THE CHUNKS AND TASKS MATRIX LIBRARY 2.0 *

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Abstract. We present a C++ header-only parallel sparse matrix library, based on sparse quadtree representation of matrices using the Chunks and Tasks programming model. The library implements a number of sparse matrix algorithms for distributed memory parallelization that are able to dynamically exploit data locality to avoid movement of data. This is demonstrated for the example of block-sparse matrix-matrix multiplication applied to three sequences of matrices with different nonzero structure, using the CHT-MPI 2.0 runtime library implementation of the Chunks and Tasks model. The runtime library succeeds to dynamically load balance the calculation regardless of the sparsity structure.

Key words. Chunks and Tasks programming model, block-sparse, parallelization, quadtree, sparse matrices, task-based programming

1. Motivation and significance. Computing the product of two matrices is one of the most fundamental operations in scientific computing [13]. Matrix-matrix multiplication is a core operation in for example combinatorics [10], deep learning [9], and electronic structure theory [7, 16]. Other commonly used linear algebra operations such as linear solves, matrix inversions and factorizations are reduced to matrix-matrix multiplications in efficient blocked implementations [12].

In the dense matrix case, efficient software typically makes use of the Basic Linear Algebra Subprograms (BLAS). This makes the code portable and gives high performance when linked to an optimized BLAS library. Parallelization schemes for dense linear algebra problems are often based on static distribution of data, such as the two-dimensional block and block-cyclic mappings of the matrix onto a two-dimensional process grid, for example used in the SUMMA algorithm for parallel matrix-matrix multiplication [20] and the HPL implementation of the HPLinpack benchmark [1], respectively. Since the matrices are dense, all computation and communication costs are known in advance and, in general, the same scheme can be used regardless of the application since the only parameters that may vary are the matrix dimensions.

Software which makes use of parallel sparse matrix-matrix multiplication, on the other hand, often resorts to specialized implementations relying on a priori information about the matrix sparsity pattern for the application at hand. Such implementations can be found in a number of electronic structure codes [14, 21]. Although great performance is often achieved, the benefits of general purpose algorithms and libraries are missing.

A class of general purpose algorithms for parallel sparse matrix-matrix multiplication is based on random permutation of rows and columns of the input matrices, with the purpose to evenly spread out the nonzero entries over the matrix [5, 6, 8]. After the random permutation some method for dense matrices is applied but with the local block products replaced by sparse products. This gives an approach that is generally applicable without need for a priori information about the sparsity pattern, but the cost you have to pay is that the nonzero structure and any data locality is

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destroyed. This inability to exploit the structure of the input matrices has serious consequences for the cost of communication [18].

Without a priori information about the sparsity pattern and without compromising on performance, the mapping of work and data to physical resources has to be done dynamically during the calculation. The development of such schemes directly on top of the standard Message Passing Interface (MPI) is an overwhelming task. This is a reason why one has been unable to combine performance and portability of algorithms and software. The use of some task-parallel framework seems like a viable approach. However, most task-parallel frameworks are primarily developed for shared memory and typically resort to static distribution or centralized management of data when extended to computer clusters with distributed memory.

We present here the Chunks and Tasks Matrix Library which can be used to implement algorithms that do not make assumptions about the structure of input matrices, but efficiently exploits data locality when available. Critical to the development of this library is its use of the Chunks and Tasks programming model [17], which provides abstractions for both work and data, and therefore makes the implementation of locality-aware parallel sparse matrix algorithms feasible. The library is written in C++ and may be used either to parallelize performance critical matrix operations of a C++ program or as part of a full-fledged Chunks and Tasks application.

The Chunks and Tasks Matrix Library has been indispensable in the development, implementation, and analysis of a number of novel parallel sparse matrix algorithms for distributed memory systems, including a general purpose parallel sparse matrix-matrix multiply efficiently exploiting locality of nonzero matrix entries [18], a sparse approximate matrix-matrix multiply for matrices with decay [2, 3], localized inverse factorization [19, 4], a new communication-avoiding divide and conquer method for inverse factorization of symmetric positive definite matrices, and density matrix purification [15].

2. Software description. The Chunks and Tasks Matrix Library is a C++ header-only library, implemented using the Chunks and Tasks programming model. To use the library in your C++ program, you need a Chunks and Tasks runtime library and an implementation of the Basic Linear Algebra Subprograms (BLAS) [11]. Open source Chunks and Tasks library implementations are publicly available at chunks-and-tasks.org.

In the Chunks and Tasks Matrix Library, matrices are represented using sparse quaternary trees (quadtrees) [22]. In this representation a matrix is either 1) identically zero, 2) stored using a data structure for small matrices, or 3) split into four quadrants, each a submatrix recursively represented by a sparse quadtree. Matrix operations are formulated as recursive algorithms traversing nonzero branches of the matrix quadtrees. Quadtrees provide an efficient way to squeeze out zero entries from the representation and to expose parallelism in both data and work.

2.1. Software Architecture. The main components of the library are the following:

- a matrix chunk template implementing the sparse quadtree representation of matrices using the Chunks and Tasks model,
- a number of task templates implementing various recursive algorithms operating on sparse quadtrees using the Chunks and Tasks model,
- and three stand-alone matrix libraries for leaf matrix representation.

The chunk template for quadtree matrix representation is parameterized with a leaf matrix type, used for matrix representation at leaf nodes. This leaf matrix type may
or may not be one of the types distributed with the Chunks and Tasks Matrix Library and may use a sparse or dense representation. A non-leaf node/chunk in the quadtree is the parent of four chunks. Each child chunk is referred to by its chunk identifier and represents a quadrant of the matrix corresponding to that non-leaf node. A Chunks and Tasks nil identifier is used to refer to submatrices that are identically zero.

The task templates for matrix operations are also parameterized with the leaf matrix type. The key component in each task implementation is an `execute` function called by the runtime library to carry out task execution. This function performs operations on a single level in the quadtree. For non-leaf input the `execute` function typically registers tasks operating on children of the input chunks. At the leaf level, leaf matrix functionality corresponding to the given task type is invoked. Matrix sparsity, i.e. zero branches in the quadtree, is handled in a fallback `execute` function, called by the Chunks and Tasks runtime library whenever one of the input matrix chunk identifiers is nil.

Three stand-alone leaf matrix types are distributed with the library, each in a subdirectory with the following names:
- `basic_matrix_lib`: Dense matrix representation using a standard column-wise layout of matrix elements [17].
- `block_sparse_matrix_lib`: Block-sparse matrix representation where submatrices (blocks) of uniform size are laid out in a two-dimensional array [18]. Zero submatrices are neither stored nor referenced.
- `hierarchical_block_sparse_lib`: Sparse quadtree matrix representation resembling the implementation at the Chunks and Tasks level [2].

The quadtree chunk template describes a data structure suitable for parallel distribution of matrices, but does not specify where data should be stored. The task templates for matrix operations describe recursive algorithms suitable for parallel execution, but do not make task scheduling decisions. The leaf matrix libraries distributed with the library are serial, unless linked to a threaded implementation of BLAS. Parallelism is achieved when the library is used together with a parallel implementation of the Chunks and Tasks model.

### 2.2. Software Functionalities

The main functionality provided by the task templates in the Chunks and Tasks Matrix Library, in combination with the leaf matrix types, can be categorized as follows:
- **Assignment from and extraction of matrix elements**: task types to construct a matrix from vectors with row and column indices and values and task types to extract elements of a matrix specified by vectors with row and column indices.
- **Matrix addition**: addition task types including regular matrix addition and addition of a matrix with a scaled identity matrix.
- **Matrix-matrix multiplication**: multiplication task types including regular and symmetric multiplication, symmetric matrix square, and symmetric rank-k construction, as well as sparse approximate multiplication.
- **Inverse factorization**: task types for inverse factorization of symmetric positive definite matrices including inverse Cholesky and localized inverse factorization.
- **Truncation**: task types for removal of small matrix elements with different variants of error control.

All task types are able to handle and exploit matrix sparsity. This list of functionality reflects the fact that the main motivation for the development of the library has been its application to large-scale electronic structure calculations. The library also includes a number of auxiliary task templates not listed here.
Weak scaling experiment setup

| Matrix Size | 10^7 | 2 × 10^7 | 4 × 10^7 | 8 × 10^7 | 1.6 × 10^8 | 3.2 × 10^8 | 6.4 × 10^8 |
|-------------|------|----------|----------|----------|------------|------------|------------|
| No. of worker processes | 2    | 4        | 8        | 16       | 32         | 64         | 128        |

**Banded**

| Size of block | 15716 | 19652 | 24621 | 30899 | 38825 | 48828 | 61446 |
| Tflop | 7.022 | 14.22 | 28.63 | 57.44 | 115.1 | 230.3 | 460.8 |

**Growing block**

| Size of block | 15716 | 19652 | 24621 | 30899 | 38825 | 48828 | 61446 |
| Tflop | 14.04 | 28.45 | 57.26 | 114.9 | 230.1 | 460.6 | 921.6 |

**Random blocks**

| Size of blocks | 15716 | 15705 | 15700 | 15697 | 15696 | 15695 | 15695 |
| No. of blocks | 1    | 2    | 4    | 8    | 16   | 32   | 64   |
| Tflop | 14.04 | 28.45 | 57.26 | 114.9 | 230.1 | 460.6 | 921.6 |

Table 1: Parameters used to set up the weak scaling experiments as described in the text. The Tflop values are the numbers of floating point operations needed for each sparse matrix-matrix multiplication measured in teraflops.

3. Illustrative Examples. We illustrate in this section the capabilities of the library as outlined earlier in this article, using the general sparse matrix-matrix multiplication as an example. We construct sequences of matrices of growing size and, for each matrix in each sequence, compute the product of the matrix with itself. For each sequence, the setup is such that the number of floating point operations needed for the products is proportional to the matrix dimension. Scaling up the computing resources with the matrix dimension gives a weak scaling experiment for each sequence. Three matrix sequences are constructed as follows:

- **Banded**: banded matrices with bandwidth $2 \times 3000 + 1$.
- **Growing block**: banded matrices, again with bandwidth $2 \times 3000 + 1$, but with a single large dense block added to the upper left corner. The size of the block is chosen so that the total number of floating point multiplications for the matrix multiply is doubled compared to the banded matrix. This gives a block size growing with matrix size.
- **Random blocks**: banded matrices, again with bandwidth $2 \times 3000 + 1$, but with a number of dense equally sized blocks placed at random positions along the main diagonal, without overlap. The number of blocks is proportional to the matrix dimension. The size of the blocks is chosen so that the total number of floating point multiplications for the matrix multiply is doubled compared to the banded matrix. The block size stays essentially constant as the matrix size increases.

The same set of matrix dimensions is used in all three experiments. The experiment setup with matrix sizes, block sizes, etc is given in Table 1.

All experiments were performed on the Beskow cluster at the PDC Center for High Performance Computing at the KTH Royal Institute of Technology in Stockholm, using the soon publicly available Chunks and Tasks library CHT-MPI 2.0\(^1\). Beskow is a Cray XC40 system with 2060 compute nodes based on Intel Haswell and Broadwell processors and a Cray Aries interconnect with Dragonfly topology. The present study made use of the Haswell nodes, each equipped with two 16-core Intel Xeon E5-2698v3 2.3 GHz CPUs and 64 gigabytes of memory. Each compute node has a theoretical

\(^1\)The release of CHT-MPI 2.0 is under preparation.
peak performance of approximately 1280 Gflop/s \([2]\). The CHT-MPI 2.0 library uses
the Message Passing Interface (MPI) for communication between nodes. The code
was compiled with GCC 9.3.0 and Cray MPICH 7.7.14. In CHT-MPI 2.0 an MPI
parent process runs the main program and spawns a number of MPI worker processes
that execute tasks. The program was configured to use 1 worker process per node
and 31 worker threads per worker process, executing tasks. Thus, one core per node
is left for threads handling communication with other nodes. The chunk cache size
for each CHT-MPI 2.0 worker process was set to 4 GB.

The leaf matrix dimension was set to \(2048 \times 2048\). Leaf matrices were represented
using the block-sparse matrix library with leaf internal blocksize \(64 \times 64\) and matrix
elements were stored in double precision. Single threaded OpenBLAS 0.3.10 \([23]\) was
used for BLAS operations on submatrices within the block-sparse leaf matrix library.
The input matrices were constructed distributed over the worker processes.

Figure 1a shows the wall time as a function of number of worker processes for the
three test cases. The figure shows the average, minimum, and maximum wall times of
4 repeated test runs. The experiment confirms previous theoretical and experimental
results for the banded matrix, showing a wall time increasing logarithmically with
the number of nodes \([18]\). We can conclude that the library succeeds in dynamically
balancing the load also in the other two cases, where the nonzero structure is not
uniform. Although the number of scalar operations is twice that of the banded
matrix test case, the wall times are considerably less than twice the wall times of
the banded matrix case. One possible explanation is that the large added blocks give
computations with larger arithmetic intensity, i.e. with more floating point operations
per nonzero element. Tasks operating on the same chunk are likely to be executed by
the same worker process. Note that CHT-MPI 2.0 makes use of work stealing between
worker processes with stolen tasks chosen from the tree of tasks based on a breadth
first strategy. The higher efficiency for the “Growing block” and “Random blocks”
test cases can also be seen in Figure 1b which shows the efficiency measured as the
ratio between the number of floating point operations per second and the theoretical
peak performance of the employed compute nodes. Note that the matrix library
dynamically balances the workload while exploiting locality in the nonzero structure
to reduce communication. The library makes no use of a priori information regarding
the nonzero structure of the matrices.

Figure 1c shows the communication measured as the amount of data received
per process during the multiply. The figure shows the average over all processes
and the four repeated test runs. The maximum (minimum) values are taken as
the maximum (minimum) over all processes and the four repeated test runs. As
a reference, we mention that the largest matrix in the banded test case has about
3.8 billion nonzero elements corresponding to 307 GB of memory in double precision
floating point representation.

4. Impact. The Chunks and Tasks Matrix Library has enabled the development
of a number of sparse matrix algorithms for distributed memory parallelization, as
discussed in Section 1 and as further described in Section 2. These algorithms have in
common their ability to dynamically exploit data locality to avoid movement of data,
as demonstrated in Section 3 for sparse matrix-matrix multiplication. They also have
in common that they are the most performance critical sparse matrix operations in
large-scale electronic structure calculations. In particular, different variants of matrix-
matrix multiplication have received ample attention among developers of methods and
software for electronic structure calculations. The Chunks and Tasks Matrix Library
Fig. 1: Performance of sparse matrix-matrix multiplication using the Chunks and Tasks Matrix Library, demonstrated for three different weak scaling test cases described in the text. Panel (a): Wall times. Panel (b): Efficiency measured as the ratio between the achieved floating point operations per second and the theoretical peak performance of the compute nodes employed. Panel (c): Data received per worker process. In both Panels (a) and (b), the solid lines show the average values over four test runs while the dashed lines show the minimum and maximum values. In Panel (c), the average, minimum and maximum values are taken not only over the four test runs but also over all worker processes.

implements task types for parallel sparse matrix-matrix multiplication that combine performance and portability in a unique way as described in Section 1. Yet the most important contribution of the Chunks and Tasks Matrix Library may be that it is showcasing new technology making the achievements above possible.

The Chunks and Tasks Matrix Library represents a paradigm shift for the parallelization of sparse matrix operations. This shift means a change in the division of responsibilities between the developer of an application and the runtime library. For any parallel programming model this division of responsibilities is basically defined by the programming interface of the library or language associated with the model. An application programmer using the Chunks and Tasks programming model worries about exposing parallelism in data and work to the runtime library but not about the mapping of this parallelism to physical resources. This means that the application
programmer does not have to think explicitly about where data should be stored, which process should execute a particular task, synchronization, or communication. At the same time we have seen that the model is expressive enough to describe complex parallel data structures and algorithms. The model imposes certain restrictions for access to data in user code, making efficient and scalable runtime implementations possible. In particular, the CHT-MPI 2.0 implementation uses a completely decentralized management of both work and data, atypical to models where the data distribution is handled by the runtime. Those properties of the Chunks and Tasks programming model are all inherited by the Chunks and Tasks Matrix Library and makes the library a potential game changer for the development and implementation of parallel sparse matrix operations.

The Chunks and Tasks Matrix Library is released under the modified BSD license and is publicly available for download at chunks-and-tasks.org.

5. Conclusions. We have presented the Chunks and Tasks Matrix Library which is a sparse matrix library based on the Chunks and Tasks programming model and sparse quadtree representation of matrices. An advantage of the quadtree representation is that large zero blocks of a sparse matrix can be skipped already at a high level, leading to improved scalability in cases with data locality. The library provides a convenient set of routines for handling large sparse matrices in a distributed setting with main focus on multiplication-heavy algorithms, which are common in electronic structure calculations. Future work and extensions of the library include continued development of algorithms for sparse matrix-matrix multiplication and the combination of outer product based matrix-matrix multiplication with the quadtree representation, to improve the scaling behavior in cases with poor data locality.

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References.
[1] HPL algorithm. http://www.netlib.org/benchmark/hpl/algorithm.html. [Online; accessed November 20, 2020].
[2] Anton G. Artemov. Approximate multiplication of nearly sparse matrices with decay in a fully recursive distributed task-based parallel framework. arXiv e-prints, art. arXiv:1906.08148, June 2019.
[3] Anton G. Artemov and Emanuel H. Rubensson. Sparse approximate matrix-matrix multiplication for density matrix purification with error control. arXiv e-prints, art. arXiv:2005.10680, May 2020.
[4] Anton G. Artemov, Elias Rudberg, and Emanuel H. Rubensson. Parallelization and scalability analysis of inverse factorization using the chunks and tasks programming model. Parallel Comput., 89:102548, 2019.
[5] Ariful Azad, Grey Ballard, Aydin Buluç, James Demmel, Laura Grigori, Oded Schwartz, Sivan Toledo, and Samuel Williams. Exploiting multiple levels of parallelism in sparse matrix-matrix multiplication. SIAM J. Sci. Comput., 38 (6):C624–C651, 2016. doi: 10.1137/15M104253X.
[6] Urban Borštnik, Joost VandeVondele, Valéry Weber, and Jürg Hutter. Sparse matrix multiplication: The distributed block-compressed sparse row library. Parallel Comput., 40(5-6):47 – 58, 2014.
[7] D. R. Bowler and T. Miyazaki. O(N) methods in electronic structure calculations. Rep. Prog. Phys., 75:036503, 2012.
[8] A. Buluç and J. R. Gilbert. Parallel sparse matrix-matrix multiplication and indexing: Implementation and experiments. *SIAM J. Sci. Comput.*, 34(4):C170–C191, 2012.

[9] Sharan Chetlur, Cliff Woolley, Philippe Vandermersch, Jonathan Cohen, John Tran, Bryan Catanzaro, and Evan Shelhamer. cuDNN: Efficient primitives for deep learning. *arXiv e-prints*, art. arXiv:1410.0759, 2014.

[10] Timothy A. Davis. Algorithm 1000: Suitesparse:graphblas: Graph algorithms in the language of sparse linear algebra. *ACM Trans. Math. Softw.*, 45(4), December 2019. doi: 10.1145/3322125.

[11] J. J. Dongarra, Jereney Du Croz, Sven Hammarling, and I. S. Duff. A set of level 3 basic linear algebra subprograms. *ACM Trans. Math. Softw.*, 16(1):1–17, March 1990. doi: 10.1145/77626.79170.

[12] Erik Elmroth, Fred Gustavson, Isak Jonsson, and Bo Kågström. Recursive blocked algorithms and hybrid data structures for dense matrix library software. *SIAM Review*, 46(1):3–45, 2004. doi: 10.1137/S0036144503428693.

[13] Jianhua Gao, Weixing Ji, Zhaonian Tan, and Yueyan Zhao. A systematic survey of general sparse matrix-matrix multiplication. *arXiv e-prints*, art. arXiv:2002.11273, February 2020.

[14] N. D. M. Hine, P. D. Haynes, A. A. Mostofi, and M. C. Payne. Linear-scaling density-functional simulations of charged point defects in Al2O3 using hierarchical sparse matrix algebra. *J. Chem. Phys.*, 133(11):114111, 2010.

[15] Anastasia Kruchinina, Elias Rudberg, and Emanuel H. Rubensson. Efficient computation of the density matrix with error control on distributed computer systems. *arXiv e-prints*, art. arXiv:1909.12533, September 2019.

[16] Roberto Olivares-Amaya, Mark A. Watson, Richard G. Edgar, Leslie Vogt, Yihan Shao, and Alán Aspuru-Guzik. Accelerating correlated quantum chemistry calculations using graphical processing units and a mixed precision matrix multiplication library. *J. Chem. Theory Comput.*, 6(1):135–144, 2010. doi: 10.1021/ct900543q. PMID: 26614326.

[17] Emanuel H. Rubensson and Elias Rudberg. Chunks and Tasks: a programming model for parallelization of dynamic algorithms. *Parallel Comput.*, 40:328–343, 2014. doi: 10.1016/j.parco.2013.09.006.

[18] Emanuel H. Rubensson and Elias Rudberg. Locality-aware parallel block-sparse matrix-matrix multiplication using the Chunks and Tasks programming model. *Parallel Comput.*, 57:87–106, 2016.

[19] Emanuel H. Rubensson, Anton G. Artemov, Anastasia Kruchinina, and Elias Rudberg. Localized inverse factorization. *IMA J. Numer. Anal.*, 2020. doi: 10.1093/imanum/drz075.

[20] R. A. Van De Geijn and J. Watts. SUMMA: scalable universal matrix multiplication algorithm. *Concurrency: Pract. Ex.*, 9(4):255–274, 1997.

[21] Valéry Weber, Teodoro Laino, Alexander Pozdneev, Irina Fedulova, and Alessandro Curioni. Semiempirical molecular dynamics (SEMD) I: Midpoint-based parallel sparse matrix-matrix multiplication algorithm for matrices with decay. *J. Chem. Theory Comput.*, 11(7):3145–3152, 2015.

[22] David S. Wise. Representing matrices as quadtrees for parallel processors: Extended abstract. *SIGSAM Bull.*, 18(3):24–25, August 1984.

[23] Zhang Xianyi. An optimized BLAS library. [http://www.openblas.net/](http://www.openblas.net/), 2020. [Online; accessed October 27, 2020].