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High Performance Technical Computing Assignment

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Abstract

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

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Chapter 1

Introduction

High-Performance Computing (HPC) is a branch of computing that uses supercomputers and server clusters to solve complex, computationally intensive problems. Unlike a personal computer with a single processor, an HPC system is made up of many processors working in parallel, considerably increasing processing capacity. This enables scientists and engineers to carry out detailed numerical simulations, such as forecasting the weather, modelling molecules for new medicines or designing aircraft.

Cranfield University has two HPC systems: CRESCENT2 and DELTA. However, this report will focus exclusively on CRESCENT2. The latter is a HPC cluster designed to provide computing power to the university community for teaching and research. The CRESCENT 2 nodes, which are like individual workstations within the cluster, are equipped with Intel Xeon E5 2620 processors. Each node contains two processors (or 'sockets'), with 16 cores and as many threads, accompanied by 16 gigabytes of RAM, enabling them to handle large workloads. Communication between the nodes is ensured by a 128 Gb/s InfiniBand EDR network, a high-speed connectivity technology that facilitates the rapid exchange of data, a crucial function for parallel processing of computer tasks.

Sparse matrix-vector multiplication is a fundamental operation in numerical linear algebra and has numerous applications in science and engineering.

1.1 Problem Description

Consider a sparse matrix M of dimensions $m \times n$ and a fat vector v of dimensions $n \times k$. The objective is to perform the multiplication $M \times v$, yielding a result that is of dimensions $m \times k$.

The matrix M is defined as:

$$M = \begin{pmatrix} m_{11} & m_{12} & \cdots & m_{1n} \\ m_{21} & m_{22} & \cdots & m_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ m_{m1} & m_{m2} & \cdots & m_{mn} \end{pmatrix} \tag{1.1}$$

where most elements of M are zeros.

The vector v is defined as:

$$v = \begin{pmatrix} v_{11} & v_{12} & \cdots & v_{1k} \\ v_{21} & v_{22} & \cdots & v_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ v_{n1} & v_{n2} & \cdots & v_{nk} \end{pmatrix} \tag{1.2}$$

Chapter 2

Methodology

2.1 Data Structures

In numerical computation and linear algebra, efficient use of memory and fast computation are crucial. This is particularly true when working with hollow matrices and fat vectors.

2.1.1 Sparse Matrix

The sparse matrix is represented in CSR (Compressed Sparse Row) format, which is particularly effective for storing and manipulating matrices where the majority of elements are zero. The CSR structure consists of three main vectors:

- **values**: A vector storing all the non-zero elements of the matrix.
- **rowPtr**: A vector storing the starting index for each element in the *values* vector.
- **colIndices**: A vector storing the column indices for each element in the vector *values*.

Here is an example of a sparse matrix in CSR format:

- `values` = $\{1, 2, 3, 4\}$
- `rowPtr` = $\{0, 2, 3, 3, 4\}$
- `colIndices` = $\{0, 2, 1, 3\}$

This hollow matrix can be visualised as:

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

The **SparseMatrix** structure is defined in Appendix B.A.

2.1.2 fat vector

Unlike a hollow matrix, a fat vector (illustrated by equation 1.2) stores all its elements, including zeros. The data structure for a fat vector is a two-dimensional array, where each row represents a separate vector. The **DenseVector** structure is defined in Appendix B.A.

2.2 Sequential Algorithm

Given a sparse matrix M in CSR format and a fat 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 $n \times k$ fat 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 $j \leftarrow 0$ **to** $k-1$ **do**
        $Result[i][l] \leftarrow Result[i][l] + (\text{value} \times v[j][l])$
      end for
    end for
  end for
  return $Result$

2.2.1 Complexity Analysis

Let M be a sparse matrix of size $m \times n$ with z non-zero elements, stored in CSR format, and v be a fat vector of size $n \times k$. The multiplication $M \times v$ can be analyzed as follows:

- For each row i of M, the algorithm iterates over its non-zero elements.
- For each non-zero element M_{ij}, the algorithm performs a multiplication with each element of column j in v, resulting in k multiplications.
- These products are accumulated in the corresponding row of the result matrix, which has dimensions $m \times k$.

2.2.1.1 Temporal Complexity

The time complexity depends on the number of non-zero elements in the hollow matrix and the dimension of the fat vector.

1. **Hollow Matrix Row Traversal:** Each row of the matrix is traversed once, so this part has complexity $O(m)$.

2. **Access to non-zero elements:** For each row, the algorithm traverses the non-zero elements, therefore the complexity of traversing all the non-zero elements in the matrix is $O(z)$.

3. **Multiplication et Accumulation:** For each non-zero element, the algorithm performs a multiplication for each column of the fat vector, so this step has complexity $O(\frac{z}{m} \times k)$. Thus, for all rows, the complexity becomes $O(z \times k)$.

Hence, the time complexity of multiplying a sparse matrix in CSR format with a fat matrix is $O(z \times k)$.

2.2.1.2 Spatial Complexity

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

- **Sparse Matrix:** The matrix is stored using three main vectors (*values*, *colIndices*, *rowPtr*). If the matrix has z non-zero elements, then the spatial complexity of the two vectors *values* and *colIndices* is $O(z)$. The vector *rowPtr* has a size of $m+1$, so its spatial complexity is $O(m)$. Thus, the space required for M in CSR format is $O(z+z+m) = O(2z+m)$.
- **Fat vector:** The fat vector has a spatial complexity of $O(n \times k)$.
- **Result Vector:** The result vector has a spatial complexity of $O(m \times k)$.

Considering the storage requirements for the sparse matrix, the dense matrix, and the result matrix, the overall spatial complexity of the multiplication operation is $O(2z+m+n \times k+m \times k)$.

2.3 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

$rowsPerProc \leftarrow m/numProcs$
$extraRows \leftarrow m(\bmod numProcs)$
$startRow \leftarrow rank \times rowsPerProc + \min(rank, extraRows)$
$endRow \leftarrow startRow + rowsPerProc + (rank < extraRows)$
$localRows \leftarrow endRow - startRow$
$Result \leftarrow$ zero matrix of size $localRows \times k$
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**
      $Result[i - startRow][l] \leftarrow Result[i - startRow][l] + (\text{value} \times v[j][l])$
    end for
  end for
end for
if $rank = 0$ **then**
  $FinalResult \leftarrow$ zero matrix of size $m \times k$
end if
Define $recvCounts[numProcs]$, $displacements[numProcs]$
Compute $recvCounts$ and $displacements$ based on $localRows$ for all processes
$MPI\_Gatherv(Result, localRows \times k, MPI\_DOUBLE, FinalResult, recvCounts, displacements, MPI\_DO$
if $rank = 0$ **then**
  for $p \leftarrow 1$ **to** $numProcs - 1$ **do**
    Integrate received partial $Results$ into $FinalResult$ based on $displacements$
  end forreturn $FinalResult$
end if

2.3.1 Complexity Analysis

2.3.1.1 Temporal Complexity

The temporal (or time) complexity analysis of the sparse matrix-fat vector multiplication using MPI in a distributed-memory parallel environment involves understanding the computational steps required for each part of the process. The main components are as follows:

1. **Initialisation and Setup**: MPI initialisation and calculation of rows per process have a negligible time complexity compared to the actual computation, so they can be considered as $O(1)$.

2. **Local Computation**:

   - Each process computes the multiplication for its assigned subset of rows.

- If the sparse matrix has z non-zero elements in total, and these elements are evenly distributed across m rows, each process handles approximately $\frac{z}{\text{worldSize}}$ non-zero elements.
- The computation for each non-zero element involves accessing the element and its corresponding column in the dense vector, followed by a multiplication and an addition. This operation is $O(1)$.
- Thus, the local computation for each process has a time complexity of $O\left(\frac{z}{\text{worldSize}}\right)$.

3. **Communication (`MPI_Gatherv`)**:
   - The complexity of the `MPI_Gatherv` operation depends on the implementation of the MPI library and the underlying network architecture.
   - In general, gathering operations can be assumed to have a logarithmic complexity with respect to the number of processes, i.e., $O(\log(\text{worldSize}))$, but this can vary.
   - The amount of data transferred per process is proportional to the size of the local result, which is $O\left(\frac{m}{\text{worldSize}} \times k\right)$.
4. **Final Assembly**:
   - The root process assembles the final result matrix. This step is essentially a concatenation of the results from each process and has a complexity linear to the total size of the result matrix, which is $O(m \times k)$.

Considering the parallel nature of the computation, the dominant factor in the time complexity is the local computation performed by each process, which is $O\left(\frac{z}{\text{worldSize}}\right)$. The communication step's complexity depends on the MPI implementation and network, but the data volume transferred per process affects this step. The final assembly in the root process is also significant but does not exceed $O(m \times k)$. Therefore, the overall time complexity of the algorithm can be approximated as $O\left(\frac{z}{\text{worldSize}} + \log(\text{worldSize}) + m \times k\right)$, with the understanding that the actual performance can be influenced by factors like network latency, bandwidth, and the distribution of non-zero elements in the sparse matrix.

2.3.1.2 Spatial Complexity

The spatial complexity analysis of the algorithm performing sparse matrix-fat vector multiplication in a distributed-memory parallel environment using MPI can be understood by considering the memory requirements for storing the sparse matrix, the dense vector, and the final result, as well as the additional storage required for parallel processing. The breakdown is as follows:

1. **Storage of Sparse Matrix (`sparseMatrix`):**
   - The sparse matrix is stored in CSR format, which includes three arrays:
     - `values`: Contains all non-zero elements of the matrix. If the matrix has z non-zero elements, this array takes $O(z)$ space.

  - `colIndices`: Stores column indices for each non-zero element, also taking $O(z)$ space.
  - `rowPtr`: Contains $m+1$ elements for an $m \times n$ matrix, requiring $O(m+1)$ space.
- Total space for the sparse matrix is therefore $O(2z+m)$.

2. **Storage of Dense Vector (`denseVector`):**
   - The dense vector (or fat vector) is a 2D array of size $n \times k$. It requires $O(n \times k)$ space.
3. **Local Result Vector (`localResult`):**
   - Each process computes a local result vector of size proportional to the number of rows it handles times the number of columns in the dense vector. In the worst case, this is $O\left(\frac{m}{\text{worldSize}} + 1 \times k\right)$ per process.
4. **Gathered Results (`gatheredResults`):**
   - In the root process, the gathered results from all processes are combined. This requires space equivalent to the size of the final result matrix, which is $O(m \times k)$.
5. **Final Result Matrix (`finalResult`):**
   - The final result matrix, which is only constructed in the root process, is of size $m \times k$, requiring $O(m \times k)$ space.
6. **Auxiliary Data for MPI Operations:**
   - Arrays like `recvCounts` and `displacements` are used for MPI communication. Their sizes are proportional to the number of processes, which is typically much smaller than the size of the matrix or vectors. Therefore, they add a relatively negligible $O(\text{worldSize})$ space complexity.

The spatial complexity of the algorithm is dominated by the storage requirements for the sparse matrix, the dense vector, and the final result matrix. Thus, the overall spatial complexity is approximately $O(2z+m+n \times k+m \times k)$. It is important to note that in a distributed-memory environment, the memory usage is distributed across multiple processes, which can reduce the memory burden on individual nodes.

2.4 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**
        $PartialResult[i][l - startCol] \leftarrow PartialResult[i][l - startCol] + (\text{value} \times v[j][l])$
      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** $FinalResult$

2.4.1 Complexity Analysis

2.4.1.1 Temporal Complexity

To analyse the temporal (or time) complexity of the sparse matrix-fat vector multiplication using a column-wise parallel approach with MPI, we need to consider the computation and communication steps involved in the process. The breakdown is as follows:

1. **Local Computation:**

- Each MPI process computes a portion of the final matrix, responsible for a subset of columns. The number of columns processed by each process is roughly colsPerProcess $= \frac{\text{vecCols}}{\text{worldSize}}$, with some processes handling extra columns if vecCols is not perfectly divisible by worldSize.
- For each column, the process computes the product with every row of the sparse matrix. If the sparse matrix has z non-zero elements in total, then, on average, each process handles approximately $\frac{z}{\text{worldSize}}$ non-zero elements.
- The computation involves accessing the element, performing a multiplication, and accumulating the result. These operations for each non-zero element are $O(1)$.
- Therefore, the local computation for each process has a time complexity of $O\left(\frac{z}{\text{worldSize}}\right)$.

2. **Communication (`MPI_Gatherv`):**

   - The `MPI_Gatherv` operation is used to gather the local results from each process into the root process. The complexity of this operation depends on the implementation of MPI and the underlying network architecture.
   - Generally, the gather operation can be assumed to have a complexity that grows with the number of processes and the amount of data being communicated. If the gathered data from each process is large, the communication time can become significant.
   - The amount of data transferred per process is proportional to the number of rows in the matrix and the number of columns processed, which is $O(m \times \text{colsPerProcess})$.

3. **Final Assembly:**

   - The root process assembles the final result matrix. This step is essentially a concatenation of results from each process and is linearly proportional to the size of the final matrix, $O(m \times k)$.

The dominant factor in the time complexity is the local computation performed by each process, which is $O\left(\frac{z}{\text{worldSize}}\right)$. The communication step can also be significant, especially if the network bandwidth is limited or if the size of the data being communicated is large. The final assembly in the root process is also linearly dependent on the size of the final result matrix. Therefore, the overall time complexity of the algorithm can be approximated as $O\left(\frac{z}{\text{worldSize}} + \text{communication cost} + m \times k\right)$, with the understanding that actual performance can vary based on factors like network performance, distribution of non-zero elements in the sparse matrix, and the specific implementation of MPI.

2.4.1.2 Spatial Complexity

The spatial complexity of the given algorithm, which performs sparse matrix-fat vector multiplication in a distributed-memory environment using a column-wise parallel approach, can be analysed by considering the memory requirements for storing the matrix, the vector, and the intermediate and final computational results. The breakdown is as follows:

1. **Sparse Matrix Storage:**
    - The sparse matrix is stored in a CSR format, which includes arrays for non-zero values, column indices, and row pointers. If the matrix has z non-zero elements, then the space required is approximately $O(z)$ for the values, $O(z)$ for the column indices, and $O(m+1)$ for the row pointers, where m is the number of rows. Therefore, the total space requirement for the sparse matrix is $O(2z+m)$.
2. **Dense Vector Storage:**
    - The dense vector (or fat vector) is a 2D array of size $n \times k$, requiring $O(n \times k)$ space.
3. **Local Result Vector:**
    - Each process computes a local result vector for its assigned columns. The size of this local result vector is proportional to the number of rows in the sparse matrix and the number of columns processed by each process. The maximum size is $O(m \times \text{colsPerProcess})$, where colsPerProcess is the number of columns processed by each process.
4. **Gathered Results:**
    - In the root process, the final gathered result needs to be stored. This is essentially the entire output matrix, which has a size of $m \times k$, hence requiring $O(m \times k)$ space.
5. **Auxiliary Arrays for MPI Operations:**
    - Arrays such as `recvCounts` and `displacements` are used in the MPI Gather operation. The size of these arrays is proportional to the number of processes (i.e., worldSize). However, this is generally small compared to the size of the matrices and vectors, so their space contribution is relatively minor.

Considering the storage requirements for the sparse matrix, the dense vector, the local results, and the final gathered results, the overall spatial complexity of the algorithm is approximately $O(2z+m+n \times k+m \times \text{colsPerProcess}+m \times k)$. It is important to note that in a distributed-memory setting, this memory usage is spread across multiple processes, reducing the memory load on any single node.

2.5 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**
      $PartialResult[i][l] \leftarrow PartialResult[i][l] + (\text{value} \times v[j][l])$
    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*

2.5.1 Complexity Analysis

2.5.1.1 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.

2.5.1.2 Spatial Complexity

- **Storage of Sparse Matrix and fat 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

Results and Discussion

3.1 HPC Environmental Impact

The LUMI supercomputer, based at the CSC-IT Center for Science in Finland, represents a milestone in the field of high-performance computing (HPC), not only because of its computing power, but also because of its approach to environmental sustainability. LUMI, one of EuroHPC's world-class supercomputers, began operating in 2021 and is expected to reach full capacity in 2023. It features an environmentally-friendly design and is considered to be one of the most energy-efficient data centres in the world.

Irina Kupiainen, who works as Programme Director for the Open Scholarship Innovation Program at the CSC, plays an important role in the development of policies relating to high-performance computing and open science. With a strong background in international policy and experience in various government and research organisations, Irina Kupiainen leads EU public affairs at the CSC, focusing on policy and international collaboration, particularly in the area of open science.

The impact of supercomputing on the environment is a major concern, not least because of the high energy demands of these systems. However, LUMI is an example of how HPC can make a positive contribution to environmental sustainability. It runs on 100% renewable energy and makes efficient use of waste heat, which can heat up to 20% of the homes in the surrounding city. This approach not only reduces the carbon footprint, but also demonstrates HPC's potential to meet climate neutrality targets.

Furthermore, sustainability measures in HPC are not limited to energy consumption and waste heat management. The entire life cycle of the machine needs to be taken into account, including construction, modularity, scalability, recycling and reuse of materials. This holistic view can contribute to the development of a circular economy, supporting sustainability to its full potential.

In conclusion, the LUMI supercomputer, led by experts such as Irina Kupiainen and others at the CSC-IT Center for Science, illustrates how supercomputing can be both a powerful tool for scientific progress and a leader in environmental sustainability. By harnessing renewable energy sources, making efficient use of waste heat and taking into account the full lifecycle of HPC systems, LUMI is setting a precedent for how high-performance computing can contribute to a greener, more sustainable future.

Chapter 4

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, partionned_df)`: Function for writing the DataFrame to the Timestream database.

Appendix B

Source Codes

Appendix B.A Data Structures

Data stuctures of the sparse matrix and fat vector.

```
#ifndef MATRIXDEFINITIONS_H
#define MATRIXDEFINITIONS_H

#include <vector>

//
/**
 * @brief Struct to represent a sparse matrix
 *
 * @param values  Non-zero values
 * @param colIndices  Column indices of non-zero values
 * @param rowPtr  Row pointers
 */
struct SparseMatrix
{
    std::vector<double> values;
    std::vector<int> colIndices;
    std::vector<int> rowPtr;
};

// Type definition for a dense vector
typedef std::vector<std::vector<double>> DenseVector;

#endif
```

Appendix B.B Sequential Algorithm

Sequential algorithm for multiplying a sparse matrix by a fat vector.

B.B.1 Declaration File

```
#ifndef SPARSEMATRIXDENSEVECTORMULTIPLY_H
#define SPARSEMATRIXDENSEVECTORMULTIPLY_H

#include "MatrixDefinitions.h"

/**
 * @brief Function to execute the sparse matrix-dense vector multiplication using
     sequential algorithm
 *
 * @param sparseMatrix  Sparse matrix
 * @param denseVector Dense vector
 * @param vecCols  Number of columns in the dense vector
 * @return DenseVector  Result of the multiplication
 */
DenseVector sparseMatrixDenseVectorMultiply(const SparseMatrix &sparseMatrix,
                                            const DenseVector &denseVector, int
                                                vecCols);

#endif
```

B.B.2 Implementation File

```
#include "SparseMatrixDenseVectorMultiply.h"

/**
 * @brief Function to execute the sparse matrix-dense vector multiplication using
     sequential algorithm
 *
 * @param sparseMatrix  Sparse matrix
 * @param denseVector Dense vector
 * @param vecCols  Number of columns in the dense vector
 * @return DenseVector  Result of the multiplication
 */
DenseVector sparseMatrixDenseVectorMultiply(const SparseMatrix &sparseMatrix,
                                            const DenseVector &denseVector, int
                                                vecCols)
{
    // Initialisation of the result vector
    DenseVector result(sparseMatrix.numRows, std::vector<double>(vecCols, 0.0));
    // Iterate over the rows of the sparse matrix
    for (int i = 0; i < sparseMatrix.numRows; ++i)
    {
        // Iterate over the non-zero elements in the current row
        for (int j = sparseMatrix.rowPtr[i]; j < sparseMatrix.rowPtr[i + 1]; ++j)
        {
            // Iterate over the columns of the dense vector
            for (int k = 0; k < vecCols; ++k)
            {
                result[i][k] += sparseMatrix.values[j] * denseVector[sparseMatrix.
                    colIndices[j]][k]; // Compute the result
            }
        }
    }
    // Return the result
    return result;
}
```

Appendix B.C Line-Based Parallelism

Parallel algorithm for multiplying a sparse matrix by a fat vector using line-based parallelism.

B.C.1 Declaration File

```
#ifndef SPARSEMATRIXDENSEVECTORMULTIPLYROWWIZE_H
#define SPARSEMATRIXDENSEVECTORMULTIPLYROWWIZE_H

#include "MatrixDefinitions.h"
#include <iostream> // std::cout

/**
 * @brief Function to multiply a sparse matrix with a dense vector using row-wise distribution
 *
 * @param sparseMatrix  The sparse matrix to be multiplied
 * @param denseVector  The dense vector to be multiplied
 * @param vecCols  Number of columns in the dense vector
 * @return DenseVector Result of the multiplication
 */
DenseVector sparseMatrixDenseVectorMultiplyRowWise(const SparseMatrix &sparseMatrix,
                                                   const DenseVector &denseVector,
                                                   int vecCols);

#endif
```

B.C.2 Implementation File

```
#include <mpi.h>
#include "SparseMatrixDenseVectorMultiplyRowWise.h"

/**
 * @brief Function to multiply a sparse matrix with a dense vector using row-wise distribution
 *
 * @param sparseMatrix  The sparse matrix to be multiplied
 * @param denseVector  The dense vector to be multiplied
 * @param vecCols  Number of columns in the dense vector
 * @return DenseVector Result of the multiplication
 */
DenseVector sparseMatrixDenseVectorMultiplyRowWise(const SparseMatrix &sparseMatrix,
                                                   const DenseVector &denseVector,
                                                   int vecCols)
{
    // MPI Initialisation
    int worldSize, worldRank;
    MPI_Comm_size(MPI_COMM_WORLD, &worldSize);
    MPI_Comm_rank(MPI_COMM_WORLD, &worldRank);

    // ============================ FOR DEBUGGING ONLY - START LOCAL COMPUTATION TIMER ================================
    // double computation_start = MPI_Wtime();
    // ============================ FOR DEBUGGING ONLY - START LOCAL COMPUTATION TIMER ================================

    // Distribute rows among processes
    int rowsCountPerProcess = sparseMatrix.numRows / worldSize;
                              // Number of rows per process
```

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

    // Gather all local results into the root process
    std::vector<double> gatheredResults;
    if (worldRank == 0)
    {
        gatheredResults.resize(recvCounts[0] * worldSize); // Resize the vector to
            hold all the results
    }
    MPI_Gatherv(localResult.data(), localSize, MPI_DOUBLE,
                gatheredResults.data(), recvCounts.data(),
                displacements.data(), MPI_DOUBLE, 0, MPI_COMM_WORLD); // Gather the
                     local results in the root process

    // ============================ FOR DEBUGGING ONLY - STOP COMMUNICATION TIMER
        ===================================
    //  double communication_end = MPI_Wtime();
    //  double local_communication_time = communication_end - communication_start;
    // ============================ FOR DEBUGGING ONLY - STOP COMMUNICATION TIMER
        ===================================

    // ============================ FOR DEBUGGING ONLY - COLLECTING AND ANALYSING
        PERFORMANCE DATA ==================
    //  double total_computation_time = 0.0, total_communication_time = 0.0;
    //  MPI_Reduce(&local_computation_time, &total_computation_time, 1, MPI_DOUBLE,
         MPI_SUM, 0, MPI_COMM_WORLD);
    //  MPI_Reduce(&local_communication_time, &total_communication_time, 1,
        MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
    // ============================ FOR DEBUGGING ONLY - COLLECTING AND ANALYSING
        PERFORMANCE DATA ==================

    // Reconstruct the final result matrix in the root process
    DenseVector finalResult;
    if (worldRank == 0)
    {
        // ============================ FOR DEBUGGING ONLY - PRINTING PERFORMANCE
            DATA ================================
        //  double avg_computation_time = total_computation_time / worldSize;
        //  double avg_communication_time = total_communication_time / worldSize;
        //  std::cout << "Row-wise Average Computation Time: " <<
            avg_computation_time << std::endl;
        //  std::cout << "Row-wise Average Communication Time: " <<
            avg_communication_time << std::endl;
        // ============================ FOR DEBUGGING ONLY - PRINTING PERFORMANCE
            DATA ================================

        finalResult.resize(sparseMatrix.numRows, std::vector<double>(vecCols, 0.0))
            ; // Resize the final result matrix

        // Iterate over the rows of the final result
        for (int i = 0, index = 0; i < sparseMatrix.numRows; ++i)
        {
            // Iterate over the columns of the final result
            for (int j = 0; j < vecCols; ++j, ++index)
            {
                finalResult[i][j] = gatheredResults[index]; // Copy the element of
                    the final result
            }
        }
    }

    // Return the final result
    return (worldRank == 0) ? finalResult : DenseVector{};
}
```

Appendix B.D Column-Wise Parallelism

Parallel algorithm for multiplying a sparse matrix by a fat vector using column-wise parallelism.

B.D.1 Declaration File

```
#ifndef SPARSEMATRIXDENSEVECTORMULTIPLYCOLUMNWIZE_H
#define SPARSEMATRIXDENSEVECTORMULTIPLYCOLUMNWIZE_H

#include "MatrixDefinitions.h"
#include <iostream> // std::cout

/**
 * @brief Function to execute the sparse matrix-dense vector multiplication using column-wise parallel algorithm
 *
 * @param sparseMatrix Sparse matrix
 * @param denseVector Dense vector
 * @param vecCols Number of columns in the dense vector
 * @return DenseVector Result of the multiplication
 */
DenseVector sparseMatrixDenseVectorMultiplyColumnWise(const SparseMatrix &sparseMatrix, const DenseVector &denseVector, int vecCols);

#endif
```

B.D.2 Implementation File

```
#include <mpi.h>
#include "SparseMatrixDenseVectorMultiplyColumnWise.h"
#include <numeric> // Pour std::accumulate

/**
 * @brief Function to execute the sparse matrix-dense vector multiplication using column-wise parallel algorithm
 *
 * @param sparseMatrix Sparse matrix
 * @param denseVector Dense vector
 * @param vecCols Number of columns in the dense vector
 * @return DenseVector Result of the multiplication
 */
DenseVector sparseMatrixDenseVectorMultiplyColumnWise(const SparseMatrix &sparseMatrix, const DenseVector &denseVector, int vecCols)
{
    // MPI Initialisation
    int worldSize, worldRank;
    MPI_Comm_size(MPI_COMM_WORLD, &worldSize);
    MPI_Comm_rank(MPI_COMM_WORLD, &worldRank);

    // ============================ FOR DEBUGGING ONLY - START LOCAL COMPUTATION TIMER ================================
    // double computation_start = MPI_Wtime();
    // ============================ FOR DEBUGGING ONLY - START LOCAL COMPUTATION TIMER ================================

    // Distribute columns among processes
    int colsPerProcess = vecCols / worldSize;                                                                          // Number of columns per process
    int extraCols = vecCols % worldSize;

        // Number of extra columns to be distributed among processes
```

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

                    // Starting column index for the current process
69              int endColThisRank = (i != worldSize - 1) ? startColThisRank +
                    colsPerProcess : startColThisRank + colsPerProcess + extraCols; //
                    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
        }
    }

    // Gather all local results into the root process
    std::vector<double> gatheredResults;
    if (worldRank == 0)
    {
        gatheredResults.resize(std::accumulate(recvCounts.begin(), recvCounts.end()
            , 0)); // Resize the vector to hold the final result
    }
    MPI_Gatherv(localResult.data(), localSize, MPI_DOUBLE,
                gatheredResults.data(), recvCounts.data(),
                displacements.data(), MPI_DOUBLE, 0, MPI_COMM_WORLD); // Gather the
                     local results in the root process

    // ============================ FOR DEBUGGING ONLY - STOP COMMUNICATION TIMER
        ===================================
    // double communication_end = MPI_Wtime();
    // double local_communication_time = communication_end - communication_start;
    // ============================ FOR DEBUGGING ONLY - STOP COMMUNICATION TIMER
        ===================================

    // ============================ FOR DEBUGGING ONLY - COLLECTING AND ANALYSING
        PERFORMANCE DATA ==================
    // double total_computation_time = 0.0, total_communication_time = 0.0;
    // MPI_Reduce(&local_computation_time, &total_computation_time, 1, MPI_DOUBLE,
        MPI_SUM, 0, MPI_COMM_WORLD);
    // MPI_Reduce(&local_communication_time, &total_communication_time, 1,
        MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
    // ============================ FOR DEBUGGING ONLY - COLLECTING AND ANALYSING
        PERFORMANCE DATA ==================

    // Reconstruct the final result matrix in the root process
    DenseVector finalResult;
    if (worldRank == 0)
    {
        // ============================ FOR DEBUGGING ONLY - PRINTING PERFORMANCE
            DATA ================================
        // double avg_computation_time = total_computation_time / worldSize;
        // double avg_communication_time = total_communication_time / worldSize;
        // std::cout << "Column-wise Average Computation Time: " <<
            avg_computation_time << std::endl;
        // std::cout << "Column-wise Average Communication Time: " <<
            avg_communication_time << std::endl;
        // ============================ FOR DEBUGGING ONLY - PRINTING PERFORMANCE
            DATA ================================

        // Reconstruct the final result matrix
        finalResult.resize(sparseMatrix.numRows, std::vector<double>(vecCols, 0.0))
            ; // Resize the final result matrix
        int resultIndex = 0;
        // Iterate over the processes
        for (int rank = 0; rank < worldSize; ++rank)
        {
            int numColsThisRank = (rank != worldSize - 1) ? colsPerProcess :
                colsPerProcess + extraCols; // Number of columns assigned to the
                current process
            int startColThisRank = rank * colsPerProcess;
                                                                // Starting column
                index for the current process

            // Iterate over the rows of the sparse matrix
            for (int row = 0; row < sparseMatrix.numRows; ++row)
            {
                // Iterate over the columns assigned to the current process
                for (int col = 0; col < numColsThisRank; ++col)
                {
                    finalResult[row][startColThisRank + col] = gatheredResults[
                        resultIndex++]; // Reconstruct the final result matrix
```

```
                }
            }
        }
    }

    // Return the final result
    return (worldRank == 0) ? finalResult : DenseVector{};
}
```

Appendix B.E Non-Zero Element Parallelism

Parallel algorithm for multiplying a sparse matrix by a fat vector using non-zero element parallelism.

B.E.1 Declaration File

```
#ifndef SPARSEMATRIXDENSEVECTORMULTIPLYNONZEROELEMENT_H
#define SPARSEMATRIXDENSEVECTORMULTIPLYNONZEROELEMENT_H

#include "MatrixDefinitions.h"
#include <iostream> // std::cout

/**
 * @brief Function to execute the sparse matrix-dense vector multiplication using non-zero element parallel algorithm
 *
 * @param sparseMatrix  Sparse matrix
 * @param denseVector  Dense vector
 * @param vecCols  Number of columns in the dense vector
 * @return DenseVector  Result of the multiplication
 */
DenseVector sparseMatrixDenseVectorMultiplyNonZeroElement(const SparseMatrix &sparseMatrix, const DenseVector &denseVector, int vecCols);

#endif
```

B.E.2 Implementation File

```
#include "SparseMatrixDenseVectorMultiplyNonZeroElement.h"
#include <mpi.h>

/**
 * @brief Function to execute the sparse matrix-dense vector multiplication using non-zero element parallel algorithm
 *
 * @param sparseMatrix  Sparse matrix
 * @param denseVector  Dense vector
 * @param vecCols  Number of columns in the dense vector
 * @return DenseVector  Result of the multiplication
 */
DenseVector sparseMatrixDenseVectorMultiplyNonZeroElement(const SparseMatrix &sparseMatrix, const DenseVector &denseVector, int vecCols)
{
    // MPI Initialisation
    int worldSize, worldRank;
    MPI_Comm_size(MPI_COMM_WORLD, &worldSize);
    MPI_Comm_rank(MPI_COMM_WORLD, &worldRank);

    // ============================ FOR DEBUGGING ONLY - START LOCAL COMPUTATION TIMER ==============================
```

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

Utility functions used by the main file.

B.F.1 Declaration File

```
#ifndef UTILS_H
#define UTILS_H

#include <iostream> // std::cout
#include <vector>   // std::vector
#include <cstdlib>  // rand() and srand()
#include <ctime>    // time()
#include <mpi.h>
#include <petsc.h>
#include <fstream>   // std::ifstream
#include <string>    // std::string
#include <sstream>   // std::stringstream
#include <utility>   // std::pair
#include <algorithm> // std::sort
#include <stdexcept> // std::runtime_error
#include <cmath>     // std::fabs
#include "MatrixDefinitions.h"

/**
 * Method to convert a PETSc matrix to a dense vector
 * @param C PETSc matrix
 * @return DenseVector Dense vector
 */
DenseVector ConvertPETScMatToDenseVector(Mat C);

/**
 * Method to compare two matrices
 * @param mat1 First matrix
 * @param mat2 Second matrix
 * @param tolerance Tolerance for comparison
 * @return bool True if the matrices are equal, false otherwise
 */
bool areMatricesEqual(const DenseVector &mat1, const DenseVector &mat2, double
    tolerance);

/**
 * Method to read a matrix from a Matrix Market file
 * @param filename Name of the file
 * @return SparseMatrix Sparse matrix
 */
SparseMatrix readMatrixMarketFile(const std::string &filename);

/**
 * Method to generate a random dense vector
 * @param n Number of rows
 * @param m Number of columns
 * @return DenseVector Dense vector
 */
DenseVector generateLargeDenseVector(int n, int k);

/**
 * @brief Method to serialize a DenseVector to a flat array
 * @param denseVec Dense vector to serialize
 * @return std::vector<double> Flat array containing the serialized data
 */
std::vector<double> serialize(const DenseVector &denseVec);

/**
 * @brief Method to deserialize a flat array to a DenseVector
 * @param flat Flat array to deserialize
 * @param rows Number of rows in the dense vector
```

```
 * @param cols Number of columns in the dense vector
 * @return DenseVector Dense vector
 */
DenseVector deserialize(const std::vector<double> &flat, int rows, int cols);

#endif
```

B.F.2 Implementation File

```
#include "utils.h"

/**
 * Method to convert a PETSc matrix to a dense vector
 * @param C PETSc matrix
 * @return DenseVector Dense vector
 */
DenseVector ConvertPETScMatToDenseVector(Mat C)
{
    PetscInt m, n;          // Number of rows and columns in the matrix
    MatGetSize(C, &m, &n); // Get the number of rows and columns in the matrix

    DenseVector denseVec(m, std::vector<double>(n, 0.0)); // Dense vector to hold
        the matrix

    // Iterate over the rows of the matrix
    for (int i = 0; i < m; ++i)
    {
        // Iterate over the columns of the matrix
        for (int j = 0; j < n; j++)
        {
            PetscScalar value;                      // Value of the element
            MatGetValue(C, i, j, &value);           // Get the value of the element
            denseVec[i][j] = PetscRealPart(value); // Copy the value of the element
        }
    }

    // Return the dense vector
    return denseVec;
}

/**
 * Method to compare two matrices
 * @param mat1 First matrix
 * @param mat2 Second matrix
 * @param tolerance Tolerance for comparison
 * @return bool True if the matrices are equal, false otherwise
 */
bool areMatricesEqual(const DenseVector &mat1, const DenseVector &mat2, double
    tolerance)
{
    // Check if the matrices have the same dimensions
    if (mat1.size() != mat2.size())
        return false;

    // Iterate over the rows of the matrices
    for (size_t i = 0; i < mat1.size(); ++i)
    {
        // Check if the rows have the same dimensions
        if (mat1[i].size() != mat2[i].size())
            return false;

        // Iterate over the columns of the matrices
        for (size_t j = 0; j < mat1[i].size(); ++j)
        {
            // Check if the elements are equal
            if (std::fabs(mat1[i][j] - mat2[i][j]) > tolerance)
            {
```

```
                return false; // Matrices are not equal
            }
        }
    }

    return true; // Matrices are equal
}

/**
 * Method to read a matrix from a Matrix Market file
 * @param filename Name of the file
 * @return SparseMatrix Sparse matrix
 */
SparseMatrix readMatrixMarketFile(const std::string &filename)
{
    std::ifstream file(filename); // Input file stream

    // Check if the file was opened successfully
    if (!file.is_open())
    {
        throw std::runtime_error("Unable to open file: " + filename);
    }

    std::string line;                           // String to hold the current line
    bool isSymmetric = false, isPattern = false; // Flags to indicate if the matrix
        is symmetric or pattern only

    // Skip the comments
    while (std::getline(file, line))
    {
        // Check if the line is a comment
        if (line[0] == '%')
        {
            // Check if the line contains the word "symmetric"
            if (line.find("symmetric") != std::string::npos)
            {
                isSymmetric = true; // Set the symmetric flag
            }

            // Check if the line contains the word "pattern"
            if (line.find("pattern") != std::string::npos)
            {
                isPattern = true; // Set the pattern flag
            }
        }
        else
        {
            break; // First non-comment line reached, break out of the loop
        }
    }

    // Read the matrix dimensions
    int numRows, numCols, nonZeros;                          // Number of rows,
        columns and non-zero elements in the matrix
    std::stringstream(line) >> numRows >> numCols >> nonZeros; // Read the
        dimensions from the line

    // Check if the file was read successfully
    if (!file)
    {
        throw std::runtime_error("Failed to read matrix dimensions from file: " +
            filename);
    }

    SparseMatrix matrix;                                                 // Sparse
        matrix to hold the data
    matrix.rowPtr.resize(numRows + 1, 0);                                // Resize
        the row pointer vector
    std::vector<std::vector<std::pair<int, double>>> tempRows(numRows); //
        Temporary vector to hold the data
```

```
120     int rowIndex, colIndex;                                         // Row and
            column indices
121     double value;                                                   // Value of
             the non-zero element
122
123     // Read the non-zero elements
124     for (int i = 0; i < nonZeros; ++i)
125     {
126         // If the matrix is pattern only, the value of the non-zero element is 1.0
127         if (isPattern)
128         {
129             file >> rowIndex >> colIndex; // Read the row and column indices
130             value = 1.0;                  // Default value for pattern entries
131         }
132         else
133         {
134             file >> rowIndex >> colIndex >> value; // Read the row and column
                    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
                temporary vector
147
148         // If the matrix is symmetric, store the data in the transpose as well
149         if (isSymmetric && rowIndex != colIndex)
150         {
151             tempRows[colIndex].emplace_back(rowIndex, value); // Store the data in
                    the temporary vector
152         }
153     }
154
155     // Sort each row by column index
156     for (auto &row : tempRows)
157     {
158         std::sort(row.begin(), row.end());
159     }
160
161     // Reconstruct SparseMatrix structure
162     int cumSum = 0; // Cumulative sum of the number of non-zero elements
163
164     // Iterate over the rows of the matrix
165     for (int i = 0; i < numRows; ++i)
166     {
167         matrix.rowPtr[i] = cumSum; // Store the cumulative sum in the row pointer
                vector
168
169         // Iterate over the non-zero elements in the current row
170         for (const auto &elem : tempRows[i])
171         {
172             matrix.values.push_back(elem.second);    // Store the value of the non-
                    zero element
173             matrix.colIndices.push_back(elem.first); // Store the column index of
                    the non-zero element
174         }
175
176         cumSum += tempRows[i].size(); // Update the cumulative sum
177     }
178
179     matrix.rowPtr[numRows] = cumSum; // Store the cumulative sum in the row pointer
             vector
180     matrix.numRows = numRows;        // Store the number of rows
```

```
    matrix.numCols = numCols;        // Store the number of columns

    // Return the sparse matrix
    return matrix;
}

/**
 * Method to generate a random dense vector
 * @param n Number of rows
 * @param m Number of columns
 * @return DenseVector Dense vector
 */
DenseVector generateLargeDenseVector(int n, int k)
{
    DenseVector denseVector(n, std::vector<double>(k)); // Dense vector to hold the
        random values

    // Iterate over the rows of the dense vector
    for (int i = 0; i < n; ++i)
    {
        // Iterate over the columns of the dense vector
        for (int j = 0; j < k; ++j)
        {
            denseVector[i][j] = rand() % 100 + 1; // Generate a random value
                between 1 and 100
        }
    }

    // Return the dense vector
    return denseVector;
}

/**
 * @brief Method to serialize a DenseVector to a flat array
 * @param denseVec Dense vector to serialize
 * @return std::vector<double> Flat array containing the serialized data
 */
std::vector<double> serialize(const DenseVector &denseVec)
{
    std::vector<double> flat; // Flat array to hold the serialized data

    // Iterate over the rows of the dense vector
    for (const auto &vec : denseVec)
    {
        flat.insert(flat.end(), vec.begin(), vec.end()); // Copy the elements
    }

    // Return the flat array
    return flat;
}

/**
 * @brief Method to deserialize a flat array to a DenseVector
 * @param flat Flat array to deserialize
 * @param rows Number of rows in the dense vector
 * @param cols Number of columns in the dense vector
 * @return DenseVector Dense vector
 */
DenseVector deserialize(const std::vector<double> &flat, int rows, int cols)
{
    DenseVector denseVec(rows, std::vector<double>(cols)); // Dense vector to hold
        the deserialized data

    // Iterate over the rows of the dense vector
    for (int i = 0; i < rows; ++i)
    {
        // Iterate over the columns of the dense vector
        for (int j = 0; j < cols; ++j)
        {
            denseVec[i][j] = flat[i * cols + j]; // Copy the element
```

```
        }
    }

    // Return the dense vector
    return denseVec;
}
```

Appendix B.G Main File

Main file for running the different algorithms and comparing their performance.

```
#include "utils.h"                                          // Utility functions
#include "SparseMatrixDenseVectorMultiply.h"                // Sequential algorithm
#include "SparseMatrixDenseVectorMultiplyRowWise.h"         // Parallel algorithm (row-wise)
#include "SparseMatrixDenseVectorMultiplyColumnWise.h"      // Parallel algorithm (column-wise)
#include "SparseMatrixDenseVectorMultiplyNonZeroElement.h" // Parallel algorithm (non-zero element)

int main(int argc, char *argv[])
{
    //
        ------------------------------------------------------------------------------------------

    // ============================================== INITIALISATION
        ================================================
    //
        ------------------------------------------------------------------------------------------


    // Initialise MPI and PETSc
    MPI_Init(&argc, &argv);
    PetscInitialize(&argc, &argv, NULL, NULL);

    // Retrieve the rank and size of the world communicator
    int worldRank, worldSize;
    MPI_Comm_rank(PETSC_COMM_WORLD, &worldRank);
    MPI_Comm_size(PETSC_COMM_WORLD, &worldSize);

    // Check if the correct number of arguments is provided
    if (argc != 3)
    {
        if (worldRank == 0)
        {
            std::cerr << "Usage: " << argv[0] << " <number of columns> <matrix file path>" << std::endl;
        }
        MPI_Abort(PETSC_COMM_WORLD, 1);
    }

    // Parse the command-line arguments
    int k = std::atoi(argv[1]);     // Convert the first argument to an integer
    std::string filename = argv[2]; // The second argument is the filename

    // Declare the sparse matrix and dense vector
    SparseMatrix M;
    DenseVector v;

    // Declare the result of the serial multiplication
    DenseVector resultSerial;

    // Declare the data for broadcasting the sparse matrix and dense vector
    std::vector<double> flatData;
    int dataSize = 0;

    // 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
            VECTOR ============================
52      //
            ----------------------------------------------------------------------------------------
53      if (worldRank == 0)
54      {
55          std::cout << "World size: " << worldSize << std::endl;   // Print the
                number of processes
56          std::cout << "Sparse matrix: " << filename << std::endl; // Print the name
                of the Matrix Market file
57
58          // Read the sparse matrix from the Matrix Market file
59          M = readMatrixMarketFile(filename);
60          std::cout << "Matrix size: " << M.numRows << "x" << M.numCols << std::endl;
61
62          // Generate a random dense vector
63          v = generateLargeDenseVector(M.numCols, k);
64          std::cout << "Vector size: " << M.numCols << "x" << k << std::endl;
65
66          // Prepare the data for broadcasting
67          flatData = serialize(v);    // Serialize the dense vector
68          dataSize = flatData.size(); // Size of the serialized data
69      }
70
71      //
            ----------------------------------------------------------------------------------------
72      // ==================================== EXECUTE THE SERIAL MULTIPLICATION
            ======================================
73      //
            ----------------------------------------------------------------------------------------
74      if (worldRank == 0)
75      {
76          // Execute the serial multiplication
77          startTime = MPI_Wtime();
78          resultSerial = sparseMatrixDenseVectorMultiply(M, v, k);
79          endTime = MPI_Wtime();
80          std::cout << "Serial Algo Execution time: " << (endTime - startTime)
81                    << std::endl;
82
83          // FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS OF THE RESULT
84          // std::cout << "Result: " << std::endl;
85          // for (int i = 0; i < 10; ++i)
86          // {
87          //     for (int j = 0; j < k; ++j)
88          //     {
89          //         std::cout << resultSerial[i][j] << " ";
90          //     }
91          //     std::cout << std::endl;
92          // }
93      }
94
95      //
            ----------------------------------------------------------------------------------------
96      // ================================ BROADCAST THE SPARSE MATRIX AND DENSE
            VECTOR ================================
97      //
            ----------------------------------------------------------------------------------------
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-
            zero elements
109     int colIndicesSize = M.colIndices.size();                   // Number of column
            indices
110     int rowPtrSize = M.rowPtr.size();                           // Number of row
            pointers
111     MPI_Bcast(&M.numRows, 1, MPI_INT, 0, MPI_COMM_WORLD);      // Broadcast the
            number of rows
112     MPI_Bcast(&M.numCols, 1, MPI_INT, 0, MPI_COMM_WORLD);      // Broadcast the
            number of columns
113     MPI_Bcast(&valuesSize, 1, MPI_INT, 0, MPI_COMM_WORLD);     // Broadcast the
            number of non-zero elements
114     MPI_Bcast(&colIndicesSize, 1, MPI_INT, 0, MPI_COMM_WORLD); // Broadcast the
            number of column indices
115     MPI_Bcast(&rowPtrSize, 1, MPI_INT, 0, MPI_COMM_WORLD);     // Broadcast the
            number of row pointers
116     // Resize the vectors for all processes
117     if (worldRank != 0)
118     {
119         M.values.resize(valuesSize);
120         M.colIndices.resize(colIndicesSize);
121         M.rowPtr.resize(rowPtrSize);
122     }
123     // Broadcast the data
124     MPI_Bcast(M.values.data(), valuesSize, MPI_DOUBLE, 0, MPI_COMM_WORLD);
125     MPI_Bcast(M.colIndices.data(), colIndicesSize, MPI_INT, 0, MPI_COMM_WORLD);
126     MPI_Bcast(M.rowPtr.data(), rowPtrSize, MPI_INT, 0, MPI_COMM_WORLD);
127
128     // Broadcast the Dense Vector to all processes
129     // Broadcast the size of the serialized data
130     MPI_Bcast(&dataSize, 1, MPI_INT, 0, MPI_COMM_WORLD);
131     // Resize flatData for all processes
132     if (worldRank != 0)
133     {
134         flatData.resize(dataSize);
135     }
136     // Broadcast the data
137     MPI_Bcast(flatData.data(), dataSize, MPI_DOUBLE, 0, MPI_COMM_WORLD);
138     // Deserialize the data
139     if (worldRank != 0)
140     {
141         v.resize(M.numCols, std::vector<double>(k));
142         v = deserialize(flatData, M.numCols, k);
143     }
144
145     // Wait for all processes to finish the broadcast
146     MPI_Barrier(MPI_COMM_WORLD);
147
148     // ============================ FOR DEBUGGING ONLY - STOP BROADCAST TIMER
            ====================================
149     // endTime = MPI_Wtime();
150     // if (worldRank == 0)
151     // {
152     //     std::cout << "Broadcast time: " << (endTime - startTime) << std::endl;
153     // }
154     // ============================ FOR DEBUGGING ONLY - STOP BROADCAST TIMER
            ====================================
155
156     //
            ----------------------------------------------------------------------------------------------------
```

```
157     // ======================== EXECUTE THE PARALLEL MULTIPLICATION (ROW-WISE)
            ====================================
158     //
            ----------------------------------------------------------------------------------------
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         // std::cout << "Result: " << std::endl;
173         // for (int i = 0; i < 10; ++i)
174         // {
175         //     for (int j = 0; j < k; ++j)
176         //     {
177         //         std::cout << resultRowWise[i][j] << " ";
178         //     }
179         //     std::cout << std::endl;
180         // }
181         // ============================ FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
                ==============================
182
183         // Compare the results of the serial and parallel multiplications
184         if (areMatricesEqual(resultSerial, resultRowWise, 1e-6)) // Tolerance = 1e
                -6
185         {
186             std::cout << "Row-wise: Results are the same!"
187                       << std::endl;
188         }
189         else
190         {
191             std::cout << "Row-wise: Results are different!"
192                       << std::endl;
193         }
194     }
195
196     //
            ----------------------------------------------------------------------------------------
197     // ======================== EXECUTE THE PARALLEL MULTIPLICATION (COLUMN-WISE)
            ====================================
198     //
            ----------------------------------------------------------------------------------------
199
200     // Wait for all processes to finish the parallel multiplication (row-wise)
201     MPI_Barrier(MPI_COMM_WORLD);
202
203     // Execute the parallel multiplication (column-wise)
204     startTime = MPI_Wtime();
205     DenseVector resultColumnWise = sparseMatrixDenseVectorMultiplyColumnWise(M, v,
            k);
206     endTime = MPI_Wtime();
207
208     // Only the main process prints the parallel execution time
209     if (worldRank == 0)
210     {
211         std::cout << "Column-wise Execution time: " << (endTime - startTime)
212                   << std::endl;
213
214         // ============================ FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
```

```
            ==============================
        // std::cout << "Result: " << std::endl;
        // for (int i = 0; i < 10; ++i)
        // {
        //     for (int j = 0; j < k; ++j)
        //     {
        //         std::cout << resultColumnWise[i][j] << " ";
        //     }
        //     std::cout << std::endl;
        // }
        // ============================ FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
            ==============================

        // Compare the results of the serial and parallel multiplications
        if (areMatricesEqual(resultSerial, resultColumnWise, 1e-6)) // Tolerance =
            1e-6
        {
            std::cout << "Column-wise: Results are the same!"
                      << std::endl;
        }
        else
        {
            std::cout << "Column-wise: Results are different!"
                      << std::endl;
        }
    }

    //
        ------------------------------------------------------------------------------------------

    // ============================ EXECUTE THE PARALLEL MULTIPLICATION (NON-ZERO
        ELEMENT) ============================
    //
        ------------------------------------------------------------------------------------------


    // Wait for all processes to finish the parallel multiplication (column-wise)
    MPI_Barrier(MPI_COMM_WORLD);

    // Execute the parallel multiplication (non-zero element)
    startTime = MPI_Wtime();
    DenseVector resultNonZeroElement =
        sparseMatrixDenseVectorMultiplyNonZeroElement(M, v, k);
    endTime = MPI_Wtime();

    // Only the main process prints the parallel execution time
    if (worldRank == 0)
    {
        std::cout << "Non-zero Elements Execution time: " << (endTime - startTime)
                  << std::endl;

        // ============================ FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
            ==============================
        // std::cout << "Result: " << std::endl;
        // for (int i = 0; i < 10; ++i)
        // {
        //     for (int j = 0; j < k; ++j)
        //     {
        //         std::cout << resultNonZeroElement[i][j] << " ";
        //     }
        //     std::cout << std::endl;
        // }
        // ============================ FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
            ==============================

        // Compare the results of the serial and parallel multiplications
        if (areMatricesEqual(resultSerial, resultNonZeroElement, 1e-6)) //
            Tolerance = 1e-6
        {
            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 (
        PETSc) ==============================
284     //
        ------------------------------------------------------------------------------------------
285
286     // Wait for all processes to finish the parallel multiplication (non-zero
        element)
287     MPI_Barrier(MPI_COMM_WORLD);
288
289     // Declare the PETSc matrix
290     Mat A, B, C;
291
292     // ========================== FOR DEBUGGING ONLY - START PETSCS SETUP TIMER
        ========================================
293     // startTime = MPI_Wtime();
294     // ========================== FOR DEBUGGING ONLY - START PETSCS SETUP TIMER
        ========================================
295
296     // Create a parallel matrix to store the sparse matrix
297     MatCreate(PETSC_COMM_WORLD, &A);
298     MatSetSizes(A, PETSC_DECIDE, PETSC_DECIDE, M.numRows, M.numCols);
299     MatSetType(A, MATMPIAIJ);
300     MatSetUp(A);
301     // Fill the PETSc matrix with the values from the sparse matrix
302     if (worldRank == 0)
303     {
304         for (int i = 0; i < M.numRows; ++i)
305         {
306             for (int j = M.rowPtr[i]; j < M.rowPtr[i + 1]; ++j)
307             {
308                 MatSetValue(A, i, M.colIndices[j], M.values[j], INSERT_VALUES);
309             }
310         }
311     }
312     // Assemble the PETSc matrix
313     MatAssemblyBegin(A, MAT_FINAL_ASSEMBLY);
314     MatAssemblyEnd(A, MAT_FINAL_ASSEMBLY);
315
316     // Create a parallel matrix to store the dense vector
317     MatCreate(PETSC_COMM_WORLD, &B);
318     MatSetSizes(B, PETSC_DECIDE, PETSC_DECIDE, M.numCols, k);
319     MatSetType(B, MATDENSE);
320     MatSetUp(B);
321     // Fill the PETSc matrix B with values from the dense matrix v
322     if (worldRank == 0)
323     {
324         for (int i = 0; i < M.numCols; ++i)
325         {
326             for (int j = 0; j < k; ++j)
327             {
328                 MatSetValue(B, i, j, v[i][j], INSERT_VALUES);
329             }
330         }
331     }
332     // Assemble the PETSc matrix
333     MatAssemblyBegin(B, MAT_FINAL_ASSEMBLY);
334     MatAssemblyEnd(B, MAT_FINAL_ASSEMBLY);
```

```
335
336     // ========================== FOR DEBUGGING ONLY - STOP PETSCS SETUP TIMER
            ========================================
337     // 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
355     // ========================== FOR DEBUGGING ONLY - START PETSCS CONVERSION
            TIMER ==================================
356     // startTime = MPI_Wtime();
357     // ========================== FOR DEBUGGING ONLY - START PETSCS CONVERSION
            TIMER ==================================
358
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
                TIMER ==================================
369         // endTime = MPI_Wtime();
370         // std::cout << "PETSc Conversion time: " << (endTime - startTime) << std::
                endl;
371         // ========================== FOR DEBUGGING ONLY - STOP PETSCS CONVERSION
                TIMER ==================================
372
373         // ========================== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
                ==============================
374         // std::cout << "Result: " << std::endl;
375         // for (int i = 0; i < 10; ++i)
376         // {
377         //     for (int j = 0; j < k; ++j)
378         //     {
379         //         std::cout << globalMatrix[i][j] << " ";
380         //     }
381         //     std::cout << std::endl;
382         // }
383         // ========================== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
                ==============================
384
385         // Compare the results of the serial and PETSc multiplications
386         if (areMatricesEqual(resultSerial, globalMatrix, 1e-6)) // Tolerance = 1e-6
387         {
388             std::cout << "PETSc: Results are the same!"
389                       << std::endl;
390         }
391         else
392         {
393             std::cout << "PETSc: Results are different!"
```

```
                        << std::endl;
        }
    }

    // Free the memory
    MatDestroy(&A);
    MatDestroy(&B);
    MatDestroy(&C);
    MatDestroy(&CSeq);

    // Finalise MPI and PETSc
    PetscFinalize();
    MPI_Finalize();

    return 0;
}
```

Appendix B.H Scripts

B.H.1 MPI Submission Script

Bash script to submit an MPI job to the cluster.

```
#!/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 mpiprocs 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 -genvall -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.H.2 Batch Test Script

Bash script to submit multiple MPI jobs to the cluster.

```
#!/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.H.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"
```