

Alexis Balayre

High Performance Technical Computing Assignment

School of Aerospace, Transport and Manufacturing Computational Software of Techniques Engineering

> MSc Academic Year: 2023 - 2024

Supervisor: Dr Irene Moulitsas 5th February 2024

Abstract

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

Table of Contents

Al	bstrac	et			ii
Tε	ible of	f Conte	nts		iii
Li	st of l	Figures			vi
Li	st of '	Fables			viii
1	Intr	oductio	n		1
2	Met	hodolog	<u>v</u>		2
	2.1	•			
		2.1.1		Matrix	
		2.1.2	-	or	
	2.2	Seque	ntial Algor	rithm	. 3
		2.2.1	_	m Flow	
		2.2.2	Tempora	al Complexity Analysis	. 3
	2.3	Line-E	-	ıllelism	
		2.3.1	Algorith	m Flow	. 4
		2.3.2	Time Co	omplexity Analysis	. 5
			2.3.2.1	Computational Complexity	
			2.3.2.2	Communication Complexity	
			2.3.2.3	Final Result Reconstruction	. 6
			2.3.2.4	Overall Time Complexity	. 6
		2.3.3	Performa	ance Analysis	. 6
			2.3.3.1	Performance Dependence	. 6
			2.3.3.2	Expected Performance	
	2.4	Colum	n-Wise Pa	arallelism	. 7
		2.4.1	Algorith	m Flow	. 7
		2.4.2	Tempora	al Complexity Analysis	. 8
			2.4.2.1	Computation Time Complexity	. 8
			2.4.2.2	Communication Time Complexity	
			2.4.2.3	Final Result Reconstruction	. 8
			2.4.2.4	Overall Time Complexity	. 8
		2.4.3	Performa	ance Analysis	. 9
			2.4.3.1	Performance Dependence	. 9
			2432	Expected Performance	C

	2.5	Non-Ze	ero Element Parallelism)
		2.5.1	Algorithm Flow)
		2.5.2	Temporal Complexity Analysis	
		2.5.3	Computation Complexity	l
		2.5.4	Communication Complexity	l
			2.5.4.1 Final Result Reconstruction	l
		2.5.5	Overall Time Complexity	
		2.5.6	Performance Analysis	2
			2.5.6.1 Performance Dependence	2
			2.5.6.2 Expected Performance	2
	2.6	Perform	mance Metrics	3
_	_			_
3			Discussion 14	_
	3.1		8	-
		3.1.1	Sparse Matrix Impact	
			3.1.1.1 Execution Time	-
			3.1.1.2 Communication Time	
			3.1.1.3 Computation Time	
			3.1.1.4 Performance	
		3.1.2	Fat Vector Impact	
			3.1.2.1 Execution Time	
			3.1.2.2 Communication Time	
			3.1.2.3 Computation Time	
			3.1.2.4 Performance	
	3.2	HPC E	Invironmental Impact	/
4	Cone	clusion	29)
Re	feren	ces	30)
Δ	Doci	ımentat	tion 31	
			tree	_
		3	g Started	
		_	ds Overview	
	11.0		Utils.h	
		11.0.1	A.C.1.1 ConvertPETScMatToFatVector	
			A.C.1.2 areMatricesEqual	
			A.C.1.3 readMatrixMarketFile	
			A.C.1.4 generateLargeFatVector	
			A.C.1.5 serialize and deserialize	
		A C 2	SparseMatrixFatVectorMultiply.h	
			A.C.2.1 sparseMatrixFatVectorMultiply	
		A.C.3	SparseMatrixFatVectorMultiplyRowWise.h	
		1 2.0.0	A.C.3.1 sparseMatrixFatVectorMultiplyRowWise	
		A.C.4	SparseMatrixFatVectorMultiplyColumnWise.h	
			A.C.4.1 sparseMatrixFatVectorMultiplyColumnWise	
			Transfer and the state of the s	L

		ce Code																				
В.		Data S																				
В.	В	Sequen			_																	
		B.B.1				tion																
		B.B.2				enta																
В.		Line-B																				
		B.C.1	D	ecl	ara	tion	ı Fi	le														
		B.C.2	In	npl	em	enta	atic	n I	File	•												
В.	D	Colum	n-V	Vis	e P	aral	llel	isn	1.			•										
		B.D.1	D	ecl	ara	tion	ı Fi	le				•										
		B.D.2	Ir	npl	em	enta	atic	n I	File	•												
В.	E	Non-Z	ero	El	em	ent	Pa	rall	eli	sm	١.											
		B.E.1	D	ecl	ara	tion	ı Fi	le														
		B.E.2	Ir	npl	em	enta	atic	n I	File	•												
В.	F	Utility	Fu	nct	ion	S																
		B.F.1	D	ecl	ara	tion	ı Fi	le														
		B.F.2	Ir	npl	em	enta	atic	n I	File	•												
B.	G	Main F	File																			
В.	Η	Scripts																				
		B.H.1	M	PΙ	Su	bmi	issi	on	Sc	rip	t.											
		B.H.2	В	atc	h T	est	Scı	ript														
		B.H.3	G	et (CS	V S	crii	ot .														

List of Figures

3.1	Cage4 matrix execution time	14
3.2	DC1 matrix execution time	15
3.3	Amazon0302 matrix execution time	15
3.4	Cop20k_A matrix execution time	15
3.5	FEM_3D_thermal1 matrix execution time	16
3.6	Cage4 matrix communication time	16
3.7	DC1 matrix communication time	16
3.8	Amazon0302 matrix communication time	17
3.9	Cop20k_A matrix communication time	17
3.10	FEM_3D_thermal1 matrix communication time	17
3.11	Cage4 matrix computation time	18
3.12	DC1 matrix computation time	18
3.13	Amazon0302 matrix computation time	18
3.14	Cop20k_A matrix computation time	19
3.15	FEM_3D_thermal1 matrix computation time	19
3.16	Cage4 matrix performance	19
3.17	DC1 matrix performance	20
	Amazon0302 matrix performance	20
	Cop20k_A matrix performance	20
3.20	FEM_3D_thermal1 matrix performance	21
3.21	Cop20k_A matrix execution time	21
3.22	Cop20k_A matrix execution time	21
3.23	Cop20k_A matrix execution time	22
3.24	Cop20k_A matrix execution time	22
3.25	Cop20k_A matrix execution time	22
3.26	Cop20k_A matrix communication time	23
3.27	Cop20k_A matrix communication time	23
3.28	Cop20k_A matrix communication time	23
3.29	Cop20k_A matrix communication time	24
3.30	Cop20k_A matrix communication time	24
3.31	Cop20k_A matrix computation time	24
3.32	Cop20k_A matrix computation time	25
3.33	Cop20k_A matrix computation time	25
	Cop20k_A matrix computation time	25
3.35	Cop20k_A matrix computation time	26
3.36	Cop20k_A matrix performance	26

3.37	Cop20k_A matrix performance												26
3.38	Cop20k_A matrix performance												27
3.39	Cop20k_A matrix performance												27
3.40	Cop20k_A matrix performance												27

List of Tables

3.1 Sparse matrix specifications	
----------------------------------	--

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 or solving structural engineering problems.

Cranfield University has two HPC systems: CRESCENT2 and DELTA. However, this report will focus exclusively on CRESCENT2, which is an HPC cluster designed to provide computing power for teaching and research. CRESCENT 2 nodes are equipped with Intel Xeon E5 2620 processors, and each node contains two 16-core processors and 16 gigabytes of RAM.

The aim of this report is to explore distributed memory parallel programming strategies for optimising the performance of sparse matrix multiplication by a fat vector, a common operation in numerical linear algebra.

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:

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

where most elements of M are zeros.

The vector *v* is defined as:

$$v = \begin{pmatrix} v_{11} & v_{12} & \cdots & v_{1k} \\ v_{21} & v_{22} & \cdots & v_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ v_{n1} & v_{n2} & \cdots & v_{nk} \end{pmatrix}$$
(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 **FatVector** structure is defined in Appendix B.A.

2.2 Sequential Algorithm

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 sequential algorithm for multiplying M by v is implemented in Appendix B.B.

2.2.1 Algorithm Flow

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 \text{ zero matrix of size } m \times k

for i \leftarrow 0 to m - 1 do

for each non-zero element (j, \text{ 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
```

The algorithmic flow can be more explicitly detailed by:

- 1. **Initialisation:** Create a zero matrix of size $m \times k$ to store the result.
- 2. **Row-wise Processing:** Iterate over each row *i* of matrix *M*, leveraging the CSR format to efficiently access non-zero elements.
- 3. **Element-wise Multiplication and Accumulation:** For each non-zero element in row i, identified by its column index j and value, conduct a nested iteration over the columns l of vector v, multiplying the non-zero element by the corresponding vector element and accumulating the result in Result[i][l].

2.2.2 Temporal Complexity Analysis

Given a sparse matrix M of size $m \times n$ with z non-zero elements and a fat vector v of size $n \times k$, the serial algorithm for multiplying $M \times v$ iterates through each non-zero element of the matrix M to compute the product.

The algorithm performs two operations (a multiplication and an addition) for each non-zero element with respect to each column of v, resulting in a total of 2zk operations.

Hence, the time complexity of the serial sparse matrix-fat vector multiplication algorithm can be expressed as:

$$T(n) = O(zk) (2.1)$$

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.

2.3.1 Algorithm Flow

```
Algorithm 2 Row-wise Parallel Sparse Matrix-Fat Vector Multiplication
Require: M is an m \times n sparse matrix
Require: v is an n \times k fat vector
Require: worldSize is the number of processes
Require: worldRank is the rank of the current process
Ensure: finalResult is an m \times k matrix, result of M \times v
  rowsPerProcess \leftarrow m/worldSize
  extraRows \leftarrow m \mod worldSize
  startRow \leftarrow worldRank \times rowsPerProcess + min(worldRank, extraRows)
  endRow \leftarrow startRow + rowsPerProcess
  if worldRank < extraRows then
      endRow \leftarrow endRow + 1
  end if
  Initialise localResult with zeros of size (endRow - startRow) \times k
  for i \leftarrow startRow to endRow - 1 do
      for each non-zero element (j, value) in row i of M do
          for k \leftarrow 0 to k-1 do
              localIndex \leftarrow (i - startRow) \times k + k
              localResult[localIndex] \leftarrow localResult[localIndex] + value \times v[j][k]
          end for
      end for
  end for
  if worldRank == 0 then
      Prepare recvCounts and displacements for gathering
  end if
  MPI_Gatherv(localResult, ...)
  if worldRank == 0 then
      Reassemble finalResult from all localResults
      return finalResult
  end if
```

The algorithmic flow can be explicitly detailed by:

- 1. **Initialisation:** Obtain MPI world size and rank to determine each process's role.
- 2. **Row Distribution:** Assign a subset of rows from the sparse matrix to each process based on the rank, ensuring an even distribution with possible adjustments for any remainder.
- 3. **Local Computation:** Each process calculates the product of its assigned rows with the fat vector, storing results in a local vector.
- 4. **Gather Results:** Use MPI_Gatherv to collect the local result vectors from all processes into a single vector at the root process.
- 5. **Final Result Reconstruction:** The root process reconstructs the final result matrix from the gathered vector.

2.3.2 Time Complexity Analysis

Given a sparse matrix M of size $m \times n$ with z non-zero elements and a fat vector v of size $n \times k$, the line-based algorithm distributes the multiplication task across p processors.

2.3.2.1 Computational Complexity

Each process computes a portion of the result vector, working on approximately m/p rows of the sparse matrix. The computation time $(T_{\rm comp})$ is therefore influenced by the distribution of non-zero elements across the rows. Assuming a uniform distribution, the computation time can be estimated as:

$$T_{\rm comp} = O\left(\frac{z \times k}{p}\right) \tag{2.2}$$

2.3.2.2 Communication Complexity

After computation, each process holds a part of the result vector that needs to be combined to form the final result. The main communication cost arises from gathering these parts at a single process or distributing them among all processes.

- Startup Overhead: The initiation of a communication incurs a latency cost, α , which is significant when the number of messages is large.
- **Data Transmission Cost:** Each process sends its portion of the result vector, incurring a cost proportional to the amount of data sent, the number of processes and the network bandwidth, denoted by β .

The communication time complexity (T_{comm}) can be approximated as:

$$T_{\text{comm}} = p \times \alpha + \beta \times \frac{m}{p} \times k \tag{2.3}$$

2.3.2.3 Final Result Reconstruction

After gathering the local results, the root process reconstructs the final result matrix. This step has a time complexity proportional to the size of the final matrix, $O(m \times k)$.

2.3.2.4 Overall Time Complexity

The overall time complexity, including both computation and communication, is given by:

$$T_{\text{overall}} = T_{\text{comp}} + T_{\text{comm}} = O\left(\frac{z \times k}{p}\right) + p \times \alpha + \beta \times \frac{m}{p} \times k + O(m \times k)$$
 (2.4)

2.3.3 Performance Analysis

2.3.3.1 Performance Dependence

- Number of processes (p): Performance improves with p until communication overhead becomes significant.
- Number of rows (*m*): Affects workload distribution. Performance optimal when $p \le m$.
- Number of non-zero elements (z): Higher z increases computation workload but mitigated by parallel execution.
- Number of columns (*k*): Increases computation linearly. Each row computation involves all columns.

2.3.3.2 Expected Performance

Optimal when $p \le m$ with even workload distribution. Performance may degrade if p > m due to idle processes or when communication overhead outweighs computation benefits.

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.

2.4.1 Algorithm Flow

Algorithm 3 Column-wise Parallel Sparse Matrix-Fat Vector Multiplication

```
Require: M is an m \times n sparse matrix
Require: v is an n \times k fat vector
Require: worldSize is the number of processes
Require: worldRank is the rank of the current process
Ensure: finalResult is an m \times k matrix, result of M \times v
  colsPerProcess \leftarrow k/worldSize
  extraCols \leftarrow k \mod worldSize
  startCol \leftarrow worldRank \times colsPerProcess
  endCol \leftarrow startCol + colsPerProcess
  if worldRank == worldSize -1 then
       endCol \leftarrow endCol + extraCols
  end if
  localSize \leftarrow m \times (endCol - startCol)
  Initialise localResult with zeros of size localSize
  for col \leftarrow startCol to endCol - 1 do
       for row \leftarrow 0 to m-1 do
          sum \leftarrow 0
          for each non-zero element (i, value) in row row of M do
               sum \leftarrow sum + value \times v[i][col]
          end for
           localResult[row][col - startCol] \leftarrow sum
      end for
  end for
  if worldRank == 0 then
       Initialise finalResult with zeros of size m \times k
  Gather localResult from all processes to finalResult at root
  if worldRank == 0 then
       State Reassemble finalResult from gathered localResults
      return finalResult
  end if
```

The algorithmic flow can be explicitly detailed by:

- 1. **Initialisation:** Obtain MPI world size and rank to determine each process's role.
- 2. **Column Distribution:** Calculate the number of columns each process will handle, distributing any extra columns to the last processes, and define the start and end column indices for each process.

- 3. **Local Computation:** Each process computes a portion of the multiplication result for its assigned columns, iterating through the sparse matrix rows and the relevant columns of the fat vector.
- 4. **Gather Results:** Use MPI_Gatherv to collect the local results from all processes into a single result vector at the root process.
- Final Result Reconstruction: The root process reassembles the gathered results into the final fat vector matrix, ensuring the elements are correctly positioned according to their original indices.

2.4.2 Temporal Complexity Analysis

Consider a sparse matrix M of size $m \times n$ with z non-zero elements and a fat vector v of size $n \times k$, the column-wise algorithm distributes the multiplication task across p processors.

2.4.2.1 Computation Time Complexity

Each process is responsible for approximately k/p columns of the fat vector. The computation time ($T_{\rm comp}$) is therefore influenced by the distribution of non-zero elements across the columns. Assuming a uniform distribution, the computation time can be estimated as:

$$T_{\text{comp}} = O\left(\frac{k \times z}{p}\right) \tag{2.5}$$

2.4.2.2 Communication Time Complexity

After local computations, partial results must be gathered at the root process. The communication time complexity (T_{comm}) can be approximated as:

$$T_{\text{comm}} = p \times \alpha + \beta \times m \times \frac{k}{p}$$
 (2.6)

2.4.2.3 Final Result Reconstruction

After gathering the local results, the root process reconstructs the final result matrix. This step has a time complexity proportional to the size of the final matrix, $O(m \times k)$.

2.4.2.4 Overall Time Complexity

The overall time complexity of the column-wise parallel sparse matrix-vector multiplication algorithm is dominated by the sum of computation and communication complexities:

$$T_{\text{overall}} = T_{\text{comp}} + T_{\text{comm}} = O\left(\frac{k \times z}{p}\right) + p \times \alpha + \beta \times m \times \frac{k}{p} + O(m \times k)$$
 (2.7)

2.4.3 Performance Analysis

2.4.3.1 Performance Dependence

- Number of processes (p): Performance improvement depends on the ratio of k to p.
- Number of rows (m): Less impact on performance scaling compared to p and k.
- Number of non-zero elements (*z*): Impacts computation time, balanced by parallel processing.
- Number of columns (k): Critical for performance. Optimal when large and divisible by p.

2.4.3.2 Expected Performance

Best when k is significantly larger than p and divisible, allowing efficient parallel processing with minimal communication overhead. Performance may degrade if p > k due to idle processes or when communication outweighs computation benefits.

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.

2.5.1 Algorithm Flow

```
Algorithm 4 Non-Zero Element Parallel Sparse Matrix-Fat Vector Multiplication
Require: M is an m \times n sparse matrix
Require: v is an n \times k fat vector
Require: worldSize is the number of processes
Require: worldRank is the rank of the current process
Ensure: finalResult is an m \times k matrix, result of M \times v
  Calculate the total number of non-zero elements and distribute them among MPI pro-
  cesses
  Determine startIdx and endIdx for non-zero elements for the current process
  Map non-zero element indices to their corresponding row indices in the sparse matrix
  Initialise localResult with zeros of size m \times k
  for idx \leftarrow startIdx to endIdx - 1 do
      Determine row, col, and value for each non-zero element
      for k \leftarrow 0 to k-1 do
          localResult[row \times k + k] \leftarrow localResult[row \times k + k] + value \times v[col][k]
      end for
  end for
  Use MPI_Reduce to sum up localResults from all processes to flatFinalResult at the
  root process
  if worldRank == 0 then
      Reconstruct finalResult from flatFinalResult
      return finalResult
  end if
```

The algorithmic flow can be explicitly detailed by:

- 1. **Initialisation:** Obtain MPI world size and rank to determine each process's role.
- 2. **Non-Zero Elements Distribution:** Calculate each process's share of non-zero elements in the sparse matrix.
- 3. **Local Computation:** Each process multiplies its assigned non-zero elements with corresponding columns in the fat vector, accumulating results locally.
- 4. **Gather Results:** Use Reduce to sum up all local results into a single vector on the root process.
- 5. **Final Result Reconstruction:** The root process reconstructs the final result matrix from the gathered vector.

2.5.2 Temporal Complexity Analysis

Given a sparse matrix M of size $m \times n$ with z non-zero elements and a fat vector v of size $n \times k$, the non-zero elements algorithm distributes the multiplication task across p processors.

2.5.3 Computation Complexity

Each process is responsible for a subset of the non-zero elements. The total computation workload is proportional to the number of non-zero elements z, distributed evenly among p processes:

$$T_{\text{comp}} = O\left(\frac{z \times k}{p}\right) \tag{2.8}$$

Given that each non-zero element computation involves a multiplication and an addition, the computation complexity remains linear with respect to the number of non-zero elements handled by each process.

2.5.4 Communication Complexity

The communication complexity involves reducing the local results from all the processes to a single result at the root process. The communication time complexity (T_{comm}) can be approximated as:

$$T_{\text{comm}} = p \times \alpha + \beta \times m \times \frac{k}{p}$$
 (2.9)

where:

- α is the latency cost of initiating a communication.
- β is the cost of data transmission.

2.5.4.1 Final Result Reconstruction

After reducing the local results, the root process reconstructs the final result matrix. This step has a time complexity proportional to the size of the final matrix, $O(m \times k)$.

2.5.5 Overall Time Complexity

The overall time complexity of the SparseMatrixFatVectorMultiplyNonZeroElement algorithm is the sum of computation and communication complexities:

$$T_{\text{overall}} = T_{\text{comp}} + T_{\text{comm}} = O\left(\frac{z \times k}{p}\right) + p \times \alpha + \beta \times m \times \frac{k}{p} + O(m \times k)$$
 (2.10)

2.5.6 Performance Analysis

2.5.6.1 Performance Dependence

- Number of processes (p): Performance improves with p, but aggregation communication can be a bottleneck.
- Number of rows (*m*): Impacts performance through non-zero element distribution.
- Number of non-zero elements (z): Directly proportional to computation workload, benefiting from parallel execution.
- Number of columns (*k*): Increases workload linearly, balanced by distributing non-zero elements across processes.

2.5.6.2 Expected Performance

Highly efficient for matrices with large and evenly distributed z, maximising parallelism. Optimal when z/p is large, minimising idle time and communication overhead.

2.6 Performance Metrics

In order to evaluate the performance of all the algorithms, they were implemented by the main program (see appendix B.G). Here is the flow of this program:

1. **Initialisation:** Start MPI and PETSc environments.

2. Matrix and Vector Preparation:

- Read the sparse matrix from a file. This feature is provided by the readMatrixMarketFile method (see appendix B.F), created thanks to the Matrix Market I/O library (1).
- Generate a random fat vector with dimensions matching the matrix and a specified number of columns.
- Distribute the matrix and vector across all processes.
- 3. **Serial Multiplication:** Perform matrix-vector multiplication using a serial algorithm and measure execution time.
- 4. **Line-Based Parallel Multiplication:** Perform matrix-vector multiplication using a line-based parallel algorithm and measure execution time.
- 5. **Column-Based Parallel Multiplication:** Perform matrix-vector multiplication using a column-based parallel algorithm and measure execution time.
- 6. **Non-Zero Element Parallel Multiplication:** Perform matrix-vector multiplication using a non-zero element parallel algorithm and measure execution time.

7. PETSc Implementation:

- Convert the sparse matrix and fat vector into PETSc formats.
- Execute matrix-vector multiplication using PETSc operations.
- Convert the result back into a Fat Vector format for comparison.
- 8. **Result Comparison:** Compare the results of serial, parallel, and PETSc implementations for correctness.
- 9. Finalisation: Clean up and close MPI and PETSc environments.

This program was executed with different sparse matrices, number of columns in the fat vector, and number of processes to evaluate the performance of the algorithms. To do so, the following performance metrics were used:

Chapter 3

Results and Discussion

3.1 Results

The performance of all algorithms was evaluated using the following five sparse matrix:

Matrix Name	Dimensions	Non-Zero Elements
Cage4	9×9	49
FEM_3D_thermal1	$17,880 \times 17,880$	430,740
DC1	$116,835 \times 116,835$	766,396
Cop20k_A	$121,192 \times 121,192$	2,624,331
Amazon0302	$262,111 \times 262,111$	1,234,877

Table 3.1: Sparse matrix specifications

3.1.1 Sparse Matrix Impact

The first set of experiments focused on the impact of the sparse matrix on the performance of the algorithms.

3.1.1.1 Execution Time

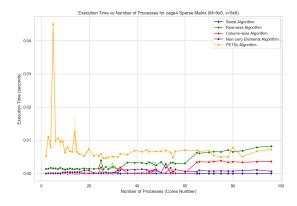


Figure 3.1: Cage4 matrix execution time

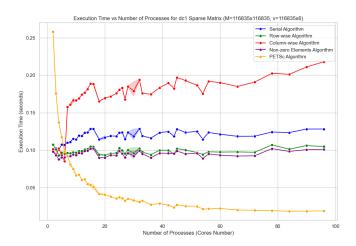


Figure 3.2: DC1 matrix execution time

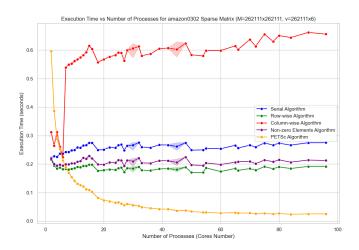


Figure 3.3: Amazon0302 matrix execution time

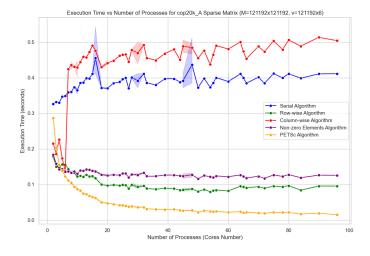


Figure 3.4: Cop20k_A matrix execution time

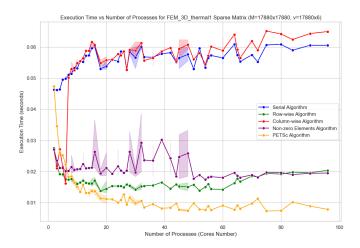


Figure 3.5: FEM_3D_thermal1 matrix execution time

3.1.1.2 Communication Time

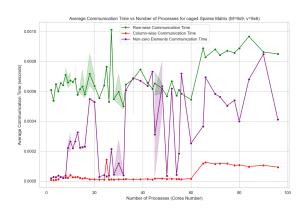


Figure 3.6: Cage4 matrix communication time

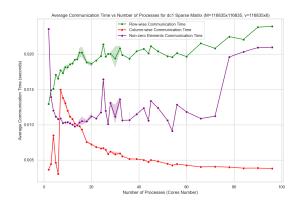


Figure 3.7: DC1 matrix communication time

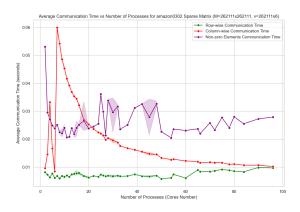


Figure 3.8: Amazon0302 matrix communication time

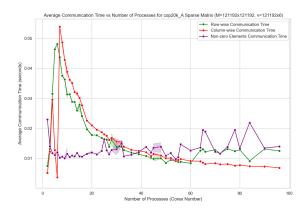


Figure 3.9: Cop20k_A matrix communication time

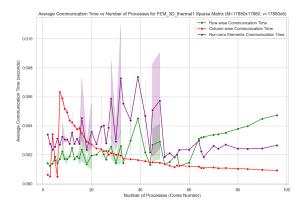


Figure 3.10: FEM_3D_thermal1 matrix communication time

3.1.1.3 Computation Time

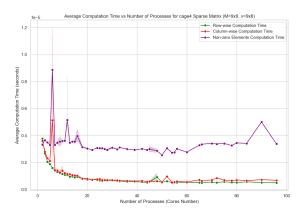


Figure 3.11: Cage4 matrix computation time

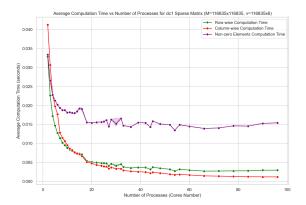


Figure 3.12: DC1 matrix computation time

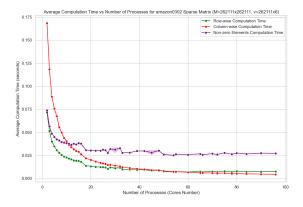


Figure 3.13: Amazon0302 matrix computation time

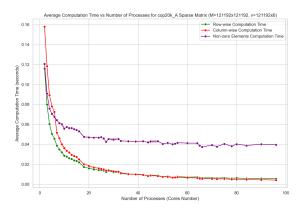


Figure 3.14: Cop20k_A matrix computation time

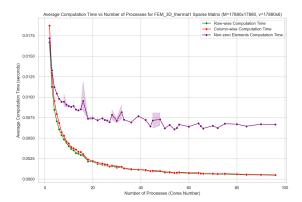


Figure 3.15: FEM_3D_thermal1 matrix computation time

3.1.1.4 Performance

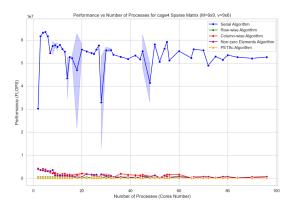


Figure 3.16: Cage4 matrix performance

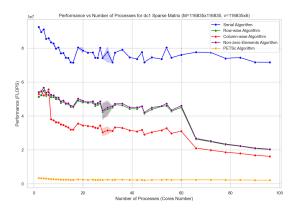


Figure 3.17: DC1 matrix performance

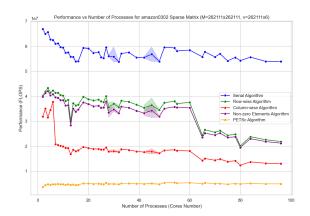


Figure 3.18: Amazon0302 matrix performance

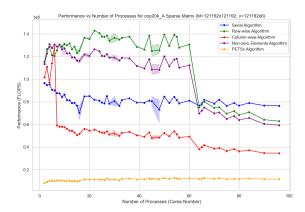


Figure 3.19: Cop20k_A matrix performance

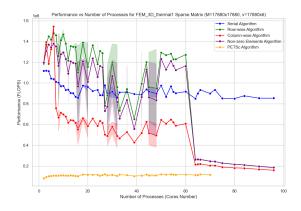


Figure 3.20: FEM_3D_thermal1 matrix performance

3.1.2 Fat Vector Impact

3.1.2.1 Execution Time

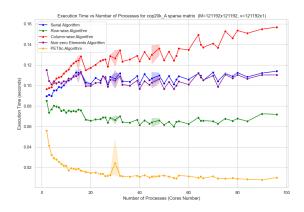


Figure 3.21: Cop20k_A matrix execution time

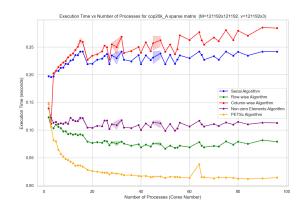


Figure 3.22: Cop20k_A matrix execution time

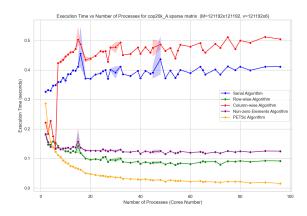


Figure 3.23: Cop20k_A matrix execution time

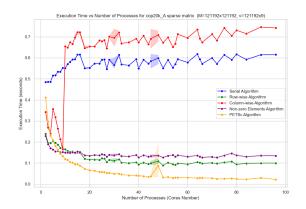


Figure 3.24: Cop20k_A matrix execution time

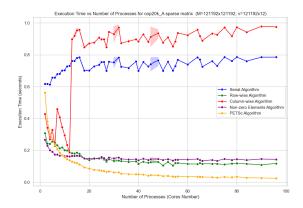


Figure 3.25: Cop20k_A matrix execution time

3.1.2.2 Communication Time

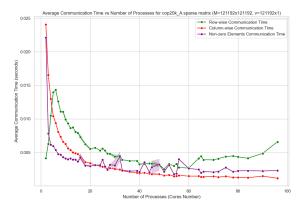


Figure 3.26: Cop20k_A matrix communication time

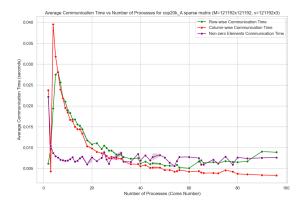


Figure 3.27: Cop20k_A matrix communication time

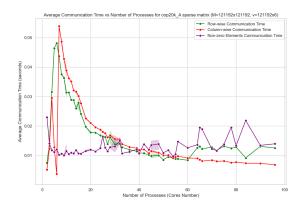


Figure 3.28: Cop20k_A matrix communication time

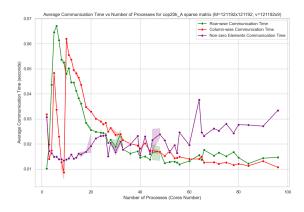


Figure 3.29: Cop20k_A matrix communication time

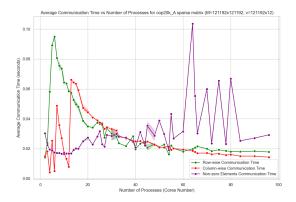


Figure 3.30: Cop20k_A matrix communication time

3.1.2.3 Computation Time

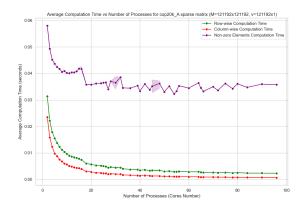


Figure 3.31: Cop20k_A matrix computation time

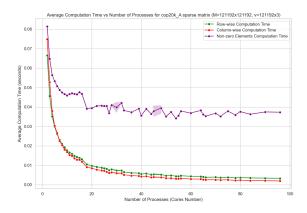


Figure 3.32: Cop20k_A matrix computation time

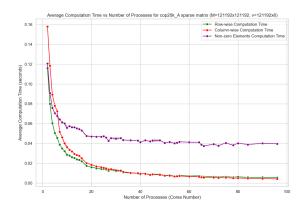


Figure 3.33: Cop20k_A matrix computation time

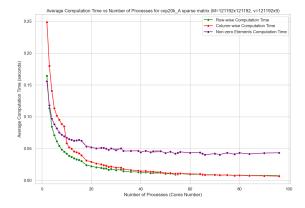


Figure 3.34: Cop20k_A matrix computation time

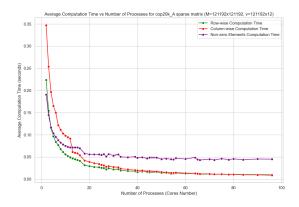


Figure 3.35: Cop20k_A matrix computation time

3.1.2.4 Performance

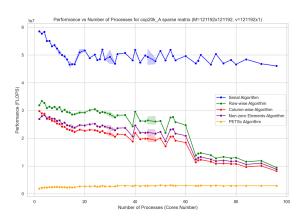


Figure 3.36: Cop20k_A matrix performance

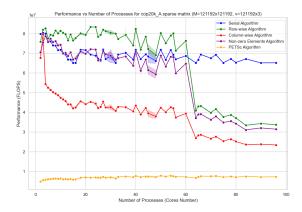


Figure 3.37: Cop20k_A matrix performance

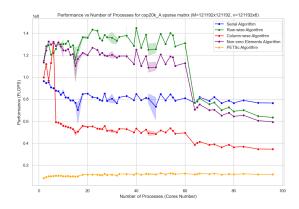


Figure 3.38: Cop20k_A matrix performance

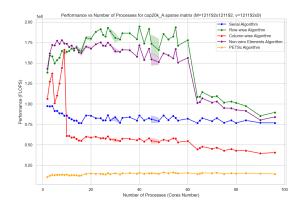


Figure 3.39: Cop20k_A matrix performance

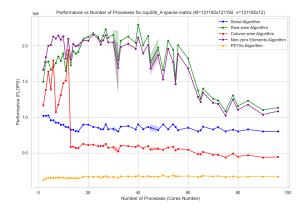


Figure 3.40: Cop20k_A matrix performance

3.2 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

References

1. Lugowski A. fast matrix market: Fast and Full-Featured Matrix Market I/O Library; 2023. Available at: https://github.com/alugowski/fast_matrix_market.(Accessed: December 28, 2023).

Appendix A

Documentation

Appendix A.A Project tree

```
Source Code/
    scripts/
        batch_test.sh
        get_csv_all.sh
        get_csv_debug.sh
        get_csv_specific.sh
        mpi.sub
    Matrix Definitions . h
    SparseMatrixFatVectorMultiply.h
    SparseMatrixFatVectorMultiply.cpp
    SparseMatrixFatVectorMultiplyRowWise.h
    SparseMatrixFatVectorMultiplyRowWise.cpp
    Sparse Matrix Fat Vector Multiply Column Wise. h \\
    Sparse Matrix Fat Vector Multiply Column Wise.cpp \\
    SparseMatrixFatVectorMultiplyNonZeroElement.h
    Sparse Matrix Fat Vector Multiply Non Zero Element. cpp\\
    utils.h
    utils.cpp
    main.cpp
results/
    fat_vector_dim/
        <sparse_matrix>_<k>_<metric>.png
    matrix_dim/
        <sparse_matrix>_-<k>_-<metric>.png
```

Appendix A.B Getting Started

To run the program, follow these steps:

- 1. Install the required libraries: mpi & petsc
- 2. Compile the main program using the following command:

```
mmpicxx -o <executable_name> -I${PETSC_DIR}/include -I${
PETSC_DIR}/${PETSC_ARCH}/include -L${PETSC_DIR}/${PETSC_ARCH}/lib -lpetsc
SparseMatrixFatVectorMultiply.cpp main_verify.cpp utils.cpp
SparseMatrixFatVectorMultiplyColumnWise.cpp
SparseMatrixFatVectorMultiplyNonZeroElement.cpp
SparseMatrixFatVectorMultiplyRowWise.cpp
```

3. Run the program using the following command:

```
mpirun -np <number_of_processes> <executable_name> <k> <
sparse_matrix_file_pathw>
```

Appendix A.C Methods Overview

A.C.1 Utils.h

A.C.1.1 ConvertPETScMatToFatVector

Description: Converts a PETSc matrix to a FatVector stucture.

Parameters:

• Mat C - PETSc matrix to be converted.

Returns: FatVector - Fat vector representation of the PETSc matrix.

A.C.1.2 areMatricesEqual

Description: Compares two matrices for equality within a specified tolerance.

Parameters:

- FatVector &mat1 First matrix.
- FatVector &mat2 Second matrix.
- double tolerance Tolerance for comparison.

Returns: bool - True if matrices are equal within the tolerance, false otherwise.

A.C.1.3 readMatrixMarketFile

Description: Reads a matrix from a Matrix Market file into a sparse matrix format.

Parameters:

• std::string &filename - Name of the Matrix Market file.

Returns: SparseMatrix - Sparse matrix read from the file.

A.C.1.4 generateLargeFatVector

Description: Generates a random Fat Vector with specified dimensions.

Parameters:

- int n Number of rows.
- int k Number of columns.

Returns: FatVector - Generated fat vector.

A.C.1.5 serialize and deserialize

Description: Serializes and descrializes a FatVector to and from a flat array, respectively.

Parameters for serialize:

• FatVector &fatVec - fat vector to serialize.

Returns: std::vector<double> - Flat array containing the serialized data.

Parameters for deserialize:

- std::vector<double> &flat Flat array to deserialize.
- int rows Number of rows in the fat vector.
- int cols Number of columns in the fat vector.

Returns: FatVector - Deserialized fat vector.

A.C.2 SparseMatrixFatVectorMultiply.h

A.C.2.1 sparseMatrixFatVectorMultiply

Description: Executes the multiplication using a sequential algorithm.

Parameters:

- SparseMatrix &sparseMatrix The sparse matrix.
- FatVector &fatVector The Fat Vector.
- int vecCols Number of columns in the Fat Vector.

Returns: FatVector - Result of the multiplication.

A.C.3 SparseMatrixFatVectorMultiplyRowWise.h

A.C.3.1 sparseMatrixFatVectorMultiplyRowWise

Description: Multiplies a sparse matrix with a Fat Vector using row-wise distribution.

Parameters:

- SparseMatrix &sparseMatrix The sparse matrix.
- FatVector &fatVector The Fat Vector.
- int vecCols Number of columns in the Fat Vector.

Returns: FatVector - Result of the multiplication.

A.C.4 SparseMatrixFatVectorMultiplyColumnWise.h

A.C.4.1 sparseMatrixFatVectorMultiplyColumnWise

Description: Executes the multiplication using column-wise parallel algorithm.

Parameters:

- SparseMatrix &sparseMatrix The sparse matrix.
- FatVector &fatVector The Fat Vector.
- int vecCols Number of columns in the Fat Vector.

Returns: FatVector - Result of the multiplication.

A.C.5 SparseMatrixFatVectorMultiplyNonZeroElement.h

A.C.5.1 sparseMatrixFatVectorMultiplyNonZeroElement

Description: Executes the multiplication using non-zero element parallel algorithm.

Parameters:

- SparseMatrix &sparseMatrix The sparse matrix.
- FatVector &fatVector The Fat Vector.
- int vecCols Number of columns in the Fat Vector.

Returns: FatVector - Result of the multiplication.

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>
   * Obrief Struct to represent a sparse matrix
9
   * @param values Non-zero values
   * Oparam colIndices Column indices of non-zero values
11
   * @param rowPtr Row pointers
*/
12
13
   struct SparseMatrix
14
15
16
       std::vector<double> values;
       std::vector<int> colIndices;
17
       std::vector<int> rowPtr;
   };
19
   // Type definition for a Fat Vector
   typedef std::vector<std::vector<double>> FatVector;
22
```

Appendix B.B Sequential Algorithm

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

B.B.1 Declaration File

```
#ifndef SPARSEMATRIXFATVECTORMULTIPLY_H
   #define SPARSEMATRIXFATVECTORMULTIPLY_H
   #include "MatrixDefinitions.h"
6
   * @brief Function to execute the sparse matrix-fat vector multiplication using
        sequential algorithm
   * @param sparseMatrix Sparse matrix
10
    * @param fatVector Fat Vector
    * @param vecCols Number of columns in the Fat Vector
   * Oreturn FatVector Result of the multiplication
14
   FatVector sparseMatrixFatVectorMultiply(const SparseMatrix &sparseMatrix,
                                                const FatVector &fatVector, int vecCols
15
                                                    );
16
   #endif
```

B.B.2 Implementation File

```
#include "SparseMatrixFatVectorMultiply.h"
2
    * @brief Function to execute the sparse matrix-Fat Vector multiplication using
4
        sequential algorithm
    * @param sparseMatrix Sparse matrix
6
    * @param fatVector Fat Vector
    * @param vecCols Number of columns in the Fat Vector
    \ast @return FatVector Result of the multiplication
10
   {\tt Fat Vector \ sparse Matrix Fat Vector Multiply (const \ Sparse Matrix \ \& sparse Matrix \ ,}
                                                   const FatVector &fatVector, int vecCols
        // Initialisation of the result vector
       FatVector result(sparseMatrix.numRows, std::vector<double>(vecCols, 0.0));
15
16
        // Iterate over the rows of the sparse matrix
       for (int i = 0; i < sparseMatrix.numRows; ++i)</pre>
18
19
            // Iterate over the non-zero elements in the current row
            for (int j = sparseMatrix.rowPtr[i]; j < sparseMatrix.rowPtr[i + 1]; ++j)</pre>
20
21
                // Iterate over the columns of the Fat Vector
23
                for (int k = 0; k < vecCols; ++k)</pre>
24
                    result[i][k] += sparseMatrix.values[j] * fatVector[sparseMatrix.
25
                         colIndices[j]][k]; // Compute the result
26
                }
27
       }
28
       // Return the result
30
       return result;
   }
31
```

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 SPARSEMATRIXFATVECTORMULTIPLYROWWIZE_H
   #define SPARSEMATRIXFATVECTORMULTIPLYROWWIZE_H
   #include "MatrixDefinitions.h"
   #include <iostream> // std::cout
    st @brief Function to multiply a sparse matrix with a Fat Vector using row-wise
        distribution
9
10
    * Oparam sparseMatrix The sparse matrix to be multiplied
    * Oparam fatVector The Fat Vector to be multiplied
    * @param vecCols Number of columns in the Fat Vector
12
    * @return FatVector Result of the multiplication
14
   {\tt Fat Vector \ sparse Matrix Fat Vector Multiply Row Wise (\verb|const| Sparse Matrix| \& sparse Matrix|,}
15
                                                          const FatVector &fatVector,
                                                          int vecCols);
17
18
   #endif
```

B.C.2 Implementation File

```
#include <mpi.h>
   #include "SparseMatrixFatVectorMultiplyRowWise.h"
   * @brief Function to multiply a sparse matrix with a Fat Vector using row-wise
5
       distribution
   st @param sparseMatrix The sparse matrix to be multiplied
   * Oparam fatVector The Fat Vector to be multiplied
    * @param vecCols Number of columns in the Fat Vector
   * @return FatVector Result of the multiplication
10
   Fat Vector \ sparse \texttt{Matrix} Fat Vector \texttt{MultiplyRowWise} (\texttt{const} \ Sparse \texttt{Matrix} \ \& \ sparse \texttt{Matrix},
                                                    const FatVector &fatVector,
                                                    int vecCols)
15
       // Retrieve the rank and size of the MPI world
17
       int worldSize, worldRank;
       MPI_Comm_size(MPI_COMM_WORLD, &worldSize);
18
       MPI_Comm_rank(MPI_COMM_WORLD, &worldRank);
20
       // =========== FOR DEBUGGING ONLY - START LOCAL COMPUTATION
21
          TIMER ===========
       // double computation_start = MPI_Wtime();
         TIMER ==========
24
       // Distribute rows among processes
       int rowsCountPerProcess = sparseMatrix.numRows / worldSize;
                              // Number of rows per process
       int extraRows = sparseMatrix.numRows % worldSize;
                                        // Number of extra rows to be distributed
         among processes
```

```
int startRow = worldRank * rowsCountPerProcess + std::min(worldRank, extraRows)
          ; // Starting row index for the current process
       int endRow = startRow + rowsCountPerProcess + (worldRank < extraRows ? 1 : 0);</pre>
29
            // Ending row index for the current process
30
31
       // Local computation
      int localSize = (endRow - startRow) * vecCols; // Number of elements in the
32
          local result vector
33
       std::vector<double> localResult(localSize);
                                                   // Local result vector
34
       // Iterate over the rows assigned to the current process
35
      for (int i = startRow; i < endRow; ++i)</pre>
37
           // Iterate over the non-zero elements in the current row
38
          for (int j = sparseMatrix.rowPtr[i]; j < sparseMatrix.rowPtr[i + 1]; ++j)</pre>
40
41
              int colIndex = sparseMatrix.colIndices[j]; // Column index of the non-
                  zero element
42
              \ensuremath{//} Iterate over the columns of the Fat Vector
43
              for (int k = 0; k < vecCols; ++k)</pre>
44
45
              {
                  int localIndex = (i - startRow) * vecCols + k;
                                                   // Index of the element in the
                      local result vector
                  localResult[localIndex] += sparseMatrix.values[j] * fatVector[
47
                      colIndex][k]; // Compute the result
              }
18
          }
49
      }
50
51
       // ============== FOR DEBUGGING ONLY - STOP LOCAL COMPUTATION
52
          // double computation_end = MPI_Wtime();
       // double local_computation_time = computation_end - computation_start;
54
55
       TIMER =========
56
       57
58
       // Start timing for communication
          double communication_start = MPI_Wtime();
       // =========== FOR DEBUGGING ONLY - START COMMUNICATION TIMER
60
          _____
61
       // Preparation for Gather operation
62
       std::vector<int> recvCounts(worldSize), displacements(worldSize);
63
      if (worldRank == 0)
64
65
      {
          int totalSize = 0; // Total number of elements to be received
66
67
68
           // Compute the number of elements to be received from each process
          for (int rank = 0; rank < worldSize; ++rank)</pre>
69
70
          {
              int startRowThisRank = rank * rowsCountPerProcess + std::min(rank,
71
                                       // Starting row index for the current
                  extraRows);
              int endRowThisRank = startRowThisRank + rowsCountPerProcess + (rank <</pre>
              extraRows ? 1 : 0); // Ending row index for the current process
recvCounts[rank] = (endRowThisRank - startRowThisRank) * vecCols;
                                         // Number of elements to be received from
                  the current process
74
              displacements[rank] = totalSize;
                                                                         11
                  Displacement for the current process
              totalSize += recvCounts[rank];
                                                                           11
                  Update the total number of elements to be received
```

```
// Gather all local results into the root process
79
       std::vector<double> gatheredResults;
80
       if (worldRank == 0)
81
82
           gatheredResults.resize(recvCounts[0] * worldSize); // Resize the vector to
83
              hold all the results
84
85
       MPI_Gatherv(localResult.data(), localSize, MPI_DOUBLE,
                  gatheredResults.data(), recvCounts.data(),
86
                   displacements.data(), MPI_DOUBLE, O, MPI_COMM_WORLD); // Gather the
87
                       local results in the root process
88
       // =========== FOR DEBUGGING ONLY - STOP COMMUNICATION TIMER
89
          double communication_end = MPI_Wtime();
90
91
          double local_communication_time = communication_end - communication_start;
92
       // =========== FOR DEBUGGING ONLY - STOP COMMUNICATION TIMER
           _____
       // =============== FOR DEBUGGING ONLY - COLLECTING AND ANALYSING
94
           PERFORMANCE DATA ===========
          double total_computation_time = 0.0, total_communication_time = 0.0;
       // MPI_Reduce(&local_computation_time, &total_computation_time, 1, MPI_DOUBLE,
96
           MPI_SUM, 0, MPI_COMM_WORLD);
97
       // MPI_Reduce(&local_communication_time, &total_communication_time, 1,
          MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
       98
          PERFORMANCE DATA =========
99
       // Reconstruct the final result matrix in the root process
100
       FatVector finalResult;
101
102
       if (worldRank == 0)
103
           // ============ FOR DEBUGGING ONLY - PRINTING PERFORMANCE
104
              DATA ===========
           // double avg_computation_time = total_computation_time / worldSize;
105
           // double avg_communication_time = total_communication_time / worldSize;
106
              std::cout << "Row-wise Average Computation Time: " <<</pre>
              avg_computation_time << std::endl;</pre>
108
           // std::cout << "Row-wise Average Communication Time: " <<
              avg_communication_time << std::endl;</pre>
           // ================== FOR DEBUGGING ONLY - PRINTING PERFORMANCE
109
              DATA ==========
110
           finalResult.resize(sparseMatrix.numRows, std::vector<double>(vecCols, 0.0))
              ; // Resize the final result matrix
113
           // Iterate over the rows of the final result
           for (int i = 0, index = 0; i < sparseMatrix.numRows; ++i)</pre>
114
115
116
               // Iterate over the columns of the final result
117
              for (int j = 0; j < vecCols; ++j, ++index)</pre>
118
              {
                   finalResult[i][j] = gatheredResults[index]; // Copy the element of
119
                      the final result
120
              }
           }
121
123
124
       // Return the final result
       return (worldRank == 0) ? finalResult : FatVector{};
125
   }
```

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 SPARSEMATRIXFATVECTORMULTIPLYCOLUMNWIZE_H
   #define SPARSEMATRIXFATVECTORMULTIPLYCOLUMNWIZE_H
   #include "MatrixDefinitions.h"
   #include <iostream> // std::cout
   * @brief Function to execute the sparse matrix-Fat Vector multiplication using
        column-wise parallel algorithm
9
10
    * Oparam sparseMatrix Sparse matrix
    * @param fatVector Fat Vector
12
    * @param vecCols Number of columns in the Fat Vector
   * @return FatVector Result of the multiplication
14
   {\tt Fat Vector \ sparse Matrix Fat Vector Multiply Column Wise ({\tt const} \ Sparse Matrix \ \& sparse Matrix, {\tt otherwise})}
        const FatVector &fatVector, int vecCols);
16
   #endif
```

B.D.2 Implementation File

```
#include <mpi.h>
   #include "SparseMatrixFatVectorMultiplyColumnWise.h"
   #include <numeric> // std::accumulate
   * @brief Function to execute the sparse matrix-Fat Vector multiplication using
6
        column-wise parallel algorithm
   * @param sparseMatrix Sparse matrix
   * @param fatVector Fat Vector
    * @param vecCols Number of columns in the Fat Vector
10
    * @return FatVector Result of the multiplication
11
   Fat Vector \ sparse \texttt{Matrix} Fat Vector \texttt{Multiply} \texttt{ColumnWise} ( \underbrace{\texttt{const}} \ \texttt{SparseMatrix} \ \& \ sparse \texttt{Matrix}),
        const FatVector &fatVector, int vecCols)
       // Retrieve the rank and size of the MPI world
15
       int worldSize, worldRank;
       MPI_Comm_size(MPI_COMM_WORLD, &worldSize);
17
       MPI_Comm_rank(MPI_COMM_WORLD, &worldRank);
18
       // ======== FOR DEBUGGING ONLY - START LOCAL COMPUTATION
20
           // double computation_start = MPI_Wtime();
       // ============= FOR DEBUGGING ONLY - START LOCAL COMPUTATION
           TIMER =============
       // Distribute columns among processes
24
       int colsPerProcess = vecCols / worldSize;
                                                                                  //
           Number of columns per process
       int extraCols = vecCols % worldSize;
           // Number of extra columns to be distributed among processes
```

```
int startCol = worldRank * colsPerProcess;
                                                                             11
          Starting column index for the current process
       int endCol = (worldRank != worldSize - 1) ? startCol + colsPerProcess :
          startCol + colsPerProcess + extraCols; // Ending column index for the
           current process
       // Local computation
30
       int localSize = sparseMatrix.numRows * (endCol - startCol); // Number of
31
           elements in the local result vector
       std::vector<double> localResult(localSize, 0.0);
32
       // Iterate over the columns assigned to the current process
33
       for (int col = startCol; col < endCol; ++col)</pre>
34
35
           // Iterate over the rows of the sparse matrix
           for (int i = 0; i < sparseMatrix.numRows; ++i)</pre>
37
38
39
               // Iterate over the non-zero elements in the current row
               double sum = 0.0;
40
               for (int j = sparseMatrix.rowPtr[i]; j < sparseMatrix.rowPtr[i + 1]; ++</pre>
41
                  j)
               {
42
43
                  int sparseCol = sparseMatrix.colIndices[j];
                      Column index of the non-zero element
                   sum += sparseMatrix.values[j] * fatVector[sparseCol][col]; //
44
                      Compute the result
45
               localResult[i * (endCol - startCol) + (col - startCol)] = sum; // Store
46
                   the result in the local result vector
          }
47
48
49
       // ============================ FOR DEBUGGING ONLY - STOP LOCAL COMPUTATION
50
          TIMER =============
       // double computation_end = MPI_Wtime();
51
52
       // double local_computation_time = computation_end - computation_start;
       // ============================ FOR DEBUGGING ONLY - STOP LOCAL COMPUTATION
53
          TIMER ==========
       // ========== FOR DEBUGGING ONLY - START COMMUNICATION TIMER
55
           _____
       // Start timing for communication
       57
58
           _____
59
       // Preparation for Gather operation
60
       std::vector<int> recvCounts(worldSize), displacements(worldSize); // Number of
61
           elements to be received from each process, Displacement for each process
       if (worldRank == 0)
62
63
       {
           // Compute the number of elements to be received from each process
64
           int displacement = 0;
65
           for (int i = 0; i < worldSize; ++i)</pre>
66
67
               int startColThisRank = i * colsPerProcess;
68
                  // Starting column index for the current process
               int endColThisRank = (i != worldSize - 1) ? startColThisRank +
69
                  colsPerProcess : startColThisRank + colsPerProcess + extraCols; //
                  Ending column index for the current process
               recvCounts[i] = sparseMatrix.numRows * (endColThisRank -
70
                  startColThisRank);
                                                                    // Number of
                   elements to be received from the current process
               displacements[i] = displacement;
                  // Displacement for the current process
               displacement += recvCounts[i];
```

```
// Update the displacement
73
74
75
       // Gather all local results into the root process
76
       std::vector<double> gatheredResults;
77
       if (worldRank == 0)
78
       {
79
           gatheredResults.resize(std::accumulate(recvCounts.begin(), recvCounts.end()
80
               , 0)); // Resize the vector to hold the final result
81
       MPI_Gatherv(localResult.data(), localSize, MPI_DOUBLE,
82
                   gatheredResults.data(), recvCounts.data(),
83
                   displacements.data(), MPI_DOUBLE, O, MPI_COMM_WORLD); // Gather the
84
                        local results in the root process
85
       // =========== FOR DEBUGGING ONLY - STOP COMMUNICATION TIMER
       // double communication_end = MPI_Wtime();
87
       // double local_communication_time = communication_end - communication_start;
       // ========== FOR DEBUGGING ONLY - STOP COMMUNICATION TIMER
89
           _____
       // ============ FOR DEBUGGING ONLY - COLLECTING AND ANALYSING
91
           PERFORMANCE DATA ===========
       // double total_computation_time = 0.0, total_communication_time = 0.0;
92
       // MPI_Reduce(&local_computation_time, &total_computation_time, 1, MPI_DOUBLE,
93
           MPI_SUM, 0, MPI_COMM_WORLD);
       // MPI_Reduce(&local_communication_time, &total_communication_time, 1,
94
           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
       FatVector finalResult:
98
00
       if (worldRank == 0)
100
       {
           // ========== FOR DEBUGGING ONLY - PRINTING PERFORMANCE
101
               DATA =========
           // double avg_computation_time = total_computation_time / worldSize;
102
103
           // double avg_communication_time = total_communication_time / worldSize;
           // std::cout << "Column-wise Average Computation Time: " <<
104
               avg_computation_time << std::endl;</pre>
           // std::cout << "Column-wise Average Communication Time: " <<
105
               avg_communication_time << std::endl;</pre>
           // ================== FOR DEBUGGING ONLY - PRINTING PERFORMANCE
106
               DATA ======
107
108
           // Reconstruct the final result matrix
           finalResult.resize(sparseMatrix.numRows, std::vector<double>(vecCols, 0.0))
109
               ; // Resize the final result matrix
           int resultIndex = 0;
110
           // Iterate over the processes
111
           for (int rank = 0; rank < worldSize; ++rank)</pre>
113
               int numColsThisRank = (rank != worldSize - 1) ? colsPerProcess :
114
                   colsPerProcess + extraCols; // Number of columns assigned to the
                   current process
               int startColThisRank = rank * colsPerProcess;
                                                                 // Starting column
                   index for the current process
116
117
               // Iterate over the rows of the sparse matrix
               for (int row = 0; row < sparseMatrix.numRows; ++row)</pre>
118
119
                   // Iterate over the columns assigned to the current process
120
                   for (int col = 0; col < numColsThisRank; ++col)</pre>
121
122
                       finalResult[row][startColThisRank + col] = gatheredResults[
123
                          resultIndex++]; // Reconstruct the final result matrix
```

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 SPARSEMATRIXFATVECTORMULTIPLYNONZEROELEMENT_H
             #define SPARSEMATRIXFATVECTORMULTIPLYNONZEROELEMENT H
             #include "MatrixDefinitions.h"
            #include <iostream> // std::cout
 6
                * @brief Function to execute the sparse matrix-Fat Vector multiplication using non
                                 -zero element parallel algorithm
                * @param sparseMatrix Sparse matrix
10
                * @param fatVector Fat Vector
               * Oparam vecCols Number of columns in the Fat Vector
               * Oreturn FatVector Result of the multiplication
13
14
             {\tt Fat Vector \ sparse Matrix Fat Vector Multiply Non Zero Element ({\tt const} \ Sparse Matrix \ \& \ Sparse Matrix \ Long Matri
                              sparseMatrix, const FatVector &fatVector, int vecCols);
              #endif
```

B.E.2 Implementation File

```
#include "SparseMatrixFatVectorMultiplyNonZeroElement.h"
2
   #include <mpi.h>
3
4
   * Obrief Function to execute the sparse matrix-Fat Vector multiplication using non
       -zero element parallel algorithm
   * Oparam sparseMatrix Sparse matrix
   * @param fatVector Fat Vector
    * @param vecCols Number of columns in the Fat Vector
   * @return FatVector Result of the multiplication
10
  FatVector sparseMatrixFatVectorMultiplyNonZeroElement(const SparseMatrix &
      sparseMatrix, const FatVector &fatVector, int vecCols)
13
      // Retrieve the rank and size of the MPI world
14
15
      int worldSize, worldRank;
      MPI_Comm_size(MPI_COMM_WORLD, &worldSize);
16
      MPI_Comm_rank(MPI_COMM_WORLD, &worldRank);
18
       // =========== FOR DEBUGGING ONLY - START LOCAL COMPUTATION
19
         TIMER ==========
```

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

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

Appendix B.F Utility Functions

Utility functions used by the main file.

B.F.1 Declaration File

```
#ifndef UTILS_H
       #define UTILS_H
 2
       #include <iostream> // std::cout
       #include <vector> // std::vector
#include <cstdlib> // rand() and srand()
 5
       #include <ctime>
                                                    // time()
       #include <mpi.h>
        #include <petsc.h>
       #include <fstream>
                                                     // std::ifstream
10
      #include <string> // std::string
#include <sstream> // std::stringstream
#include <utility> // std::pair
#include <cli>#include <cli>#inc
11
13
       #include <algorithm> // std::sort
15
       #include <stdexcept> // std::runtime_error
      #include <cmath> // std::fabs
16
       #include "MatrixDefinitions.h"
17
18
19
        * Method to convert a PETSc matrix to a fat vector
         * @param C PETSc matrix
21
        * @return FatVector fat vector
22
       FatVector ConvertPETScMatToFatVector(Mat C);
24
26
         * Method to compare two matrices
27
        * Oparam mat1 First matrix
        * @param mat2 Second matrix
29
30
        * Oparam tolerance Tolerance for comparison
         * Oreturn bool True if the matrices are equal, false otherwise
32
       bool areMatricesEqual(const FatVector &mat1, const FatVector &mat2, double
33
              tolerance);
34
35
        * Method to read a matrix from a Matrix Market file

* @param filename Name of the file
36
37
        * Oreturn SparseMatrix Sparse matrix
39
40
       SparseMatrix readMatrixMarketFile(const std::string &filename);
41
42
         * Method to generate a random fat vector
43
        * @param n Number of rows
44
         * @param m Number of columns
45
         * @return FatVector fat vector
47
48
       FatVector generateLargeFatVector(int n, int k);
50
         * Obrief Method to serialize a FatVector to a flat array
51
52
         * @param denseVec fat vector to serialize
        * @return std::vector<double> Flat array containing the serialized data
53
       std::vector<double> serialize(const FatVector &denseVec);
55
57
       * @brief Method to deserialize a flat array to a FatVector * @param flat Flat array to deserialize
58
* @param rows Number of rows in the fat vector
```

```
# @param cols Number of columns in the fat vector
# @return FatVector fat vector
# /
# FatVector deserialize(const std::vector<double> &flat, int rows, int cols);
# endif
# endif
```

B.F.2 Implementation File

```
#include "utils.h"
2
3
    * Method to convert a PETSc matrix to a fat vector
4
    * @param C PETSc matrix
    * @return FatVector fat vector
6
   FatVector ConvertPETScMatToFatVector(Mat C)
9
                              // Number of rows and columns in the matrix
10
       PetscInt m, n;
       MatGetSize(C, &m, &n); // Get the number of rows and columns in the matrix
       FatVector denseVec(m, std::vector<double>(n, 0.0)); // fat vector to hold the
14
15
       // Iterate over the rows of the matrix
       for (int i = 0; i < m; ++i)</pre>
16
17
18
            // Iterate over the columns of the matrix
           for (int j = 0; j < n; j++)</pre>
19
20
21
                PetscScalar value;
                                                         // Value of the element
                                                        // Get the value of the element
                MatGetValue(C, i, j, &value);
22
                denseVec[i][j] = PetscRealPart(value); // Copy the value of the element
24
25
       // Return the fat vector
27
28
       return denseVec;
   }
30
31
    * Method to compare two matrices
32
33
    * @param mat1 First matrix
    * @param mat2 Second matrix
34
    * Oparam tolerance Tolerance for comparison
35
36
    * Oreturn bool True if the matrices are equal, false otherwise
37
   bool areMatricesEqual(const FatVector &mat1, const FatVector &mat2, double
38
       tolerance)
39
       // Check if the matrices have the same dimensions
40
       if (mat1.size() != mat2.size())
41
           return false:
42
43
       // Iterate over the rows of the matrices
       for (size_t i = 0; i < mat1.size(); ++i)</pre>
45
46
            // Check if the rows have the same dimensions
47
            if (mat1[i].size() != mat2[i].size())
48
                return false;
49
50
51
            \ensuremath{//} Iterate over the columns of the matrices
            for (size_t j = 0; j < mat1[i].size(); ++j)</pre>
53
                // Check if the elements are equal
54
                if (std::fabs(mat1[i][j] - mat2[i][j]) > tolerance)
55
```

```
return false; // Matrices are not equal
58
            }
59
        }
61
        return true; // Matrices are equal
62
   }
63
64
65
    * Method to read a matrix from a Matrix Market file
66
    * @param filename Name of the file
67
    * @return SparseMatrix Sparse matrix
    */
69
    SparseMatrix readMatrixMarketFile(const std::string &filename)
70
71
        std::ifstream file(filename); // Input file stream
72
73
74
        // Check if the file was opened successfully
75
        if (!file.is_open())
76
77
            throw std::runtime_error("Unable to open file: " + filename);
        }
78
79
                                                        // String to hold the current line
        std::string line;
80
81
        bool isSymmetric = false, isPattern = false; // Flags to indicate if the matrix
             is symmetric or pattern only
82
83
        // Skip the comments
        while (std::getline(file, line))
84
85
            // Check if the line is a comment
86
            if (line[0] == '%')
87
88
                // Check if the line contains the word "symmetric"
89
                if (line.find("symmetric") != std::string::npos)
90
91
                {
                     isSymmetric = true; // Set the symmetric flag
92
                }
93
94
                // Check if the line contains the word "pattern"
95
96
                if (line.find("pattern") != std::string::npos)
97
                     isPattern = true; // Set the pattern flag
98
00
                }
            }
100
101
            else
            {
102
103
                break; // First non-comment line reached, break out of the loop
104
            }
105
106
107
        // Read the matrix dimensions
        int numRows, numCols, nonZeros;
                                                                       // Number of rows,
108
            columns and non-zero elements in the matrix
        std::stringstream(line) >> numRows >> numCols >> nonZeros; // Read the
109
            dimensions from the line
110
        // Check if the file was read successfully
111
        if (!file)
        {
            throw std::runtime_error("Failed to read matrix dimensions from file: " +
114
                filename);
115
        }
116
                                                                                // Sparse
        SparseMatrix matrix;
           matrix to hold the data
        matrix.rowPtr.resize(numRows + 1, 0);
                                                                                // Resize
118
            the row pointer vector
        std::vector<std::vector<std::pair<int, double>>> tempRows(numRows); //
          Temporary vector to hold the data
```

```
int rowIndex, colIndex;
                                                                            // Row and
120
           column indices
       double value;
                                                                            // Value of
121
            the non-zero element
122
123
       // Read the non-zero elements
       for (int i = 0; i < nonZeros; ++i)</pre>
124
125
126
            // If the matrix is pattern only, the value of the non-zero element is 1.0
127
           if (isPattern)
           {
128
               file >> rowIndex >> colIndex; // Read the row and column indices
129
               value = 1.0;
                                              // Default value for pattern entries
130
           }
131
           else
           {
133
               file >> rowIndex >> colIndex >> value; // Read the row and column
134
                   indices and the value
           }
135
136
137
           // Check if the file was read successfully
138
           if (!file)
139
           {
               throw std::runtime_error("Failed to read data from file: " + filename);
140
141
           }
142
           rowIndex--; // Adjusting from 1-based to 0-based indexing
143
144
           colIndex --; // Adjusting from 1-based to 0-based indexing
145
           tempRows[rowIndex].emplace_back(colIndex, value); // Store the data in the
146
               temporary vector
147
148
           // If the matrix is symmetric, store the data in the transpose as well
           if (isSymmetric && rowIndex != colIndex)
149
           {
150
                tempRows[colIndex].emplace_back(rowIndex, value); // Store the data in
151
                   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
        // Reconstruct SparseMatrix structure
161
162
       int cumSum = 0; // Cumulative sum of the number of non-zero elements
163
       // Iterate over the rows of the matrix
164
       for (int i = 0; i < numRows; ++i)</pre>
165
166
           matrix.rowPtr[i] = cumSum; // Store the cumulative sum in the row pointer
167
168
           // Iterate over the non-zero elements in the current row
169
170
           for (const auto &elem : tempRows[i])
               zero element
               matrix.colIndices.push_back(elem.first); // Store the column index of
173
                   the non-zero element
174
           }
175
           cumSum += tempRows[i].size(); // Update the cumulative sum
176
177
178
       matrix.rowPtr[numRows] = cumSum; // Store the cumulative sum in the row pointer
179
       180
```

```
matrix.numCols = numCols;  // Store the number of columns
181
182
        // Return the sparse matrix
183
        return matrix;
184
   }
185
186
187
    * Method to generate a random fat vector
188
    * @param n Number of rows
189
190
    * @param m Number of columns
    * @return FatVector fat vector
191
    */
192
   FatVector generateLargeFatVector(int n, int k)
193
194
        FatVector denseVector(n, std::vector<double>(k)); // fat vector to hold the
           random values
196
197
        // Iterate over the rows of the fat vector
        for (int i = 0; i < n; ++i)</pre>
198
199
            // Iterate over the columns of the fat vector
200
201
            for (int j = 0; j < k; ++ j)
202
                 denseVector[i][j] = rand() % 100 + 1; // Generate a random value
203
                    between 1 and 100
204
            }
        }
205
206
207
        // Return the fat vector
208
        return denseVector;
   }
209
210
211
    * Obrief Method to serialize a FatVector to a flat array
    * @param denseVec fat vector to serialize
213
214
    * @return std::vector<double> Flat array containing the serialized data
215
216
    std::vector <double > serialize(const FatVector &denseVec)
217
        std::vector<double> flat; // Flat array to hold the serialized data
218
219
220
        // Iterate over the rows of the fat vector
        for (const auto &vec : denseVec)
            flat.insert(flat.end(), vec.begin(), vec.end()); // Copy the elements
223
224
225
226
        // Return the flat array
        return flat;
   }
228
229
230
    * Obrief Method to deserialize a flat array to a FatVector
231
    * @param flat Flat array to deserialize
232
    * Oparam rows Number of rows in the fat vector
233
    * @param cols Number of columns in the fat vector
234
235
    * @return FatVector fat vector
    */
236
   FatVector deserialize(const std::vector<double> &flat, int rows, int cols)
237
238
239
        FatVector denseVec(rows, std::vector <double > (cols)); // fat vector to hold the
            deserialized data
240
        // Iterate over the rows of the fat vector
241
242
        for (int i = 0; i < rows; ++i)</pre>
243
            // Iterate over the columns of the fat vector
244
245
            for (int j = 0; j < cols; ++j)
246
            {
                denseVec[i][j] = flat[i * cols + j]; // Copy the element
247
```

Appendix B.G Main File

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

```
#include "utils.h"
                                                          // Utility functions
   #include "SparseMatrixFatVectorMultiply.h"
2
                                                        // Sequential algorithm
   #include "SparseMatrixFatVectorMultiplyRowWise.h"
3
                                                        // Parallel algorithm (row
      -wise)
   #include "SparseMatrixFatVectorMultiplyColumnWise.h"
                                                       // Parallel algorithm (
      column-wise)
   #include "SparseMatrixFatVectorMultiplyNonZeroElement.h" // Parallel algorithm (non
      -zero element)
6
7
   int main(int argc, char *argv[])
8
   {
9
       10
          _____
      // Initialise MPI and PETSc
      MPI_Init(&argc, &argv);
14
      PetscInitialize(&argc, &argv, NULL, NULL);
15
      // Retrieve the rank and size of the world communicator
17
18
      int worldRank, worldSize;
      MPI_Comm_rank(PETSC_COMM_WORLD, &worldRank);
19
      MPI_Comm_size(PETSC_COMM_WORLD, &worldSize);
20
21
      // Check if the correct number of arguments is provided
22
      if (argc != 3)
23
24
          if (worldRank == 0)
25
26
              std::cerr << "Usage: " << argv[0] << " <number of columns> <matrix file
27
                  path>" << std::endl;</pre>
28
          MPI_Abort(PETSC_COMM_WORLD, 1);
29
30
31
      // Parse the command-line arguments
32
      33
      std::string filename = argv[2]; // The second argument is the filename
35
36
      // Declare the sparse matrix and Fat Vector
37
      SparseMatrix M;
      FatVector v;
38
39
      // Declare the result of the serial multiplication
40
41
      FatVector resultSerial;
42
      // Declare the data for broadcasting the sparse matrix and Fat Vector
43
44
      std::vector<double> flatData;
45
      int dataSize = 0;
46
      // Declare the variables for timing the execution of the algorithms
```

```
48
       double startTime, endTime;
50
51
       // =============== READ THE SPARSE MATRIX AND GENERATE THE Fat
           Vector ==============
52
       if (worldRank == 0)
53
           std::cout << "World size: " << worldSize << std::endl; // Print the
55
               number of processes
           std::cout << "Sparse matrix: " << filename << std::endl; // Print the name
              of the Matrix Market file
58
           // Read the sparse matrix from the Matrix Market file
           M = readMatrixMarketFile(filename);
59
           std::cout << "Matrix size: " << M.numRows << "x" << M.numCols << std::endl;
61
           // Generate a random Fat Vector
62
63
           v = generateLargeFatVector(M.numCols, k);
           std::cout << "Vector size: " << M.numCols << "x" << k << std::endl;
64
65
           // Prepare the data for broadcasting
66
           flatData = serialize(v); // Serialize the Fat Vector
67
           dataSize = flatData.size(); // Size of the serialized data
68
       }
69
70
       // ============ EXECUTE THE SERIAL MULTIPLICATION
72
73
       if (worldRank == 0)
75
76
           \ensuremath{//} Execute the serial multiplication
77
           startTime = MPI_Wtime();
           resultSerial = sparseMatrixFatVectorMultiply(M, v, k);
78
79
           endTime = MPI_Wtime();
           std::cout << "Serial Algo Execution time: " << (endTime - startTime)
80
                     << std::endl;
81
83
           // FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS OF THE RESULT
           // std::cout << "Result: " << std::endl;
84
           // for (int i = 0; i < 10; ++i)
           // {
86
           //
                  for (int j = 0; j < k; ++j)
87
           11
88
           //
                      std::cout << resultSerial[i][j] << " ";</pre>
89
90
           //
           //
                  std::cout << std::endl;</pre>
91
           // }
92
       }
93
94
95
       // ======= MATRIX AND Fat Vector
97
98
       // Wait for the main process to finish the serial multiplication
       MPI_Barrier(MPI_COMM_WORLD);
100
```

```
101
       // ============ FOR DEBUGGING ONLY - START BROADCAST TIMER
102
           _____
       // startTime = MPI_Wtime();
103
       // =============== FOR DEBUGGING ONLY - START BROADCAST TIMER
104
           _____
       // Broadcast the Sparse Matrix to all processes
106
       // Prepare the data for broadcasting
107
       int valuesSize = M.values.size();
                                                                  // Number of non-
108
           zero elements
       int colIndicesSize = M.colIndices.size();
                                                                  // Number of column
           indices
       int rowPtrSize = M.rowPtr.size();
                                                                  // Number of row
       MPI_Bcast(&M.numRows, 1, MPI_INT, 0, MPI_COMM_WORLD);
                                                                 // Broadcast the
           number of rows
       MPI_Bcast(&M.numCols, 1, MPI_INT, 0, MPI_COMM_WORLD);
                                                                 // Broadcast the
           number of columns
       MPI_Bcast(&valuesSize, 1, MPI_INT, 0, MPI_COMM_WORLD);
                                                                 // Broadcast the
           number of non-zero elements
       MPI_Bcast(&colIndicesSize, 1, MPI_INT, 0, MPI_COMM_WORLD); // Broadcast the
114
           number of column indices
       MPI_Bcast(&rowPtrSize, 1, MPI_INT, 0, MPI_COMM_WORLD);
                                                                // Broadcast the
115
           number of row pointers
       // Resize the vectors for all processes
116
       if (worldRank != 0)
       {
118
           M.values.resize(valuesSize);
119
120
           M.colIndices.resize(colIndicesSize);
           M.rowPtr.resize(rowPtrSize);
       }
       // Broadcast the data
       MPI_Bcast(M.values.data(), valuesSize, MPI_DOUBLE, 0, MPI_COMM_WORLD);
124
       MPI_Bcast(M.colIndices.data(), colIndicesSize, MPI_INT, 0, MPI_COMM_WORLD);
125
126
       MPI_Bcast(M.rowPtr.data(), rowPtrSize, MPI_INT, 0, MPI_COMM_WORLD);
127
128
       // Broadcast the Fat Vector to all processes
       // Broadcast the size of the serialized data
129
       MPI_Bcast(&dataSize, 1, MPI_INT, 0, MPI_COMM_WORLD);
130
131
       // Resize flatData for all processes
       if (worldRank != 0)
       {
134
           flatData.resize(dataSize);
135
       // Broadcast the data
136
       MPI_Bcast(flatData.data(), dataSize, MPI_DOUBLE, 0, MPI_COMM_WORLD);
137
138
       // Deserialize the data
       if (worldRank != 0)
139
140
       {
           v.resize(M.numCols, std::vector<double>(k));
141
142
           v = deserialize(flatData, M.numCols, k);
143
144
       // Wait for all processes to finish the broadcast
145
       MPI_Barrier(MPI_COMM_WORLD);
146
147
       // ========== FOR DEBUGGING ONLY - STOP BROADCAST TIMER
       // endTime = MPI_Wtime();
149
150
       // if (worldRank == 0)
       // {
151
152
       //
              std::cout << "Broadcast time: " << (endTime - startTime) << std::endl;</pre>
153
       // ================ FOR DEBUGGING ONLY - STOP BROADCAST TIMER
154
156
```

```
// ========= EXECUTE THE PARALLEL MULTIPLICATION (ROW-WISE)
157
158
159
       // Execute the parallel multiplication (row-wise)
160
       startTime = MPI_Wtime();
161
162
       FatVector resultRowWise = sparseMatrixFatVectorMultiplyRowWise(M, v, k);
163
       endTime = MPI_Wtime();
164
        // Only the main process prints the parallel execution time
165
       if (worldRank == 0)
166
       {
167
           std::cout << "Row-wise Execution time: " << (endTime - startTime)
                     << std::endl;
169
170
           // ============== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
171
            // std::cout << "Result: " << std::endl;
           // for (int i = 0; i < 10; ++i)
173
           // {
174
175
           //
                  for (int j = 0; j < k; ++j)
           //
176
177
           //
                       std::cout << resultRowWise[i][j] << " ";</pre>
178
           //
           //
                  std::cout << std::endl:
179
           // }
180
           // ============= FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
181
182
           // Compare the results of the serial and parallel multiplications
183
184
           if (areMatricesEqual(resultSerial, resultRowWise, 1e-6)) // Tolerance = 1e
           {
185
               std::cout << "Row-wise: Results are the same!"</pre>
186
                         << std::endl;
187
188
           }
           else
189
           {
190
               std::cout << "Row-wise: Results are different!"</pre>
191
                         << std::endl;
192
           }
193
       }
194
195
196
        // ========== EXECUTE THE PARALLEL MULTIPLICATION (COLUMN-WISE)
197
            _____
198
199
        // Wait for all processes to finish the parallel multiplication (row-wise)
200
       MPI_Barrier(MPI_COMM_WORLD);
201
202
       // Execute the parallel multiplication (column-wise)
203
       startTime = MPI_Wtime();
204
       FatVector resultColumnWise = sparseMatrixFatVectorMultiplyColumnWise(M, v, k);
205
206
       endTime = MPI_Wtime();
207
208
       \ensuremath{//} Only the main process prints the parallel execution time
       if (worldRank == 0)
209
210
       {
           std::cout << "Column-wise Execution time: " << (endTime - startTime)
                     << std::endl:
212
           // =========== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
214
```

```
// std::cout << "Result: " << std::endl;
215
           // for (int i = 0; i < 10; ++i)
216
           // {
217
           //
                  for (int j = 0; j < k; ++ j)
218
           //
219
           //
                      std::cout << resultColumnWise[i][j] << " ";</pre>
220
221
           //
                  std::cout << std::endl:
           // }
223
224
           // =========== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
                 ______
225
           // Compare the results of the serial and parallel multiplications
226
           if (areMatricesEqual(resultSerial, resultColumnWise, 1e-6)) // Tolerance =
227
               1e-6
           {
228
               std::cout << "Column-wise: Results are the same!"</pre>
229
230
                        << std::endl;
231
           }
232
           else
233
           {
               std::cout << "Column-wise: Results are different!"</pre>
234
235
                         << std::endl;
           }
236
237
       }
238
239
       // ============= EXECUTE THE PARALLEL MULTIPLICATION (NON-ZERO
240
           ELEMENT) ==========
241
242
       // Wait for all processes to finish the parallel multiplication (column-wise)
243
       MPI_Barrier(MPI_COMM_WORLD);
244
245
246
       // Execute the parallel multiplication (non-zero element)
       startTime = MPI_Wtime();
247
248
       FatVector resultNonZeroElement = sparseMatrixFatVectorMultiplyNonZeroElement(M,
           v, k);
       endTime = MPI Wtime():
249
250
251
       // Only the main process prints the parallel execution time
       if (worldRank == 0)
252
253
254
           std::cout << "Non-zero Elements Execution time: " << (endTime - startTime)</pre>
255
                     << std::endl;
           // =========== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
257
           // std::cout << "Result: " << std::endl;
258
           // for (int i = 0; i < 10; ++i)
259
           // {
260
           //
                  for (int j = 0; j < k; ++ j)
261
262
           //
           //
                      std::cout << resultNonZeroElement[i][j] << " ";</pre>
263
           11
264
265
           //
                  std::cout << std::endl;</pre>
           // }
266
           267
                 _____
268
           // Compare the results of the serial and parallel multiplications
269
           if (areMatricesEqual(resultSerial, resultNonZeroElement, 1e-6)) //
               Tolerance = 1e-6
271
272
               std::cout << "Non-zero Elements: Results are the same!"</pre>
                   << std::endl;
273
```

```
274
            }
            else
275
            {
276
277
                std::cout << "Non-zero Elements: Results are different!"</pre>
                           << std::endl;
278
279
            }
        }
280
281
        //
282
        // =================== EXECUTE THE PARALLEL MULTIPLICATION (
            PETSc) ============
284
285
        // Wait for all processes to finish the parallel multiplication (non-zero
286
            element)
        MPI_Barrier(MPI_COMM_WORLD);
287
288
        // Declare the PETSc matrix
289
290
        Mat A, B, C;
291
292
        // ============= FOR DEBUGGING ONLY - START PETSCS SETUP TIMER
            _____
        // startTime = MPI_Wtime();
293
        // ================== FOR DEBUGGING ONLY - START PETSCS SETUP TIMER
294
            _____
295
        // Create a parallel matrix to store the sparse matrix
296
        MatCreate(PETSC_COMM_WORLD, &A);
297
298
        MatSetSizes(A, PETSC_DECIDE, PETSC_DECIDE, M.numRows, M.numCols);
        MatSetType(A, MATMPIAIJ);
299
        MatSetUp(A);
300
        // Fill the PETSc matrix with the values from the sparse matrix
301
        if (worldRank == 0)
302
303
        {
            for (int i = 0; i < M.numRows; ++i)</pre>
304
305
                for (int j = M.rowPtr[i]; j < M.rowPtr[i + 1]; ++j)</pre>
306
307
                    MatSetValue(A, i, M.colIndices[j], M.values[j], INSERT_VALUES);
308
309
                }
310
            }
311
        // Assemble the PETSc matrix
312
313
        MatAssemblyBegin(A, MAT_FINAL_ASSEMBLY);
314
        MatAssemblyEnd(A, MAT_FINAL_ASSEMBLY);
315
        // Create a parallel matrix to store the Fat Vector {\tt MatCreate(PETSC\_COMM\_WORLD} , &B);
316
317
        MatSetSizes(B, PETSC_DECIDE, PETSC_DECIDE, M.numCols, k);
318
        MatSetType(B, MATDENSE);
319
320
        MatSetUp(B);
        // Fill the PETSc matrix B with values from the dense matrix \boldsymbol{v}
321
322
        if (worldRank == 0)
323
            for (int i = 0; i < M.numCols; ++i)</pre>
324
325
                for (int j = 0; j < k; ++j)
326
327
                {
328
                     MatSetValue(B, i, j, v[i][j], INSERT_VALUES);
329
330
            }
331
        // Assemble the PETSc matrix
332
        MatAssemblyBegin(B, MAT_FINAL_ASSEMBLY);
333
334
        MatAssemblyEnd(B, MAT_FINAL_ASSEMBLY);
335
```

```
336
       // endTime = MPI_Wtime();
337
       // if (worldRank == 0)
338
       // {
339
       //
// }
             std::cout << "PETSc Setup time: " << (endTime - startTime) << std::endl;</pre>
340
341
       // ===
             ==================== FOR DEBUGGING ONLY - STOP PETSCS SETUP TIMER
342
          343
       // Create a parallel matrix to store the result of the multiplication
344
       startTime = MPI_Wtime();
345
       MatProductCreate(A, B, NULL, &C);
346
       MatMatMult(A, B, MAT_INITIAL_MATRIX, PETSC_DEFAULT, &C);
347
       endTime = MPI_Wtime();
348
       if (worldRank == 0)
349
350
351
          // Print the execution time
          std::cout << "PETSc Execution time: " << (endTime - startTime) << std::endl
352
353
354
355
       // ========= FOR DEBUGGING ONLY - START PETSCS CONVERSION
          TIMER ===========
356
       // startTime = MPI_Wtime();
       // ========= FOR DEBUGGING ONLY - START PETSCS CONVERSION
357
          TIMER ============
358
       // Create a sequential matrix to retrieve the result
359
360
       Mat CSeq;
       MatCreateRedundantMatrix(C, worldSize, MPI_COMM_NULL, MAT_INITIAL_MATRIX, &CSeq
361
          );
362
       if (worldRank == 0)
363
364
           // Convert the result matrix C to a FatVector
365
          FatVector globalMatrix = ConvertPETScMatToFatVector(CSeq);
366
367
          // ============ FOR DEBUGGING ONLY - STOP PETSCS CONVERSION
              // endTime = MPI_Wtime();
369
370
          // std::cout << "PETSc Conversion time: " << (endTime - startTime) << std::
              endl;
           // ============ FOR DEBUGGING ONLY - STOP PETSCS CONVERSION
371
              TIMER ===========
372
          // =============== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
          // std::cout << "Result: " << std::endl;
374
          // for (int i = 0; i < 10; ++i)
375
          // {
376
          //
                 for (int j = 0; j < k; ++j)
377
378
          //
          //
                    std::cout << globalMatrix[i][j] << " ";</pre>
379
           //
380
          //
                 std::cout << std::endl;</pre>
381
          // }
382
          // ========== FOR DEBUGGING ONLY - PRINT 10 FIRST ELEMENTS
383
384
          // Compare the results of the serial and PETSc multiplications
385
          if (areMatricesEqual(resultSerial, globalMatrix, 1e-6)) // Tolerance = 1e-6
386
387
              std::cout << "PETSc: Results are the same!"</pre>
388
389
                       << std::endl;
          }
391
          else
392
          {
393
              std::cout << "PETSc: Results are different!"</pre>
                  << std::endl;
394
```

```
395
396
397
398
         // Free the memory
         MatDestroy(&A);
399
400
         MatDestroy(&B);
401
         MatDestroy(&C);
         MatDestroy(&CSeq);
402
403
404
         // Finalise MPI and PETSc
         PetscFinalize();
405
406
         MPI_Finalize();
407
408
         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 -1 select line
## 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
               - 24 hours
## one_day
## two_day
               - 48 hours
## five_day
               - 120 hours
               - 240 hours (by special arrangement)
## ten_day
#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.500@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 -1'
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 Fat 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-ZO-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|" "$temp_script" # Set the number of chunks and cpus per
                    # Submit the job and get the job id
                    job_id=$(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
                        \# 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, Fat 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
                            # Extract the row-wise average computation time from
    | awk '{print $5}')
   the file
       row_wise_execution_time=$(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 |
                                      # Extract the non-zero elements execution
   awk '{print $5}')
   time from the file
       nonzero_result=$(grep "Non-zero Elements: Results are" $file | awk '{print
   $6}')
                                    # Extract the non-zero elements result from the
       nonzero_result=$(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,
   \verb| $row_wise_communication_time|, \verb| $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"
```