FAST MATLAB COMPATIBLE SPARSE ASSEMBLY ON MULTICORE COMPUTERS

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ABSTRACT. We develop and implement in this paper a fast sparse assembly algorithm, the fundamental operation which creates a compressed matrix from raw index data. Since it is often a quite demanding and sometimes critical operation, it is of interest to design a highly efficient implementation. We show how to do this, and moreover, we show how our implementation can be parallelized to utilize the power of modern multicore computers. Our freely available code, fully Matlab compatible, achieves about a factor of $5 \times$ in speedup on a typical 6-core machine and $10 \times$ on a dual-socket 16-core machine compared to the built-in serial implementation.

1. INTRODUCTION

The popular Matlab programming environment was originally built around the insight that most computing applications in some way or the other rely on storage and manipulations of one fundamental object — the matrix. In the early 90s an important update was made with the support of a sparse storage format as presented in [7]. In that paper the way sparse matrices are managed in an otherwise dense storage matrix environment is described, including the initial creation of a sparse matrix, some basic manipulations and operations, and fundamental matrix factorizations in sparse format.

As a guiding principle the authors formulate the “time is proportional to flops”-rule [7, p. 334]:

The time required for a sparse matrix operation should be proportional to the number of arithmetic operations on nonzero quantities.

The situation is somewhat different today since flops often can be considered to be “free” while memory transfers are, in most cases, the real bottlenecks of the program. With the multicore era here to stay programs need to be threaded in order to utilize all hardware resources efficiently. This is a non-trivial task and requires some careful design [1].

In this paper we consider a sole sparse operation, namely the initial assembly operation as implemented by the Matlab function sparse;

$\texttt{>> S = sparse(i,j,s,m,n,nzmax);}$
After the call, $S$ contains a sparse representation of the matrix defined by $S(i_k,j_k) = s_k$ for $k$ a range of indices pointing into the vectors $\{i,j,s\}$, and where repeated indices imply that the corresponding elements are to be summed together. Many applications naturally lead to substantial repetitions of indices and the implied reduction must be detected and handled efficiently. For example, in the important case of assembly in linear finite element methods for partial differential equations, the resulting sparse matrix has a sparsity pattern which is identical to that of the matrix representation of the underlying triangular or tetrahedral mesh when viewed as a graph. The number of collisions during the assembly then corresponds exactly to the connectivity of the nodes in this graph.

Since the assembly must be performed before any other matrix operations are executed, the performance may become a bottleneck. The typical example is for dynamic nonlinear partial differential equations (PDEs), where re-assembly occurs many times as a numerical time integration proceeds, including during the iterations of the nonlinear solver. Thus, with the assembly process a quite time-consuming operation which is repeatedly performed, it cannot always be amortized over subsequent operations. Notably, in the truly large case presented in [9, §5.1.2–5.1.3], the performance of the sparse assembly is found to be the reason behind the loss of strong scaling beyond a few thousands of cores.

Algorithms for sparse assembly have caught the attention also by others. General assembly via an intermediate hashed data format is considered in [2], where serial performance experiment in the PETSc library are also reported. As a follow-up on [7], in [15] the design of sparse matrices in Matlab$^\text{P}$, a kind of parallel version of Matlab, is discussed. Unfortunately, little information about the current status of this language is available. More recently, a “graphBLAS” [10] has been suggested, where one of the operations, BuildMatrix, corresponds to the sparse function.

As mentioned, finite element methods naturally lead to the assembly of large sparse matrices. A stack based representation specially designed for this application is suggested in [8], and is also implemented there using a hybrid parallel programming model on a Cray XE6. Another approach is reported in [4], where the assembly of finite element sparse matrices in both Matlab and Octave is considered using these high-level languages directly.

Using the “time is proportional to flops”-rule as a guiding principle - but paying close attention to memory accesses - we provide a fast re-implementation of the sparse function. The resulting function fsparse is Matlab compatible, memory efficient, and parallelizes well on modern multicore computers. Moreover, it is well tested and has been freely available in the public domain for quite some time.

In §2 we describe in some detail the algorithm proposed, which can be understood as an efficient index-based sorting rule. In §3 parallelization aspects are discussed and performance experiments are made in §4, where the memory bound character of the operation is also highlighted. In general, with most sparse algorithms, there are not enough non-trivial arithmetic operations to hide the format overhead and data transfer costs [3]. A summarizing discussion around these issues is found in §5.

1.1. Availability of software. The code discussed in the paper is publicly available and the performance experiments reported here can be repeated through the Matlab-scripts we distribute. Refer to §5.1 for details.
2. A fast general algorithm for sparse assembly

In this section we lay out a fast algorithm for assembling sparse matrices from the standard index triplet data. A description of the problem is first offered in §2.1, where some alternative approaches and extensions of the problem are also briefly mentioned. The formats of input and output are detailed in §2.2 after which the algorithm is presented stepwise in §2.3. A concluding complexity analysis in §2.4 demonstrates that the algorithm proposed has a favorable memory access pattern without requiring large amounts of auxiliary memory.

2.1. Description of the problem. The column compressed sparse (CCS)\(^1\) is the sparse matrix storage format supported by Matlab but has also enjoyed a widespread use in several other packages. Given a 4-by-4 matrix \(S\) defined by

\[
S = \begin{pmatrix}
10 & 0 & 0 & -2 \\
3 & 9 & 0 & 0 \\
0 & 7 & 8 & 7 \\
3 & 0 & 8 & 5 \\
\end{pmatrix},
\]

the three required CCS arrays read as follows

\[
\begin{align*}
\text{prS} &= [10 \ 3 \ 3 \ 9 \ 7 \ 8 \ 8 \ -2 \ 7 \ 5], \\
\text{irS} &= [0 \ 1 \ 3 \ 1 \ 2 \ 2 \ 3 \ 0 \ 2 \ 3], \\
\text{jcS} &= [0 \ 3 \ 5 \ 7 \ 10],
\end{align*}
\]

where \(\text{prS}\) contains the nonzero values column-wise, \(\text{irS}\) the zero-offset row indices, and where \(\text{jcS}\) points to the columns in both \(\text{prS}\) and \(\text{irS}\). For an \(M\)-by-\(N\) sparse matrix we always have that \(\text{jcS}[0] = 0\) and that \(\text{jcS}[N] = \text{nnz}\), the total number of nonzero elements.

In Matlab we may form a representation of \(S\) by

\[
\begin{align*}
\text{>> s} &= [10 \ 3 \ 3 \ 9 \ 7 \ 8 \ 8 \ -2 \ 7 \ 5]; \\
\text{>> i} &= [1 \ 2 \ 4 \ 2 \ 3 \ 3 \ 4 \ 1 \ 3 \ 4]; \\
\text{>> j} &= [1 \ 1 \ 1 \ 2 \ 2 \ 3 \ 3 \ 4 \ 4 \ 4]; \\
\text{>> S} &= \text{sparse}(\text{i}, \text{j}, \text{s}); \% \text{size(S)} = [4,4] \text{ is implicit}
\end{align*}
\]

The assembly problem, therefore, is to transform the triplet \((i, j, s)\) into the CCS triplet \((\text{irS}, \text{jcS}, \text{prS})\). Generally, the difficulties lie in that (i) the data is unordered, and (ii), the values in \(s\) of equivalent pairs \((i, j)\) are to be summed together. For example, the above matrix may also be constructed from the triplet data

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**Listing 1. Sample input (running example)**

\[
\begin{align*}
\text{>> s} &= [4 \ 4 \ 5 \ 7 \ 3 \ 5 \ 5 \ 4 \ 3 \ 4 \ 9 \ 7 \ -2]; \\
\text{>> i} &= [3 \ 4 \ 1 \ 3 \ 2 \ 1 \ 4 \ 4 \ 4 \ 3 \ 2 \ 3 \ 1]; \\
\text{>> j} &= [3 \ 3 \ 1 \ 4 \ 1 \ 1 \ 4 \ 3 \ 1 \ 3 \ 2 \ 2 \ 4];
\end{align*}
\]

---

Below we will use the sample input of Listing 1 as a running example to demonstrate the effects of the code snippets shown.

The complexity of the assembly operation can be bounded from above as follows. Consider first sorting the triplet with respect to column indices, then sorting each column with respect to rows. In a final sweep over all columns, equivalent indices

\(^1\)Note that the abbreviation “CSC” is also in widespread use.
are summed together. If the initial triplet has length \( L \), then the complexity is that of sorting and hence bounded by \( L \log L \). Additionally, using an in-place sorting algorithm, it is easy to see that the whole operation can in fact be done in-place. In practice, sorting algorithms using auxiliary memory are generally faster and also parallelize better.

While these are generally applicable remarks they do not take into account the fact that the indices are bounded integers and hence can be sorted more efficiently. In fact, the algorithm presented in §2.3 below can be seen as a version of the “Distribution counting sort” [11, Algorithm D, §5.2]. Notably with this approach, speedup up to a factor of 4.8 on 8 cores was reported in [12].

The algorithm in §2.3 is quite general in that it can readily be extended to allow for various more powerful input and output combinations. Relevant examples include the case when not all input is available at the first call (“delayed assembly”), or when the output must be formed in a distributed setting. Another case is supported by the full code \texttt{fsparse} but not detailed here; this is an extension of the Matlab syntax which allows for row- and/or column-indices to be counted several times as dictated by the dimensions of the inputs.

One should keep in mind that repeated assembly can often be done efficiently by saving various types of information between successive calls. However, the possibility of “quasi assembly” is clearly very strongly problem dependent. Thus in what follows, we remain in the general setting.

### 2.2. Format of input and output.

In the following we stepwise explain the algorithm by giving snippets of actual C-code in an imagined environment which contains an increasing number of variables. The final serial version of the code with all pieces taken together is found in Listing 15 in Appendix A.

In the example above the dimensions of the final matrix are implicitly defined as the largest row- and column index. Hence as the first step, these arrays must be parsed for the maximum values and we also conveniently translate them into integers (recall that an array in Matlab by default is a \texttt{double} array). Code for this pre-processing is found in Listing 13 in Appendix A and the result is the equivalence of Listing 2. Note that the input index arrays remain in unit-offset.

#### Listing 2. Input format

```c
const double *sr; // pointer to values
const int *ii,*jj; // pointers to row- and column indices (unit-offset)
int len; // length of arrays ii, jj, sr
int M,N; // sparse matrix dimensions
```

Given the input in Listing 2, the algorithm detailed in §2.3 below produces an intermediate format which is very close to the final matrix. This format is stated in Listing 3 and contains two arrays. One of these, \( \text{jCS} \), belongs to the final output and has been discussed previously. The other one, \( \text{irrank} \), the inverse rank, contains information as to how the remaining CCS-arrays \( \text{prS} \) and \( \text{irS} \) are to be formed from the raw triplet data. The relation is that for \( i = 0...\text{len} - 1 \) (recall that zero-offset
is used here),

\begin{equation}
\text{irS}[j] = \text{ii}[i] - 1, \quad \text{where } \text{irank}[i] = j, \tag{2.2}
\end{equation}

\begin{equation}
\text{prS}[j] = \sum_{i: \text{irank}[i] = j} \text{sr}[i]. \tag{2.3}
\end{equation}

In plain language, \text{irank}[i] points to the final position in \((\text{irS}, \text{prS})\) for the corresponding pair \((\text{ii}[i], \text{sr}[i])\). Code for finalizing the representation according to these relations is found in Listing 14 in Appendix A. Note that as a consequence of (2.2), \(\text{nnz} = 1 + \max_i \text{irank}[i]\).

### Listing 3. Intermediate output format

```c
int *irank; // inverse rank array of length len
int *jcS; // final column pointer for sparse matrix S

jcS = calloc(N+1,sizeof(jcS[0]));
irank = malloc(len*sizeof(irank[0]));
```

2.3. **Index-based sparse assembly.** The task at hand is now to arrive at the intermediate output of Listing 3, given the parsed input of Listing 2. We will do this incrementally in four parts detailed in §2.3.1–2.3.4 below. The first part estimates the number of nonzeros per row, the second part constructs a rank-array which provides with the ability for a row-wise traversal. The most complex part of the algorithm is the third part in which the unique row indices of each column are found. Finally, in the fourth part the required intermediate outputs \text{irank} and \text{jcS} can be determined.

#### 2.3.1. Part 1. **This part builds a kind of row pointer with the same structure as \text{jcS}, but for rows instead of for columns. “Kind of” because there is no data available to actually point into, the input still being unordered. In Listing 4, note also that the resulting pointer \text{jrS} ignores collisions and hence that the estimated number of nonzeros per row is an upper bound.**

### Listing 4. Part 1: count rows

```c
int *jrS; // accumulated row counter
jrS = calloc(M+1,sizeof(jrS[0]));

// count and accumulate indices to rows
for (int i = 0; i < len; i++) jrS[ii[i]]++;
for (int r = 2; r <= M; r++) jrS[r] += jrS[r-1];
```

**Example.** Given the arrays defined in Listing 1 as inputs, Listing 4 produces the pointer to rows

\[
\text{jrS} = [0 \ 3 \ 5 \ 9 \ 13].
\]

That collisions are ignored at this stage can be seen from the fact that \(S\) in (2.1) has 10 nonzero elements, whereas \(\text{jrS}\) has reserved space for 13 elements. □
2.3.2. Part 2. With an upper bound on the number of nonzeros per row available it is now straightforward to create a rank-array \textbf{rank} such that \( i = \text{rank}[j] \) points to the \( i \)th triplet \((ii[i], jj[i], sr[i])\) ordered with respect to row indices (that is, with \( ii[i] \) non-decreasing). Hence the key feature with \textbf{rank} is that it allows for the data to be traversed in an ordered row-by-row fashion.

\begin{verbatim}
Listing 5. Part 2: build rank-array
int *rank; // rank-array for rows
rank = malloc(len*sizeof(rank[0]));

// build rank with the active use of jrS
jrS--; /* (unit-offset in ii) */
for (int i = 0; i < len; i++) rank[jrS[ii[i]]]++ = i;
\end{verbatim}

Example. Continuing with the sample input from Listing 1, Listing 5 produces
\[
\text{rank} = [2 \ 5 \ 12 \ 4 \ 10 \ 0 \ 3 \ 9 \ 11 \ 1 \ 6 \ 7 \ 8],
\]
\[
\text{jrS} = [∗ \ 3 \ 5 \ 9 \ 13 \ 13],
\]
where the notation indicates that \( \text{jrS} \) is now in unit-offset. The defining relation is
\[
\text{ii}[\text{rank}[i]] = [1 \ 1 \ 1 \ 2 \ 2 \ 3 \ 3 \ 3 \ 4 \ 4 \ 4 \ 4],
\]
such that \textbf{rank} indeed provides for a row-wise traversal of the data. 

2.3.3. Part 3. In this part of the algorithm, the program loops over the input and makes each column unique with respect to row indices, building both the index array \textbf{irank} and the column pointer \textbf{jcS} at the same time. This is made feasible by the row-wise traversal of the input data and a small cache memory for column indices.

\begin{verbatim}
Listing 6. Part 3: uniqueness
int *hcol; // cache memory for columns
hcol = calloc(N,sizeof(hcol[0]));

// loop over all row indices
for (int row = 1,i = 0; row <= M; row++)
// loop over single row
for ( ; i < jrS[row]; i++) {
    const int ixijs = rank[i]; // index into input data triplet (ii,jj,sr)
    const int col = jj[ixijs]; // column index

    // new element?
    if (hcol[col] < row) {
        hcol[col] = row; // remembered by the row index
        jcS[col]++; // count it
    }

    // irank keeps track of where it should go
    irank[ixijs] = jcS[col]-1;
}
\end{verbatim}
// done: deallocate auxiliary variables
free(++hcol);
free(rank);
free(++jrS);

Example. Our sample input in Listing 1 yields

\[ \text{irank} = [0 \ 1 \ 0 \ 1 \ 0 \ 2 \ 1 \ 2 \ 0 \ 0 \ 1 \ 0], \]
\[ \text{jcS} = [0 \ 3 \ 2 \ 2 \ 3], \]

which is not very informative due to the missing final accumulation of indices.  

2.3.4. Part 4. In the final part of the algorithm the column pointer \( \text{jcS} \) is finalized by an accumulating sum. Since there is a dependency between \( \text{irank} \) and \( \text{jcS} \), the former must be updated analogously.

Listing 7. Part 4: finalize intermediate format

```
// accumulate pointer to columns
for (int c = 2; c <= N; c++) jcS[c] += jcS[c-1];

// irank must account for the previous accumulation
jcS--; /* (again, unit-offset in jj) */
for (int i = 0; i < len; i++) irank[i] += jcS[jj[i]];
jcS++;
```

Example. The final part of the algorithm transforms our running example into

\[ \text{irank} = [5 \ 6 \ 0 \ 8 \ 1 \ 0 \ 9 \ 6 \ 2 \ 5 \ 3 \ 4 \ 7], \]
\[ \text{jcS} = [0 \ 3 \ 5 \ 7 \ 10]. \]

While \( \text{rank} \) is a permutation, \( \text{irank} \) is a combination and has no inverse. However, if we define \( \text{JJ} \) by executing the assignment

\[ \text{JJ}[\text{irank}[i]] = \text{jj}[i], \]

from \( i = 0 \) and upwards, then,

\[ \text{JJ} = [1 \ 1 \ 1 \ 2 \ 2 \ 3 \ 3 \ 4 \ 4 \ 4]. \]

That is, \( \text{irank} \) has sorted the data according to columns and detected all collisions in the process. Note also that, as required, \( \text{JJ} \) is indexed by \( \text{jcS} \).

2.4. Complexity. The assembly process clearly has a memory bound character and the single most important complexity metric is therefore the number of memory accesses made. Since sparse matrices are used to avoid excessive memory use, it is also of interest to look at the amount of working memory allocated. We estimate these both characteristics in turn.

Thanks to the deterministic character of all loops, it is straightforward to determine the number of memory accesses; this amounts to little more than just counting the pointer evaluations in Listings 4–7. The result is found in Table 2.1 and it shows that the number of indirect accesses is about \( SL \) (with \( L := \text{len} \) for brevity), that is, the equivalence of an array of size \( L \) is looped over in random order a total of 8
Table 2.1. Memory access complexity in Listings 4–7 and in terms of $L = \text{len}$. Included is the number of data accesses, the number of indirect (hence possibly non-contiguous) accesses, and the number of indirect accesses to data arrays of size $L$ (assuming $L \gg M, N$).

| Part 1 | $2L + M$ | $L$ | 0 |
| Part 2 | $3L$ | $2L$ | $L$ |
| Part 3 | $5L + M$ | $4L$ | $2L$ |
| Part 4 | $3L + N$ | $L$ | 0 |
| Total | $13L + 2M + N$ | $8L$ | $3L$ |

times. The most common case is that $M$ and $N$ are much smaller than $L$ such that indirect accesses to an array of size $L$ are more expensive than to arrays of sizes $M$ or $N$. For this situation we see that a size $L$ array is looped over randomly a total of 3 times only.

When it comes to allocated memory it is also easy to follow the explicit allocations made by the program. The result is that the maximal allocation will take place in one of two places. The first candidate is in Listing 6 just after the array $\text{hcol}$ has been allocated. Here the equivalence of an integer array of size

$$S_1 = 2N + 1 + M + 1 + 2L$$  \hspace{1cm} (2.4)

has been allocated in total. A second candidate is when the final output has been allocated. Here only the intermediate result array $\text{irank}$ remains allocated and assuming $\text{sizeof(double)} = 2 \times \text{sizeof(int)}$ the effective data size is

$$S_2 = N + 1 + 3nnz + L,$$  \hspace{1cm} (2.5)

where usually $S_2 > S_1$. Hence the maximal memory ever allocated by the algorithm is generally the size of the output plus a size $L$ integer array.

As we will see in §4 these theoretical performance metrics do imply a respectable performance for the algorithm, with about a factor of two times speedup compared to the built-in Matlab version. We now proceed to parallelize the algorithm in a shared memory environment.

3. Parallel sparse assembly in shared memory

In this section we present and analyze the threaded version of the assembly algorithm outlined in §2. The obvious approach to parallelizing the algorithm is to evenly distribute the input data among the cores and perform a local assembly, then finalize the result by summing these local matrices together. We advocate against this for two reasons: the required amount of working memory is substantially larger with this approach and the final gather operation is a quite complicated task in itself. Our OpenMP implementation was developed in an incremental fashion starting from the serial version. After several design leaps along the way the final version achieves a competitive performance as we shall see, while still requiring only a small amount of working memory.
3.1. **Revisited: format of input and output.** The effective input data in Listing 2 is the same in the threaded implementation although the associated code is somewhat more involved, see Listing 16 in Appendix B.

The intermediate output format, however, differs considerably between the two versions. To begin with, for the threaded version a *permuted* version \( \text{irankP} \) of \( \text{irank} \) is preferred. Formally, the arrays are related through

\[
\text{irankP}[\text{rank}]=\text{irank}
\]

for \( i = 0 \ldots \text{len} - 1 \). This implies that (compare (2.2)–(2.3))

\[
\text{irS}[j]=\text{ii}[k]-1, \quad \text{where } (\text{irankP}[i],\text{rank}[i])=(j,k),
\]

\[
\text{prS}[j]=\sum_{i; (\text{irankP}[i],\text{rank}[i])=(j,k)} \text{sr}[k].
\]

As we shall see the main benefits with this seemingly more complicated setup is that (i) it opens up for more parallelism in the post-processing part, and (ii) it simplifies the memory access pattern in Part 3 and 4.

Code for finalizing the representation according to (3.2)–(3.3) is found in Listing 17 in Appendix B. The logic for increasing the degree of parallelism is fairly clear and builds on the fact that \( \text{rank} \) allows for a row-wise traversal; hence data can be distributed according to row indices.

Finally, two minor details present in Listing 8 deserve to be mentioned. Firstly, since \( \text{rank} \) is used in the post-processing part we now need to store the row pointers \( \text{jrS} \) throughout the whole algorithm. Secondly, the algorithm is considerably streamlined when those pointers are kept in thread-private copies. For the same reason this design was also used for the column pointer \( \text{jcS} \).

----

Listing 8. Intermediate output format, parallel version

```c
// rank-array and inverse permuted rank-array
int *rank,*irankP;
rank = malloc(len*sizeof(rank[0]));
irankP = malloc(len*sizeof(irankP[0]));

const int nThreads = omp_get_max_threads();
int **jrS; // row counters, one per thread
jrS = malloc((nThreads+1)*sizeof(jrS[0]));
for (int k = 0; k <= nThreads; k++) {
    jrS[k] = calloc(M+1,sizeof(jrS[k][0]));
    jrS[k]--; /* (unit-offset in ii) */
} /* (final result will appear in jrS[nThreads-1]) */

int **jcC; // column counters, one per thread
jcS = malloc((nThreads+1)*sizeof(jcS[0]));
for (int k = 0; k <= nThreads; k++)
    jcS[k] = calloc(N+1,sizeof(jcS[k][0]));
/* (final result will appear in jcS[0]) */
```
3.2. **An index-based multithreaded algorithm.** The threaded version follows closely the pattern laid out in §2, the main difference being found in Parts 3 and 4 which are now merged into one parallel region.

3.2.1. **Part 1.** Counting rows in parallel is straightforward since each thread has its own local counter. Accumulation has to be done in two steps, the last of which is strictly serial, but which runs over a length $M$ array only (where usually $M \ll L$). A feature with the code in Listing 9 is the final block in which the thread-private pointers $jrS$ are finalized. The format used here supports each thread to continue to process data in a fully independent manner.

**Listing 9. Part 1: count rows, parallel version**
```c
#pragma omp parallel
{
    // count local portion
    const int myId = omp_get_thread_num();
    const int istart = len*myId/nThreads;
    const int iend = len*(myId+1)/nThreads;
    for (int i = istart; i < iend; i++)
        jrS[myId+1][ii[i]]++;

#pragma omp barrier
    // accumulate jrS over the threads
    #pragma omp for
    for (int r = 1; r <= M; r++)
        for (int k = 1; k < nThreads; k++)
            jrS[k+1][r] += jrS[k][r];

    // serial accumulation in jrS[0]
    #pragma omp single
    for (int r = 1; r <= M; r++)
        jrS[0][r+1] += jrS[0][r]+jrS[nThreads][r];

    // determine a private jrS for each thread
    #pragma omp for
    for (int r = 1; r <= M; r++)
        for (int k = 1; k < nThreads; k++)
            jrS[k][r] += jrS[0][r];
} // end parallel
```

3.2.2. **Part 2.** With thread-private pointers to rows available, constructing the rank-array is trivially parallel yet follows the logic of its serial counterpart.

**Listing 10. Part 2: build rank-array, parallel version**
```c
#pragma omp parallel
{
    // rank-array for local portion
    for (int i = istart; i < iend; i++)
        rank[jrS[myId][ii[i]]++] = i;
} // end parallel
```
3.2.3. *Part 3 and 4.* Since each thread may loop over rows independently, the
double for-loop construction in the serial code in Listing 6 can still be used. Thanks to
the modified intermediate output format, with a permuted version \( \text{irankP} \) replacing \( \text{irank} \), the access pattern is actually slightly simplified. The final accumulation
of \( \text{jcS} \) follows closely the logic for \( \text{jrS} \) in Listing 10.

```
Listing 11. Part 3+4: uniqueness and final format, parallel version
#pragma omp parallel
{
    int *hcol; // cache memory for columns
    hcol = calloc(N,sizeof(hcol[0]));
    hcol--; /* (unit-offset in jj) */

    const int rstart = 1+N*myId/nThreads;
    const int rend = M*(myId+1)/nThreads;
    int istart = 0;
    if (rstart > 1)
        istart = jrS[nThreads-1][rstart-1];

    // loop over segment of row indices
    for (int row = rstart,i = istart; row <= rend; row++)
        // loop over single row
        for ( ; i < jrS[nThreads-1][row]; i++) {
            const int col = jj[rank[i]]; // column index

            // new element?
            if (hcol[col] < row) {
                hcol[col] = row; // store row index
                jcS[myId+1][col]++; // count it
            }

            // irankP keeps track of where it should go
            irankP[i] = jcS[myId+1][col]-1;
        }
    free(++hcol);

#pragma omp barrier
    // accumulate jcS over the threads
#pragma omp for
    for (int c = 1; c <= N; c++)
        for (int k = 1; k < nThreads; k++)
            jcS[k+1][c] += jcS[k][c];

    // serial accumulation in jcS[0]
#pragma omp single
{
    for (int c = 1; c <= N; c++)
        jcS[0][c] += jcS[0][c-1]+jcS[nThreads][c];
    jcS[0]--; /* (unit-offset in jj) */
}  
```
3.3. Parallel complexity. The memory complexity of the parallel algorithm can be estimated as before and provides us with some insight. Under the reasonable assumption that the number of threads $p$ is small compared to the other array sizes, for simplicity we ignore all accesses made to size $p$ arrays. Table 3.1 lists the total number of memory accesses performed concurrently.

Compared to Table 2.1 the total number of indirect accesses is the same in the serial and in the parallel version. However, the number of expensive indirect accesses in size $L$ arrays has increased from $3L$ to $4L$ which can be attributed to the final block in Part 4 where there is now one more addressing in the rank-array than before. This is by design as it saves an even more expensive final permutation of $\text{irankP}$ as well as opens up for more parallelism in the final post-processing.

For large enough data sizes the maximal memory allocation occurs when the final data is being allocated and is equal to the equivalent of an integer array of size

$$S_3 = N + 1 + (M + 1)(p + 1) + 3\text{nnz} + 2L.$$  

Compared to the serial memory footprint (2.5) one more size $L$ array is required and we also see the extra allocation of the thread-private pointer to rows $\text{jrS}$.

4. Performance Experiments

In this section we present results of performance experiments of both the proposed serial and parallel algorithms. To get some baseline results for our index-based sorting algorithm we start by profiling our serial version and briefly compare it with the built-in Matlab function $\text{sparse}$. The results for our threaded version
are presented in §4.3, where we look at the speedup for the different parts of the assembly process. Although we clearly observe the bandwidth bound character of the algorithm, the parallel efficiency we obtain is on par with similar algorithms [12]. Thanks to the properties of the proposed index-based algorithm we are able to achieve a significant speedup when compared to the serial implementation.

4.1. **Hardware and benchmark configuration.** We performed our experiments on two different hardware platforms. The first one is a standard workstation based on an Intel Xeon W3680 CPU with 6 cores, 24 GB of memory and 12 MB of cache, and is denoted ‘C1’. The second system is a server with a dual socket Intel Xeon E5-2680 CPU, where each CPU has 8 cores and 20 MB of cache, 64GB of total memory, and is denoted ‘C2’. On both systems we run 64 bit Linux OS; Matlab R2014b (8.4.0.150421) on C1 and Matlab R2012b (8.0.0.783) on C2. To avoid OS noise and caching effects, all tests were performed 40 times and the average time was determined as the arithmetic mean.

There are essentially three parameters which can vary in the input data for the sparse assembly procedure — the dimensions of the output matrix, the number of nonzero elements per row of the output matrix, and the number of collisions per row. Formally, the latter two parameters may of course vary per row according to some empirical distribution. For convenience we considered constant or almost constant values only. While others have benchmarked sparse assembly algorithms using classes of matrices ranging from highly structured to highly unstructured cases [2], on balance we find it difficult to characterize this structure in a meaningful way. Some preliminary tests performed by us using matrices from the UF-collection [6], indicated that the actual structure of the final matrix does not strongly influence the algorithmic performance. We therefore ran all our tests with matrices of random structure relying on uniform random numbers for the indices. In Listing 12 we show the generation of experimental data according to these considerations.

### Listing 12. Benchmark data generator

```matlab
function [ii,jj,ss,siz] = ransparse(siz,nnz_row,nrep)
    % input: size, nonzeros per row, and collisions per final element
    % output: row and column indices, sparse values, and size

    nnz = nnz_row*siz; % number of nonzeros
    ii = repmat((1:siz)',[1 nnz_row]);
    jj = ceil(rand(siz,nnz_row)*siz);
    ii = repmat(ii(:),[1 nrep]);
    jj = repmat(jj(:),[1 nrep]); % (some jj's might be the same)
    p = randperm(numel(ii));
    ii = ii(p);
    jj = jj(p);
    ss = ones(size(ii));
```

For the experiments we focus on three different data sets. All sets consists of 2,500,000 elements of raw input. The first data set is to be accumulated into a sparse matrix with size 10,000 and 50 elements per row (yielding effectively 500,000 nonzero elements in total). The next two data sets are larger in terms of matrix size,
but data set #2 contains less collisions and data set #3 contains more collisions than nonzero elements per row. The configuration is presented in Table 4.1.

| Set   | matrix size | nnz | collisions |
|-------|-------------|-----|------------|
| Data 1| 10,000      | 50  | 50         |
| Data 2| 50,000      | 50  | 10         |
| Data 3| 50,000      | 10  | 50         |

Table 4.1. Benchmark data sets. Number of nonzeros per row and number of collisions per nonzero element.

These data could mimic different problems. For example, with finite element methods in 3D and higher order elements, the matrices contain a relatively large number of nonzero elements per row and the collision pattern and resulting number of nonzero entries per row will be fairly large (as in data set 1). The second data set could mimic high-dimensional problems discretized with a lower order element, and the last data set represents problems in low spatial dimension but modeled again by higher order elements. However, the reader could map various other scenarios from stochastic processes, data mining, and so on to similar data sets. As a concrete example, a Laplace problem in 3D with linear Lagrange elements and discretized with tetrahedron elements results in 12–48 collisions and about 7 nonzero elements per row.

4.2. Serial assembly. In order to facilitate the understanding of the parallel behavior of the proposed index-based sorting algorithm, we start with profiling each part of the serial code. As expected the different data sets put somewhat different loads at each section of the code, see Figure 4.1.

The behavior observed in the figure can be explained fairly intuitively as follows. If the problem contains more nonzero elements per row (relative to the matrix size), then this puts extra pressure on the post-processing procedure (Listing 17 in Appendix B) since it needs to perform more reduction operations. As a by-product to this, naturally, the other parts take less time in a relative sense. An important feature with the proposed parallel algorithm is that the reduction of duplicate elements can be done in a fully independent manner. This allows us to perform this computation completely in parallel without any locks or atomic operations. Counting the number of nonzero elements (Part 1) takes under 5% for all data sets and is proportional to the size of the matrix and to the number of collisions per row. The operations for achieving uniqueness (Part 2 and 3) using row-wise traversal via \texttt{rank} are more expensive for matrices with large number of collisions per row. The performance of the serial \texttt{fsparse} can of course vary between CPUs, however, the relative time for each part is likely to remain fairly stable with fluctuations mainly due to different cache configurations.

Although we do not have access to Matlab’s built-in \texttt{sparse} function, by monitor the processes we can conclude that this function is serial. Loren Shure in a blog-post explains that \texttt{sparse} is based on quicksort [16]. She remarks that quicksort has a higher complexity compared to other algorithms such as bucket sort, but argues that it performs fairly well in practice. For all tests performed here, our proposed serial version outperforms Matlab’s \texttt{sparse} convincingly, see Table 4.2.
4.3. **Parallel assembly.** Due to the fact that essentially all operations in the sparse assembly process are memory bounded, it is unreasonable to expect a linear speedup even in the ideal case. The reason is that the memory bus of the CPU can be utilized efficiently already with a single core, hence additional memory accesses associated with an increasing number of cores can generally not utilize the bandwidth to linear scaling. Following the STREAM benchmark test suite [13, 14], a very simple parallel copy function can demonstrate this phenomenon,

```c
#pragma omp parallel for
for (int j = 0; j < N; j++) a[j] = b[j];
```

With $N = 100,000,000$ this bandwidth test shows that the OpenMP section can speedup the copy up to $4.3\times$ on the workstation (using 6 threads/cores) and up to $6.3\times$ (using 16 threads) on the dual socket server. However, this is only a pure streaming test which does not take into account the cache — with more cores the aggregated cache is, of course, larger.

Before starting the actual assembly, the function determines the maximum values of the index arrays and converts them to integers (Listing 16 in Appendix B). This operation contains only contiguous memory accesses and is purely parallel. Thus the speedup for this function does not depend on data and is around $7\times$ (on C2), see Figure 4.3. Note that Figures 4.1 and 4.2 present only the fraction of the total time, while the actual measured speedup of course also takes into account the real execution time.

For both implementations, Part 1 takes below 5% of the total execution time. The parallelism in this part and thus the total speedups depend mainly on the size of the matrix, due to the fact that all loops are performed over rows, and where the reductions are computed element-wise per thread.
The situation is similar for the computation of the forward mapping, the rank-array (Part 2). The whole computation is basically a single loop over all input entries and since the indirect mapping depends on the number of rows in the resulting matrix, the overhead of looping over a larger matrix reduces the speedup due to additional memory accesses.

In the parallel version we combine Part 3 and 4 into one. Although the memory access pattern is complex, the number of contiguous and indirect memory accesses are proportional to the total size of the input data arrays. Thus, the speedup factors for all test cases are in fact similar, around 5×.

All speedup factors, for all parts of the code, are presented in Figure 4.3. The overall speedups comparing the serial and parallel versions are 4.7×, 6.3× and 4.0× on C2.

The final accumulation of the results (Listing 17 in Appendix B) heavily depends on the number of nonzero elements which need to be computed. Thanks to the fact that with our approach all of the main computations can be performed in parallel, for all data sets this computation takes between 25–35% of the total time. Thus, we observe that the OpenMP implementation gives the highest speedup for the problem with the most nonzero elements per row (normalized by the matrix size).

Finally, we also briefly compare the full parallel fsparse against the built-in Matlab sparse. The results are presented in Table 4.2 for hardware C1 and C2. Our implementation outperforms the Matlab version by 4–5× on C1 and 9–10× on C2.

5. Conclusions

In this paper we devised an index-based implicit sorting algorithm for the assembly of sparse matrices in CCS format given raw index-triplet data. The algorithm
was shown to be efficient in terms of memory accesses and does not require much auxiliary memory. We also showed how the algorithm could be modified and parallelized on multicore CPUs with shared memory. The characteristic in terms of memory accesses for our parallel version is reminiscent of the serial one and results in a good overall performance. As shown by our experiments, compared to the standard serial Matlab implementation, we are able to assemble a matrix up to 10× faster on a dual-socket system and about 5× faster on a 6 core system.

The approach taken in the code is a good example of how to avoid locks by computing and storing slightly more temporary results, resulting in a more streamlined parallel implementation and a higher efficiency.

5.1. **Reproducibility.** Our implementation of fsparse as described in this paper is available for download via the first author’s web-page\(^2\). The code comes with a

\(^2\)http://user.it.uu.se/~stefane/freeware
convenient Matlab mex-interface and along with the code, automatic Matlab-scripts that repeat the numerical experiments presented here are also distributed.

The matrix assembly functions in the PARALUTION\textsuperscript{3} library (ver.0.7.0) are based on this implementation. PARALUTION is a library for iterative sparse methods targeting multicore CPUs and accelerators.

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\textsuperscript{3}http://www.paralution.com
Appendix A. Additional serial codes

The identical code producing \( jj \) and \( N \) has been omitted for brevity.

Listing 13. Pre-processing: input of index \( ii/jj \)

```c
const double *ival = mxGetPr(I); // Matlab input vector I
int *ii = malloc(len*sizeof(int));
int M = 0;
for (int i = 0; i < len; i++) {
    // error: bad index
    if (ival[i] < 1.0 || ival[i] != ceil(ival[i])) return false;
    if ((ii[i] = ival[i]) > M) M = ival[i];
}
```

Listing 14. Post-processing: finalize CCS format

```c
for (int i = 0; i < len; i++) {
    irS[irank[i]] = ii[i]-1; // switch to zero-offset
    prS[irank[i]] += sr[i];
}
```
void sparse(const int *ii, const int *jj, const double *sr,
            int len, int M, int N)
{
    // output
    int *jcS; // column pointer for sparse matrix S
    int *irank; // inverse rank array of length len

    int *jrS; // accumulated "pessimistic" row counter
    int *rank; // rank-array for rows
    int *hcol; // cache memory for columns

    // Part 1: count and accumulate indices to rows
    jrS = calloc(M+1, sizeof(jrS[0]));
    for (int i = 0; i < len; i++) jrS[ii[i]]++;
    for (int r = 2; r <= M; r++) jrS[r] += jrS[r-1];

    // Part 2: build rank with the active use of jrS
    rank = malloc(len * sizeof(rank[0]));
    jrS--; /* (unit-offset in ii) */
    for (int i = 0; i < len; i++) rank[jrS[ii[i]]++] = i;

    /* Part 3: loop over input and make each column unique with respect
       to rowindices, building both an index vector irank and the final
       column pointer at the same time */
    jcS = calloc(N+1, sizeof(jcS[0]));
    hcol = calloc(N, sizeof(hcol[0]));
    hcol--; /* (unit-offset in jj) */
    irank = malloc(len * sizeof(irank[0]));
    for (int row = 1, i = 0; row <= M; row++)
        for (; i < jrS[row]; i++) {
            const int ixijs = rank[i]; // index into input data triplet (ii,jj,sr)
            const int col = jj[ixijs]; // column index

            // new element?
            if (hcol[col] < row) {
                hcol[col] = row; // remembered by the row index
                jcS[col]++; // count it
            }

            // irank keeps track of where it should go
            irank[ixijs] = jcS[col]-1;
        }
    free(++hcol);
    free(rank);
    free(++jrS);

    // Part 4: accumulate pointer to columns
    for (int c = 2; c <= N; c++) jcS[c] += jcS[c-1];

    // irank must account for the previous accumulation
    jcS--; /* (again, unit-offset in jj) */
}
for (int i = 0; i < len; i++) irank[i] += jcS[jj[i]];
jcS++;

#include <algorithm>

for (int i = 0; i < len; i++) irank[i] += jcS[jj[i]];
jcS++;

/* allocate output and insert data: code not shown */

// deallocate intermediate format
free(irank);

APPENDIX B. ADDITIONAL PARALLEL CODES

Listing 16. Pre-processing in parallel

const double *ival = mxGetPr(I); // Matlab input vector
int *ii = malloc(len*sizeof(int));
int M = 0;
#pragma omp parallel shared (M)
{
    int myM = M; // local version of M
    #pragma omp for
    for (int i = 0; i < len; i++) {
        if (ival[i] < 1.0 || ival[i] != ceil(ival[i]))
            ok = false; // no harm in continuing
        else if ((ii[i] = ival[i]) > myM)
            myM = ival[i];
    }

    if (M < myM)
        #pragma omp critical
        // ensure nothing changed, then make the swap:
        if (M < myM) M = myM;
} // end parallel

Listing 17. Post-processing in parallel

#pragma omp parallel
{
    const int myId = omp_get_thread_num();
    const int rstart = 1+M*myId/nThreads;
    const int rend = M*(myId+1)/nThreads;
    int istart;
    if (rstart == 1)
        istart = 0;
    else
        istart = jrS[nThreads-1][rstart-1];

    if (rend >= 1) {
        for (int i = istart; i < jrS[nThreads-1][rend]; i++)
            irS[irankP[i]] = ii[rank[i]]-1;
        for (int i = istart; i < jrS[nThreads-1][rend]; i++)
            prS[irankP[i]] += sr[rank[i]];
    }
} // end parallel

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