 // Number of extra columns to be distributed among processes
29 int startCol = worldRank * colsPerProcess;
30 //
31 // Starting column index for the current process
32 int endCol = (worldRank != worldSize - 1) ? startCol + colsPerProcess :
33 startCol + colsPerProcess + extraCols; // Ending column index for the
34 current process
35
36 // Local computation
37 int localSize = sparseMatrix.numRows * (endCol - startCol); // Number of
38 elements in the local result vector
39 std::vector<double> localResult(localSize, 0.0);
40 // Iterate over the columns assigned to the current process
41 for (int col = startCol; col < endCol; ++col)
42 {
43     // Iterate over the rows of the sparse matrix
44     for (int i = 0; i < sparseMatrix.numRows; ++i)
45     {
46         // Iterate over the non-zero elements in the current row
47         double sum = 0.0;
48         for (int j = sparseMatrix.rowPtr[i]; j < sparseMatrix.rowPtr[i + 1]; ++
49             j)
50         {
51             int sparseCol = sparseMatrix.colIndices[j]; //
52             Column index of the non-zero element
53             sum += sparseMatrix.values[j] * denseVector[sparseCol][col]; //
54             Compute the result
55         }
56         localResult[i * (endCol - startCol) + (col - startCol)] = sum; // Store
57         the result in the local result vector
58     }
59 }
60
61 // ===== FOR DEBUGGING ONLY - STOP LOCAL COMPUTATION
62 // TIMER =====
63 // double computation_end = MPI_Wtime();
64 // double local_computation_time = computation_end - computation_start;
65 // ===== FOR DEBUGGING ONLY - STOP LOCAL COMPUTATION
66 // TIMER =====
67
68 // ===== FOR DEBUGGING ONLY - START COMMUNICATION TIMER
69 // =====
70 // Start timing for communication
71 // double communication_start = MPI_Wtime();
72 // ===== FOR DEBUGGING ONLY - START COMMUNICATION TIMER
73 // =====
74
75 // Preparation for Gather operation
76 std::vector<int> recvCounts(worldSize), displacements(worldSize); // Number of
77 elements to be received from each process, Displacement for each process
78 if (worldRank == 0)
79 {
80     // Compute the number of elements to be received from each process
81     int displacement = 0;
82     for (int i = 0; i < worldSize; ++i)
83     {
84         int startColThisRank = i * colsPerProcess;
85
86         // Starting column index for the current process
87         int endColThisRank = (i != worldSize - 1) ? startColThisRank +
88 colsPerProcess : startColThisRank + colsPerProcess + extraCols; //
89 Ending column index for the current process

```

```

70         recvCounts[i] = sparseMatrix.numRows * (endColThisRank -
            startColThisRank);
                                                    // Number of
            elements to be received from the current process
71         displacements[i] = displacement;

            // Displacement for the current process
72         displacement += recvCounts[i];

            // Update the displacement
73     }
74 }

75 // Gather all local results into the root process
76 std::vector<double> gatheredResults;
77 if (worldRank == 0)
78 {
79     gatheredResults.resize(std::accumulate(recvCounts.begin(), recvCounts.end()
80         , 0)); // Resize the vector to hold the final result
81 }
82 MPI_Gatherv(localResult.data(), localSize, MPI_DOUBLE,
83     gatheredResults.data(), recvCounts.data(),
84     displacements.data(), MPI_DOUBLE, 0, MPI_COMM_WORLD); // Gather the
            local results in the root process
85
86 // ===== FOR DEBUGGING ONLY - STOP COMMUNICATION TIMER
87 // =====
88 // double communication_end = MPI_Wtime();
89 // double local_communication_time = communication_end - communication_start;
90 // ===== FOR DEBUGGING ONLY - STOP COMMUNICATION TIMER
91 // =====
92
93 // ===== FOR DEBUGGING ONLY - COLLECTING AND ANALYSING
94 // PERFORMANCE DATA =====
95 // double total_computation_time = 0.0, total_communication_time = 0.0;
96 // MPI_Reduce(&local_computation_time, &total_computation_time, 1, MPI_DOUBLE,
97 //     MPI_SUM, 0, MPI_COMM_WORLD);
98 // MPI_Reduce(&local_communication_time, &total_communication_time, 1,
99 //     MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
100 // ===== FOR DEBUGGING ONLY - COLLECTING AND ANALYSING
101 // PERFORMANCE DATA =====
102
103 // Reconstruct the final result matrix in the root process
104 DenseVector finalResult;
105 if (worldRank == 0)
106 {
107     // ===== FOR DEBUGGING ONLY - PRINTING PERFORMANCE
108     // DATA =====
109     // double avg_computation_time = total_computation_time / worldSize;
110     // double avg_communication_time = total_communication_time / worldSize;
111     // std::cout << "Column-wise Average Computation Time: " <<
112     //     avg_computation_time << std::endl;
113     // std::cout << "Column-wise Average Communication Time: " <<
114     //     avg_communication_time << std::endl;
115     // ===== FOR DEBUGGING ONLY - PRINTING PERFORMANCE
116     // DATA =====
117
118     // Reconstruct the final result matrix
119     finalResult.resize(sparseMatrix.numRows, std::vector<double>(vecCols, 0.0))
120         ; // Resize the final result matrix
121     int resultIndex = 0;
122     // Iterate over the processes
123     for (int rank = 0; rank < worldSize; ++rank)
124     {
125         int numColsThisRank = (rank != worldSize - 1) ? colsPerProcess :
126             colsPerProcess + extraCols; // Number of columns assigned to the
127             current process
128         int startColThisRank = rank * colsPerProcess;
129
130             // Starting column
131             index for the current process

```

```

116         // Iterate over the rows of the sparse matrix
117         for (int row = 0; row < sparseMatrix.numRows; ++row)
118         {
119             // Iterate over the columns assigned to the current process
120             for (int col = 0; col < numColsThisRank; ++col)
121             {
122                 finalResult[row][startColThisRank + col] = gatheredResults[
123                     resultIndex++]; // Reconstruct the final result matrix
124             }
125         }
126     }
127 }
128
129 // Return the final result
130 return (worldRank == 0) ? finalResult : DenseVector{};
131 }

```

Appendix B.D Non-Zero Element Parallelism

B.D.1 Declaration File

```

1  #ifndef SPARSEMATRIXDENSEVECTORMULTIPLYNONZEROELEMENT_H
2  #define SPARSEMATRIXDENSEVECTORMULTIPLYNONZEROELEMENT_H
3
4  #include "MatrixDefinitions.h"
5  #include <iostream> // std::cout
6
7  /**
8   * @brief Function to execute the sparse matrix-dense vector multiplication using
9   *        non-zero element parallel algorithm
10   *
11   * @param sparseMatrix Sparse matrix
12   * @param denseVector Dense vector
13   * @param vecCols Number of columns in the dense vector
14   * @return DenseVector Result of the multiplication
15   */
16 DenseVector sparseMatrixDenseVectorMultiplyNonZeroElement(const SparseMatrix &
17     sparseMatrix, const DenseVector &denseVector, int vecCols);
18
19 #endif

```

B.D.2 Implementation File

```

1  #include "SparseMatrixDenseVectorMultiplyNonZeroElement.h"
2  #include <mpi.h>
3
4  /**
5   * @brief Function to execute the sparse matrix-dense vector multiplication using
6   *        non-zero element parallel algorithm
7   *
8   * @param sparseMatrix Sparse matrix
9   * @param denseVector Dense vector
10   * @param vecCols Number of columns in the dense vector
11   * @return DenseVector Result of the multiplication
12   */
13 DenseVector sparseMatrixDenseVectorMultiplyNonZeroElement(const SparseMatrix &
14     sparseMatrix, const DenseVector &denseVector, int vecCols)
15 {
16     // MPI Initialisation
17     int worldSize, worldRank;
18     MPI_Comm_size(MPI_COMM_WORLD, &worldSize);

```

```

17 MPI_Comm_rank(MPI_COMM_WORLD, &worldRank);
18
19 // ===== FOR DEBUGGING ONLY - START LOCAL COMPUTATION
20 // double computation_start = MPI_Wtime();
21 // ===== FOR DEBUGGING ONLY - START LOCAL COMPUTATION
22 // =====
23 // Distribute non-zero elements among processes
24 int totalNonZeroElements = sparseMatrix.values.size(); // Total number of
25 // non-zero elements
26 int elementsPerProcess = totalNonZeroElements / worldSize; // Number of non-
27 // zero elements per process
28 int extraElements = totalNonZeroElements % worldSize; // Number of extra
29 // non-zero elements to be distributed among processes
30 int startIdx, endIdx; // Starting and
31 // ending indices of the non-zero elements for the current process
32
33 // Determine the starting and ending indices of the non-zero elements for the
34 // current process
35 if (worldRank < extraElements)
36 {
37     startIdx = worldRank * (elementsPerProcess + 1); // Add 1 to account for
38     // the extra non-zero elements
39     endIdx = startIdx + elementsPerProcess + 1; // Add 1 to account for
40     // the extra non-zero elements
41 }
42 else
43 {
44     startIdx = worldRank * elementsPerProcess + extraElements; // Add
45     // extraElements to account for the extra non-zero elements
46     endIdx = startIdx + elementsPerProcess; // Add
47     // extraElements to account for the extra non-zero elements
48 }
49
50 // Map the indices of the non-zero elements to their corresponding row indices
51 std::vector<int> rowIndexMap(sparseMatrix.values.size());
52 // Iterate over the rows of the sparse matrix
53 for (int row = 0, idx = 0; row < sparseMatrix.rowPtr.size() - 1; ++row)
54 {
55     // Iterate over the non-zero elements in the current row
56     for (; idx < sparseMatrix.rowPtr[row + 1]; ++idx)
57     {
58         rowIndexMap[idx] = row; // Map the index of the non-zero element to its
59         // corresponding row index
60     }
61 }
62
63 // Local computation
64 std::vector<double> localResult(sparseMatrix.numRows * vecCols, 0.0);
65 // Iterate over the non-zero elements assigned to the current process
66 for (int idx = startIdx; idx < endIdx; ++idx)
67 {
68     int row = rowIndexMap[idx]; // Row index of the non-zero
69     // element
70     int col = sparseMatrix.colIndices[idx]; // Column index of the non-zero
71     // element
72     double value = sparseMatrix.values[idx]; // Value of the non-zero element
73
74     // Iterate over the columns of the dense vector
75     for (int k = 0; k < vecCols; ++k)
76     {
77         localResult[row * vecCols + k] += value * denseVector[col][k]; //
78         // Compute the result
79     }
80 }
81
82 // ===== FOR DEBUGGING ONLY - STOP LOCAL COMPUTATION
83 // double computation_end = MPI_Wtime();
84 // =====

```

```

71 // double local_computation_time = computation_end - computation_start;
72 // ===== FOR DEBUGGING ONLY - STOP LOCAL COMPUTATION
    TIMER =====
73
74 // ===== FOR DEBUGGING ONLY - START COMMUNICATION TIMER
    =====
75 // FOR DEBUGGING ONLY - START COMMUNICATION TIMER
76 // double communication_start = MPI_Wtime();
77 // ===== FOR DEBUGGING ONLY - START COMMUNICATION TIMER
    =====
78
79 // Initialise the final result only in the root process
80 DenseVector finalResult;
81 if (worldRank == 0)
82 {
83     finalResult.resize(sparseMatrix.numRows, std::vector<double>(vecCols, 0.0))
        ;
84 }
85
86 // Gather the local results in the root process
87 std::vector<double> flatFinalResult(sparseMatrix.numRows * vecCols, 0.0);
        // Flat vector to
    hold the final result
88 MPI_Reduce(localResult.data(), flatFinalResult.data(), sparseMatrix.numRows *
    vecCols, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD); // Gather the local
    results in the root process
89
90 // ===== FOR DEBUGGING ONLY - STOP COMMUNICATION TIMER
    =====
91 // double communication_end = MPI_Wtime();
92 // double local_communication_time = communication_end - communication_start;
93 // ===== FOR DEBUGGING ONLY - STOP COMMUNICATION TIMER
    =====
94
95 // ===== FOR DEBUGGING ONLY - COLLECTING AND ANALYSING
    PERFORMANCE DATA =====
96 // double total_computation_time = 0.0, total_communication_time = 0.0;
97 // MPI_Reduce(&local_computation_time, &total_computation_time, 1, MPI_DOUBLE,
    MPI_SUM, 0, MPI_COMM_WORLD);
98 // MPI_Reduce(&local_communication_time, &total_communication_time, 1,
    MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
99 // ===== FOR DEBUGGING ONLY - COLLECTING AND ANALYSING
    PERFORMANCE DATA =====
100
101 // Reconstruct the finalResult from flatFinalResult in the root process
102 if (worldRank == 0)
103 {
104     // ===== FOR DEBUGGING ONLY - PRINTING PERFORMANCE
        DATA =====
105     // double avg_computation_time = total_computation_time / worldSize;
106     // double avg_communication_time = total_communication_time / worldSize;
107     // std::cout << "Non-zero elements Average Computation Time: " <<
        avg_computation_time << std::endl;
108     // std::cout << "Non-zero elements Average Communication Time: " <<
        avg_communication_time << std::endl;
109     // ===== FOR DEBUGGING ONLY - PRINTING PERFORMANCE
        DATA =====
110
111     // Iterate over the rows of the final result
112     for (int i = 0; i < sparseMatrix.numRows; ++i)
113     {
114         std::copy(flatFinalResult.begin() + i * vecCols, flatFinalResult.begin
            () + (i + 1) * vecCols, finalResult[i].begin()); // Copy the row of
            the final result
115     }
116 }
117
118 // Return the final result
119 return (worldRank == 0) ? finalResult : DenseVector{};
120 }

```

Appendix B.E Utility Functions

B.E.1 Declaration File

```

1  #ifndef UTILS_H
2  #define UTILS_H
3
4  #include <iostream> // std::cout
5  #include <vector>   // std::vector
6  #include <cstdlib>  // rand() and srand()
7  #include <ctime>    // time()
8  #include <mpi.h>
9  #include <petsc.h>
10 #include <fstream>   // std::ifstream
11 #include <string>    // std::string
12 #include <sstream>   // std::stringstream
13 #include <utility>   // std::pair
14 #include <algorithm> // std::sort
15 #include <stdexcept> // std::runtime_error
16 #include <cmath>     // std::fabs
17 #include "MatrixDefinitions.h"
18
19 /**
20  * Method to convert a PETSc matrix to a dense vector
21  * @param C PETSc matrix
22  * @return DenseVector Dense vector
23  */
24 DenseVector ConvertPETScMatToDenseVector(Mat C);
25
26 /**
27  * Method to compare two matrices
28  * @param mat1 First matrix
29  * @param mat2 Second matrix
30  * @param tolerance Tolerance for comparison
31  * @return bool True if the matrices are equal, false otherwise
32  */
33 bool areMatricesEqual(const DenseVector &mat1, const DenseVector &mat2, double
    tolerance);
34
35 /**
36  * Method to read a matrix from a Matrix Market file
37  * @param filename Name of the file
38  * @return SparseMatrix Sparse matrix
39  */
40 SparseMatrix readMatrixMarketFile(const std::string &filename);
41
42 /**
43  * Method to generate a random dense vector
44  * @param n Number of rows
45  * @param m Number of columns
46  * @return DenseVector Dense vector
47  */
48 DenseVector generateLargeDenseVector(int n, int k);
49
50 /**
51  * @brief Method to serialize a DenseVector to a flat array
52  * @param denseVec Dense vector to serialize
53  * @return std::vector<double> Flat array containing the serialized data
54  */
55 std::vector<double> serialize(const DenseVector &denseVec);
56
57 /**
58  * @brief Method to deserialize a flat array to a DenseVector
59  * @param flat Flat array to deserialize
60  * @param rows Number of rows in the dense vector
61  * @param cols Number of columns in the dense vector
62  * @return DenseVector Dense vector
63  */
64 DenseVector deserialize(const std::vector<double> &flat, int rows, int cols);

```

```

65
66 #endif

```

B.E.2 Implementation File

```

1  #include "utils.h"
2
3  /**
4   * Method to convert a PETSc matrix to a dense vector
5   * @param C PETSc matrix
6   * @return DenseVector Dense vector
7   */
8  DenseVector ConvertPETScMatToDenseVector(Mat C)
9  {
10     PetscInt m, n;           // Number of rows and columns in the matrix
11     MatGetSize(C, &m, &n); // Get the number of rows and columns in the matrix
12
13     DenseVector denseVec(m, std::vector<double>(n, 0.0)); // Dense vector to hold
14     // the matrix
15
16     // Iterate over the rows of the matrix
17     for (int i = 0; i < m; ++i)
18     {
19         // Iterate over the columns of the matrix
20         for (int j = 0; j < n; j++)
21         {
22             PetscScalar value;           // Value of the element
23             MatGetValues(C, i, j, &value); // Get the value of the element
24             denseVec[i][j] = PetscRealPart(value); // Copy the value of the element
25         }
26     }
27
28     // Return the dense vector
29     return denseVec;
30 }
31
32 /**
33 * Method to compare two matrices
34 * @param mat1 First matrix
35 * @param mat2 Second matrix
36 * @param tolerance Tolerance for comparison
37 * @return bool True if the matrices are equal, false otherwise
38 */
39 bool areMatricesEqual(const DenseVector &mat1, const DenseVector &mat2, double
40 tolerance)
41 {
42     // Check if the matrices have the same dimensions
43     if (mat1.size() != mat2.size())
44         return false;
45
46     // Iterate over the rows of the matrices
47     for (size_t i = 0; i < mat1.size(); ++i)
48     {
49         // Check if the rows have the same dimensions
50         if (mat1[i].size() != mat2[i].size())
51             return false;
52
53         // Iterate over the columns of the matrices
54         for (size_t j = 0; j < mat1[i].size(); ++j)
55         {
56             // Check if the elements are equal
57             if (std::fabs(mat1[i][j] - mat2[i][j]) > tolerance)
58             {
59                 return false; // Matrices are not equal
60             }
61         }
62     }
63 }

```



```

61
62     return true; // Matrices are equal
63 }
64
65 /**
66  * Method to read a matrix from a Matrix Market file
67  * @param filename Name of the file
68  * @return SparseMatrix Sparse matrix
69  */
70 SparseMatrix readMatrixMarketFile(const std::string &filename)
71 {
72     std::ifstream file(filename); // Input file stream
73
74     // Check if the file was opened successfully
75     if (!file.is_open())
76     {
77         throw std::runtime_error("Unable to open file: " + filename);
78     }
79
80     std::string line; // String to hold the current line
81     bool isSymmetric = false, isPattern = false; // Flags to indicate if the matrix
82     // is symmetric or pattern only
83
84     // Skip the comments
85     while (std::getline(file, line))
86     {
87         // Check if the line is a comment
88         if (line[0] == '%')
89         {
90             // Check if the line contains the word "symmetric"
91             if (line.find("symmetric") != std::string::npos)
92             {
93                 isSymmetric = true; // Set the symmetric flag
94             }
95
96             // Check if the line contains the word "pattern"
97             if (line.find("pattern") != std::string::npos)
98             {
99                 isPattern = true; // Set the pattern flag
100             }
101         }
102         else
103         {
104             break; // First non-comment line reached, break out of the loop
105         }
106     }
107
108     // Read the matrix dimensions
109     int numRows, numCols, nonZeros; // Number of rows,
110     // columns and non-zero elements in the matrix
111     std::stringstream(line) >> numRows >> numCols >> nonZeros; // Read the
112     // dimensions from the line
113
114     // Check if the file was read successfully
115     if (!file)
116     {
117         throw std::runtime_error("Failed to read matrix dimensions from file: " +
118             filename);
119     }
120
121     SparseMatrix matrix; // Sparse
122     // matrix to hold the data
123     matrix.rowPtr.resize(numRows + 1, 0); // Resize
124     // the row pointer vector
125     std::vector<std::vector<std::pair<int, double>>> tempRows(numRows); //
126     // Temporary vector to hold the data
127     int rowIndex, colIndex; // Row and
128     // column indices
129     double value; // Value of
130     // the non-zero element

```

```

122 // Read the non-zero elements
123 for (int i = 0; i < nonZeros; ++i)
124 {
125     // If the matrix is pattern only, the value of the non-zero element is 1.0
126     if (isPattern)
127     {
128         file >> rowIndex >> colIndex; // Read the row and column indices
129         value = 1.0; // Default value for pattern entries
130     }
131     else
132     {
133         file >> rowIndex >> colIndex >> value; // Read the row and column
134         indices and the value
135     }
136
137     // Check if the file was read successfully
138     if (!file)
139     {
140         throw std::runtime_error("Failed to read data from file: " + filename);
141     }
142
143     rowIndex--; // Adjusting from 1-based to 0-based indexing
144     colIndex--; // Adjusting from 1-based to 0-based indexing
145
146     tempRows[rowIndex].emplace_back(colIndex, value); // Store the data in the
147     temporary vector
148
149     // If the matrix is symmetric, store the data in the transpose as well
150     if (isSymmetric && rowIndex != colIndex)
151     {
152         tempRows[colIndex].emplace_back(rowIndex, value); // Store the data in
153         the temporary vector
154     }
155
156     // Sort each row by column index
157     for (auto &row : tempRows)
158     {
159         std::sort(row.begin(), row.end());
160     }
161
162     // Reconstruct SparseMatrix structure
163     int cumSum = 0; // Cumulative sum of the number of non-zero elements
164
165     // Iterate over the rows of the matrix
166     for (int i = 0; i < numRows; ++i)
167     {
168         matrix.rowPtr[i] = cumSum; // Store the cumulative sum in the row pointer
169         vector
170
171         // Iterate over the non-zero elements in the current row
172         for (const auto &elem : tempRows[i])
173         {
174             matrix.values.push_back(elem.second); // Store the value of the non-
175             zero element
176             matrix.colIndices.push_back(elem.first); // Store the column index of
177             the non-zero element
178         }
179
180         cumSum += tempRows[i].size(); // Update the cumulative sum
181     }
182
183     matrix.rowPtr[numRows] = cumSum; // Store the cumulative sum in the row pointer
184     vector
185     matrix.numRows = numRows; // Store the number of rows
186     matrix.numCols = numCols; // Store the number of columns
187
188     // Return the sparse matrix
189     return matrix;

```

```

185 }
186
187 /**
188  * Method to generate a random dense vector
189  * @param n Number of rows
190  * @param m Number of columns
191  * @return DenseVector Dense vector
192  */
193 DenseVector generateLargeDenseVector(int n, int k)
194 {
195     DenseVector denseVector(n, std::vector<double>(k)); // Dense vector to hold the
196     // random values
197
198     // Iterate over the rows of the dense vector
199     for (int i = 0; i < n; ++i)
200     {
201         // Iterate over the columns of the dense vector
202         for (int j = 0; j < k; ++j)
203         {
204             denseVector[i][j] = rand() % 100 + 1; // Generate a random value
205             // between 1 and 100
206         }
207     }
208
209     // Return the dense vector
210     return denseVector;
211 }
212
213 /**
214  * @brief Method to serialize a DenseVector to a flat array
215  * @param denseVec Dense vector to serialize
216  * @return std::vector<double> Flat array containing the serialized data
217  */
218 std::vector<double> serialize(const DenseVector &denseVec)
219 {
220     std::vector<double> flat; // Flat array to hold the serialized data
221
222     // Iterate over the rows of the dense vector
223     for (const auto &vec : denseVec)
224     {
225         flat.insert(flat.end(), vec.begin(), vec.end()); // Copy the elements
226     }
227
228     // Return the flat array
229     return flat;
230 }
231
232 /**
233  * @brief Method to deserialize a flat array to a DenseVector
234  * @param flat Flat array to deserialize
235  * @param rows Number of rows in the dense vector
236  * @param cols Number of columns in the dense vector
237  * @return DenseVector Dense vector
238  */
239 DenseVector deserialize(const std::vector<double> &flat, int rows, int cols)
240 {
241     DenseVector denseVec(rows, std::vector<double>(cols)); // Dense vector to hold
242     // the deserialized data
243
244     // Iterate over the rows of the dense vector
245     for (int i = 0; i < rows; ++i)
246     {
247         // Iterate over the columns of the dense vector
248         for (int j = 0; j < cols; ++j)
249         {
250             denseVec[i][j] = flat[i * cols + j]; // Copy the element
251         }
252     }
253
254     // Return the dense vector

```

```

252     return denseVec;
253 }

```

Appendix B.F Main File

```

1  #include "utils.h" // Utility functions
2  #include "SparseMatrixDenseVectorMultiply.h" // Sequential algorithm
3  #include "SparseMatrixDenseVectorMultiplyRowWise.h" // Parallel algorithm (
   row-wise)
4  #include "SparseMatrixDenseVectorMultiplyColumnWise.h" // Parallel algorithm (
   column-wise)
5  #include "SparseMatrixDenseVectorMultiplyNonZeroElement.h" // Parallel algorithm (
   non-zero element)
6
7  int main(int argc, char *argv[])
8  {
9      //
10     // ===== INITIALISATION
11     // =====
12
13     // Initialise MPI and PETSc
14     MPI_Init(&argc, &argv);
15     PetscInitialize(&argc, &argv, NULL, NULL);
16
17     // Retrieve the rank and size of the world communicator
18     int worldRank, worldSize;
19     MPI_Comm_rank(PETSC_COMM_WORLD, &worldRank);
20     MPI_Comm_size(PETSC_COMM_WORLD, &worldSize);
21
22     // Check if the correct number of arguments is provided
23     if (argc != 3)
24     {
25         if (worldRank == 0)
26         {
27             std::cerr << "Usage: " << argv[0] << " <number of columns> <matrix file
               path>" << std::endl;
28         }
29         MPI_Abort(PETSC_COMM_WORLD, 1);
30     }
31
32     // Parse the command-line arguments
33     int k = std::atoi(argv[1]); // Convert the first argument to an integer
34     std::string filename = argv[2]; // The second argument is the filename
35
36     // Declare the sparse matrix and dense vector
37     SparseMatrix M;
38     DenseVector v;
39
40     // Declare the result of the serial multiplication
41     DenseVector resultSerial;
42
43     // Declare the data for broadcasting the sparse matrix and dense vector
44     std::vector<double> flatData;
45     int dataSize = 0;
46
47     // Declare the variables for timing the execution of the algorithms
48     double startTime, endTime;
49
50     //
   -----

```

```

51 // ===== READ THE SPARSE MATRIX AND GENERATE THE DENSE
52 // VECTOR =====
53
54 if (worldRank == 0)
55 {
56     std::cout << "World size: " << worldSize << std::endl; // Print the
57     // number of processes
58     std::cout << "Sparse matrix: " << filename << std::endl; // Print the name
59     // of the Matrix Market file
60
61     // Read the sparse matrix from the Matrix Market file
62     M = readMatrixMarketFile(filename);
63     std::cout << "Matrix size: " << M.numRows << "x" << M.numCols << std::endl;
64
65     // Generate a random dense vector
66     v = generateLargeDenseVector(M.numCols, k);
67     std::cout << "Vector size: " << M.numCols << "x" << k << std::endl;
68
69     // Prepare the data for broadcasting
70     flatData = serialize(v); // Serialize the dense vector
71     dataSize = flatData.size(); // Size of the serialized data
72 }
73
74 // ===== EXECUTE THE SERIAL MULTIPLICATION =====
75
76 if (worldRank == 0)
77 {
78     // Execute the serial multiplication
79     startTime = MPI_Wtime();
80     resultSerial = sparseMatrixDenseVectorMultiply(M, v, k);
81     endTime = MPI_Wtime();
82     std::cout << "Serial Algo Execution time: " << (endTime - startTime)
83     << std::endl;
84
85     // FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS OF THE RESULT
86     // std::cout << "Result: " << std::endl;
87     // for (int i = 0; i < 10; ++i)
88     // {
89     //     for (int j = 0; j < k; ++j)
90     //     {
91     //         std::cout << resultSerial[i][j] << " ";
92     //     }
93     //     std::cout << std::endl;
94     // }
95 }
96
97 // ===== BROADCAST THE SPARSE MATRIX AND DENSE VECTOR =====
98
99 // Wait for the main process to finish the serial multiplication
100 MPI_Barrier(MPI_COMM_WORLD);
101
102 // ===== FOR DEBUGGING ONLY - START BROADCAST TIMER =====
103 // startTime = MPI_Wtime();

```

```

104 // ===== FOR DEBUGGING ONLY - START BROADCAST TIMER
105 // =====
106 // Broadcast the Sparse Matrix to all processes
107 // Prepare the data for broadcasting
108 int valuesSize = M.values.size(); // Number of non-
109 // zero elements
110 int colIndicesSize = M.colIndices.size(); // Number of column
111 // indices
112 int rowPtrSize = M.rowPtr.size(); // Number of row
113 // pointers
114 MPI_Bcast(&M.numRows, 1, MPI_INT, 0, MPI_COMM_WORLD); // Broadcast the
115 // number of rows
116 MPI_Bcast(&M.numCols, 1, MPI_INT, 0, MPI_COMM_WORLD); // Broadcast the
117 // number of columns
118 MPI_Bcast(&valuesSize, 1, MPI_INT, 0, MPI_COMM_WORLD); // Broadcast the
119 // number of non-zero elements
120 MPI_Bcast(&colIndicesSize, 1, MPI_INT, 0, MPI_COMM_WORLD); // Broadcast the
121 // number of column indices
122 MPI_Bcast(&rowPtrSize, 1, MPI_INT, 0, MPI_COMM_WORLD); // Broadcast the
123 // number of row pointers
124 // Resize the vectors for all processes
125 if (worldRank != 0)
126 {
127     M.values.resize(valuesSize);
128     M.colIndices.resize(colIndicesSize);
129     M.rowPtr.resize(rowPtrSize);
130 }
131 // Broadcast the data
132 MPI_Bcast(M.values.data(), valuesSize, MPI_DOUBLE, 0, MPI_COMM_WORLD);
133 MPI_Bcast(M.colIndices.data(), colIndicesSize, MPI_INT, 0, MPI_COMM_WORLD);
134 MPI_Bcast(M.rowPtr.data(), rowPtrSize, MPI_INT, 0, MPI_COMM_WORLD);
135
136 // Broadcast the Dense Vector to all processes
137 // Broadcast the size of the serialized data
138 MPI_Bcast(&dataSize, 1, MPI_INT, 0, MPI_COMM_WORLD);
139 // Resize flatData for all processes
140 if (worldRank != 0)
141 {
142     flatData.resize(dataSize);
143 }
144 // Broadcast the data
145 MPI_Bcast(flatData.data(), dataSize, MPI_DOUBLE, 0, MPI_COMM_WORLD);
146 // Deserialize the data
147 if (worldRank != 0)
148 {
149     v.resize(M.numCols, std::vector<double>(k));
150     v = deserialize(flatData, M.numCols, k);
151 }
152
153 // Wait for all processes to finish the broadcast
154 MPI_Barrier(MPI_COMM_WORLD);
155
156 // ===== FOR DEBUGGING ONLY - STOP BROADCAST TIMER
157 // =====
158 // endTime = MPI_Wtime();
159 // if (worldRank == 0)
160 // {
161 //     std::cout << "Broadcast time: " << (endTime - startTime) << std::endl;
162 // }
163 // ===== FOR DEBUGGING ONLY - STOP BROADCAST TIMER
164 // =====
165
166 // -----
167
168 // ===== EXECUTE THE PARALLEL MULTIPLICATION (ROW-WISE)
169 // =====
170 // -----

```

```

159
160 // Execute the parallel multiplication (row-wise)
161 startTime = MPI_Wtime();
162 DenseVector resultRowWise = sparseMatrixDenseVectorMultiplyRowWise(M, v, k);
163 endTime = MPI_Wtime();
164
165 // Only the main process prints the parallel execution time
166 if (worldRank == 0)
167 {
168     std::cout << "Row-wise Execution time: " << (endTime - startTime)
169         << std::endl;
170
171     // ===== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
172     // =====
173     // std::cout << "Result: " << std::endl;
174     // for (int i = 0; i < 10; ++i)
175     // {
176     //     for (int j = 0; j < k; ++j)
177     //     {
178     //         std::cout << resultRowWise[i][j] << " ";
179     //     }
180     //     std::cout << std::endl;
181     // }
182     // ===== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
183     // =====
184
185     // Compare the results of the serial and parallel multiplications
186     if (areMatricesEqual(resultSerial, resultRowWise, 1e-6)) // Tolerance = 1e
187         -6
188     {
189         std::cout << "Row-wise: Results are the same!"
190             << std::endl;
191     }
192     else
193     {
194         std::cout << "Row-wise: Results are different!"
195             << std::endl;
196     }
197 }
198
199 // ===== EXECUTE THE PARALLEL MULTIPLICATION (COLUMN-WISE)
200 // =====
201
202 // Wait for all processes to finish the parallel multiplication (row-wise)
203 MPI_Barrier(MPI_COMM_WORLD);
204
205 // Execute the parallel multiplication (column-wise)
206 startTime = MPI_Wtime();
207 DenseVector resultColumnWise = sparseMatrixDenseVectorMultiplyColumnWise(M, v,
208     k);
209 endTime = MPI_Wtime();
210
211 // Only the main process prints the parallel execution time
212 if (worldRank == 0)
213 {
214     std::cout << "Column-wise Execution time: " << (endTime - startTime)
215         << std::endl;
216
217     // ===== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
218     // =====
219     // std::cout << "Result: " << std::endl;
220     // for (int i = 0; i < 10; ++i)
221     // {

```

```

218 //     for (int j = 0; j < k; ++j)
219 //     {
220 //         std::cout << resultColumnWise[i][j] << " ";
221 //     }
222 //     std::cout << std::endl;
223 // }
224 // ===== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
225 // =====
226 // Compare the results of the serial and parallel multiplications
227 if (areMatricesEqual(resultSerial, resultColumnWise, 1e-6)) // Tolerance =
    1e-6
228 {
229     std::cout << "Column-wise: Results are the same!"
230     << std::endl;
231 }
232 else
233 {
234     std::cout << "Column-wise: Results are different!"
235     << std::endl;
236 }
237 }
238 //
239 // -----
240 // ===== EXECUTE THE PARALLEL MULTIPLICATION (NON-ZERO
241 // ELEMENT) =====
242 // -----
243 // Wait for all processes to finish the parallel multiplication (column-wise)
244 MPI_Barrier(MPI_COMM_WORLD);
245 // Execute the parallel multiplication (non-zero element)
246 startTime = MPI_Wtime();
247 DenseVector resultNonZeroElement =
248     sparseMatrixDenseVectorMultiplyNonZeroElement(M, v, k);
249 endTime = MPI_Wtime();
250 // Only the main process prints the parallel execution time
251 if (worldRank == 0)
252 {
253     std::cout << "Non-zero Elements Execution time: " << (endTime - startTime)
254     << std::endl;
255     // ===== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
256     // =====
257     // std::cout << "Result: " << std::endl;
258     // for (int i = 0; i < 10; ++i)
259     // {
260     //     for (int j = 0; j < k; ++j)
261     //     {
262     //         std::cout << resultNonZeroElement[i][j] << " ";
263     //     }
264     //     std::cout << std::endl;
265     // }
266     // }
267     // ===== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
268     // =====
269 // Compare the results of the serial and parallel multiplications
270 if (areMatricesEqual(resultSerial, resultNonZeroElement, 1e-6)) //
    Tolerance = 1e-6
271 {
272     std::cout << "Non-zero Elements: Results are the same!"
273     << std::endl;
274 }
275 else
276 {

```



```

277         std::cout << "Non-zero Elements: Results are different!"
278         << std::endl;
279     }
280 }
281
282 //
283 // ===== EXECUTE THE PARALLEL MULTIPLICATION (
284 // PETSc) =====
285
286 // Wait for all processes to finish the parallel multiplication (non-zero
287 // element)
288 MPI_Barrier(MPI_COMM_WORLD);
289
290 // Declare the PETSc matrix
291 Mat A, B, C;
292
293 // ===== FOR DEBUGGING ONLY - START PETSCS SETUP TIMER
294 // =====
295 // startTime = MPI_Wtime();
296 // ===== FOR DEBUGGING ONLY - START PETSCS SETUP TIMER
297 // =====
298
299 // Create a parallel matrix to store the sparse matrix
300 MatCreate(PETSC_COMM_WORLD, &A);
301 MatSetSizes(A, PETSC_DECIDE, PETSC_DECIDE, M.numRows, M.numCols);
302 MatSetType(A, MATMPIAIJ);
303 MatSetUp(A);
304 // Fill the PETSc matrix with the values from the sparse matrix
305 if (worldRank == 0)
306 {
307     for (int i = 0; i < M.numRows; ++i)
308     {
309         for (int j = M.rowPtr[i]; j < M.rowPtr[i + 1]; ++j)
310         {
311             MatSetValue(A, i, M.colIndices[j], M.values[j], INSERT_VALUES);
312         }
313     }
314 }
315 // Assemble the PETSc matrix
316 MatAssemblyBegin(A, MAT_FINAL_ASSEMBLY);
317 MatAssemblyEnd(A, MAT_FINAL_ASSEMBLY);
318
319 // Create a parallel matrix to store the dense vector
320 MatCreate(PETSC_COMM_WORLD, &B);
321 MatSetSizes(B, PETSC_DECIDE, PETSC_DECIDE, M.numCols, k);
322 MatSetType(B, MATDENSE);
323 MatSetUp(B);
324 // Fill the PETSc matrix B with values from the dense matrix v
325 if (worldRank == 0)
326 {
327     for (int i = 0; i < M.numCols; ++i)
328     {
329         for (int j = 0; j < k; ++j)
330         {
331             MatSetValue(B, i, j, v[i][j], INSERT_VALUES);
332         }
333     }
334 }
335 // Assemble the PETSc matrix
336 MatAssemblyBegin(B, MAT_FINAL_ASSEMBLY);
337 MatAssemblyEnd(B, MAT_FINAL_ASSEMBLY);
338
339 // ===== FOR DEBUGGING ONLY - STOP PETSCS SETUP TIMER
340 // =====
341 // endTime = MPI_Wtime();

```

```

338 // if (worldRank == 0)
339 // {
340 //     std::cout << "PETSc Setup time: " << (endTime - startTime) << std::endl;
341 // }
342 // ===== FOR DEBUGGING ONLY - STOP PETSCS SETUP TIMER
343 // =====
344 // Create a parallel matrix to store the result of the multiplication
345 startTime = MPI_Wtime();
346 MatProductCreate(A, B, NULL, &C);
347 MatMatMult(A, B, MAT_INITIAL_MATRIX, PETSC_DEFAULT, &C);
348 endTime = MPI_Wtime();
349 if (worldRank == 0)
350 {
351     // Print the execution time
352     std::cout << "PETSc Execution time: " << (endTime - startTime) << std::endl;
353 }
354 // ===== FOR DEBUGGING ONLY - START PETSCS CONVERSION
355 // TIMER =====
356 // startTime = MPI_Wtime();
357 // ===== FOR DEBUGGING ONLY - START PETSCS CONVERSION
358 // TIMER =====
359 // Create a sequential matrix to retrieve the result
360 Mat CSeq;
361 MatCreateRedundantMatrix(C, worldSize, MPI_COMM_NULL, MAT_INITIAL_MATRIX, &CSeq);
362
363 if (worldRank == 0)
364 {
365     // Convert the result matrix C to a DenseVector
366     DenseVector globalMatrix = ConvertPETScMatToDenseVector(CSeq);
367
368     // ===== FOR DEBUGGING ONLY - STOP PETSCS CONVERSION
369     // TIMER =====
370     // endTime = MPI_Wtime();
371     // std::cout << "PETSc Conversion time: " << (endTime - startTime) << std::endl;
372     // ===== FOR DEBUGGING ONLY - STOP PETSCS CONVERSION
373     // TIMER =====
374
375     // ===== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
376     // =====
377     // std::cout << "Result: " << std::endl;
378     // for (int i = 0; i < 10; ++i)
379     // {
380     //     for (int j = 0; j < k; ++j)
381     //     {
382     //         std::cout << globalMatrix[i][j] << " ";
383     //     }
384     //     std::cout << std::endl;
385     // }
386     // ===== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
387     // =====
388
389     // Compare the results of the serial and PETSc multiplications
390     if (areMatricesEqual(resultSerial, globalMatrix, 1e-6)) // Tolerance = 1e-6
391     {
392         std::cout << "PETSc: Results are the same!"
393         << std::endl;
394     }
395     else
396     {
397         std::cout << "PETSc: Results are different!"
398         << std::endl;
399     }
400 }

```

```

398 // Free the memory
399 MatDestroy(&A);
400 MatDestroy(&B);
401 MatDestroy(&C);
402 MatDestroy(&CSeq);
403
404 // Finalise MPI and PETSc
405 PetscFinalize();
406 MPI_Finalize();
407
408 return 0;
409 }

```

Appendix B.G Scripts

B.G.1 MPI Submission Script

```

#!/bin/bash
##
## MPI submission script for PBS on CR2
## -----
##
## "MPI-sub2022v1"
## Follow the 6 steps below to configure your job
##
## STEP 1:
##
## Enter a job name after the -N on the line below:
##
#PBS -N mpi_assessment_test_8_cores_16_425500
##
## STEP 2:
##
## Select the number of cpus/cores required by modifying the #PBS -l select line
## below
##
## Normally you select cpus in chunks of 16 cpus
## The Maximum value for ncpus is 16 and mpirprocs MUST be the same value as ncpus.
##
## If more than 16 cpus are required then select multiple chunks of 16
## e.g. 16 CPUs: select=1:ncpus=16:mpiprocs=16
##      32 CPUs: select=2:ncpus=16:mpiprocs=16
##      ..etc..
##
#PBS -l select=2:ncpus=16:mpiprocs=16
##
## STEP 3:
##
## Select the correct queue by modifying the #PBS -q line below
##
## half_hour      - 30 minutes
## one_hour       - 1 hour
## three_hour     - 3 hours
## six_hour       - 6 hours
## half_day       - 12 hours
## one_day        - 24 hours
## two_day        - 48 hours
## five_day       - 120 hours
## ten_day        - 240 hours (by special arrangement)
##
#PBS -q half_hour
##
## STEP 4:
##
## Replace the hpc@cranfield.ac.uk email address

```

```

## with your Cranfield email address on the #PBS -M line below:
## Your email address is NOT your username
##
#PBS -m abe
#PBS -M alexis.balayre@cranfield.ac.uk
##
## =====
## DO NOT CHANGE THE LINES BETWEEN HERE
## =====
#PBS -j oe
#PBS -W sandbox=PRIVATE
#PBS -k n
ln -s $PWD $PBS_O_WORKDIR/$PBS_JOBID
## Change to working directory
cd $PBS_O_WORKDIR
## Calculate number of CPUs
export cpus='cat $PBS_NODEFILE | wc -l'
sort -u $PBS_NODEFILE -o mpi_nodes.$$
export I_MPI_HYDRA_IFACE=ib0
export I_MPI_HYDRA_BOOTSTRAP=ssh
export I_MPI_HYDRA_RMK=pbs
export K_VALUE=1
export MATRIX_PATH=/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/cop20k_A.
    mtx
## Debug options - only enable when instructed by HPC support
##export I_MPI_HYDRA_DEBUG=1
##export I_MPI_DEBUG=6
##export I_MPI_DEBUG_OUTPUT=%h-%r-%p-debug.out
## set some MPI tuning parameters to use the correct transport
## =====
## AND HERE
## =====
##
## STEP 5:
##
## Load the default application environment
## For a specific version add the version number, e.g.
## module load intel/2016b
##
module use /apps/modules/all
module load intel/2021b
##
## STEP 6:
##
## Run MPI code
##
## The main parameter to modify is your mpi program name
## - change YOUR_EXECUTABLE to your own filename
##

mpirun -genval1 -hostfile mpi_nodes.$$ -np ${cpus} ../my_program_final_debug ${
    K_VALUE} ${MATRIX_PATH}

## Tidy up the log directory
## DO NOT CHANGE THE LINE BELOW
## =====
rm $PBS_O_WORKDIR/$PBS_JOBID
#

```

B.G.2 Batch Test Script

```
#!/bin/bash

# Script to submit a batch of jobs to the cluster

# Path to the original script
original_script="mpi.sub"

# Maximum number of cores used for the job
max_cores=96

# Define a set of k values to test (Number of columns in the dense vector)
k_values=(1 3 6 9 12)

# Define a set of paths to test
paths=(
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/cop20k_A.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/adder_dcop_32.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/bcsstk17.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/af23560.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/amazon0302.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/cavity10.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/cage4.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/dc1.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/FEM_3D_thermal1.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/mac_econ_fwd500.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/mcfe.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/mhd4800a.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/olafu.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/raefsky2.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/rdist2.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/thermal1.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/thermomech_TK.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/west2021.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/lung2.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/olm1000.mtx"
    "/mnt/beegfs/home/s425500/hpc/assignment/sparse-matrix/roadNet-PA.mtx"
)

# Loop over the k values
for k_value in "${k_values[@]"; do
    # Loop over the paths of MTX files
    for path in "${paths[@]"; do
        # Loop over the number of chunks
        for chunks in $(seq 1 $((max_cores / 16))); do
            # Loop over the number of cpus per chunk
            for cpus in $(seq 2 16); do
                # Calculate the total number of cores
                total_cores=$((chunks * cpus))
                # Check if the total number of cores is less than the maximum
                number of cores
                if [ $total_cores -le $max_cores ]; then
                    echo "Submitting job with $total_cores cores, $chunks chunks
                    and $cpus cpus per chunk"
                    echo "Path: $path"

                    # Create a unique job name
                    matrix_name=$(basename "$path") # Remove the path
                    sanitized_matrix_name=${matrix_name//[~a-zA-Z0-9_]/_} # Replace
                    all non-alphanumeric characters with underscores
                    job_name="${sanitized_matrix_name}_k${k_value}_cores${
                    total_cores}_chunks${chunks}_cpus${cpus}" # Add the k value to the job name

                    # Create a temporary submission script
                    temp_script="temp_${job_name}.sub"
                    cp "$original_script" "$temp_script"

                    # Replace the variables in the temporary script
```

```

sed -i "s|export k_value=.*|export k_value=${k_value}|" "
$temp_script" # Export the k value
sed -i "s|export MATRIX_PATH=.*|export MATRIX_PATH=${path}|" "
$temp_script" # Export the path to the MTX file
sed -i "s|#PBS -N .*/#PBS -N $job_name|" "$temp_script" # Set
the job name
sed -i "s|#PBS -l select=.*|#PBS -l select=${chunks}:ncpus=
$cpus:mpiprocs=$cpus|" "$temp_script" # Set the number of chunks and cpus per
chunk

# Submit the job and get the job id
job_id=$(qsub "$temp_script")
echo "Job id: $job_id"

# Wait until the job is finished
while true; do
    # Get the job status and duration
    job_status=$(qstat -f "$job_id" | grep job_state | awk '{
print $3}') # Get the job status
    job_duration=$(qstat -f "$job_id" | grep resources_used.
walltime | awk '{print $3}') # Get the job duration
    job_duration_seconds=$(echo $job_duration | awk -F: '{
print ($1 * 3600) + ($2 * 60) + $3 }') # Convert the job duration to seconds
    echo "Job status: $job_status"
    echo "Job duration: $job_duration"

    # If the job is finished, break the loop
    if [ -z "$job_status" ]; then
        break
    fi

    # if the job is running for more than 4 minutes, cancel it
    if [ "$job_duration_seconds" -gt 240 ]; then
        echo "Job is running for more than 4 minutes.
Cancelling it."
        qdel "$job_id"
        break
    fi

    # Wait for 1 second
    sleep 1
done

# Remove the temporary script
rm "$temp_script"
fi
done
done
done
done

```

B.G.3 Get CSV Script

Bash script to analyse all job results files and extract the relevant information to create a CSV file.

```
#!/bin/bash

# Name of the CSV file to write the data to
output_csv="results.csv"

# Headers for the CSV file
echo "file Name,Cores Number,Sparse Matrix,Dense Vector,Serial Algo Execution time,
Row-wise Average Communication Time,Row-wise Average Computation Time,Row-wise
Execution time,Row-wise Result,Column-wise Average Communication Time,Column-
wise Average Computation Time,Column-wise Execution time,Column-wise Result,Non
-zero elements Average Communication Time,Non-zero elements Average Computation
Time,Non-zero Elements Execution time,Non-zero Elements Result,PETSc Execution
time,PETSc Result" >$output_csv

# Loop over the output files
for file in *.o*; do
    # Check that the file is valid and that it is a result file
    if [[ -s $file && $file == *mtx* ]]; then
        # Extract the job name and the number of cores from the file name
        job_name=$(basename "$file" | sed -e 's/\.([^.]*$)//') # Remove file
        extension
        num_cores=$(echo $file | grep -oP '(?<=_cores)\d+') # Extract the number
        of cores from the file name

        # Extract the matrix size and the vector size from the file
        matrix_size=$(grep "Matrix size" $file | awk '{print $3}' | sed 's/size://')
        ) # Extract the matrix size from the file
        vector_size=$(grep "Vector size" $file | awk '{print $3}' | sed 's/size://')
        ) # Extract the vector size from the file

        # Extract the serial execution time from the file
        serial_time=$(grep "Serial Algo Execution time" $file | awk '{print $5}')

        # Row-wise Data
        row_wise_communication_time=$(grep "Row-wise Average Communication Time"
$file | awk '{print $5}') # Extract the row-wise average communication time
from the file
        row_wise_computation_time=$(grep "Row-wise Average Computation Time" $file
| awk '{print $5}') # Extract the row-wise average computation time from
the file
        row_wise_execution_time=$(grep "Row-wise Execution time" $file | awk '{
print $4}') # Extract the row-wise execution time from the file
        row_wise_result=$(grep "Row-wise: Results are" $file | awk '{print $5}')
        # Extract the row-wise result from the file
        row_wise_result=$(if [ $row_wise_result == "same!" ]; then echo "same";
else echo "different"; fi) # Convert the row-wise result to a boolean

        # Column-wise Data
        col_wise_communication_time=$(grep "Column-wise Average Communication Time"
$file | awk '{print $6}') # Extract the column-wise average communication time
from the file
        col_wise_computation_time=$(grep "Column-wise Average Computation Time"
$file | awk '{print $6}') # Extract the column-wise average computation
time from the file
        col_wise_execution_time=$(grep "Column-wise Execution time" $file | awk '{
print $4}') # Extract the column-wise execution time from the
file
        col_wise_result=$(grep "Column-wise: Results are" $file | awk '{print $5}')
        # Extract the column-wise result from the file
        col_wise_result=$(if [ $col_wise_result == "same!" ]; then echo "same";
else echo "different"; fi) # Convert the column-wise result to a boolean

        # Non-zero element Data
        nonzero_communication_time=$(grep "Non-zero elements Average Communication
Time" $file | awk '{print $6}') # Extract the non-zero elements average
```

```

communication time from the file
    nonzero_computation_time=$(grep "Non-zero elements Average Computation Time
" $file | awk '{print $6}') # Extract the non-zero elements average
computation time from the file
    nonzero_execution_time=$(grep "Non-zero Elements Execution time" $file |
awk '{print $5}') # Extract the non-zero elements execution
time from the file
    nonzero_result=$(grep "Non-zero Elements: Results are" $file | awk '{print
$6}') # Extract the non-zero elements result from the
file
    nonzero_result=$(if [ $nonzero_result == "same!" ]; then echo "same"; else
echo "different"; fi) # Convert the non-zero elements result to a
boolean

# PETSc Data
    petsc_execution_time=$(grep "PETSc Execution time" $file | awk '{print $4}'
) # Extract the PETSc execution time from the file
    petsc_result=$(grep "PETSc: Results are" $file | awk '{print $5}')
# Extract the PETSc result from the file
    petsc_result=$(if [ $petsc_result == "same!" ]; then echo "same"; else echo
"different"; fi) # Convert the PETSc result to a boolean

# Write the extracted data to the CSV file
    echo "$job_name,$num_cores,$matrix_size,$vector_size,$serial_time,
$row_wise_communication_time,$row_wise_computation_time,
$row_wise_execution_time,$row_wise_result,$col_wise_communication_time,
$col_wise_computation_time,$col_wise_execution_time,$col_wise_result,
$nonzero_communication_time,$nonzero_computation_time,$nonzero_execution_time,
$nonzero_result,$petsc_execution_time,$petsc_result" >>$output_csv
fi
done

echo "The data was successfully written in $output_csv"

```