Model-guided Performance Analysis of the Sparse Matrix-Matrix Multiplication

Tobias Scharpf*, Klaus Iglberger†, Georg Hager* and Ulrich Rüde*

*Chair for System Simulation, University Erlangen-Nuremberg, Erlangen, Germany
Email: {tobias.scharpf,klaus.iglberger,uli.ruede}@fau.de
†Erlangen Regional Computing Center, University Erlangen-Nuremberg, Erlangen, Germany
Email: georg.hager@fau.de

Abstract—Achieving high efficiency with numerical kernels for sparse matrices is of utmost importance, since they are part of many simulation codes and tend to use most of the available compute time and resources. In addition, especially in large scale simulation frameworks the readability and ease of use of mathematical expressions are essential components for the continuous maintenance, modification, and extension of software.

In this context, the sparse matrix-matrix multiplication is of special interest. In this paper we thoroughly analyze the single-core performance of sparse matrix-matrix multiplication kernels in the Blaze Smart Expression Template (SET) framework. We develop simple models for estimating the achievable maximum performance, and use them to assess the efficiency of our implementations. Additionally, we compare these kernels with several commonly used SET-based C++ libraries, which, just as Blaze, aim at combining the requirements of high performance with an elegant user interface.

For the different sparse matrix structures considered here, we show that our implementations are competitive or faster than those of the other SET libraries for most problem sizes on a current Intel multicore processor.

I. Motivation

Various popular simulation algorithms in high performance computing (HPC), such as computational dynamics for rigid bodies, rely on sparse matrix-matrix multiplication (spMMM) as one of their computational kernels. Due to its central role in the applications and its computational complexity it is of vital importance to have highly optimized implementations. However, apart from performance, other metrics such as programmability, readability and foremost maintainability are crucial for a successful long-term software development effort. Yet these metrics usually play only a minor role in HPC software development. Although there exist several approaches to provide fast spMMM implementations, these libraries, like most HPC software efforts, strictly focus on high performance but do not so well in most other software metrics (see also [1]). This neglect especially endangers complex, long-term software developments due to impeded maintenance work. However, the maintainability of software should be of major interest: on average, 60% of the total software development costs is spent in maintenance, where long-term projects usually lean towards higher maintenance costs [2]. Improving the maintainability immediately leads to less effort in software modification and extension and subsequently to fewer software defects.

This realization is the driving force behind several C++ Smart Expression Template (SET) math libraries. These libraries attempt to combine highly optimized math kernels for vector and matrix operations with the advantages of a domain-specific language. They include an intuitive formulation of mathematical operations, high readability, and easy modification of operations (see for instance Listing 1).

In this paper we focus on the optimization of the sequential spMMM algorithm in the Blaze SET library, and compare the resulting performance characteristics for two chosen sparse matrices with similar high-performance SET-based frameworks. It will be clear that such a comparison can only make sense when the analysis is performed over a wide range of problem sizes, which rules out an extensive survey of popular matrix collections. We recognize that such a survey would be desirable. In this work we prefer a deeper analysis with more insight, however, and leave the survey to future research.

This paper is organized as follows. In Section II we give a short overview of other C++ math libraries that follow an approach similar to Blaze, before Section III briefly summarizes the details of our benchmark platform and benchmarking strategy. In Section IV we describe basic tasks and necessary steps for spMMM, together with appropriate performance models. Here we also demonstrate the general suitability of the SET methodology for HPC in terms of performance and the advantages in terms of software development. The optimized kernels are benchmarked and compared to several other SET-based C++ math libraries in Section V. Section VI concludes the paper and provides suggestions for future work.

II. Related Work

The C++ programming language provides the feature to directly overload mathematical operators, which enables a very intuitive application of mathematical operations. However, due to the necessary creation of a temporary in each operation, the performance of classic C++ operator overloading cannot compete with other approaches. A reputed solution are Expression Templates (ET), which due to lazy evaluation...
of the result promise optimized performance. The first ET-based C++ library for dense arithmetic was Blitz++ \[1\]. This framework, written by the inventor of ETs, Todd Veldhuizen, has been recognized as a pioneer in the area of C++ template metaprogramming \[4\]. The Boost uBLAS library \[5\] is one of the most widespread ET math libraries since it is distributed together with the Boost library \[6\]. In contrast to Blitz++, it additionally provides sparse matrices and vectors. However, in \[1\] we have demonstrated that the assumption that ETs are a performance optimization is not justified, and have introduced an improved solution by the Smart Expression Template (SET) methodology. Among other features, SETs encapsulate performance-optimized compute kernels like those provided by the BLAS and LAPACK standards. An early example for a SET library is Armadillo \[7\], which is restricted to dense linear algebra operations, but employs SETs to integrate BLAS and LAPACK for optimized performance. The same feature is provided by MTLA, which additionally includes sparse matrix operations. An alternative with similar functionality is the GMM++ library \[8\], which allows to use ATLAS \[9\] as BLAS backend. Numerics involving dense and sparse matrices and vectors, the use of optimized kernels, and the advanced SET features of intrinsics-based vectorization of non-BLAS operations and automatic expression optimization are supported by the Eigen3 \[10\] and the Blaze \[11\] libraries. In contrast to Eigen3, which provides optimized kernels for all basic operations, Blaze uses BLAS subroutines for BLAS level 2 and 3 operations.

In \[1\] we have analyzed several of these ET implementations in detail and have introduced the notion of SETs and our SET library Blaze in particular. In \[12\] we have extended our analysis to more ET-based libraries, focused on the optimization and vectorization capabilities for dense arithmetic, and presented performance results for the CG algorithm, which is fundamental for many applications. In this work we expand our analysis to sparse arithmetic and the sparse matrix-matrix multiplication (spMMM) in particular.

Much work has been devoted to sparse matrix based algorithms and efficient implementations in the past. However, most publications deal with parallel sparse matrix-vector multiplication \[13\], \[14\], \[15\], since it is of pivotal importance in solving sparse linear systems and sparse eigenvalue problems. While there has also been substantial work on sparse matrix-matrix multiplication, it mostly deals with execution and communication efficiency in the parallel case \[16\], \[17\]. Here, however, we only cover the sequential kernel any try to understand its features in a well-defined setting, and especially in the context of SET frameworks. Consequently, issues of load and communication balancing, which would be crucial in the parallel case, do not arise.

### III. Benchmark Platform and Test-Cases

An Intel Sandy Bridge i7-2600 CPU was used for all benchmarks. Using only one of the four cores it runs at 3.8 GHz with 8 MB of shared L3 cache, 256 KB of L2 cache and 32 KB of L1 data cache. The maximum achievable main memory bandwidth (as measured by the STREAM benchmark \[18\]) is about 18.5 GB/s. For each non-zero element of a sparse matrix we store the value as double precision floating point number and an index as a 64-bit integral value. Since we concentrate on general sparse matrices and there is no vector gather instruction in current x86 designs, we do not utilize SIMD vectorization but run scalar code. This means that the CPU is capable of performing one double precision floating point multiplication and one double precision floating point addition as well as either two load or one load (LD) and one store (ST) instruction per cycle \[19\]. Therefore the theoretical peak performance is 7.6 GFlop/s.

The benchmark platform runs an openSuse 12.1 and we use the GNU g++ compiler with the following compiler flags: `-Wall -Werror -ansi -pedantic -O3 -mavx -DNDEBUG`

We use the Blazemark benchmark suite, which ships with Blaze, for a direct comparison of the different libraries. It uses the same random seed for all libraries and care is taken that randomly generated numbers and structures are identical for all tested libraries. We extended the Blazemark to have the option to compare not only different libraries but also multiple implementations of the Blaze spMMM kernels. To make sure that all measured times are accurate the Blazemark runs short test-cases several times until the total runtime exceeds two seconds. Furthermore, each test is performed at least 5 times and the best result is taken as the final measurement. The number of floating point operations per second (Flops/s) for the spMMM are calculated as follows: The number of required multiplications is

\[
\sum_{k=0}^{n-1} \tilde{a}_k \ast \tilde{b}_k,
\]

where \(\tilde{a}_k\) is the number of non-zeros in the \(k\)-th column of \(A\), and \(\tilde{b}_k\) is the number of non-zeros in the \(k\)-th row of \(B\). The number of additions required is always bounded by the required number of multiplications. We always use the worst case assumption to calculate the Flops, which means that the overall number of floating point operations is approximately twice the number of multiplications.

Two different input matrices over a range of problem sizes are used to review the outcome of our analysis. The first test-case multiplies two five-band matrices, which are created by using a 5-point stencil resulting from a finite difference discretization of a Dirichlet boundary value problem on a square. All graphs showing the result of multiplying two of these five-band matrices are marked with (FD). The second test-case uses two randomly generated quadratic matrices. For each matrix five random numbers are placed on random locations in each row. This allows for a good comparability between the two test-cases in terms of the fill rate of the matrices. Whenever a graph shows the outcome of the multiplication of two randomly generated matrices it is marked with (random).
IV. IMPLEMENTATION AND PERFORMANCE ANALYSIS OF THE spM MM KERNEL

For a thorough analysis it has turned out to be convenient to split the spMMM kernel in two logically independent parts: The pure computation and the actual storing of the results.

A. The pure spMMM computation kernel

Looking only at the pure computation of the spMMM allows to implement this part of the kernel and be sure that it works at the highest possible performance without any interference of additional data accesses for storing the result. In Blaze we use implementations of the two well known formats “compressed sparse row” (CSR) and “compressed sparse column” (CSC) [20]. These formats usually show good performance for general matrices on general-purpose cache-based microprocessors. Both formats use an array of pointers, which provides an immediate access to a specific row (CSR) or column (CSC).

The classic way of calculating a matrix-matrix product $C = A \ast B$ is to perform a dot product-like operation between a row of $A$ and a column of $B$ for each element in the resulting matrix. To achieve optimal performance with this approach, the format should be CSR for matrix $A$ and CSC for $B$, while the format of $C$ is irrelevant. The problem is that both vectors are sparse and therefore the operation suffers from all known issues of sparse vector-vector multiplications. Furthermore the results of these “dot products” are zero most of the time. Optimizations such as unrolling or blocking, which would lead to increased computational intensity [21], [14], rely on exploiting specific matrix structures and will not be explored here.

Another algorithm, optimized for a set of three CSR or three CSC matrices, was introduced in [22]. As shown in Figure 1 it multiplies each non-zero value $a_{r,c}$ of row $r$ of matrix $A$ with all non-zero entries $b_{c,s}$ of matrix $B$. The intermediate results are collected in a dense temporary vector, which is initially filled with zeros, by just adding each result to the current value at the position $x$ of the temporary vector. If this is done for all non-zero values of row $r$ of matrix $A$, the vector is a dense representation of the $r$th row of the resulting matrix. Note that the approach can also be applied to column-major matrices in the spMMM with three CSC matrices.

Figure 1: Sketch of a spMMM with the row-major algorithm.

In case one of the two matrices is available in CSR format and the other in CSC format it turns out to be more efficient to convert one of the matrices to the other format instead of providing a fallback to the “classic” algorithm. The effort to convert the format is linear in the number of non-zero entries. Therefore it is not necessary to implement a total of eight computation kernels for all eight possible combinations. It is sufficient to convert one of the two matrices to be able to use the row-major or column-major algorithm.

In order to arrive at a realistic upper performance limit for our computational kernels we employ a simple bandwidth-based performance model [23], [21]: The maximum performance for a loop is

$$ P = \max \left( P_{\text{max}}, \frac{b_{\text{max}}}{B_c} \right), $$

where $b_{\text{max}}$ is the bandwidth of the relevant data path in bytes/s and $B_c$ is the loop’s code balance:

$$ B_c = \frac{\text{Data traffic [Bytes]}}{\text{Floating point operations [Flops]}} $$

This model works well if the performance of the loop is dominated by the data transfers to and from a single data path. Other effects, such as dependencies, abundant branch mispredictions, or the general inability of a single core to saturate the bandwidth of some memory hierarchy levels, may cause significant deviations from the model [24]. However, it is still a valuable starting point for a loop-based performance analysis, since it provides a “light speed” estimate. We concentrate here on modeling the more advanced implementations of the spMMM kernel, since the naive version is plagued by conditional branches and erratic access patterns, which are not easily modeled.

Listing 2: The row-major computation kernel without storing the result to the matrix $C$.

```cpp
void compute(
    CSRMatrix& C, 
    const CSRMatrix& A, 
    const CSRMatrix& B )
{
    typedef CSRMatrix::const_iterator iterator;

    // Estimate the number of elements in matrix C
    nnzEstimation( C, A, B );

    // Temporary vector to store the result row-wise
    std::vector<double> temp( C.columns(), 0.0 );

    // Loop over all rows of the target matrix
    for( std::size_t cy = 0; cy < C.rows(); ++cy )
    {
        iterator ait( A.begin(cy) );
        iterator aend( A.end(cy) );

        // Loop over the non-zero entries of the
        // current row of A
        for( ; ait!=aend; ++ait )
        {
            std::size_t const indexA( ait->index() );
            double const valueA( ait->value() );

            iterator bit( B.begin(indexA) );
            iterator bend( B.end(indexA) );

            // Loop over the non-zero entries of the
            // current row of B
```
Listing 2 shows the code for the row-major computation kernel. The inner loop between lines 32 and 39 has a code balance of 16 Bytes/Flop. We assume that the update to the temp[] vector causes a load and a store to the relevant memory hierarchy level, but ignores non-consecutive accesses, which would lead to excess data traffic. Hence, the predictions of the balance model must be seen as best-case values. Within the L1 cache this leads to a maximum theoretical performance of 3800 MFlops/sec at 3.8 GHz clock frequency, whereas in memory the limit is 1140 MFlops/sec.

Figure 2 shows performance results versus problem size (number of matrix rows) for the 5-point finite difference stencil matrices. The row-major algorithm (CSR × CSR) clearly achieves the best results for CSR × CSR and even comes close to the theoretical performance of 1140 MFlops/sec beyond the L3 cache limit. Even if the right-hand side operand is given as a CSC matrix and is therefore internally converted to CSR (CSR × CSC (with conversion)), still about 50% of the original performance is achieved. The classic CSR × CSC kernel cannot compete with the the row-major approach due to the problems mentioned before. The fact that the row-major algorithm’s performance only drops slightly for matrices that do not fit into the L3 cache anymore shows that the balance model is problematic for in-cache situations, and more advanced modeling techniques would be required [24]. All data of the left-hand side matrix is traversed with stride one. For the right-hand side operand the prefetcher can easily predict which data to load, thanks to the fixed five-band pattern of the matrix.

Figure 3 shows the results for the test case which uses randomly generated spares matrices. The classic CSR × CSC algorithm is not influenced by the structure of the matrices and therefore shows the same bad performance we saw in Figure 2. The row-major approach clearly achieves better results. However, because of the random structure of the left-hand side operand the prefetcher does not work optimally for the right-hand side matrix; thus, performance goes down with growing problem sizes. The classic approach does not show any significant performance for problem sizes greater than \( N = 200 \). Compared to this the row-major approach shows a much better performance even for huge matrices that do not fit into the L3 cache anymore, and also if the right-hand side matrix has to be converted to the other format. Due to the cache-unfriendly access patterns the calculated performance limits cannot nearly be reached for this matrix.

Note that the general guideline to have a regular matrix structure for best performance is valid predominantly in view of the left-hand side matrix \( A \); the performance is largely independent of the structure of \( B \).

B. Storing the spMMM result

The algorithm in Listing 2 only calculates all the entries for the result matrix, but never actually stores them to the object. Therefore all further optimization is driven by the requirement to access the memory when storing the result in the most efficient way.

In this context, estimating the number of non-zero entries in the resulting matrix is an essential aspect. It is of highest importance to prevent frequent dynamic memory allocations during the calculation. Therefore an estimation of the final number of non-zero entries is required that never underestimates and, if possible, only slightly overestimates the needed memory. We found that the number of multiplications required to perform the spMMM (see III) is a good estimate. Each intermediate result either takes a place which is still zero or is added to another intermediate result. Due to this fact the number is always equal or higher than the number of non-
zeros in the resulting matrix. Using this estimation the memory allocation is only done once at the beginning of the kernel.

Another performance-critical part is the interface for storing the values in the resulting matrix. Our implementation of the CSR/CSC formats provides two low-level functions for this. First the append function, which appends an entry. It is the programmer’s responsibility to append values in increasing row order and, within each row, in increasing column order. The second function is finalize, which marks the end of a row after all values have been appended. It has to be called after each row and leaves the matrix in a consistent state (note that the CSC format is handled accordingly). Streaming the results in this way has the advantage that all the values are stored in one successive memory block, and the underlying data structure for the row access is only modified once per spMMM.

We have shown above that the row-major algorithm (see Listing 2) is very efficient. It calculates a dense representation of each result row, which subsequently has to be stored in the sparse result matrix. However, the way the temporary vector is converted to a sparse row is crucial. A first alternative is a brute force approach, which iterates over the double values of the temporary vector and appends all non-zero values to the resulting matrix (“Brute Force”-double). To reduce the amount of memory that has to be traversed the second approach is to use an additional lookup vector, either of type bool (“Brute Force”-bool) or char (“Brute Force”-char). In the STL a std::vector<bool> is implemented as a bit field [25] and can therefore hold information for 512 positions per cache line instead of 8 doubles or 64 chars. Figure 4 shows the performance results for the CSR × CSR “brute force” kernels for the 5-point finite difference stencils and Figure 5 shows the corresponding results for the randomly created matrices.

**Figure 4:** Comparison of different “Brute Force” and “MinMax” kernels (FD) for the complete spMMM.

Despite the fact that “Brute Force”-bool accesses the least memory it has to perform additional Boolean operations for each entry, which leads to the worst performance in both cases. Also in both cases the additional char vector increases the performance slightly compared with the “Brute Force”-double approach without die additional lookup vector. Also shown are our “MinMax” kernels, which basically do the same as the “Brute Force” kernels, but additionally keep track of the lowest and highest index of the non-zero entries in the temporary vector. Especially in the test-case with the five-band matrices this optimization gives a considerable performance boost. Notably, using the additional char vector hurts the performance of “MinMax” considerably. With the “MinMax” kernel each checked entry of temporary vector is more likely a non-zero value and therefore the advantage of the lookup vector is not big enough to compensate the extra effort.

Even though the “MinMax” approach is better than “Brute Force,” both influence the performance significantly. In addition, the bigger the problem sizes the more the performance suffers compared to the pure computation kernel. With the problem size also the length of the temporary vector and the number of elements in the minimum-maximum range increases, but the absolute number of non-zeros does not change significantly.

The next approach is to store all indices for non-zero elements within a row in a separate vector, which is usually small enough to fit into any cache level. After the complete row is calculated the few entries of the vector that hold the indices are sorted using std::sort, and then only these positions of the temporary vector are appended to the resulting matrix. Figure 6 shows the performance results for the CSR × CSR for the five-point finite difference stencils with the sorting kernel (Sort) and Figure 7 illustrates the corresponding results for the test-case with the randomly generated matrices. It shows that the performance drawback of the sorting approach does not significantly increase with the problem size.

**Figure 5:** Comparison of different “Brute Force” and “MinMax” kernels (random) for the complete spMMM.

For both test-cases the “MinMax” approach still performs better at small problem sizes. Hence, the final approach is to combine the “MinMax” and “Sort” kernels to the new “Combined” kernel. The decision which of the two storing strategies to use is performed for every single row. Note that it is more important that the decision can be done quickly than that it is precise, as it is performed for every row separately. The current implementation uses “MinMax” if its region is...
smaller than twice the number of non-zero values in this row and “Sort” in all other cases. In Figure 7 the switch from “MinMax” to “Sort” is clearly visible between $N = 49$ and $N = 64$. We found that as long as the storing method is not about to change, the “Combined” kernel is at most 5% less efficient than the kernels with only a single strategy. Overall, the “Combined” kernel reaches 35% of the pure computation performance for the CSR $\times$ CSR test case using the five-point finite difference stencils.

All previously shown test-cases used matrices with a fixed number of non-zero entries in each row. This means that the fill ratio decreases with increasing problem size. The benchmark shown in Figure 8 uses the same matrix generation algorithm as for the random case, but the fill ratio is 0.1% for each row instead of the fixed five elements. With the increasing absolute number of non-zero entries in each row the fill ratio of the result matrix increases. At $N \approx 38000$ the “MinMax” approach exceeds the performance of the “Combined” kernel, which uses the “Sort” storing strategy. At this point the fill ratio of the result matrix is 3.7% or about 1400 non-zero entries per row. For the “MinMax” kernel this means that on average every third cache line loaded actually contains one non-zero entry. Our conclusion is that there is a break-even point in terms of problem size for which the “MinMax” approach is faster than sorting because of the growing probability that loaded data is actually stored in the result matrix.

V. PERFORMANCE COMPARISON OF SET LIBRARIES

In this section we compare the performance of the Blaze library to other expression template based C++ libraries. We selected the most common libraries that provide the according kernels for the multiplication of two CSR matrices and the multiplication of a CSR and a CSC matrix. We use the Boost uBLAS library in version 1.51, MTL4 in version 4.0.8883 (open source edition), Eigen3 in version 3.1.1, and Blaze in version 1.1, the latter employing the fastest “Combined” kernel from Section IV-B. All libraries were benchmarked as given. We only present double precision results in MFlop/s graphs for each test case. For all in-cache benchmarks we make sure that the data has already been loaded to the cache.

Figure 9 shows the comparison of the results of the CSR $\times$ CSR kernels for sparse matrices resulting from five-point finite difference stencils. The Blaze library achieves roughly twice the performance of Eigen3 and MTL4. uBLAS cannot compete with the others, since it abstracts from the actual storage order of the operands and traverses the right-hand side operand in a column-wise fashion despite it being stored in row-major order. It becomes apparent that with a proper implementation of the kernel the size of the matrix hardly influences the performance. Only a small drop can be observed for matrices that do not fit into the L3 cache anymore and have to be loaded from main memory.

Figure 10 summarizes the results for the CSR $\times$ CSR kernels for randomly created sparse matrices. Again, Blaze shows a higher performance than the Eigen3 and MTL4 libraries, and uBLAS falls far behind. In comparison to sparse matrices resulting from finite difference stencils, though, the performance clearly depends on the size of the matrix and degrades with growing matrix sizes.

The results for the CSR $\times$ CSC kernels for sparse matrices resulting from five-point finite difference stencils are presented
in Figure 11. The performance of the Blaze and MTL4 libraries drop due to the creation of a temporary CSR matrix and converting the storage order of the right-hand side operand. The performance of Eigen3 slightly increases in comparison to the CSR × CSR kernel. Also the performance of the uBLAS library increases since the strategy of multiplying a row and a column fits the given storage orders. However, still the performance drops quickly with growing problem size and prohibits the multiplication of large sparse matrices.

Finally, Figure 12 shows the results for CSR × CSC kernels for random sparse matrices. Again, the performance of the Blaze and MTL4 libraries drop to the creation of a converted temporary and the performance of Eigen3 slightly increases. Consequently, the performance of Eigen3 can even surpass the Blaze performance for medium-sized matrices. For small and large sparse matrices Blaze exhibits the best performance.

VI. CONCLUSION AND FUTURE WORK

We have conducted the first thorough performance analysis of several spMMM kernels on a modern standard processor. Employing a simple performance model we have demonstrated that our implementations can come close to the maximum predicted performance in the computational part of the kernel for out-of-cache situations with matrices leading to streaming memory access patterns. Due to further optimizations in the memory management and storage strategy, we can provide the currently fastest C++-based spMMM as part of the Blaze C++ library. Blaze combines high maintainability, which proves to be of essential importance for large scale software development, with HPC-grade performance that matches or exceeds the capabilities of other commonly used C++ math libraries.

With the single core performance optimized the next step to improve the Blaze library is to include shared memory parallelization to exploit many- and multicore architectures. We expect that the typical contention and saturation effects seen with these architectures will add many new effects to the results presented here. Additionally, more work has to be invested in further improving the single core performance. Exploiting the given structure of the sparse matrix operands might be a possible approach. Alternative sorting algorithms which are better suited to sort short lists of unique integral numbers may also be advantageous. Finally, the decision criterion for which of the two storing strategies to use might be further improved.
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