Chapter 10

Parallel Patterns: Sparse Matrix Computation

An introduction to data compression and regularization

CHAPTER OUTLINE

Our next parallel pattern is sparse matrix computation. In a sparse matrix, the majority of the elements are zeros. Storing and processing these zero elements are wasteful in terms of memory capacity, memory bandwidth, time and energy. Many important real-world problems involve sparse matrix computation. Due to the importance of these problems, several sparse matrix storage formats and their corresponding processing methods have been proposed and widely used in the field. All of these methods employ some type of compaction techniques to avoid storing or processing zero elements at the cost of introducing some level of irregularity into the data representation. Unfortunately, such irregularity can lead to underutilization of memory bandwidth, control flow divergence, and load imbalance in parallel computing. It is therefore important to strike a good balance between compaction and regularization. Some storage formats achieve a higher level of compaction at a high-level of irregularity. Others achieve a more modest level of compaction while keeping the representation more regular. The parallel computation performance of their corresponding methods is known to be heavily dependent on the distribution of non-zero elements in the sparse matrices. Understanding the wealth of work in sparse matrix storage formats and their corresponding parallel algorithms gives a parallel programmer important background for addressing compaction and regularization challenges in solving related problems.

10.1. Background

A sparse matrix is a matrix where the majority of the elements are zeros. Sparse matrices arise in many science, engineering and financial modeling problems. For example, as we saw in Chapter 6, matrices can be used to represent the coefficients in a linear system of equations. Each row of the matrix represents one equation of the linear system. In many science and engineering problems, the large number of variables and equations involved are sparsely coupled. That is, each equation only involves a small number of variables. This is illustrated in Figure 10.1, where each column of the matrix corresponds to the coefficients for a variable: column 0 for x_0, column 1 for x_1, etc. For example, the fact that row 0 has non-zero elements in columns 0 and 2 indicates that variables x_0 and x_2 are involved in equation 0. It should be clear that none of the variables are present in equation 1, variables x_1, x_2 and x_3 are present in equation 2, and finally variables x_0 and x_3 are present in equation 3.

$$\begin{array}{l|cccc|} \text{Row 0} & 3 & 0 & 1 & 0 \\ \text{Row 1} & 0 & 0 & 0 & 0 \\ \text{Row 2} & 0 & 2 & 4 & 1 \\ \text{Row 3} & 1 & 0 & 0 & 1 \end{array}$$

Figure 10.1: A simple sparse matrix example

Sparse matrices are typically stored in a format, or representation, that avoids storing zero elements. We will start with the Compressed Sparse Row (CSR) storage format, which is illustrated in Figure 10.2. CSR stores only non-zero values in a one dimensional data storage, shown as data[] in Figure 10.2. Array data[] stores all the non-zero values in the sparse matrix in Figure 10.1. This is done by storing the non-zero elements of Row 0 (3 and 1) first, followed by the non-zero elements of Row 1 (none), followed by the non-zero elements of Row 2 (2, 4, 1), and finally the non-zero elements of Row 3 (1, 1). The format compresses away all the zero elements.

			Row 0	Row 2	Row 3	
Nonzero values	data[7]	{	3, 1,	2, 4, 1,	1, 1	}
Column indices	col_index[7]	{	0, 2,	1, 2, 3,	0, 3	}
Row Pointers	row_ptr[5]	{	0, 2, 2, 5, 7 }			

Figure 10.2: Example of Compressed Sparse Row (CSR) format.

With the compressed format, we need to put in two sets of markers to preserve the structure of the original sparse matrix in the compressed representation. The first set of markers form a column index array, col_index[] in Figure 10.2, that gives the column index of every non-zero value in the original sparse matrix. Since we have squeezed away non-zero elements of each row, we need to use these markers to remember where the remaining elements were in the original rows of the sparse matrix. For example, value 3 and 1 came from columns 0 and 2 of row 0 in the original sparse matrix. The col_index[0] and col_index[1] elements are assigned to store the column indices for these two elements. For another example, values 2, 4, and 1 came from columns 1, 2, and 3 of row 2 in the original sparse matrix. Therefore, col_index[2], col_index[3], and col_index[4] store indices 1, 2, and 3.

The second set of markers give the starting location of every row in the compressed format. This is because the size of each row becomes variable after zero elements are removed. It is no longer possible to use indexing based on the fixed row size to find the starting location of each row in the compressed storage. In Figure 10.2, we show a row_ptr[] array whose elements are the indices for the beginning locations of each row. That is, row_ptr[0] indicates that Row 0 starts at location 0 of the data[] array, row_ptr[1] indicates that Row 1 starts at location 2, etc. Note that row_ptr[1] and row_ptr[2] are both 2. This means that none of the elements of the Row 1 is stored in the compressed format. This makes sense since Row 1 in Figure 10.1 consists entirely of zero values. Note also that row_ptr[4] stores the starting location of a non-existing "Row 4". This is for convenience, as some algorithms need to use the starting location of the next row to delineate the end of the current row. This extra marker gives a convenient way to locate the ending location of Row 3.

As we discussed in Chapter 6, matrices are often used in solving linear system of N equations of N variables in the form of A*X + Y = 0, where A is an N×N matrix, X is a vector of N variables, and Y is a vector of N constant values. The objective is to solve for the X variable values that will satisfy all the equations. An intuitive approach is to inverse the matrix so that X = A^{-1} * (-Y). This can be done for matrices of moderate size through methods such as Guassian elimination, as we illustrated in Chapter 6. While it is theoretically possible to use these methods to solve equations represented in sparse matrices, the sheer size of many sparse matrices can simply overwhelm this intuitive approach. Furthermore, an inversed sparse matrix is often much larger than the original due the fact that the inversion process tends to generate a large number of addition non-zero elements called fill-in. As a result, it is often impractical to compute and store the inversed matrix in solving real-world problems.

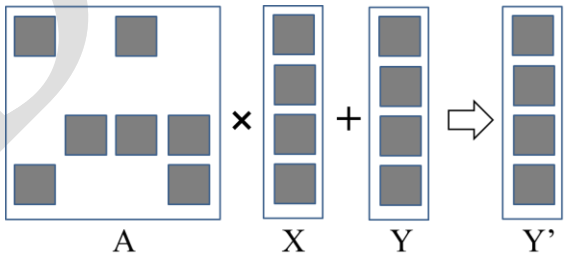


Figure 10.3: A small example of matrix-vector multiplication and accumulation

Instead, linear systems of equations represented in sparse matrices can be better solved with an iterative approach. When the sparse matrix A is positive-definite (i.e., $x^TAx > 0$ for all non-zero vectors x in R^n), one can use Conjugate Gradient methods to iteratively solve the corresponding linear system with guaranteed convergence to a solution [Hest1952]. Conjugate Gradient methods guess a solution for X and perform A*X+Y and see if the result is close to a 0 vector. If not, we can use a gradient vector formula to refine the guessed X and perform another iteration of A*X+Y.

The most time consuming part of such iterative approaches is in the evaluation of A*X+Y, which is a sparse matrix-vector multiplication and accumulation. Figure 10.3 shows a small example of matrix-vector multiplication and accumulation, where A is a sparse matrix. The dark squares in A represent non-zero elements. In contrast, both X and Y are typically dense vectors. That is, most of the elements of X and Y hold non-zero values. Due to its importance, standardized library function interfaces have been created to perform this operation under the name SpMV (Sparse Matrix Vector multiplication and accumulate). We will use SpMV to illustrate the important tradeoffs between different storage formats in parallel sparse matrix computation.

```
1.   for (int row = 0; row < num_rows; row++) {
2.     float dot = 0;
3.     int row_start = row_ptr[row];
4.     int row_end =   row_ptr[row+1];
5.     for (int elem = row_start; elem < row_end; elem++) {
6.         dot += data[elem] * x[col_index[elem]];
       }
7.     y[row] += dot;
     }
```
Figure 10.4: a sequential loop that implements SpMV based on the CSR format

A sequential implementation of SpMV based on the CSR format is quite straightforward, which is shown in Figure 10.4. We assume that the code has access to (1) num_rows, a function argument that specifies the number of rows in the sparse matrix, (2) a floating point data array of A elements (via the data[] input parameter), two floating-point x[] and y[] arrays of X and Y elements, and two integer row_ptr and col_index arrays as described in Figure 10.2. There are only seven lines of code. Line 1 is a loop that iterates through all rows of the matrix, with each iteration calculating a dot product of the current row and the vector x.

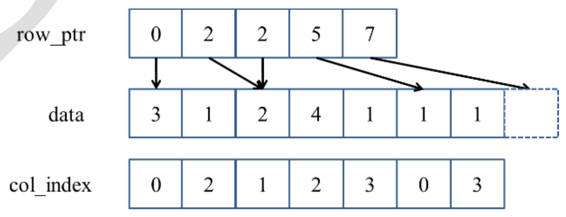


Figure 10.5: Sequential loop SpMV ~~loop~~ operating on the sparse matrix example in Figure 10.1

In each row, Line 2 first initializes the dot product to zero. It then sets up the range of data[] array elements that belong to the current row. The starting and ending locations can be loaded from the row_ptr[] array. Figure 10.5 illustrates this for the small sparse matrix in Figure 10.1. For row=0, row_ptr[row] is 0 and row_ptr[row+1] is 2. Note that the two elements from Row 0 reside in data[0] and data[1]. That is, row_ptr[row] gives the starting position of the current row and row_ptr[row+1] gives the starting position of the next row, which is one after the ending position of the current row. This is reflected in the loop in Line 5, where the loop index iterates from position given by row_ptr[row] to row_ptr[row+1]-1.

The loop body in Line 6 calculates the dot product for the current row. For each element, it uses the loop index elem to access the matrix A element in data[elem]. It also uses elem to retrieve the column index for the element from col_index[elem]. This column index is then used to access the appropriate x element for multiplication. For example, The element in data[0] and data[1] are form column 0 (col_index[0]=0) and column 2 (col_index[1]=2). So the inner loop will perform the dot product for row 0 as data[0]*x[0]+data[1]*x[2]. The reader is encouraged to work out the dot product for other rows as an exercise.

CSR completely removes all zero elements from the storage. It does incur storage overhead by introducing the col_index and row_ptr arrays. In our small example where the number of zero elements is not much larger than the number of non-zero elements, the storage overhead is actually more than the space saved by not storing the zero elements. However, it should be clear that for sparse matrices where the vast majority of elements are zeros, the overhead introduced is far less than the space saved by not storing zeros. For example, in a sparse matrix where only 1% of the elements are non-zero values, the total storage for the CSR representation including all the overhead would be around 2% of the space required to store both zero and non-zero elements.

Removing all zero elements from the storage also eliminates the need to fetch these zero elements from memory or perform useless multiplication operations on these zero elements. This can significantly reduce the consumption of memory bandwidth and computation resources.

It should be obvious that any SpMV computation code will reflect the storage format assumed. Therefore, we will add the storage format to the name of a code to clarify the combination used. We will refer to the SpMV code in Figure 10.4 as sequential SpMV/CSR. With a good understanding of sequential SpMV/CSR, we are now ready to discuss parallel sparse computation.

10.2. Parallel SpMV Using CSR

Note that the dot product calculation for each row of the sparse matrix is independent of that for other rows. That is, all iterations of the outer loop (Line 1) in Figure 10.4 are logically independent of each other. We can easily convert this sequential SpMV/CSR into a parallel

CUDA kernel by assigning each iteration of the outer loop to a thread. That is, each thread calculates the inner product for a row of the matrix, which is illustrated in Figure 10.6, where Thread 0 calculates the dot product for row 0, Thread 1 for row 1, and so on.

$$\begin{array}{l|cccc|}
\text{Thread 0} & 3 & 0 & 1 & 0 \\
\text{Thread 1} & 0 & 0 & 0 & 0 \\
\text{Thread 2} & 0 & 2 & 4 & 1 \\
\text{Thread 3} & 1 & 0 & 0 & 1
\end{array}$$

Figure 10.6: Example of mapping threads to rows in parallel SpMV/CSR

In a real-world sparse matrix application, there are usually thousands to millions of rows, each of which contains tens to hundreds of non-zero elements. This makes the mapping shown in Figure 10.6 seem very appropriate: there are many threads and each thread has a substantial amount of work. We show a parallel SpMV/CSR in Figure 10.7.

```
1.  __global__ void SpMV_CSR(int num_rows, float *data, int *col_index,
      int *row_ptr, float *x, float *y) {

2.    int row = blockIdx.x * blockDim.x + threadIdx.x;

3.    if (row < num_rows) {
4.      float dot = 0;
5.      int row_start = row_ptr[row];
6.      int row_end =   row_ptr[row+1];
7.      for (int elem = row_start; elem < row_end; elem++) {
8.        dot += data[elem] * x[col_index[elem]];
        }
9.      y[row] = dot;
      }

    }
```

Figure 10.7: A parallel SpMV/CSR kernel

It should be clear that the kernel looks almost identical to the sequential SpMV/CSR loop. The outermost loop construct has been removed since it is replaced by the thread grid. In Line 2, the row index assigned to a thread is calculated as the familiar expression blockIdx.x*blockDim.x + threadIdx.x. Also, due to the need to handle any arbitrary number of rows, Line 3 checks if the row index of a thread exceeds the number of rows. This handles the situation where the number of rows is not a multiple of the thread block size.

While the parallel SpMV/CSR kernel is quite simple, it has two major shortcomings. First the kernel does not make coalesced memory accesses. If the reader examines Figure 10.5, it should be cl ear that adjacent threads will be making simultaneous non-adjacent memory accesses. In our small example, threads 0, 1, 2, and 3 will access data[0], none, data[2], and data[5] in the first iteration of their dot product loop. They will then access data[1], none, data[3], and data[6] in the second iteration, and so on. As a result, the parallel SpMV/CSR kernel in Figure 10.7 does not make efficient use of memory bandwidth.

The second shortcoming of the SpMV/CSR kernel is that it can potentially have significant control flow divergence in all warps. The number of iterations taken by a thread in the dot product loop depends on the number of non-zero elements in the row assigned to the thread. Since the distribution of non-zero elements among rows can be random, adjacent rows can have very different number of non-zero elements. As a result, there can be wide spread control flow divergence in most or even all warps.

It should be clear that both the execution efficiency and memory bandwidth efficiency of the parallel SpMV kernel depends on the distribution of the input data matrix. This is quite different from most of the kernels we have studied so far. However, such data-dependent performance behavior is quite common in real-world applications. This is one of the reasons why parallel SpMV is such an important parallel pattern, it is simple and yet it illustrates an important behavior in many complex parallel applications. We will discuss three important techniques in the next sections to address the non-coalesced memory accesses and control flow divergence in the parallel SpMV/CSR kernel.

10.3. Padding and Transposition

The problems of non-coalesced memory accesses and control divergence can be addressed by applying data padding and transposition on the sparse matrix data. These ideas were used in the ELL storage format, whose name came from the sparse matrix package in ELLPACK a package for solving elliptic boundary value problems [Rice1984] A simple way to understand the ELL format is to start with CSR format, as is illustrated in Figure 10.8.

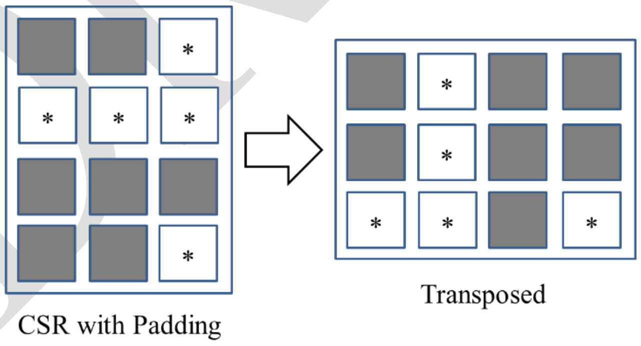


Figure 10.8. ELL Storage Format

From a CSR representation, we first determine the rows with the maximal number of non-zero elements. We then add **dummy** (zero) elements to all other rows after the non-zero elements to make them the same length as the maximal rows. This makes the matrix a rectangular matrix. For our small sparse matrix example, we determine that row 2 has the maximal number of elements. We then add one zero element to row 0, three zero elements to row 1, and one zero element to row 3 to make all them the same length. These additional zero elements are shown as squares with an * in Figure 10.8. Now the matrix has become a rectangular matrix. Note that the col_index array also needs to be padded the same way to preserve their correspondence to the data values.

We can now lay the padded matrix out in column major order. That is, we will place all elements of column 0 in consecutive memory locations, followed by all elements of column 1, and so on. This is equivalent to **transposing** the rectangular matrix in the row major order used by the C language. In terms of our small example, after the transposition, data[0] through data[3] now contain 3, *, 2, 1, the 0th elements of all rows. This is illustrated in the bottom portion of Figure 10.9. Similarly, col_index[0] through col_index[3] contain the column positions of 0th elements of all rows. Note that we no longer need the row_ptr since the beginning of row i is now simply data[i]. With the padded elements, it is also very easy to move from the current element of row i to the next element by simply adding the number of rows in the original matrix to the index. For example, the 0th element of row 2 is in data[2] and the next element is in data[2+4]=data[6], where 4 is the number of rows in the original matrix in our small example.

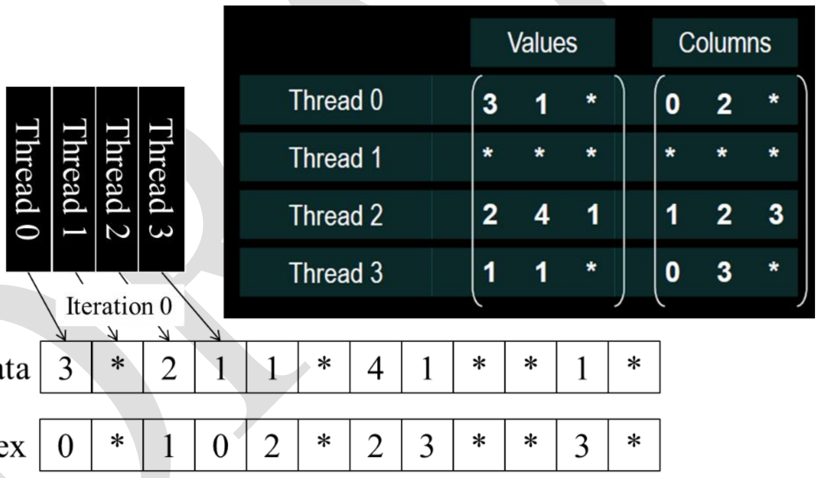


Figure 10.9: More details of our small example in ELL

Using the ELL format, we show a parallel SpMV_ELL kernel in Figure 10.10. The kernel receives slightly different arguments. It no longer needs the row_ptr. Instead, it needs an argument num_elem to know the number of elements in each row after padding. Recall that num_elem is the maximal number of non-zero elements among all rows in the original sparse matrix.

```
1.  __global__ void SpMV_ELL(int num_rows, float *data, int *col_index,
      int num_elem, float *x, float *y) {

2.    int row = blockIdx.x * blockDim.x + threadIdx.x;
3.    if (row < num_rows) {
4.      float dot = 0;
5.      for (int i = 0; i < num_elem; i++) {
6.        dot += data[row+i*num_rows] * x[col_index[row+i*num_rows]];
        }
7.      y[row] = dot;
      }
    }
```

Figure 10.10: A parallel SpMV/ELL kernel.

A first observation is that the SpMV/ELL kernel code is simpler than that of SpMV/CSR. With padding, all rows are now of the same length. In the dot-product loop in Line 5, all threads can simply loop through the number of elements given by num_elem. As a result, there is no longer control flow divergence in warps: all threads now iterate exactly the same number of times in the dot-product loop. In the case where a dummy element is used in a multiplication and accumulation step, it will not affect the final result because its value is 0.

A second observation is that in the dot-product loop body, each thread accesses its 0th element in data[row] and in general, its ith element in data[row+i*num_rows]. As we have seen in Figure 10.9, by arranging the elements in column major order all adjacent threads are now accessing adjacent memory locations, enabling memory coalescing and thus making more efficient use of memory bandwidth.

By eliminating control flow divergence and enabling memory coalescing, SpMV/ELL should run faster than SPMV/CSR. Furthermore, SpMV/ELL is simpler. This seems to make SpMV/ELL an all-around winning approach. Unfortunately, it does have a potential downside. In situations where one or a small number of rows have an exceedingly large number of non-zero elements, the ELL format will result in excessive number of padded elements. These padded elements will take up storage, need to be fetched, and take part in calculations even though they do not contribute to the final result. They consume memory storage, memory bandwidth, and execution cycles. Consider our sample matrix, in the ELL format we have replaced a 4x4 matrix with a 4x3 matrix, and with the overhead from the column indices we are storing more data than contained in the original 4x4 matrix.

For example, if a 1000x1000 sparse matrix has 1% of its elements of non-zero value. This means that on average, each row has 10 non-zero elements. With the overhead, the size of a CSR representation would about 2% of the uncompressed total size. Assume that one of the rows has 200 non-zero values while all other rows have less than 10. Using the ELL format, we would pad all other rows to 200 elements. This makes the ELL representation about 40% of the uncompressed total size and 20 times larger than the CSR representation. While the excessively long row will make only one of the warps of the SpMV/CSR kernel run for a long time, the padding will make all warps of the SpMV/ELL kernel run for a long time. With so many padded dummy elements, an SpMV/ELL kernel can actually run more slowly than an SpMV/CSR kernel. This calls for a method to control the number of padded elements when we convert from the CSR format to the ELL format.

10.4. Using a Hybrid Approach to Regulate Padding

The root of the problem with excessive padding in the ELL representation is that one or a small number of rows have exceedingly large number of non-zero elements. If we have a mechanism to "take away" some elements from these rows, we can reduce the number of padded elements in ELL. The Coordinate (COO) format provides such a mechanism.

			Row 0	Row 2	Row 3	
Nonzero values	data[7]	{	3, 1,	2, 4, 1,	1, 1	}
Column indices	col_index[7]	{	0, 2,	1, 2, 3,	0, 3	}
Row indices	row_index[7]	{	0, 0,	2, 2, 2,	3, 3	}

Figure 10.11: Example of Coordinate (COO) format

The COO format is illustrated in Figure 10.11, where each non-zero element is stored with both its column index and row index. We have both col_index and row_index arrays to accompany the data array. For example A[0,0] of our small example is now stored with both its column index (0 in col_index[0]) and its row index (0 in row_index[0]). With the COO format, one can look at any element in the storage and know where the element came from in the original sparse matrix. Like the ELL format, there is no need for row_ptr since each element self-identifies its column and row position.

While the COO format does come with the cost of additional storage for the row_index array, it also comes with the additional benefit of flexibility. We can arbitrarily re-order the elements in a COO format without losing any information as long as we re-order the data, col_index, and row_index arrays the same way. This is illustrated using our small example in Figure 10.12.

Nonzero values	data[7]	{	1	1,	2,	4,	3,	1	1	}
Column indices	col_index[7]	{	0	2,	1,	2,	0,	3,	3	}
Row indices	row_index[7]	{	3	0,	2,	2,	0,	2,	3	}

Figure 10.12 Re-ordering Coordinate (COO) format.

In Figure 10.12, we have reordered the elements of data, col_index, and row_index. Now data[0] actually contains an element from row 3 and column 0 of the original sparse matrix. Because we have also shifted the row index and column index values along with the data value, we can correctly identify this element's location in the original sparse matrix. The reader may ask why we would want to reorder these elements. Such reordering would disturb the locality and sequential patterns that are important for efficient use of memory bandwidth.

The answer lies in an important use case for the COO format. It can be used to curb the length of rows in the CSR or ELL format. First, we make an important observation. In the COO format, we can process the elements in any order we want. For each element in data[i], we can simply perform a y[row_index[i]] += data[i] * x[col_index[i]] operation. The correct y element identified by row_index[i] will receive the correct contribution from the product of data[i] and x[col_index]. If we make sure somehow we perform this operation for all elements of data, we will calculate the correct final answer regardless of the order in which we process these elements.

Before we convert from a sparse matrix from CSR to ELL, we can take away some of the elements from the rows with exceedingly large number of non-zero elements and place them into a separate COO storage. We can use SpMV/ELL on the remaining elements. With excess elements removed from the extra-long rows, the number of padded elements for other rows can be significantly reduced. We can then use a SpMV/COO to finish the job. This approach of employing two formats to collaboratively complete a computation is often referred to as a hybrid method.

Let's illustrate a hybrid ELL and COO method for SpMV using our small sparse matrix, as shown in Figure 10.13. We see that row 2 has the most number of non-zero elements. We remove the last non-zero element of row 2 from the ELL representation and move it into a separate COO representation. By removing the last element of row 2, we reduce the maximal number of non-zero elements among all rows in the small sparse matrix from 3 to 2. As shown in Figure 10.13, we reduced the number of padded elements from 5 to 2. More importantly, all threads now only need to take 2 iterations rather than 3. This can give a 50% acceleration to the parallel execution of the SpMV/ELL kernel.

A typical way of using an ELL-COO hybrid method is for the host to convert the format from something like a CSR format into ELL. During the conversion, the host removes some non-zero elements form the rows with exceedingly large number of non-zero elements. The host places these elements into a COO representation. The host then transfers the ELL representation of the data to a device. When the device completes the SpMV/ELL kernel, it transfers the resulting y values back to the host. These values are missing the contributions from the elements in the COO representation. The host performs a sequential SpMV/COO kernel on the COO elements and finishes their contributions to the y element values.

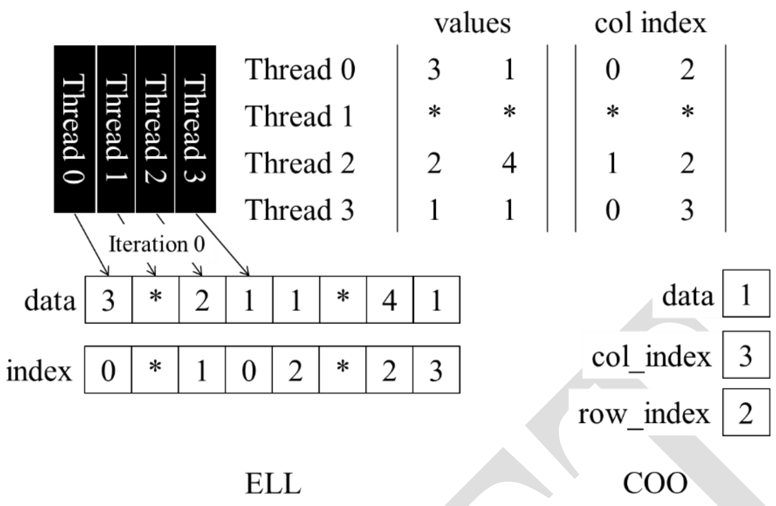


Figure 10.13: Our Small example in ELL and COO Hybrid

The user may question whether the additional work done by the host to separate COO elements from an ELL format could incur too much overhead. The answer is it depends. In situations where a sparse matrix is only used in one SpMV calculation, this extra work can indeed incur significant overhead. However, in many real-work applications, the SpMV is performed on the same sparse kernel repeatedly in an iterative solver. In each iteration of the solver, the x and y vectors vary but the sparse matrix remains the same since its elements correspond to the coefficients of the linear system of equations being solved and these coefficients do not change from iteration to iteration. So, the work done to produce both the hybrid ELL and COO representation can be amortized across many iterations. We will come back to this point in the next section.

In our small example, the device finishes the SpMV/ELL kernel on the ELL portion of the data. The y values are then transferred back to the host. The host then add the contribution of the COO element with the operation y[2] += data[0] * x[col_index[0]] = 1*x[3]. Note that there are in general multiple non-zero elements in the COO format. So, we expect that the host code to be a loop as shown in Figure 10.14.

```
for (int i = 0; i < num_elem; row++)
  y[row_index[i]] += data[i] * x[col_index[i]];
```

Figure 10.14: a sequential loop that implements SpMV/COO

The loop is extremely simple. It iterates through all the data elements and perform the multiply and accumulate operation on the appropriate x and y elements using the accompanying col_index and row_index elements. We will not present a parallel SpMV/COO kernel. It can be easily constructed using each thread to process a portion of the data elements and use an atomic operation to accumulate the results into y elements. This is because the threads are no longer mapped to a particular row. In fact, many rows will likely be missing from the COO representation; only the rows that have exceedingly large number of non-zero elements will have elements in the COO representation. Therefore, it is better just to have each thread to take a portion of the data element and use atomic operation to make sure that none of the threads will trample the contribution of other threads.

The hybrid SpMV/ELL-COO method is a good illustration of productive use of both CPUs and GPUs in a heterogeneous computing system. The CPU can perform SpMV/COO fast using its large cache memory. The GPU can perform SpMV/ELL fast using its coalesced memory accesses and large number of hardware execution units. The removal of some elements from the ELL format is a form of regularization technique: it reduces the disparity between long and short rows and makes the workload of all threads more uniform. Such improved uniformity results in benefits such as less control divergence in a SpMV/CSR kernel or less padding in a SpMV/ELL kernel.

10.5. Sorting and Partitioning for Regularization

While COO helps to regulate the amount of padding in an ELL representation, we can further reduce the padding overhead by sorting and partitioning the rows of a sparse matrix. The idea is to sort the rows according to their length, say from the longest to the shortest. This is illustrated with our small sparse matrix in Figure 10.15. Since the sorted matrix looks largely like a triangular matrix, the format is often referred to as Jagged Diagonal Storage (JDS) format. As we sort the rows, we typically maintain an additional jds_row_index array that preserves the original index of the row. For CSR, this is similar to the row_ptr array in that ~~there is~~both arrays have one element ~~per~~ for each row of the matrix. Whenever we exchange two rows in the sorting process, we also exchange the corresponding elements of the jds_row_index array. This way, we can always keep track the original position of all rows.

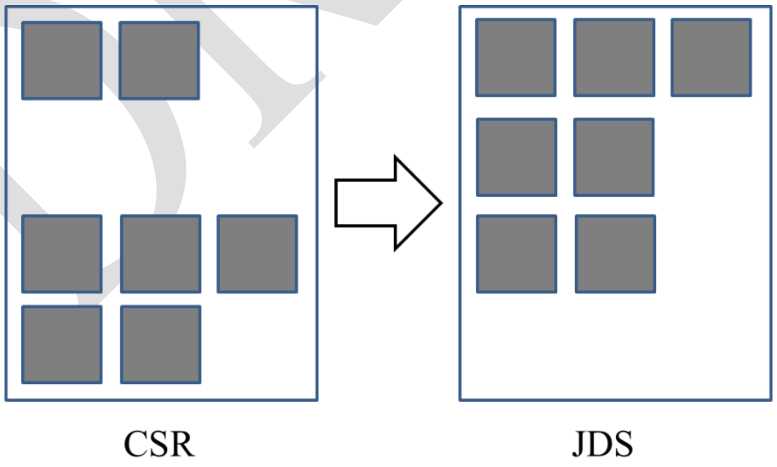
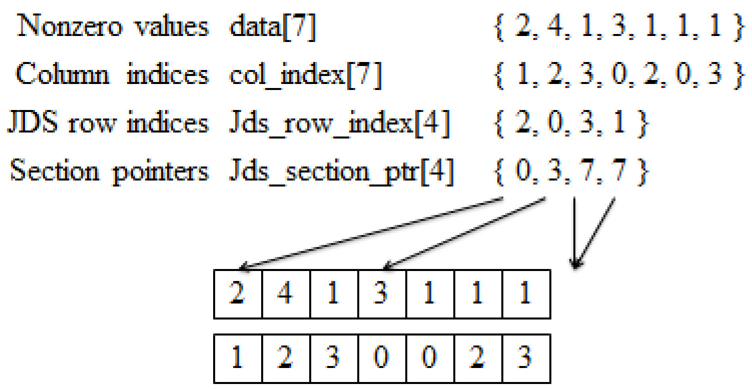


Figure 10.15: Sorting rows according to their length

Once a sparse matrix is in JDS format, we can partition the matrix into sections of rows. Since the rows have been sorted, all rows in a section will likely have more or less uniform number of non-zero elements. In Figure 10.15, we can divide the small matrix into three sections: the first section consists of the one row that has three elements. The second section consists of the two rows with two elements each. The third section consists of one row without any element. We can then generate ELL representation for each section. Within each section, we only need to pad the rows to match the row with the maximal number of elements in that section. This would reduce the number of padded elements. In our example, we do not even need to pad within any of the three sections. We can then transpose each section independently and launch a separate kernel on each section. In fact, we do not even need to launch a kernel for the section of rows with no non-zero elements.



Nonzero values	data[7]	{ 2, 4, 1, 3, 1, 1, 1 }
Column indices	col_index[7]	{ 1, 2, 3, 0, 2, 0, 3 }
JDS row indices	Jds_row_index[4]	{ 2, 0, 3, 1 }
Section pointers	Jds_section_ptr[4]	{ 0, 3, 7, 7 }

Figure 10.16 JDS format and sectioned ELL

Figure 10.16 shows a JDS-ELL representation of our small sparse matrix. It assumed the same sorting and partitioning results shown in Figure 10.15. Out of the three sections, the first section has only one row so the transposed layout is the same as the original. The second section is a 2×2 matrix and has been transposed. The third section consists of Row 1, which does not have any non-zero element. This is reflected in the fact that its starting location and the next section's starting position are identical.

We will not show a SpMV/JDS kernel. The reason is that we would be just using either an SpMV/CSR kernel on each section of the CSR, or a SpMV/ELL kernel on each section of the ELL after padding. The host code required to create a JDS representation and to launch SpMV kernels on each section of the JDS representation is left as an exercise.

Note that we want each section to have a large number of rows so that its kernel launch will be worthwhile. In the extreme cases where a very small number of rows have extremely large number of non-zero elements, we can still use the COO hybrid with JDS to allow us to have more rows in each section.

Once again, the reader should ask whether sorting rows will result into incorrect solutions to the linear system of equations. Recall that we can freely re-order equations of a linear system without changing the solution. As long as we re-order the y elements along with the rows, we are effectively re-ordering the equations. Therefore, we will end up with the correct solution. The only extra step is to reorder the final solution back to the original order using the jds_row_index array.

The other question is whether sorting will incur significant overhead. The answer is similar to what we saw in the hybrid method. As long as the SpMV/JDS kernel is used in an iterative solver, one can afford to perform such sorting as well as the re-ordering of the final solution x elements and amortize the cost among many iterations of the solver.

In more recent devices, the memory coalescing hardware has relaxed the address alignment requirement. This allows one to simply transpose a JDS-CSR representation. Note that we do need to adjust the jds_section_ptr array after transposition. This further eliminates the need to pad rows in each section. As memory bandwidth becomes increasingly the limiting factor of performance, eliminating the need to store and fetch padded elements can be a significant advantage. Indeed, we have observed that while sectioned JDS-ELL tend to give the best performance on older CUDA devices, transposed JDS-CSR tend to give the best performance on Fermi and Kepler.

We would like to make an additional remark on the performance of sparse matrix computation as compared to dense matrix computation. In general, the FLOPS rating achieved by either CPUs or GPUs are much lower for sparse matrix computation than for dense matrix computation. This is especially true for SpMV, where there is no data re-use in the sparse matrix. The CGMA value (Chapter 4) is essentially 1, limiting the achievable FLOPS rate to a small fraction of the peak performance. The various formats are important for both CPUs and GPUs since both are limited by memory bandwidth when performing SpMV. Many folks have been surprised by the low FLOPS rating of this type of computation on both CPUs and GPUs in the past. After reading this chapter, one should be no longer be surprised.

10.6. Summary

In this chapter, we presented sparse matrix computation as an important parallel pattern. Sparse matrices are important in many real-world applications that involve modeling complex phenomenon. Furthermore, sparse matrix computation is a simple example of data-dependent performance behavior of many large real-world applications. Due to the large amount of zero elements, compaction techniques are used to reduce the amount of storage, memory accesses and computation performed on these zero elements. Unlike most other kernels presented in this book so far, the SpMV kernels are sensitive to the distribution of data, specifically the non-zero elements in sparse matrices. Not only can the performance of each kernel vary significantly across matrices, their relative merit can also change significantly. Using this pattern, we introduce the concept of regularization using hybrid methods and sorting/partitioning. These regularization methods are used in many real-world applications. Interestingly, some of the regularization techniques re-introduce zero elements into the compacted representations. We use hybrid methods to mitigate the pathological cases where we could introduce too many zero elements. Readers are referred to [Bell2009] and encouraged to experiment with different sparse data sets to gain more insight into the data dependent performance behavior of the various SpMV kernels presented in this chapter.

References

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[Hest1952] Hestenes, Magnus R.; Stiefel, Eduard (December 1952). "Methods of Conjugate Gradients for Solving Linear Systems" (PDF). *Journal of Research of the National Bureau of Standards* **49** (6)

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10.7. Exercises

1. Complete the host code to produce the hybrid ELL-COO format, launch the ELL kernel on the device, and complete the contributions of the COO elements.

2. Complete the host code for producing JDS-ELL and launch one kernel for each section of the representation.

3. Consider the following sparse matrix:

$$\begin{matrix} 1 & 0 & 7 & 0 \\ 0 & 0 & 8 & 0 \\ 0 & 4 & 3 & 0 \\ 2 & 0 & 0 & 1 \end{matrix}$$

Represent it in each of the following formats: (a) COO, (b) CSR, and (c) ELL.

4. Given a sparse matrix of integers with m rows, n columns, and z non-zeros. How many integers are needed to represent the matrix in (a) COO, (b) CSR, and (c) ELL. If the information provided is not enough, indicate what information is missing.