Efficient Distributed-Memory Parallel Matrix-Vector Multiplication with Wide or Tall Unstructured Sparse Matrices

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Abstract—This paper presents an efficient technique for matrix-vector and vector-transpose-matrix multiplication in distributed-memory parallel computing environments, where the matrices are unstructured, sparse, and have a substantially larger number of columns than rows or vice versa. Our method allows for parallel I/O, does not require extensive preprocessing, and has the same communication complexity as matrix-vector multiplications with column or row partitioning. Our implementation of the method uses MPI. We partition the matrix by individual nonzero elements, rather than by row or column, and use an “overlapped” vector representation that is matched to the matrix. The transpose multiplies use matrix-specific MPI communicators and reductions that we show can be set up in an efficient manner. The proposed technique achieves a good work per processor balance even if some of the columns are dense, while keeping communication costs relatively low.

Index Terms—Linear algebra, Sparse matrices, Parallel algorithms, Distributed algorithms

I. INTRODUCTION AND MOTIVATION

The sparse matrix-vector multiply (SpMV) operation multiplies a sparse matrix $A \in \mathbb{R}^{m \times n}$ by a dense vector $x \in \mathbb{R}^n$, resulting in a dense vector $y \in \mathbb{R}^m$, $Ax = y$. The sparse vector-transpose-matrix (SpVTM) operation multiplies $A$ by the transpose of a dense vector $v \in \mathbb{R}^m$ resulting in the transpose of a dense vector $u \in \mathbb{R}^n$, $v^T A = u^T$. The sequential implementation of these operations is straightforward and possibly easily parallelizable on shared-memory computers, for example, using pragma directives [5]. However, implementing large-scale SpMVs and SpVTMs on distributed-memory supercomputers requires careful attention to detail. Various approaches exist if $A$ has some structure, for example, if it is block-diagonal [15][14]. If $A$ lacks such structure, standard row or column partitioning techniques may have difficulty producing an even load balance, or may require extensive preprocessing of $A$ in order to do so [4][2]. For example, some document-term matrices arising in text classification problems [13] are sparse and wide, i.e. have $m \ll n$, and contain a small number of highly dense columns. A natural way of partitioning wide matrices is to assign subsets of the columns to individual processors. However, this approach may result in a very uneven load balance in the presence of dense columns. This paper describes a nonzero partitioning technique that avoids this issue by assigning subsets of nonzero matrix entries, instead of columns, to individual processors, and adjusting the representation of vectors to match the representation of the matrix.

II. DATA DISTRIBUTION

For the sake of brevity, we will assume throughout this paper that $A$ has many more columns than rows, that is, $m \ll n$, and is stored in column major order [7]. By reversing the roles of rows and columns, our method may be applied analogously to “tall” matrices with $m \gg n$, stored in row major order. Our partitioning method distributes the nonzero elements of $A$ evenly between processors and can result in one column of $A$ being “owned” by multiple processors; the details will be covered below. Coefficients of vectors of length $n$, such as $x$ and $u$ above, are also distributed across processors. On the other hand, we replicate vectors of length $m$, such as $y$ and $v$ above, in the memory of all processors. Since these vectors are much shorter than $x$ or $u$, the memory usage impact of this replication is limited. Throughout the discussion, we treat each processor as having its own memory; this does not prevent the method from being implemented on a system in which physical memory is (partially) shared.

Suppose that there are $P$ processors denoted $p_0$ through $p_{P-1}$, and let $\{J_0, \ldots, J_{P-1}\}$ be a collection of subsets of $\{1, \ldots, n\}$, with $J_i$ denoting the set of
partitioning, spreading the 21 nonzeros of an 8-column matrix across 7 processors, leaving each processor with exactly 3 nonzeros (this matrix does not have $m \ll n$, but we still use it for purposes of illustration). As Fig. 2 suggests, this technique can assign parts of the same column to different processors; if a local matrix $A_{(i)}$ has a partial column, then the missing elements are locally treated as being zero. For example, consider the first two local matrices in Fig. 2, $A_{(0)}$ and $A_{(1)}$. The first of these local matrices, $A_{(0)}$, is stored in $p_0$ and is represented as a sparse matrix with 2 columns, having 2 nonzeros in the first column and 1 nonzero in the second. The second local matrix, $A_{(1)}$, is stored in $p_1$ and is represented as a sparse matrix with 1 column containing 3 nonzeros. Thus, global column $A_2$ is split between processors $p_0$ and $p_1$. As a consequence, both $J_0$ and $J_1$ contain the index 2; specifically, $J_0 = \{1, 2\}$ and $J_1 = \{2\}$.

Whenever two or more processors are responsible for one column, we call that column’s index an overlap zone. If index $j$ is an overlap zone, then global column $A_j$ is the sum of the corresponding columns stored on each processor in the overlap zone. When storing $n$-dimensional vectors such as $x$ and $u$ above, each processor $p_i$ stores all the vector elements whose indices fall in $J_i$. Thus, vector coefficients in overlap zone columns will be replicated in multiple processors. In the example of Fig. 2, a vector $x \in \mathbb{R}^8$ will have the replication pattern shown in Fig. 3 with three overlap zones corresponding to matrix columns 2, 4, and 6. The vector element $x_2$ is replicated twice, $x_4$ three times, and $x_6$ twice.

In this scheme, every processor receives the same number of matrix nonzeros, give or take 1, regardless of the sparsity pattern of $A$. However, $n$-vectors are represented in a possibly unbalanced manner.

### III. SpMVs with Nonzero Partitioning

Given our vector and matrix distribution scheme, we may calculate $Ax$ as follows, using the terminology of MPI (11):

1) Each processor $p_i$ locally calculates $A_{(i)}x_{(i)} = y_{(i)}$

2) We sum the vectors $y_{(i)} \in \mathbb{R}^m$ over all processors using the MPI _Allreduce_ operation. Every processor thus receives the vector $\sum_{i=0}^{P-1} y_{(i)} = y = Ax$.

Fig. 4 illustrates this procedure. SpMVs with nonzero partitioning are straightforward to implement and work in essentially the same manner as they would with column partitioning. The complexity of the first step is $O(Z/P)$ and the complexity of the second step is $O(m \log P)$ using standard parallel reduction algorithms. Thus, the overall complexity is $O(Z/P + m \log P)$.
IV. **SpVTMs with Nonzero Partitioning**

A. Calculations

We now consider calculations of the form \( v^\top A = u^\top \). If we were to use a column-partitioned representation of \( A \), then this operation would require no communication, assuming that we are replicating the length-\( m \) vector \( v \) on all processors as we have already supposed. In our nonzero-based partitioning scheme, however, some communication is needed, because overlap-zone columns are split between different processors. Specifically, suppose that \( j \) is the \( k \)th zone (counting from left to right) and the storage for \( A_j \) is split among the processors in \( S_k = \{ p_{\ell}, p_{\ell+1}, \ldots, p_r \} \). Each processor \( p \in S_k \) stores a partial column \( A^p_j \) such that \( A_j = \sum_{p \in S_k} A^p_j \). Globally, we need to compute \( u_j = v^\top A_j \), and then replicate this value among all processors serving the overlap zone. Locally, however, each processor is only able to compute \( u^p_j = v^\top A^p_j \), but if we sum these values we obtain

\[
\sum_{p \in S_j} v^\top A^p_j = v^\top \left( \sum_{p \in S_j} A^p_j \right) = v^\top A_j = u_j.
\]

So, among the processors for each overlap zone, we simply need to sum the scalars \( u^p_j = v^\top A^p_j \) and then broadcast the result. We thus arrive at the following algorithm:

1) Each processor \( p_i \) locally computes \( v^\top A_{(i)} = u_{(i)} \).
2) The processors \( p \in S_k \) corresponding to each overlap zone \( j_k \) compute the sum \( \sum_{p \in S_k} u^p_{j_k} \) and broadcast it throughout \( S_k \).

Fig. 5 illustrates this procedure for the first overlap zone in the example above. In general, the local matrix multiplication step has complexity \( O(Z/P) \), just as in the previous algorithm. In MPI, we implement the second step by using `MPI_Allreduce` operations on specialized communicators, one for each overlap zone.

In general, we let \( z \) be the number of overlap zones and denote them \( j_0 < j_2 < \cdots < j_{z-1} \), with respective associated processor sets \( S_0, \ldots, S_{z-1} \). Table I shows the zones and sets for the example matrix of Fig. 1.
required to set up the overlap zone communicators is relatively insignificant: using appropriate parallel computations, they can be created in \( O(\log P) \) time, which is of lower order than a single multiplication.

To accomplish this, we must be careful in our use of MPI primitives. MPI contains the powerful, general communicator-creation primitive \( \text{MPI_Comm_split} \), but it uses all-to-all communication operations and therefore has complexity \( \Omega(P) \); we explicitly avoid such operations.

Throughout this section, we consider the processors to be ordered from “left” to “right”, that is, processor \( p_{i-1} \) is considered to be to the left of processor \( p_i \), and processor \( p_{i+1} \) to be on the right. At the beginning of the procedure, each processor \( p_i \), \( i = 1, \ldots, P - 1 \), determines the index of its first column \( j_i^1 \in J_i \) and the index of its last column \( j_i^2 \in J_i \); this step requires only constant time if the matrix elements are stored in column major order. The communicator setup procedure operates as follows:

1) Determine overlap zones: Using the primitive \( \text{MPI_Sendrecv} \), each processor \( p_i \) (except the last) sends \( j_i^1 \) to processor \( p_{i+1} \). Conversely, also using \( \text{MPI_Sendrecv} \), each processor \( p_i \) (except the first) sends \( j_i^2 \) to processor \( p_{i-1} \). Then each processor \( p_i \) computes the variables \( \text{needLeft} \) and \( \text{needRight} \), flags respectively indicating whether a processor shares responsibility for its first column with the previous processor, or responsibility for its last column with the next processor. Specifically,

\[
\text{needLeft} = \begin{cases} 
1, & \text{if } j_i^1 = j_{i-1}^1, \quad i = 1, \ldots, P - 1 \\
0, & \text{otherwise}
\end{cases}
\]

\[
\text{needRight} = \begin{cases} 
1, & \text{if } j_i^2 = j_{i+1}^2, \quad i = 0, \ldots, P - 2 \\
0, & \text{otherwise}
\end{cases}
\]

We set \( \text{needLeft} = 0 \) in \( p_0 \) and \( \text{needRight} = 0 \) in \( p_{P-1} \).

2) Determine ranks of overlap groups: A processor’s “left group” is the set of processors sharing responsibility for its first column, and its “right group” is the set of processors sharing responsibility for its last column. A processor may be in two groups if it shares its first column and last column with other processors, but these columns are not the same, as occurs for processor 4 in the example above. As already established, a processor cannot be in more than two groups.

We next assign a unique rank from 0 to \( z - 1 \) to each group (\( z \) being the number of overlap zones), progressing from the lowest to highest-ranked processors. In our example matrix of Fig. 1, the ranks are as shown in Table I. Group 0, with \( S_0 = \{ p_0, p_1 \} \) is the right group of \( p_0 \) and the left group of \( p_1 \). Group 1, with \( S_1 = \{ p_2, p_3, p_4 \} \) is the right group of \( p_2 \), both the left and right group of \( p_3 \), and the left group of \( p_4 \). Finally, group 2, with \( S_2 = \{ p_4, p_5 \} \), is the right group of \( p_4 \) and the left group of \( p_5 \).

To create this ranking and identify all left and right groups, each processor first computes an integer variable \( \text{leftGroupEnd} \) that is 1 if the processor has a left group and is the highest-rank processor in that group; otherwise, it is 0. The value assigned to \( \text{leftGroupEnd} \) on processor \( p_i \) is

\[
(\text{needLeft} = 1) \land ((\text{needRight} = 0) \lor (j_i^1 \neq j_i^2)).
\]

Next, we perform an additive forward scan (or parallel prefix operation, see for example [1, Chapter 4 and Appendix A]) on \( \text{leftGroupEnd} \). The resulting value is the number of complete groups up to and including each processor’s left group. We call this value \( \text{rightGroup} \), because it is the rank, from 0 to \( z - 1 \), of the processor’s right group, if it has one (otherwise its value is immaterial). We then calculate the rank of each processor’s left group (if it has one), by

\[
\text{leftGroup} = \text{rightGroup} - \text{leftGroupEnd}.
\]

3) Determine group extents: Consider a segmented addition operator \( \circ \) operating on pairs of integers in the following manner:

\[
\begin{pmatrix} s \\ k \end{pmatrix} \circ \begin{pmatrix} t \\ l \end{pmatrix} = \begin{cases} 
\begin{pmatrix} s + t \\ l \end{pmatrix}, & \text{if } k = l \\
\begin{pmatrix} t \\ l \end{pmatrix}, & \text{if } k \neq l.
\end{cases}
\]

This operator is noncommutative, but easily shown to be associative; it is therefore suitable for parallel prefix operations.

We next perform a forward scan using the \( \circ \) operator on the pairs

\[
\begin{pmatrix} \text{needLeft} \\ \text{leftGroup} \end{pmatrix}.
\]

In each processor \( p_i \), let \( \text{procsOnLeft} \) denote the first element of the result; it is the number of lower-ranked processors in the current processor’s left group. Next, we perform a backward scan, using the same operator \( \circ \), on the pairs

\[
\begin{pmatrix} \text{needRight} \\ \text{rightGroup} \end{pmatrix}.
\]

In each processor, let \( \text{procsOnRight} \) denote the first element of the result; this value is the number of higher-ranked processors in the current processor’s right group.

Each processor now has sufficient information to determine the full extent of its left and right groups (which may be the same group, or empty). Table I shows all the calculations for the example matrix of Fig. 1; note that value of \( \text{procsOnLeft} \) is unused in processors for which \( \text{needLeft} = 0 \) and similarly the
value of procsOnRight is unused in processors for which needRight = 0.

4) Create communicators: Each processor now uses MPI_Group_range_incl to create MPI group objects corresponding to its left and right groups; if these groups are the same, only one MPI group object is created. Every processor now simultaneously calls MPI_Comm_create with the group argument set to the MPI group object for the even-ranked group it participates in, if any. Each processor can be in at most one even-ranked group. If it is not in such a group, the processor supplies the argument MPI_GROUP_NULL. This operation simultaneously creates all even-numbered groups. Next, in a similar manner, we simultaneously create all odd-numbered groups. This operation completes the communicator setup.

To summarize the complexity of the operations above, all the numeric calculations require constant time, while the scans require O(log P) time. The MPI groups created may each be described by a single range-stride triplet, so their creation needs only constant time. Finally, creating an MPI communicator requires O(log S) time, where S is the size of the communicator. Therefore, simultaneous creation of the even communicators requires O(log V) \subseteq O(log P) time, and the same goes for the creation of the odd communicators. Therefore, the entire communicator creation process has complexity O(log P).

V. IMPLEMENTATION DETAILS

We created a C++ implementation consisting of two driver programs ColP and NzP, a class implementing our nonzero partitioning techniques, and a standard local sparse-matrix-multiply kernel default_dcscmv. The ColP driver implements the column partitioning technique: each processor reads in a contiguous span of the columns of the matrix stored in Intel MKL’s BLAS CSC format [12], and then performs 1,000 wraps of SpMV-SpVTM pairs. This pattern is meant to reflect that algorithms involving wide or tall matrices must typically perform equal numbers of matrix-vector and vector-transpose-matrix multiplications. We implement the local matrix-vector multiplies with the default_dcscmv kernel, and the sums needed by the SpMV operations with MPI_Allreduce reduction primitives.

The NzP driver implements the nonzero partitioning approach. For this technique, we store the matrix as a stream of (row, column, value) triples in column major order, and each processor core reads in a contiguous span of that data. After reading in the data, we use our nonzero partitioning class to determine the overlap zones and creates the necessary communicators as described in Section IV-B. Then, similarly to ColP, NzP performs 1,000 wraps of SpMV-SpVTM pairs. The multiplies consists of local sparse matrix-vector and vector-transpose-matrix multiplies, again executed by the kernel default_dcscmv, and MPI reduction operations, which include reductions performed across overlap zones in the case of the SpVTM calculations.

VI. EXPERIMENTAL RESULTS

Using an HPC system [10] with Xeon e5-2694v4 processors, the Intel Omni-Path interconnect fabric, the GNU C++ compilers, and MPICH, we tested both approaches with a highly unstructured wide matrix obtained from the UCI “Twenty Newsgroups” (News20) data set [6, 9]. The problem’s document-term matrix A has 19,996 rows, 1,355,191 columns and a total of 9,097,916 nonzero coefficients. While the average density is approximately 7 nonzeros per column, the matrix has 25 columns having at least 9,998 nonzero elements, with the 10 densest columns ranging between 11,872 and 18,531 nonzeros.

For our first set of tests, we arranged the columns of A in descending order based on their density, which is the worst-case scenario for the column partitioning approach. Figure 6 is a strong scaling graph for both techniques, with the number of processor cores appearing on the horizontal axis and the program running time, including I/O time, on the vertical axis. Clearly, the NzP algorithm exhibits much better scaling than ColP, since it does not have to contend with work-load imbalances between processor cores. NzP exhibits good scaling behavior through 128 processor cores, after which little further speedup is obtained, however, at that point, the total computation time is less than 1 second for 1,000 multiplication pairs. Table IV shows the nonzero imbalance (expressed as a percentage) for ColP and the number of overlap zones for NzP. The nonzero imbalance (\(\Delta\)) is calculated by dividing the difference between the maximum (\(\Xi\)) and minimum (\(\xi\)) number of nonzeros assigned to a single processor core by the average number of nonzeros per core (\(Z/P\)), i.e. \(\Delta = (\Xi - \xi)/(Z/P) = P(\Xi - \xi)/Z\).

Figure 7 shows the performance of both methods on the News20 dataset with its columns in the “native” order as obtained from the UCI repository. Although this order

| TABLE II | Communicator setup variable values for matrix in Fig. 1 |
|----------|-------------------------------------------------------|
| variable | 0 | 1 | 0 | 1 | 1 | 0 |
| needLeft | 1 | 0 | 1 | 1 | 1 | 0 |
| needRight| 0 | 1 | 0 | 1 | 1 | 0 |
| leftGroupEnd | 0 | 1 | 0 | 1 | 1 | 1 |
| rightGroup | 0 | 1 | 1 | 2 | 3 | 3 |
| leftGroup | 0 | 0 | 1 | 1 | 1 | 2 |
| procsOnLeft | 0 | 1 | 0 | 1 | 1 | 0 |
| procsOnRight | 1 | 2 | 2 | 1 | 1 | 0 |
is no longer the worst possible for column partitioning. Table IV indicates that the resulting imbalance is very substantial. As a result, the NzP code still performs significantly better than the ColP.

Finally, we tested both approaches on a 2,000 × 100,000 randomly generated matrix generated by the following procedure:

1) Based on initial density (ρ) and imbalance (ι−, ι+) parameters, we compute respective lower and upper bounds

\[ l = \lfloor \rho m \rfloor - \iota^- \quad u = \lceil \rho m \rceil + \iota^+ \]

on the number of nonzeros per column.

2) Randomly generate the number of nonzeros for each column from the uniform distribution on the interval \([l, u]\).

3) Specify row indices using a shuffle procedure assuring that all rows have at least one nonzero element.

This matrix (denser than News20) has 54,797,477 nonzeros nearly evenly balanced between columns and requires a large number of overlap zones for NzP, as illustrated in Table V. This situation is essentially the best case for column partitioning. As can be seen from Fig. 8, the codes achieve essentially identical scaling through 128 cores, after which NzP’s scaling starts to degrade faster than ColP’s. However, at that point, the total computation time is approximately 1 second.

In summary, we conclude that NzP is relatively insensitive the sparsity pattern of the matrix, as expected. It is far more robust than column partitioning, performing much better for unbalanced sparsity patterns but matching column partitioning’s performance on well balanced matrices, except at the very highest processor counts.

### VII. Final Remarks

First-order numerical algorithms involving sparse matrices typically alternate between matrix-vector multiplications and simple vector operations such as addition, scaling, and inner products. As illustrated in Fig. 4, the nonzero partitioning approach causes the workload

| Processor cores | ColP Imbalance % | NzP Overlap Zones |
|-----------------|-----------------|-------------------|
| 1               | 0%              | 0                 |
| 2               | 144%            | 1                 |
| 4               | 272%            | 3                 |
| 8               | 498%            | 6                 |
| 16              | 898%            | 12                |
| 32              | 1,585%          | 27                |
| 64              | 2,758%          | 54                |
| 128             | 4,735%          | 111               |
| 256             | 7,995%          | 186               |
| 512             | 13,287%         | 408               |
of such simple vector operations to become somewhat unbalanced, because the number of stored vector coefficients varies between processors. The worst possible case for these simple operation occurs when one processor owns \([Z/P]\) columns, each with a single nonzero. In this case, local vector operations have complexity \(O(Z/P)\) and inner products have complexity \(O(Z/P + \log P)\). In balanced column partitioning, the respective complexity of these operations is \(O(n/P)\) and \(O(n/P + \log P)\). With column partitioning, however, the complexity of SpMV and SpVTM operations could be respectively as bad as \(O(nm/P + m \log P)\) and \(O(nm/P)\), as compared to \(O(Z/P + m \log P)\) and \(O(Z/P + \log P)\) for nonzero partitioning.

If we suppose that there is a constant bound on the ratio between the number of matrix multiplication and the number of other operations, as is typically the case, then the effect of using nonzero partitioning is to improve the complexity of the dominant matrix multiplication operations at the cost of worsening the complexity of some nondominant operations. The highest complexity non-multiplication operation is the calculation of inner products, which becomes \(O(Z/P + \log P)\), the same as the SpVTM operation and lower than the SpMV operation. Therefore, while non-multiplication operations become more time consuming, they cannot become dominant in worst-case complexity terms. Meanwhile, the multiplication operations, which typically dominate running time, generally become more balanced than in the column partitioning approach, and remain so even for pathological sparsity structures. In general, we are trading off far better load balance in dominant operations for somewhat inferior load balancing of non-dominant operations. We have used the nonzero partitioning technique to implement various first-order optimization methods, such as spectral gradient and conjugate gradient, and have observed that the extra time required for simple vector operations does not have a significant impact on overall computation time.

A natural topic for further research is whether similar techniques may be used when \(m\) and \(n\) are of comparable magnitudes and both \(m\)-vectors and \(n\)-vectors are stored in a distributed manner. Such situations appear to be considerably more complicated.

**ACKNOWLEDGMENTS**

This research was supported in part by National Science Foundation grant CCF-1115638. This research used resources from the Rutgers Discovery Informatics Institute (RDF), a user facility supported by the Rutgers University Office of Research and Economic Development (ORED) [10]. The authors acknowledge the Texas Advanced Computing Center (TACC) at The University of Texas at Austin for providing HPC resources that have contributed to the research results reported within this paper. See [http://www.tacc.utexas.edu](http://www.tacc.utexas.edu).

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