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Small Scale Parallel Programming Assignment

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MSc
Academic Year: 2023 - 2024

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26th February 2024

Abstract

This paper explores the effectiveness of different parallelization strategies for multiplying sparse matrices by fat vectors, focusing on the use of MPI in High Performance Computing (HPC). It compares the performance of sequential and parallel methods, including row-by-row, column-by-column, and non-zero element approaches. The results highlight the implications of each strategy on execution time and efficiency, while considering the environmental impact of HPC, suggesting avenues towards more sustainable computing systems.

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Chapter 1

Introduction

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

Chapter 2

Methodology

2.1 Problem Statement

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:

$$M = \begin{pmatrix} m_{11} & m_{12} & \cdots & m_{1n} \\ m_{21} & m_{22} & \cdots & m_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ m_{m1} & m_{m2} & \cdots & m_{mn} \end{pmatrix} \quad (2.1)$$

where most elements of M are zeros.

The vector v is defined as:

$$v = \begin{pmatrix} v_{11} & v_{12} & \cdots & v_{1k} \\ v_{21} & v_{22} & \cdots & v_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ v_{n1} & v_{n2} & \cdots & v_{nk} \end{pmatrix} \quad (2.2)$$

2.2 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.

2.2.1 Sparse Matrix

Matrix Name	M	NZ	Avg_NZ	Max_NZ	Symmetric
cavity10	2597	76367	29.4	62	False
PR02R	161070	8185136	50.8	92	False
nlpkkt80	1062400	28704672	27.0	28	True
Cube_Coup_dt0	2164760	127206144	58.8	68	True
roadNet-PA	1090920	3083796	2.8	9	True
ML_Laplace	377002	27689972	73.4	74	False
bcssstk17	10974	428650	39.1	150	True
mhda416	416	8562	20.6	33	False
af_1_k101	503625	17550675	34.8	35	True
thermal1	82654	574458	7.0	11	True
thermomech_TK	102158	711558	7.0	10	True
cage4	9	49	5.4	6	False
cant	62451	4007383	64.2	78	True
dc1	116835	766396	6.6	114190	False
raefsky2	3242	294276	90.8	108	False
rdist2	3198	56934	17.8	61	False
mcf	765	24382	31.9	81	False
olm1000	1000	3996	4.0	6	False
lung2	109460	492564	4.5	8	False
webbase-1M	1000005	3105536	3.1	4700	False
mhd4800a	4800	102252	21.3	33	False
west2021	2021	7353	3.6	12	False
thermal2	1228045	8580313	7.0	11	True
adder_dcop_32	1813	11246	6.2	100	False
mac_econ_fwd500	206500	1273389	6.2	44	False
FEM_3D_thermal1	17880	430740	24.1	27	False
amazon0302	262111	1234877	4.7	5	False
cop20k_A	121192	2624331	21.7	81	True
olafu	16146	1015156	62.9	89	True
af23560	23560	484256	20.6	21	False

Table 2.1: Summary of sparse matrices

2.2.1.1 Compressed Sparse Row (CSR) Format

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, 2, 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 **SparseMatrixCRS** structure is defined in Appendix B.A.

2.2.1.2 ELLPACK

The ELLPACK sparse matrix representation has gained wide usage thanks to its storage and computational efficiency. Within the ELLPACK format, the matrix is stored in arrays that possess two dimensions. Each row of the array contains a set number of non-zero elements, with the non-zero values being stored in the values array, and the corresponding column indices being stored in the column index array as represented in Figure 4. The void entries in the matrix are filled with zeroes in AS and -1 in JA. This format is optimized for parallel computation, particularly for matrices with uniform sparsity patterns, and is well-suited for use with CUDA frameworks.

Compared to the CRS format, the ELLPACK format provides a fixed-length representation for each row, which can significantly improve computational efficiency by using caches and registers. Moreover, the ELLPACK format is more memory-efficient compared to the CSR format, particularly for matrices with uniform sparsity patterns.

However, it's important to note that the ELLPACK format may not be the most efficient representation for matrices with irregular sparsity patterns. This may result in significant storage overhead and inefficient memory access. Additionally, the fixed-length representation for each row may not be optimal for matrices with variable sparsity patterns, where a lot of unnecessary data will be stored.

2.2.2 Fat Vector

Unlike a hollow matrix, a fat vector (illustrated by equation 2.2) 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.

2.3 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 ??.

2.3.1 Algorithm Flow

Algorithm 1 Sparse Matrix-Dense Vector Multiplication (CRS)

Require: A is an $m \times n$ sparse matrix in CRS format

Require: X is an $n \times k$ fat vector

Ensure: Y is an $m \times k$ fat vector, result of $A \times X$

```

for  $i = 0$  to  $A.numRows - 1$  do
    for  $j = A.rowPtr[i]$  to  $A.rowPtr[i + 1] - 1$  do
         $colIndex \leftarrow A.colIndices[j]$ 
         $value \leftarrow A.values[j]$ 
        for  $k = 0$  to  $X.numCols - 1$  do
             $yIndex \leftarrow i \times X.numCols + k$ 
             $xIndex \leftarrow colIndex \times X.numCols + k$ 
             $Y.values[yIndex] \leftarrow Y.values[yIndex] + value \times X.values[xIndex]$ 
        end for
    end for
end for

```

Algorithm 2 Sparse Matrix-Dense Vector Multiplication (ELLPACK)

Require: A is an $m \times n$ sparse matrix in ELLPACK format

Require: X is an $n \times k$ fat vector

Ensure: Y is an $m \times k$ fat vector, result of $A \times X$

```

for  $i = 0$  to  $A.numRows - 1$  do
    for  $j = 0$  to  $A.maxNonZerosPerRow - 1$  do
         $colIndex \leftarrow A.colIndices[i \times A.maxNonZerosPerRow + j]$ 
         $value \leftarrow A.values[i \times A.maxNonZerosPerRow + j]$ 
        if  $colIndex \neq -1$  then
            for  $k = 0$  to  $X.numCols - 1$  do
                 $yIndex \leftarrow i \times X.numCols + k$ 
                 $xIndex \leftarrow colIndex \times X.numCols + k$ 
                 $Y.values[yIndex] \leftarrow Y.values[yIndex] + value \times X.values[xIndex]$ 
            end for
        end if
    end for
end for

```

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 $Result[i][l]$.

2.3.2 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:

$$T(n) = O(zk) \quad (2.3)$$

2.4 Line-Based Parallelism

This algorithm distributes the rows of the sparse matrix across multiple processes for parallel computation in a line-based manner. The implementation is detailed in Appendix ??.

2.4.1 Algorithm Flow

Algorithm 3 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  $M \times v$ 

 $rowsPerProcess \leftarrow m/worldSize$ 
 $extraRows \leftarrow m \bmod worldSize$ 
 $startRow \leftarrow worldRank \times rowsPerProcess + \min(worldRank, extraRows)$ 
 $endRow \leftarrow startRow + rowsPerProcess$ 
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( $localResult, \dots$ )
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.

2.4.2 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.

2.4.2.1 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_{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:

$$T_{\text{comp}} = O\left(\frac{z \times k}{p}\right) \quad (2.4)$$

2.4.2.2 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:

$$T_{\text{comm}} = p \times \alpha + \beta \times \frac{m}{p} \times k \quad (2.5)$$

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, including both computation and communication, is given by:

$$T_{\text{overall}} = T_{\text{comp}} + T_{\text{comm}} = O\left(\frac{z \times k}{p}\right) + p \times \alpha + \beta \times \frac{m}{p} \times k + O(m \times k) \quad (2.6)$$

2.4.3 Performance Analysis

2.4.3.1 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 $p \leq m$.
- 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.

2.4.3.2 Expected Performance

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

2.5 Column-Wise Parallelism

This algorithm distributes the columns of the fat vector across multiple processes for parallel computation in a column-based manner. The implementation is detailed in Appendix ??.

2.5.1 Algorithm Flow

Algorithm 4 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  $M \times v$ 

 $colsPerProcess \leftarrow k/worldSize$ 
 $extraCols \leftarrow k \bmod worldSize$ 
 $startCol \leftarrow worldRank \times colsPerProcess$ 
 $endCol \leftarrow startCol + colsPerProcess$ 
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  $m \times k$ 
end if
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.
5. **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.

2.5.2 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.

2.5.2.1 Computation Time Complexity

Each process is responsible for approximately k/p columns of the fat vector. The computation time (T_{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:

$$T_{\text{comp}} = O\left(\frac{k \times z}{p}\right) \quad (2.7)$$

2.5.2.2 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:

$$T_{\text{comm}} = p \times \alpha + \beta \times m \times \frac{k}{p} \quad (2.8)$$

2.5.2.3 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, $O(m \times k)$.

2.5.2.4 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:

$$T_{\text{overall}} = T_{\text{comp}} + T_{\text{comm}} = O\left(\frac{k \times z}{p}\right) + p \times \alpha + \beta \times m \times \frac{k}{p} + O(m \times k) \quad (2.9)$$

2.5.3 Performance Analysis

2.5.3.1 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 .

2.5.3.2 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.

2.6 Non-Zero Element Parallelism

This algorithm distributes the non-zero elements of the sparse matrix across multiple processes for parallel computation. The implementation is detailed in Appendix ??.

2.6.1 Algorithm Flow

Algorithm 5 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 processes

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.

2.6.2 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.

2.6.3 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:

$$T_{\text{comp}} = O\left(\frac{z \times k}{p}\right) \quad (2.10)$$

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.

2.6.4 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:

$$T_{\text{comm}} = p \times \alpha + \beta \times m \times \frac{k}{p} \quad (2.11)$$

where:

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

2.6.4.1 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, $O(m \times k)$.

2.6.5 Overall Time Complexity

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

$$T_{\text{overall}} = T_{\text{comp}} + T_{\text{comm}} = O\left(\frac{z \times k}{p}\right) + p \times \alpha + \beta \times m \times \frac{k}{p} + O(m \times k) \quad (2.12)$$

2.6.6 Performance Analysis

2.6.6.1 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.

2.6.6.2 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.

2.7 Performance Metrics

The evaluation of algorithm performance within the main program (detailed in appendix ??) involves a systematic approach to assess efficiency across various implementations. In addition, the PETSc library (1) is used to compare the performance of the parallel algorithms with a highly optimised parallel sparse matrix-vector multiplication implementation. The program's workflow is structured as follows:

1. **Initialisation:** Initial setup of MPI and PETSc environments to enable distributed computation and matrix operations.
2. **Matrix and Vector Preparation:**
 - *Matrix Reading:* Sparse matrices are sourced from files utilising the `readMatrixMarketFile` method (refer to appendix ??), leveraging the Matrix Market I/O library (2) for efficient data handling.
 - *Fat Vector Generation:* Creation of fat vectors, with dimensions tailored to the corresponding matrices and predetermined column counts, ensuring compatibility for multiplication.
 - *Distribution:* Uniform distribution of matrices and vectors across processes for parallel computation.
3. **Serial Multiplication:** Execution and timing of matrix-vector multiplication in a serial context to establish a performance baseline.
4. **Parallel Multiplication Variants:** Application of distinct parallel multiplication strategies—line-based, column-based, and non-zero element—to measure execution times and identify efficiency variances.
5. **PETSc Implementation:**
 - *Conversion:* Adaptation of matrices and vectors to PETSc formats to utilise its optimized operations.
 - *Execution:* Conducting matrix-vector multiplication within the PETSc framework.
 - *Result Conversion:* Reformatting PETSc output back to Fat Vector for uniform result comparison.
6. **Result Comparison:** Validation of output correctness across serial, parallel, and PETSc implementations to ensure computational integrity.
7. **Finalisation:** Termination of MPI and PETSc environments and release of resources.

Comprehensive testing, facilitated by the `batch_test.sh` script (see appendix ??), was conducted to evaluate algorithmic performance under varying conditions—spanning different sparse matrix characteristics, fat vector column numbers, and process counts. These tests were categorised into three batches to pinpoint performance influencers:

- **Matrix Impact:** Examining how variations in sparse matrix properties affect algorithm efficiency.
- **Fat Vector Influence:** Assessing the performance implications of altering fat vector column quantities.
- **Execution Time Measurement:** Repeating the second batch tests without tracking average communication and computation times to capture precise execution durations.

This structured approach enables a thorough understanding of each algorithm's behavior under diverse computational scenarios and establishes a foundation for optimising sparse matrix-vector multiplication operations.

Chapter 3

Results and Discussion

3.1 Results

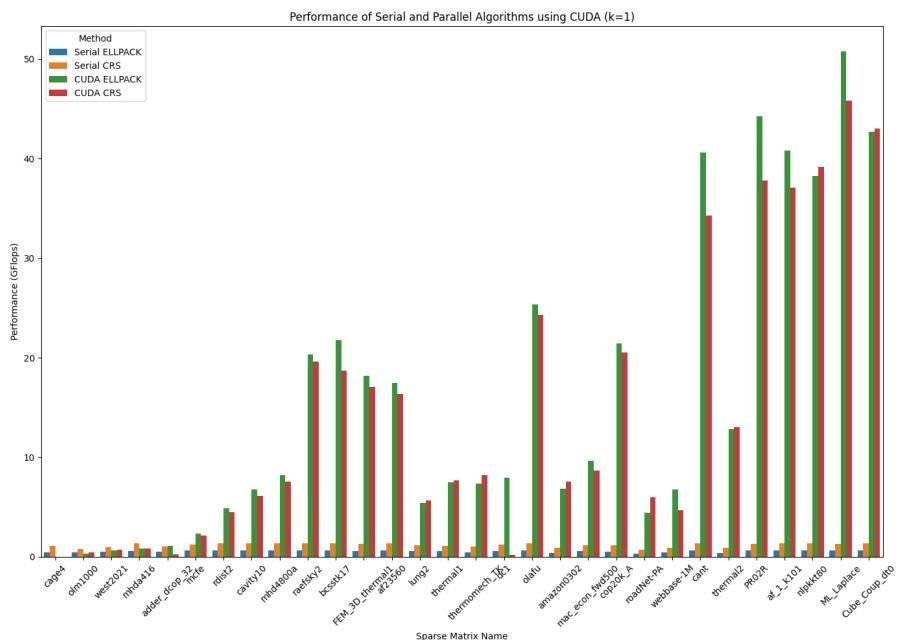
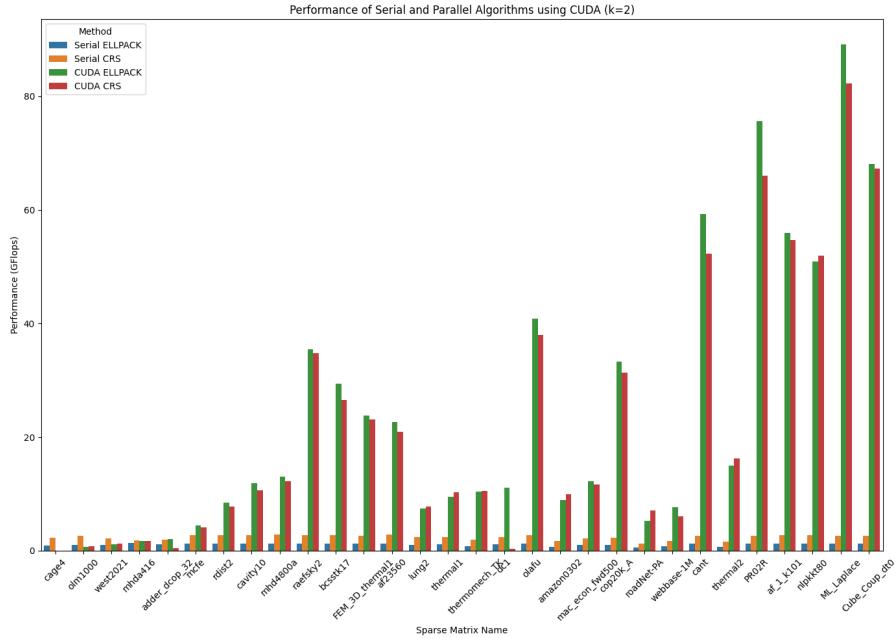
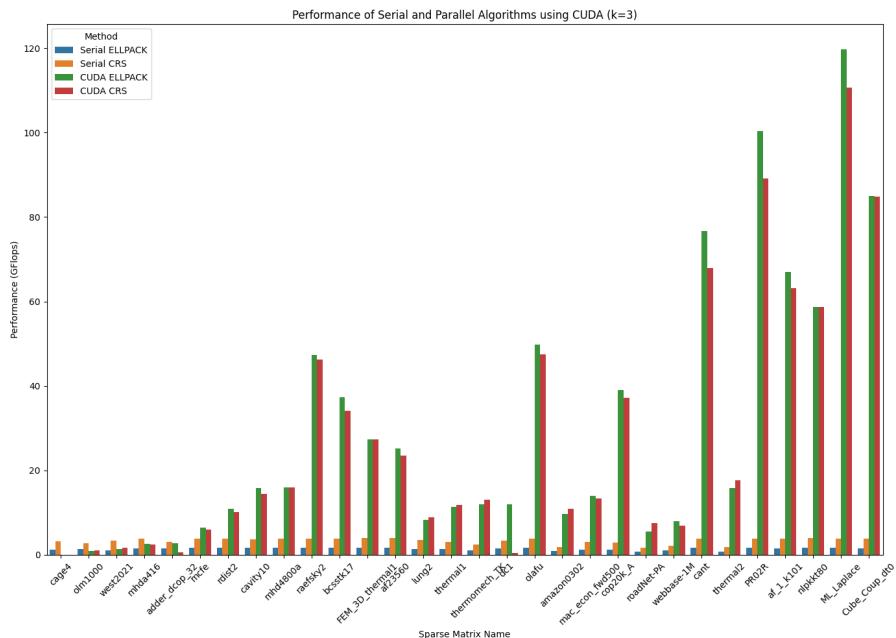


Figure 3.1: Performance of Serial and Parallel Algorithms using CUDA for $k = 1$

Figure 3.2: Performance of Serial and Parallel Algorithms using CUDA for $k = 2$ Figure 3.3: Performance of Serial and Parallel Algorithms using CUDA for $k = 3$

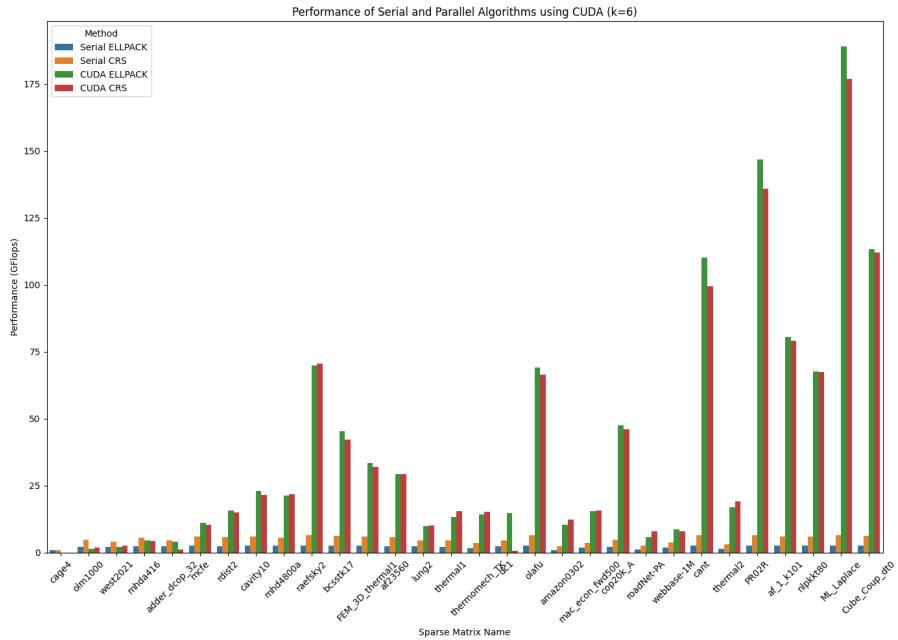
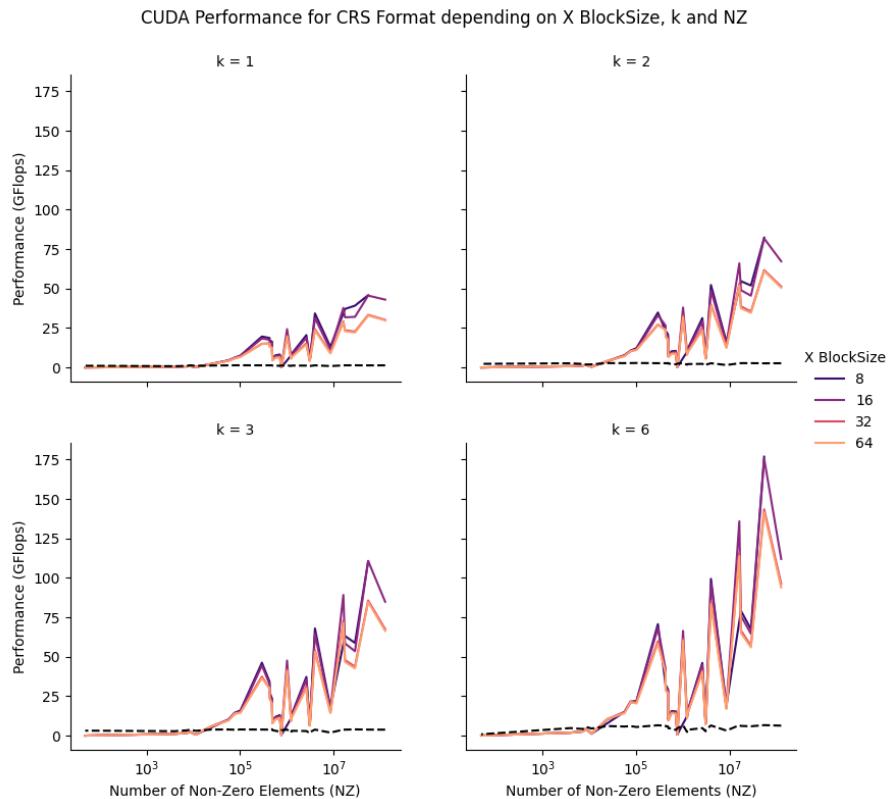
Figure 3.4: Performance of Serial and Parallel Algorithms using CUDA for $k = 6$ 

Figure 3.5: CUDA Performance for CRS Format depending on X BlockSize

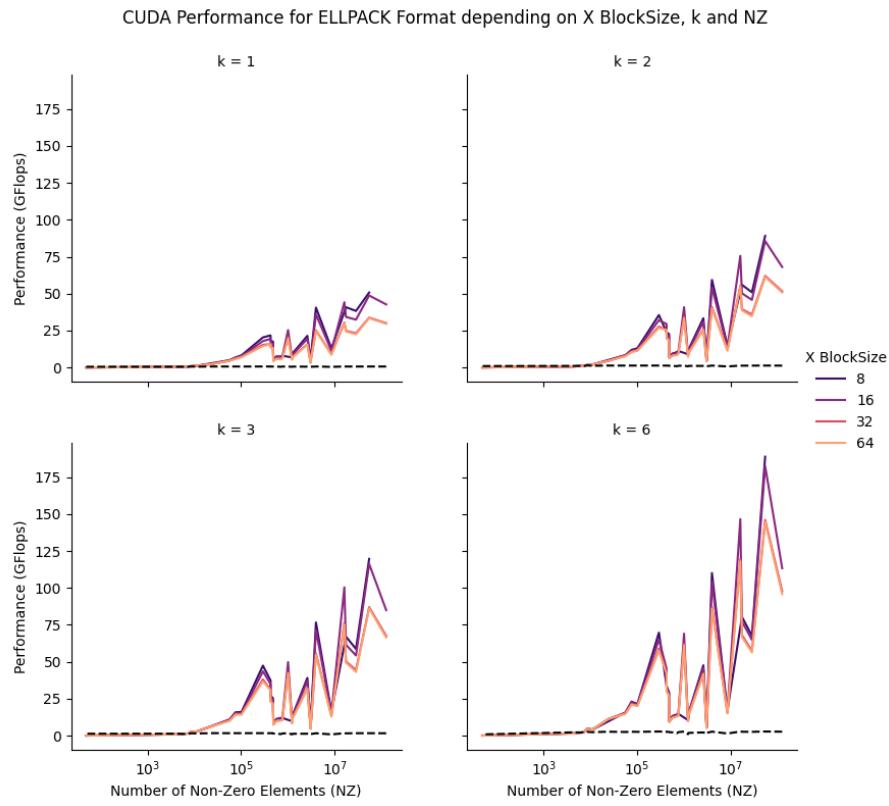


Figure 3.6: CUDA Performance for ELLPACK Format depending on X BlockSize

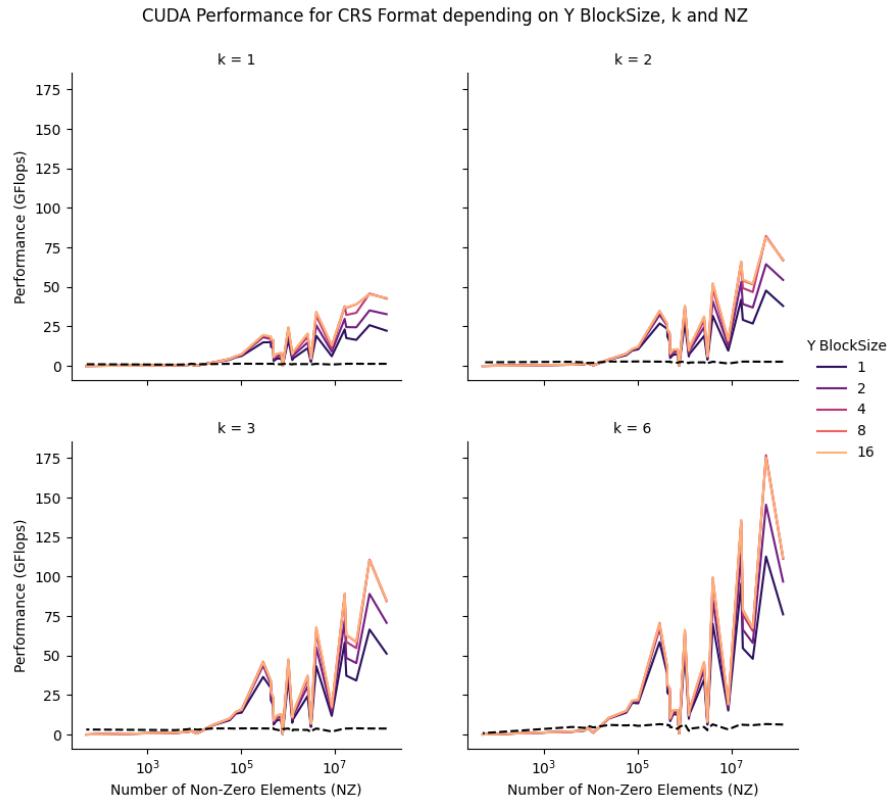


Figure 3.7: CUDA Performance for CRS Format depending on Y BlockSize

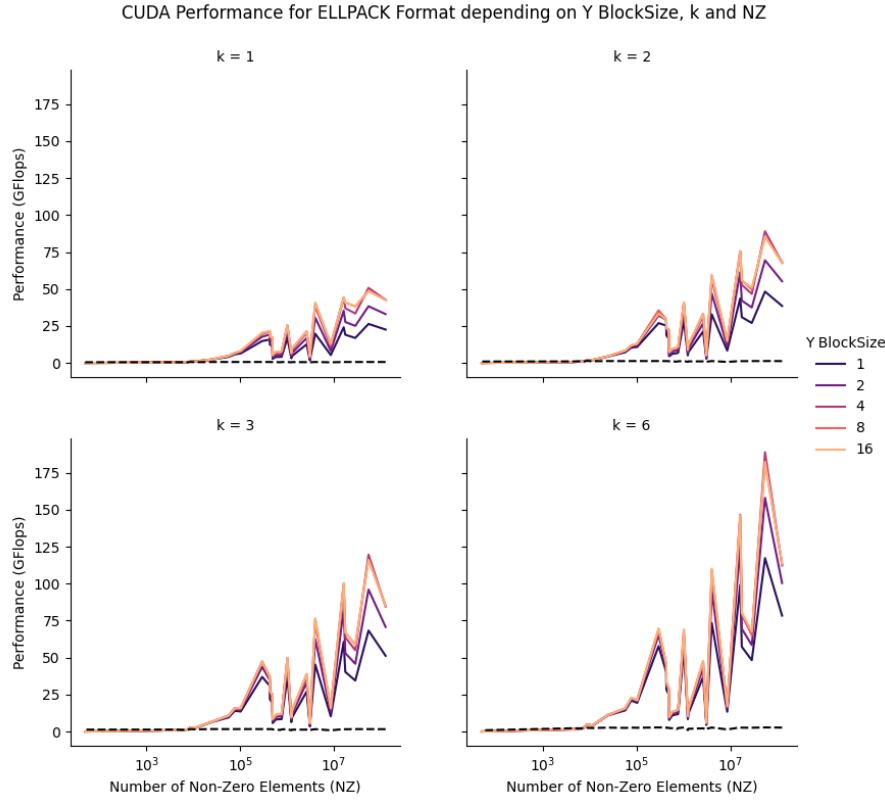
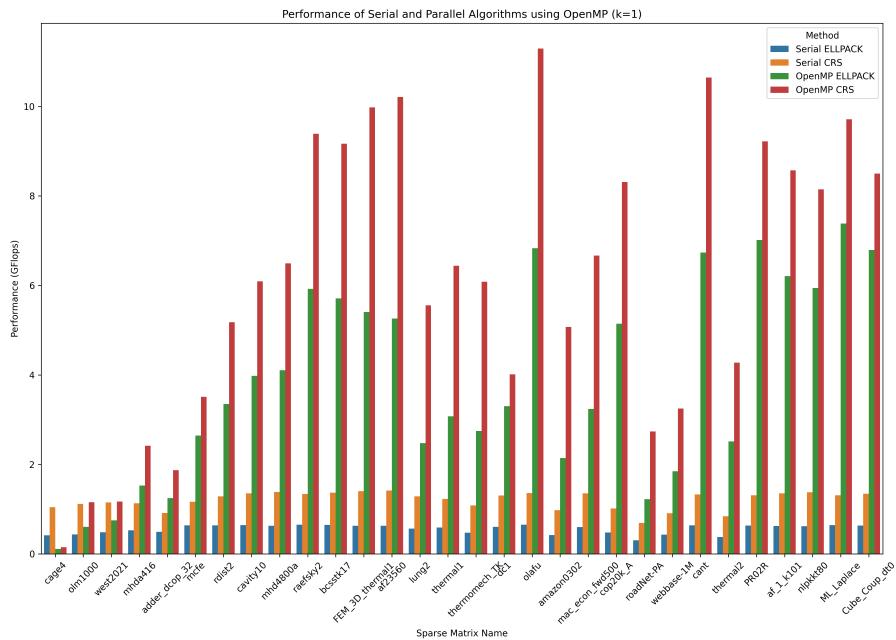
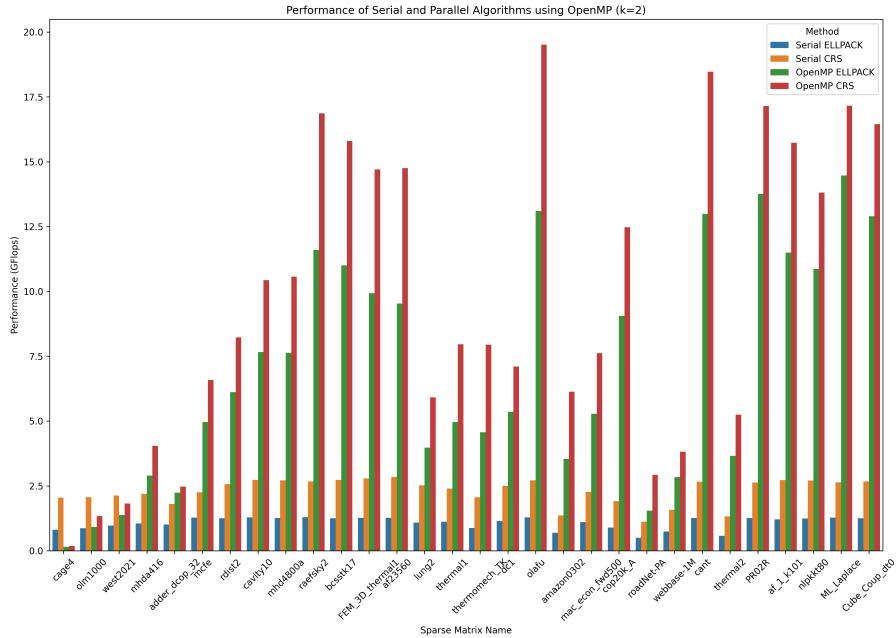
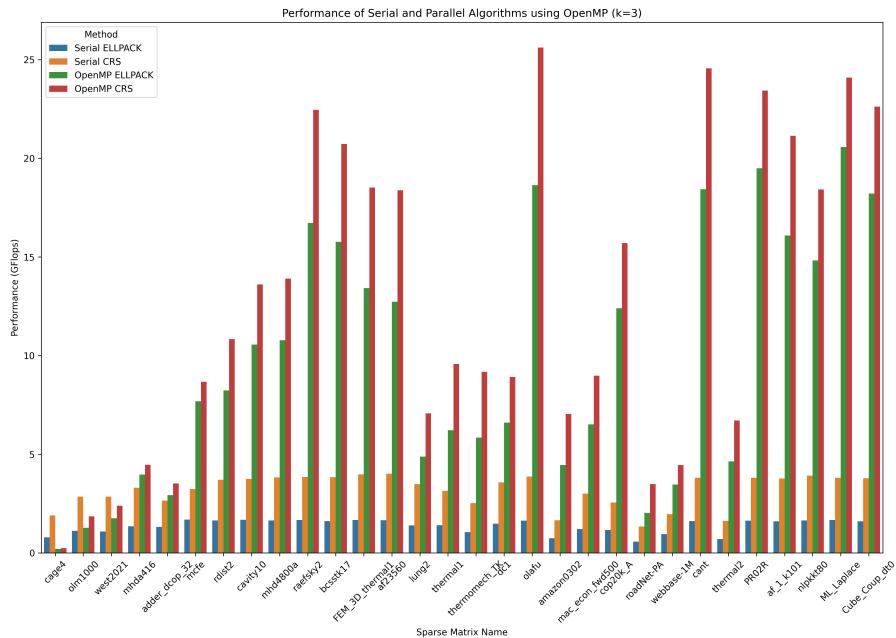


Figure 3.8: CUDA Performance for ELLPACK Format depending on Y BlockSize

Figure 3.9: Performance of Serial and Parallel Algorithms using OpenMP for $k = 1$

Figure 3.10: Performance of Serial and Parallel Algorithms using OpenMP for $k = 2$ Figure 3.11: Performance of Serial and Parallel Algorithms using OpenMP for $k = 3$

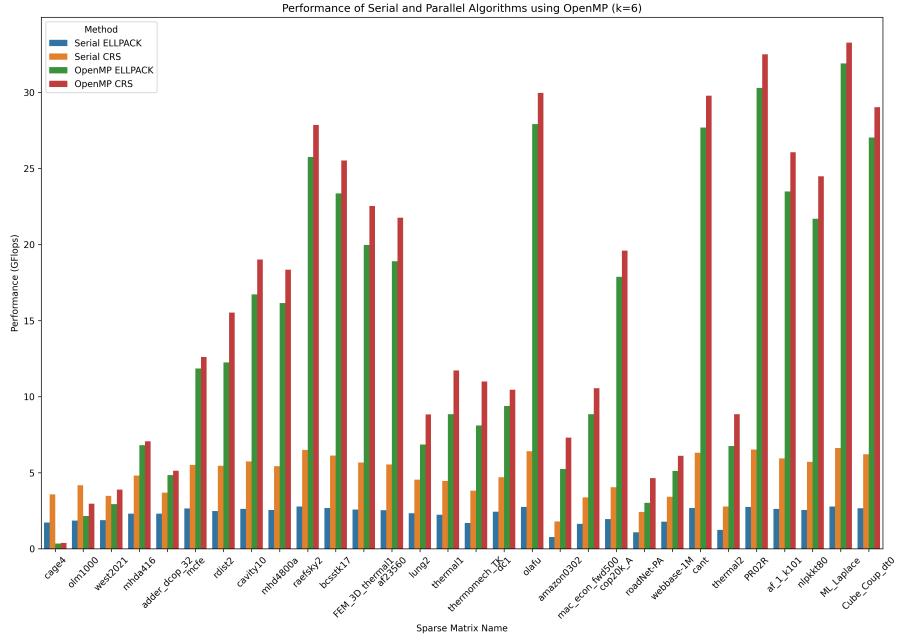
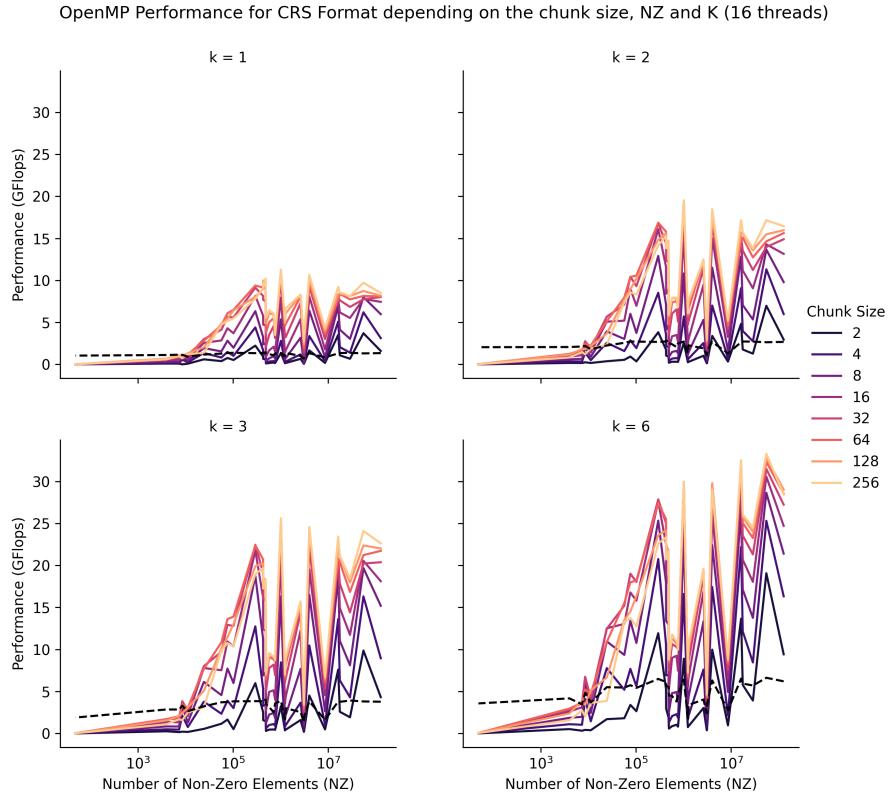
Figure 3.12: Performance of Serial and Parallel Algorithms using OpenMP for $k = 6$ 

Figure 3.13: OpenMP Performance for CRS Format depending on Chunk Size

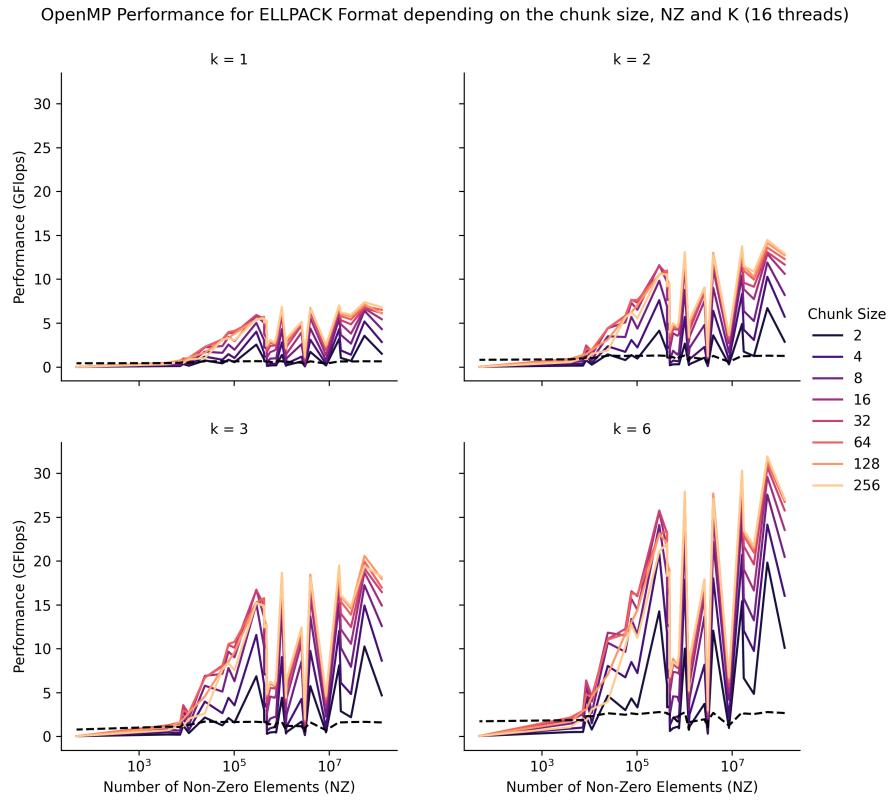


Figure 3.14: OpenMP Performance for ELLPACK Format depending on Chunk Size

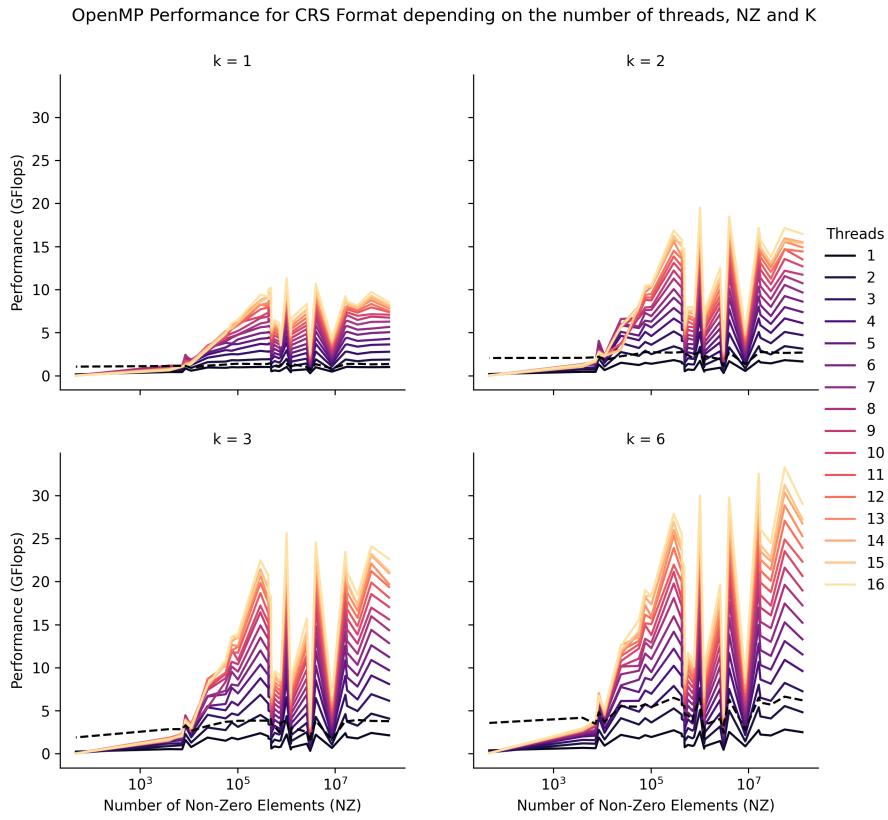


Figure 3.15: OpenMP Performance for CRS Format depending on Threads

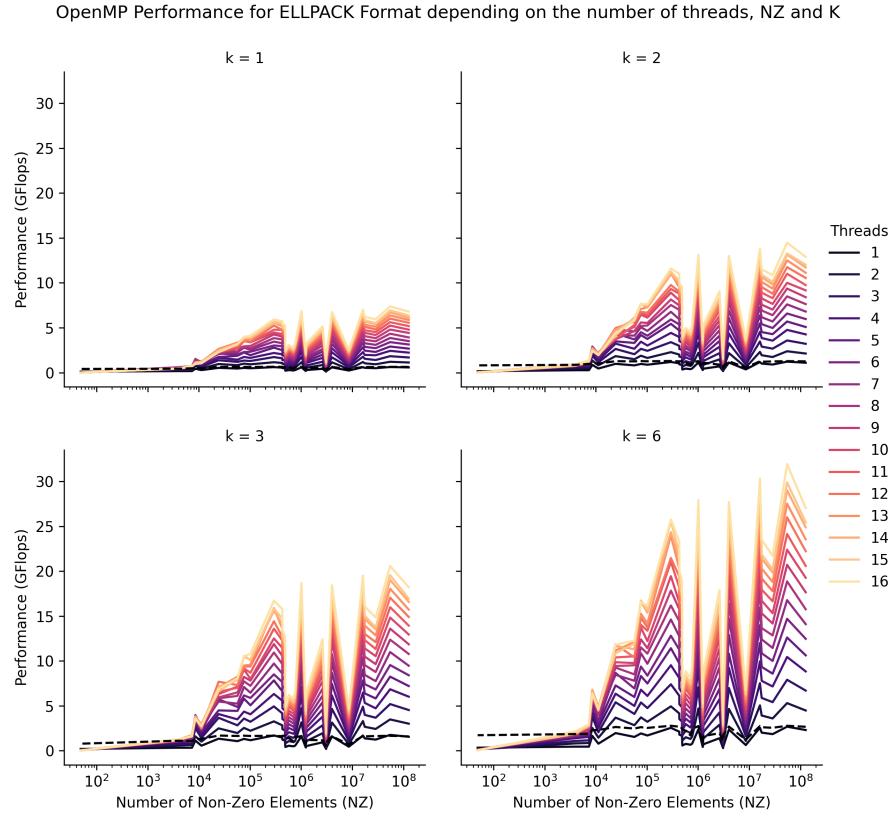
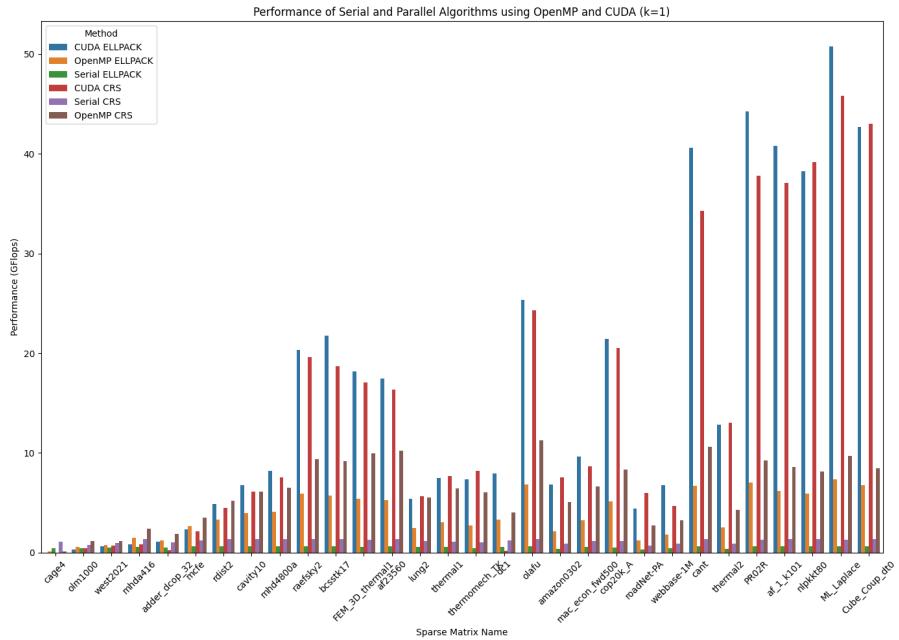
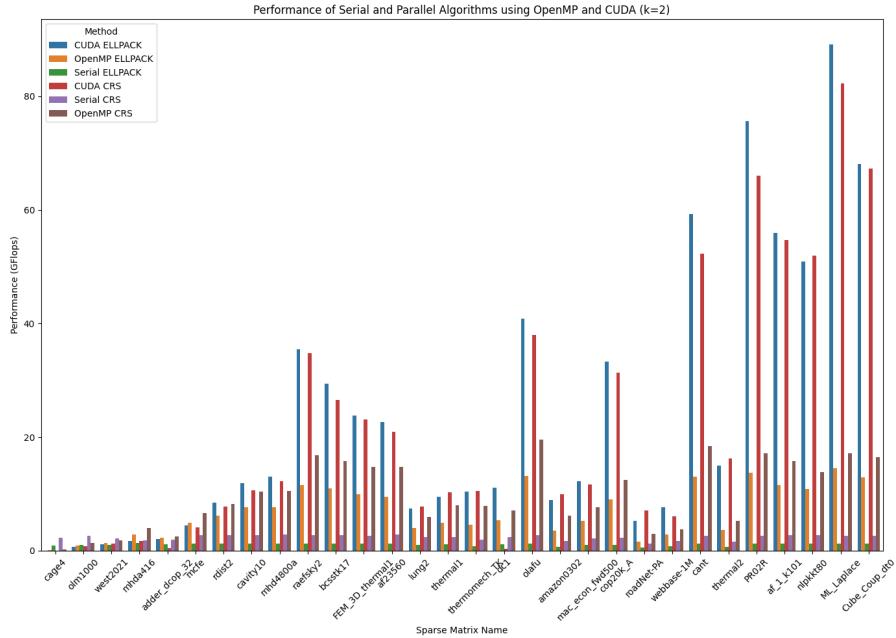
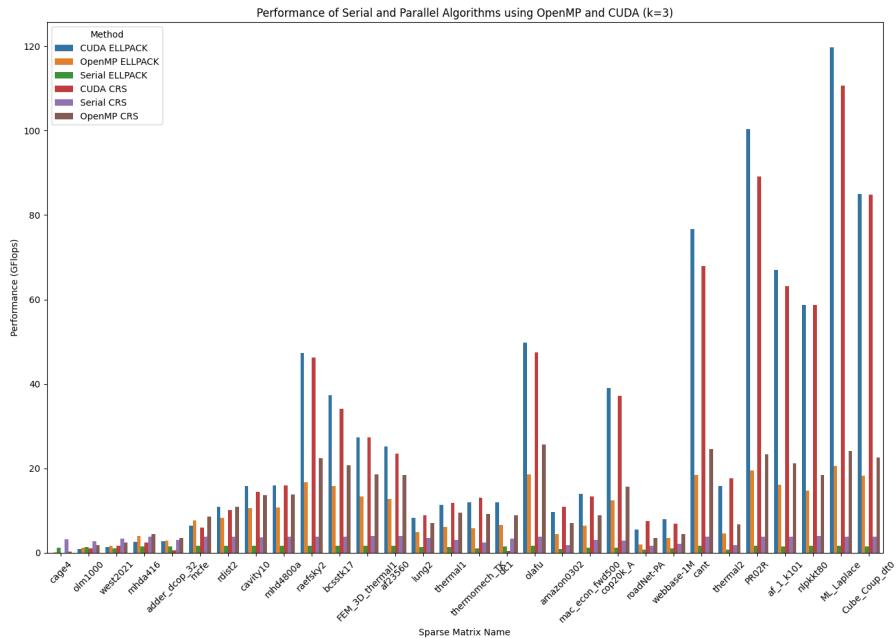
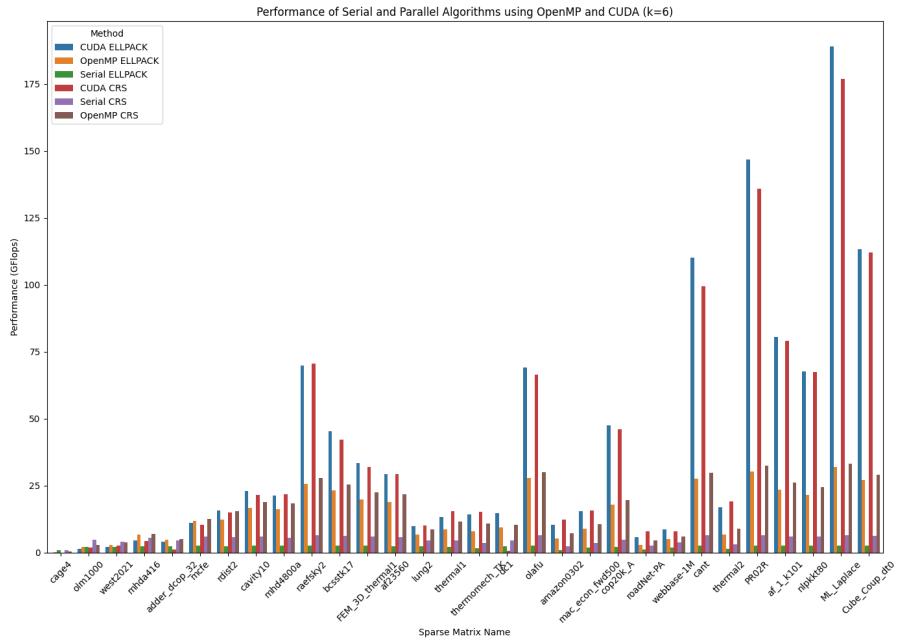


Figure 3.16: OpenMP Performance for ELLPACK Format depending on Threads

Figure 3.17: OpenMP vs CUDA Performance for $k = 1$

Figure 3.18: OpenMP vs CUDA Performance for $k = 2$ Figure 3.19: OpenMP vs CUDA Performance for $k = 3$

Figure 3.20: OpenMP vs CUDA Performance for $k = 6$

Chapter 4

Conclusion

In conclusion, this report has meticulously analysed various parallelization strategies for fat matrix vector multiplication, based on the MPI and PETSc frameworks, and through extensive experimentation and comparison, highlights the importance of choosing an appropriate parallelization approach based on matrix characteristics and computational resources. The results highlight the trade-offs between computational and communication overheads, emphasising the need for a balanced distribution of workloads to maximise efficiency. As expected the PETSc library outperforms the custom implementations in terms of execution time but not in terms of performance, as the matrices stay distributed even after the multiplication. The custom implementations are more efficient to reconstruct the final result from the gathered vector. In addition, the discussion of the environmental impact of HPC practices, with a nod to sustainable computing, reflects a broader perspective on the implications of computational research. Future directions could explore adaptive parallelization techniques, further optimizing specific models and matrix sizes, possibly integrating AI for dynamic algorithm selection based on real-time performance metrics. This study not only contributes to the field of HPC by providing insight into efficient algorithmic implementations, but also paves the way for more energy-efficient HPC systems, in line with global sustainable development goals.

References

1. Balay S, Abhyankar S, Adams MF, Benson S, Brown J, Brune P, et al.. PETSc Web page; 2023. <https://petsc.org/>. Available at: <https://petsc.org/>. (Accessed: December 28, 2023).
2. 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
  MatrixDefinitions.h
  SparseMatrixFatVectorMultiply.h
  SparseMatrixFatVectorMultiply.cpp
  SparseMatrixFatVectorMultiplyRowWise.h
  SparseMatrixFatVectorMultiplyRowWise.cpp
  SparseMatrixFatVectorMultiplyColumnWise.h
  SparseMatrixFatVectorMultiplyColumnWise.cpp
  SparseMatrixFatVectorMultiplyNonZeroElement.h
  SparseMatrixFatVectorMultiplyNonZeroElement.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_path>
```

Appendix A.C Methods Overview

A.C.1 Utils.h

A.C.1.1 ConvertPETScMatToFatVector

Description: Converts a PETSc matrix to a FatVector structure.

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 deserializes 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.