Performance of Distributed and Shared Memory Parallel Sparse Matrix Vector Multiplication

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Acknowledgements

To err is human; but to really foul things up requires a computer.

Paul R. Ehrlich

Abstract

Sparse Matrix Vector Multiplication is an important kernel used in scientific computing. It is a problem that lends itself well to parlallization. The problem is bounded by, and scales with the memory bandwidth of the system. Therefore in order to efficiently perform *SpMV* on large distributed memory systems, it is important to reduce the communication between nodes, in order to extract as much as possible out of the memory bandwidth of the system.

This thesis aims to investigate the results of *SpMV* when ran using different communication strategies.

Contents

Chapter 1

Theory

1.1 Sparse Matrix-Vector Multiplication

Sparse Matrix-Vector Multiplication (SpMV) is a fundamental operation encountered in many areas of scientific computing. It is especially prominent in solving large systems of linear equations and in large-scale simulations. The matrices involved are typically both very large and very sparse.

A matrix can in theory be considered sparse if it is worthwhile to treat zero values separately. In theory, this translates to a matrix being less than full, i.e. less than $\mathcal{O}\left(n^2\right)$ nonzeros for a $n \times n$ matrix. However, in the context of sparse linear algebra, sparse means that there is a constant number of nonzeros per row, i.e. $\mathcal{O}(n)$ nonzeros per row. The matrices used in scientific computing, such as matrices based on meshes, or graphs such as social networks all have this property. Optimizing the performance of SpMV, particularly through parallel computing techiniques, is crucial for enhancing the efficiency of many scientific applications.

However, SpMV is notoriously difficult to optimize, both in sequential and parallel implementations. One major reason is its inherently low computational intensity.

1.2 Definitions

Term	Definition
Node	A node, or a compute node, is a computeunit within a larger parallel computing system.
Dual/single socket	A dual or single socket node refers to the amount of processors on a node. Dual socketed nodes have two processors, that are connected through an interconnect.

1.3 Latency

The execution time of computational operations can vary significantly, and it is important to have some understanding of the latency times associated with typical operations. Referencing these latency numbers can be valuable when interpreting benchmark results and the performance of different programs.

Operation	Time [ns]
L1 cache reference	1
Branch misprediction	3
L2 cache reference	4
Mutex lock/unlock	17
Main memory reference	100
Compress 1K bytes with Zippy	2000
Send 2kB over 10 Gbps network	1600
Send 1K bytes over 1 Gbps network	10 000
Read 4K bytes randomly from SSD*	20 000
Round trip within same datacenter	500 000
Read 1MB sequentially from memory	1 000 000
Disk seek	10 000 000
Read 1MB sequentially form disk	10 000 000
TCP packet round trip between continents	150 000 000

Figure 1.1: Latency numbers for common operation, adapted from [4]

1.4 Parallel Architectures

There are two main architectures used in the parallel computing industry: Shared Memory Architecture and Distributed Memory Architecture. The following sections gives an overview of the key difference between the two.

1.4.1 Shared Memory Architecture

On a system with shared memory architecture, every processing unit (PU) have access to the same memory, treat it as a global address space. On such systems, the biggest challenge is that of *cache coherency*, where in order to prevent race conditions, every read of the cache must reflect the latest write (adapted from [3]).

1.4.2 Distributed Memory Architecture

On systems with distributed memory architecture, every processor have their own local memory, not accesible by other processors. When a process needs to access memory from another process, explicit communication of the data stored at that memory address needs to occur, and happens through whichever network the processors are connected with (adapted from [3]). Figure 1.2 shows the difference between shared and distributed memory architectures.

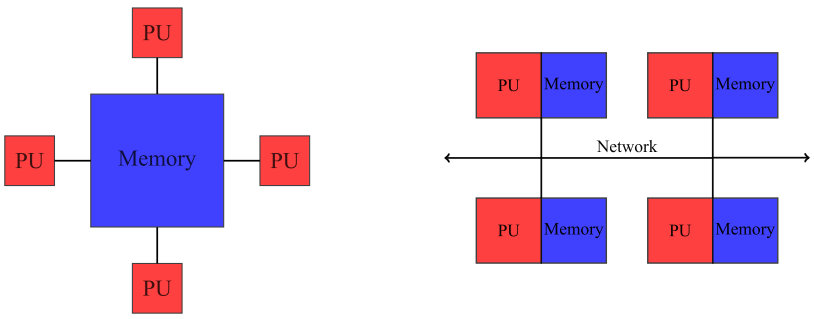


Figure 1.2: Shared and Distributed Memory Architecture (adapted from [2])

1.4.3 Non-Uniform Memory Access

Non-Uniform Memory Access (NUMA) refers to a multiprocessor system architecture in which memory access latencies depend on the location of the memory relative to a given processor. Unlike traditional symmetric multiprocessing (SMP) systems, where all processors share equal access times to a centralized memory pool, NUMA architectures consist of multiple processor sockets or nodes, each directly connected to its own local memory. These nodes are interconnected by a high-speed communication network, typically an interconnect, facilitating access to remote memory residing on other nodes.

Chapter 2

Background

2.1 CSR Storage Format

CSR (Compressed Sparse Row) is the most widely used storage format for sparse matrices. As its name suggests, it compresses the amount of memory used to store a matrix without loss of information. It does so by utilizing three vectors A_p, A_j, A_x. Figure 2.1 shows an example of a matrix stored in CSR format, adapted from [1].

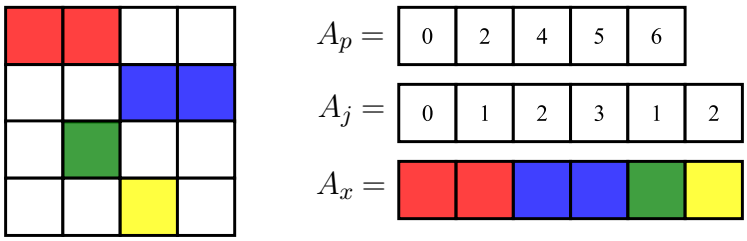


Figure 2.1: Matrix represented in the CSR format.

The first vector, A_p stores the indices of the first non-zero in the vectors A_p and A_x. For a given entry $A_p[i]$, $A_p[i]$ is the index of the first non-zero in the i^{th} row. $A_j[j]$ and $A_x[j]$ denotes the column index and value of the j^{th} non-zero, respectively.

Throughout the remainder of this thesis, we operate under the assumption that all matrices are represented in CSR format, unless explicitly noted otherwise.

2.1.1 Computational Intensity

The *computational intensity* of an operation describes the relation between the number of floating-point operations (FLOPS) and the number of memory accesses required. It is formally defined as:

$$\text{Computational intensity} = \frac{\text{FLOPS}}{\text{Memory accesses}} \tag{2.1}$$

Operations with low computational intensity, such as SpMV, are often *memory bound* rather than *compute bound*. This means that increasing the computational power of a system (e.g., faster processors) does not necessarily lead to proportional speedups in SpMV performance, as memory bandwidth remains the limiting factor.

2.2 Other storage formats

There exists many other lesser used storage formats for matrices

2.2.1 COO Format

The Coordinate List (COO) format stores the matrix as a set of triples on the form i, j, x, where i is the row index, j is the column index, and x is the value stored at (i, j) in the matrix. In this format all 0 entries are ignored.

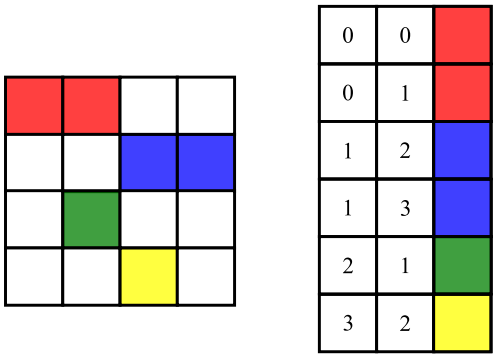


Figure 2.2: Example Matrix represented in the COO format.

2.2.2 CSC Format

The Compressed Sparse Column (CSC) format is similar to the CSR format, but instead of compressing the rows, we compress the columns. In this matrix format, we have irregular memory writes, but the reads are more regular. This can however be a problem

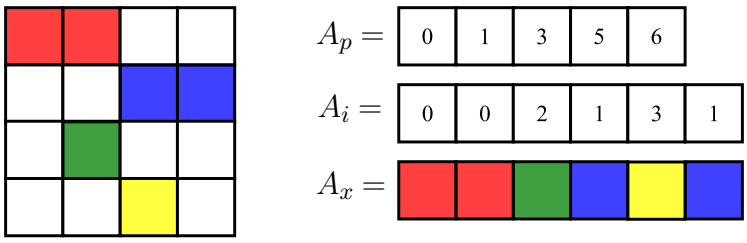


Figure 2.3: Matrix represented in the CSC format.

2.2.3 ELLPack Format

For an $M \times N$ matrix with a maximum of K non-zeros per row, the ELLPack format stores the non-zeros in an $M \times K$ matrix `data`, and an $M \times K$ matrix `indices`. The `data` matrix store the values of the non-zeros, and `indices` store the column index of every element. Rows that have fewer than K non-zeros are padded with zeros. Adapted from [5].

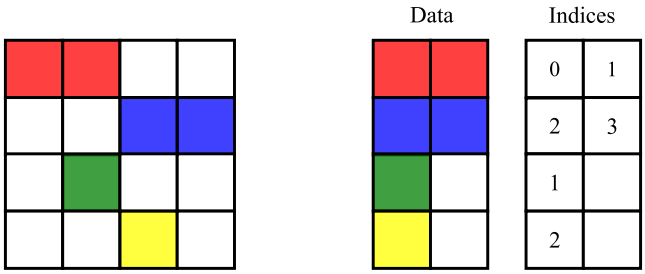


Figure 2.4: Matrix Represented in the ELLPACK format.

2.3 Sequential SpMV

A sequential implementation of SpMV on a matrix stored in the CSR format can be implemented in the following manner:

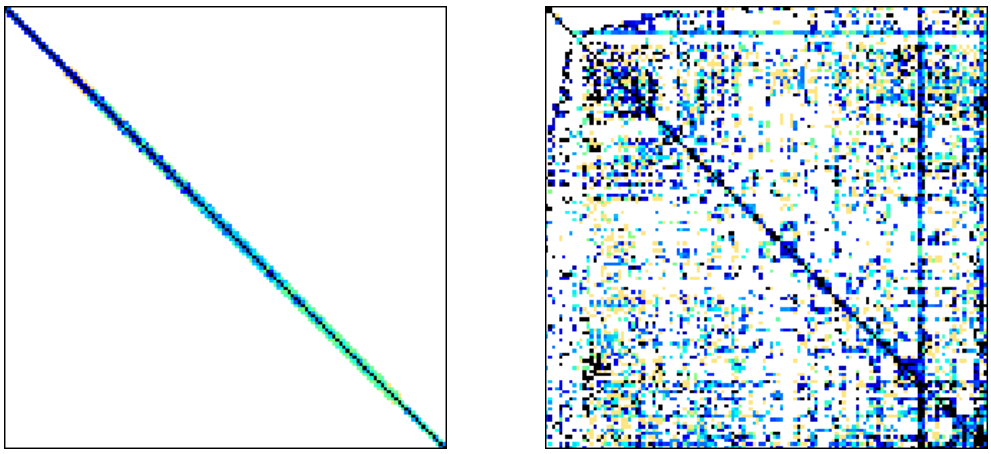
Algorithm 1: Sequential CSR-based SpMV

Input : A_p, A_j, A_x, x
Output : y

for $i \leftarrow 0$ **to** n **do**
  sum $\leftarrow 0$
  for $j \leftarrow A_p[i]$ **to** $A_p[i+1]$ **do**
    sum $=$ sum $+ A_x[j] \cdot x[A_j[j]]$
  $y[i] \leftarrow$ sum

For SpMV on well structured matrices such as those similar to the matrix illustrated in Figure 2.5, each non-zero element typically incurs a data movement cost of approximately 12 bytes and results in 2 floating-point operations (FLOPs). This estimation may appear inconsistent with the data access pattern described in algorithm 2.3, where two double-precision values and one integer are accessed per non-zero, corresponding to a total of 20 bytes. The apparent discrepancy arises from the caching behavior of the input vector x: after the initial access, elements of x are frequently reused and thus remain in cache, reducing the effective memory traffic associated with subsequent accesses.

In contrast, for highly unstructured matrices, the absence of data locality can significantly degrade cache reuse. In the worst case scenario, each non-zero may trigger the loading of an entire 64 byte cache line, with only a small fraction of it being used. Consequently, the effective data movement can increase to as much as 76 bytes per 2 FLOPs.



(a) Cube_Coup_dt0 (b) shermanACd

Figure 2.5: Well structured (a) and poorly structured (b) matrices.

2.4 Shared Memory SpMV

SpMV can be parallelized using the OpenMP directive `#pragma omp parallel for`. By default, this tells OpenMP to use `static` scheduling when parallelizing the outer iteration loop. When static scheduling is used, the span of the iteration that each thread will execute is precomputed, and stays static, as the naming suggests. There are other scheduling options, such as `dynamic` and `guided`, which will be discussed in later sections.

An implementation of shared memory SpMV is outlined below.

Algorithm 2: Shared Memory CSR-based SpMV

Input : A_p, A_j, A_x, x
Output : y

```
#pragma omp parallel for
for i ← 0 to n do
    sum ← 0
    for j ← A_p[i] to A_p[i+1] do
        sum = sum + A_x[j] · x[A_j[j]]
    y[i] ← sum
```

2.4.1 Scheduling options

As seen in algorithm 2, the outer loop is parallelized, which translates to dividing the rows of the matrix evenly among the threads. This work fine for well structured matrices, but for matrices with dense rows, such as the matrix shown in Figure 2.6, we obtain large imbalances in the computational load for each thread, which impacts performance.

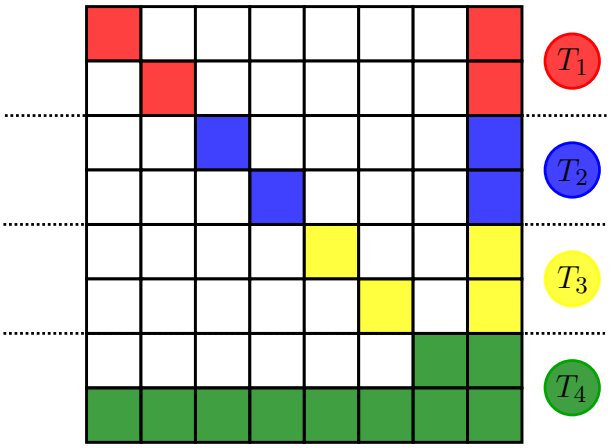


Figure 2.6: Row distribution among threads under static scheduling.

2.4.2 Dynamic Scheduling

Dynamic scheduling in OpenMP involves precomputing the range of iterations without assigning specific iteration subsets to individual threads

in advance. Under static scheduling, if thread A receives sparse rows and thread B receives dense rows, thread A will become idle prematurely while thread B remains computationally engaged. In contrast, dynamic scheduling allocates iterations at runtime to threads as they become available, thus potentially balancing the computational load more effectively, particularly when iteration workloads vary significantly.

At first glance, dynamic scheduling appears to resolve the workload imbalance inherent in static scheduling, even though it comes with more overhead. While this assumption holds true on smaller systems, such as personal laptops equipped with fewer physical cores and a single processor socket, it does not readily apply to larger, dual-socket systems utilized in this thesis. Here, the first-touch memory policy becomes particularly significant.

2.4.3 First-Touch Policy

The first-touch policy stipulates that the initial thread accessing a memory page allocates this page to its local memory domain. Consequently, if thread first accesses a memory page, it is stored locally to thread . Subsequent accesses by thread to this page result in non-local memory access, compelling thread to retrieve the data from either remote or main memory. Such accesses incur performance penalties due to significantly higher latency compared to local memory access.

2.4.4 Performance Implications of the First-Touch Policy

Table 1.1 illustrates that accesses to main memory exhibit substantially higher latency compared to local cache (e.g., L1 cache) accesses. In dual-socket configurations, accessing memory residing on the remote socket involves inter-socket communication through an interlink, further exacerbating latency. Consequently, dynamic (or guided) scheduling alone does not mitigate the performance degradation arising from poorly structured matrices, as it inadvertently exacerbates memory locality issues inherent to the first-touch policy on NUMA architectures.

2.5 Distributed Memory SpMV

In distributed memory systems, the computational workload is distributed across multiple nodes, each typically comprising a dual-socket architecture

with local memory. Unlike shared memory systems, data access across nodes is non-trivial and requires explicit communication, most commonly implemented using the Message Passing Interface (MPI).

For distributed sparse matrix-vector multiplication (SpMV), the computation proceeds similarly to the shared memory case (algorithm 2). The sparse matrix is divided across nodes, and each node computes its local segment of the output vector y. At the end of each iteration, partial results are assembled to produce the global vector, necessitating inter-node communication.

While the thread scheduling and memory locality issues discussed in 2.4.1 remain relevant, distributed memory systems introduce the additional challenge of communication overhead. As shown in Table 1.1, inter-node communication is significantly more expensive than memory accesses. Consequently, minimizing the total communication volume per SpMV iteration is critical for performance.

2.5.1 Load Balancing

To reduce communication volume, the matrix must be partitioned effectively across processing units. Typically, this involves assigning subgraphs or matrix blocks to either nodes or sockets. The quality of the partition is dependent upon finding a balance between creating parts that are roughly equal in size, and creating parts that minimize the communication load. Enforcing the size of each partition is usually done by specifing some imbalance thershold (e.g. 3%). However, minimizing the communication load is more difficult.

The communication volume between two partitions is determined by the size of the edge-cut of the subgraphs assigned to each partition. Given two subgraphs $G_1(V_1, E_1)$ and $G_2(V_2, E_2)$, the edge-cut is the set $e \in E_1 \cap E_2$, and the communication volume between these two partitions is given by $2 \cdot |e|$, because both of endpoints of the edges in this set needs to be communicated.

Finding a partition that minimizes the sizes of all edge-cuts between partitions is an NP-Hard problem and therefore all partitions produced are approximations. Finding partitions that optimize for either criteria is trivial. For the size criteria it is possible to simply assign a node to the part that currently has the fewest nodes, until every node is assigned to some part. For the edge-cut criteria it is possible to assign all nodes to a single part of the partition, which effectively brings the communication

volume to zero.

There are no fixed criterion of the imbalance value that leads to optimal communication reduction. It is possible to assign the entire graph to one part, leaving the other parts of the partitions empty, which effectively eliminates all communication, but this is clearly not optimal as the entire computational workload is assigned to a single process, leaving all other processes with no work. Usually an imabalence value of around 3% is sufficient for most matrices.

2.5.2 Graph Partitioners

There are many options when it comes to picking which graph partitioner to use, each with their own benefits and drawbacks. For the experiments performed in this thesis, the METIS graph partitioner has been used. The algorithms used in for graph partitioning in METIS are based on multilevel recursive-bisection. These kinds of algorithms optimize for communication reduction by minimizing the edge-cut, while trying to keep the size difference between partitions within the constraint given by the imbalance value.

It is worth mentioning that the problem graph partitioners are trying to solve, mainly that of a perfect bisection, is NP-Hard. Therefore the best these tools can provide us are approximations. They are however very reliable and produce good partitions that are sufficient for our usage

The following algorithm outlines how a graph (or matrix) is partitioned and reordered. Given a matrix g stored in the CSR Format, the number of partitions n_p, and a partition vector p of size $n_p + 1$, that is to store the size of the partition such that the size of the i^{th} ranks size is given by $p[i+1] - p[i]$.

Algorithm 3: Partitioning and reordering a matrix.

```
Input  : g, n_p, p
Output : Partitioned and reordered g

if n_p = 1 then
    p[0] ← 0
    p[1] ← g.n_r
    return g
partitionVector ← METIS_PartGraphKway(arguments
 specifying constraints for partition)
newId ← [0] · g.n_r
oldId ← [0] · g.n_r
id ← 0
p[0] ← 0
for r ∈ {0,...r} do
    for i ∈ {0,...,g.n_r} do
        if partitionVector[i] = r then
            oldId[id] ← i
            newId[i] ← id
            id ← id + 1
    partitionVector[r+1] ← id
newRowPtr ← [0] · g.n_r + 1
newColIdx ← [0] · g.n_c
newValues ← [0] · g.n_c
for i ∈ {0,...,g.n_r − 1} do
    d ← g.rowPtr[oldId[i]+1] - g.rowPtr[oldId[i]]
    newRowPtr[i + 1] ← newRowPtr[i] + d
    for j ∈ {0,...,d−1} do
        newColIdx[newRowPtr[i] + j] ← g.colIdx[g.rowPtr[oldId[i]]
         + j]
        newValues[newRowPtr[i] + j] ← g.values[g.rowPtr[oldId[i]]
         + j]
    for j ∈ {newRowPtr[i],...,newRowPtr[i+1]−1} do
        newColIdx[j] ← newId[newColIdx[j]]
g.rowPtr ← newRowPtr
g.colIdx ← newColIdx
g.values ← newValues
return g
```

Chapter 3

Communication Strategies

In parallel implementations of Sparse Matrix-Vector Multiplication (SpMV), effective communication management is critical due to its significant influence on overall performance. Communication often emerges as a bottleneck in distributed-memory systems because the speed at which data moves between nodes is significantly lower than within-node memory access speeds. Consequently, reducing communication volume and optimizing communication patterns can yield substantial performance improvements.

This chapter evaluates a series of progressively optimized communication strategies employed in distributed-memory parallel SpMV. Starting from the simplest method, exchanging the entire result vector between all nodes, the strategies become increasingly selective and efficient, focusing specifically on exchanging only the essential data elements required by each node. These approaches leverage knowledge of the matrix structure, partitioning methods, and computational dependencies to minimize communication overhead.

3.1 Exchange entire vector

The most straightforward approach is to have each rank send all of its computed values of y to every other rank. This ensures that all processes possess a complete and updated copy of the output vector before the next iteration. This strategy can be implemented using MPI's collective communication operation `MPI_Allgatherv`, which accommodates variable message sizes from each rank. Figure 3.2 illustrates the state of the y vector before and after communication using this strategy.

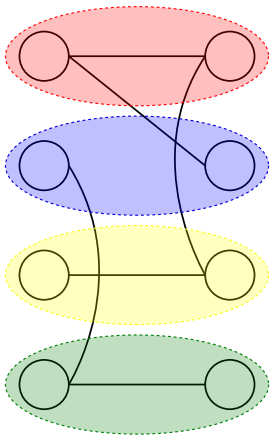


Figure 3.1: examplegraph

Algorithm 4: 1a - Exchange entire vector

for *each iteration* **do**
  spmv(g,x,y)
  MPI_Allgatherv(local_y, sendcount, MPI_DOUBLE, y,
   recvcounts, displs, MPI_DOUBLE, MPI_COMM_WORLD)
  swap pointers of x and y

3.2 Exchange only separators

An improvement to the previous strategy can be achieved by recognizing that only separator values, those required by multiple processes, must be communicated. Non-separator values are used exclusively by the process that computed them and therefore do not need to be communicated.

To facilitate this strategy, separator values are reordered such that they appear at the beginning of each process's local segment of y. Once this structure is established, communication is performed using `MPI_Allgatherv`, transmitting only the subset of y that contains separator values. The number of separators on each process must be known beforehand, which can be computed by counting the number of elements that have neighbours belonging to a different partition.

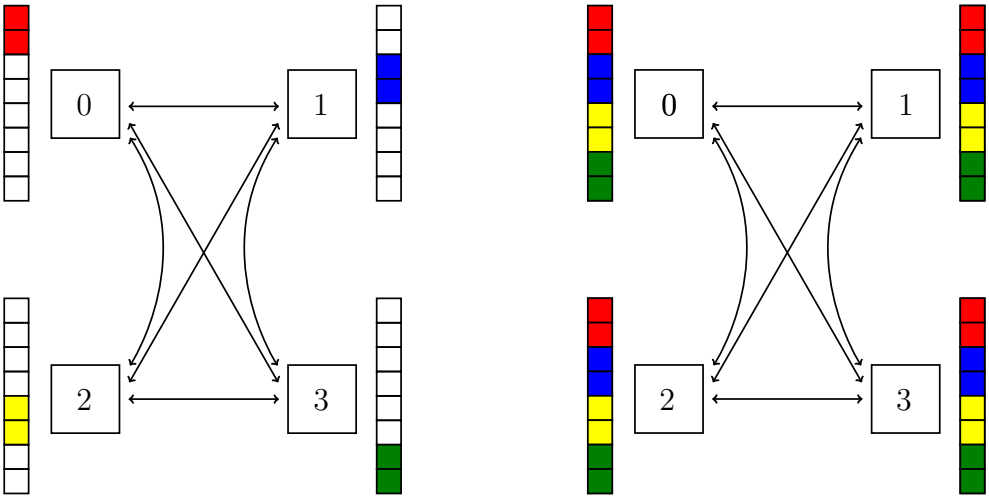


Figure 3.2: 1acomm 2

3.2.1 Reordering

After partitioning the matrix into different parts, we obtain a partition vector p, where the $p[i]$ stores the index of the partition the i^{th} entry in A_p. It is necessary to reorder the entries in A_p in accordance with the partition vector, such that all entries belonging to the same partition are stored in sequence. The algorithm below gives an outline of how this can be achieved. Here n_p is the number of partitions, n_r is the size of A_p, and n_c is the size of A_j and A_x.

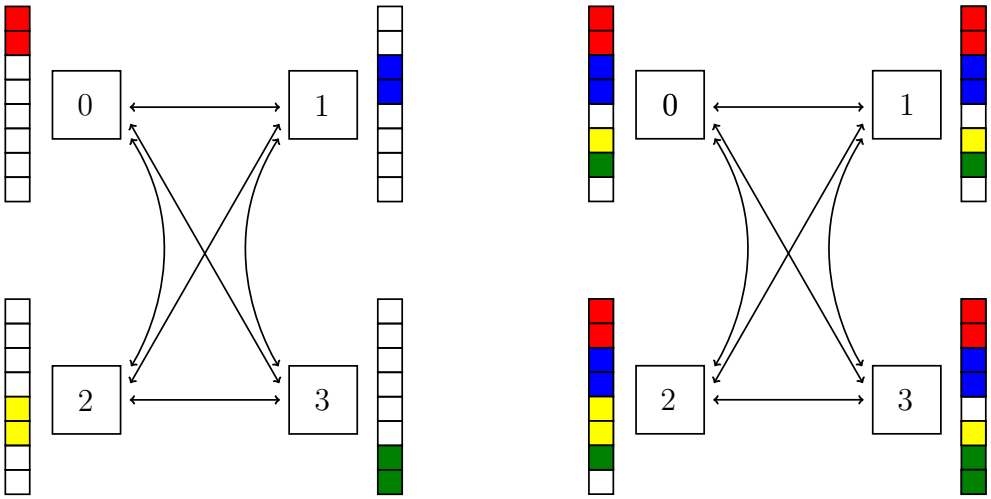


Figure 3.3: 1bcomm

Algorithm 5: Reordering of Separators

Input : $n_p, n_r, n_c, p, A_p, A_j, A_x$
Output : Reordered A_p, A_j, A_x

```
newId ← [0] · n_r
oldId ← [0] · n_r
id ← 0
p_0 ← 0

for r ∈ {0,...,n_p − 1} do
    for i ∈ {0,...,n_r − 1} do
        if p[i] = r then
            oldId[id] ← i
            newId[i] ← id
            id ← id + 1
    p[r + 1] ← id

newV ← [0] · (n_r + 1)
newE ← [0] · n_c
newA ← [0] · n_c

for i ∈ {0,...,n_r − 1} do
    degree ← A_p[oldId[i] + 1] − A_p[oldId[i]]
    newV[i + 1] ← newV[i] + degree

for i ∈ {0,...,n_r − 1} do
    degree ← A_p[oldId[i] + 1] − A_p[oldId[i]]
    for j ∈ {0,..., degree − 1} do
        newE[newV[i]+j] ← A_j[A_p[oldId[i]] + j]
        newA[newV[i]+j] ← A_x[A_p[oldId[i]] + j]
    for j ∈ {newV[i],...,newV[i + 1] − 1} do
        newE[j] ← newId[newE[j]]
```

3.3 Exchange only required separators

Further reduciton to the communication volume can be achieved by observing that not all separator values are required by every process. As the number of partitions increases, the set of dependencies between partitions tends towards sparcity. As a consequence of this, certain sets of separators may only need to be communicated to a given subset of processes. Using this strategy, each process only communicates its set of separator values to the processes that require them.

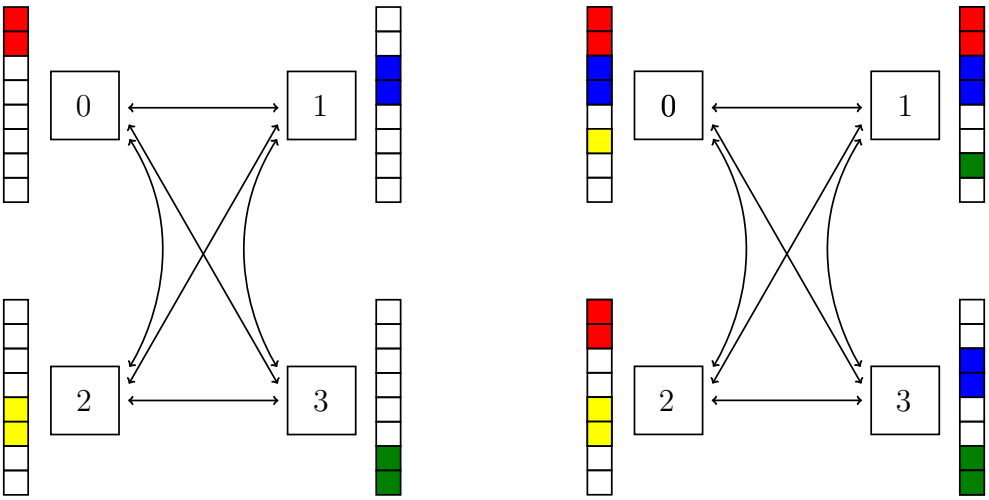


Figure 3.4: 1ccomm

3.4 Exchange only required separator values

The final strategy aims to minimize communication overhead by transmitting only the exact subset of separator values that are both computed by and required for inter-process computation. If a specific separator value computed by one process is needed by exactly one other process, then only that single recipient receives the value.

This approach eliminates all unnecessary data transfers but introduces additional complexity in managing communication schedules. Dependencies must be mapped at a fine-grained level, and communication patterns must be explicitly tailored to the structure of the matrix and its partitioning.

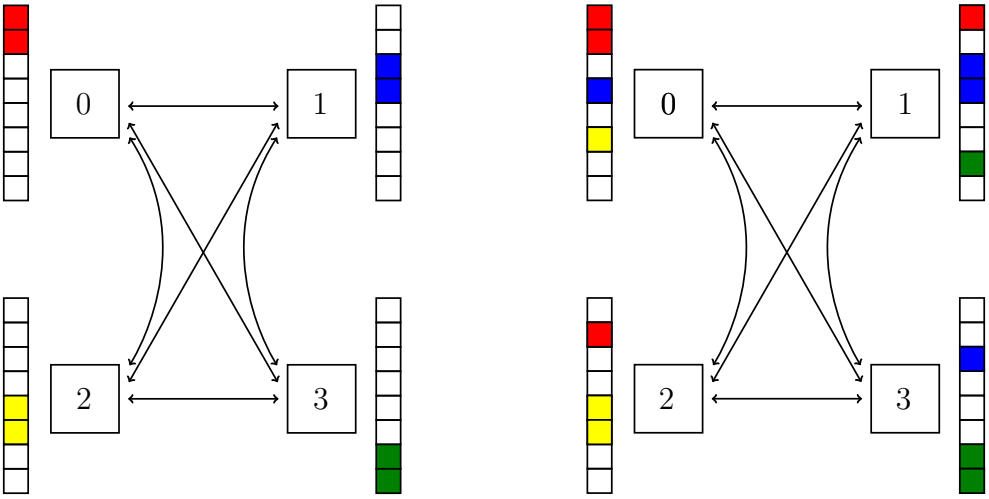


Figure 3.5: 1dcomm

3.5 Exchange Required Elements - Memory Scalable

The communication strategies discussed so far all have a common problem that prevents them from scaling to large matrices. These strategies all store the entire vector x, and will run into performance issues when x is so large that it doesn't fit into memory. Usually, this is not a problem when SpMV is ran on CPUs, as they have large amounts of memory. Even on GPUs this problem might not be encountered, as modern GPUs have sufficient memory for large matrices.

3.5.1 Intelligence processing units

paragraph on IPUs goes here

3.5.2 Memory Scalable

Instead of storing the entire vector, each rank only stores its local part of the vector. In addition, it is necessary to allocate enough space for the separators elements that are needed from the other ranks. In order to achieve this, x is renumbered such that every ranks part of the vector is.

Figure 3.6: 2dcomm

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