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Introducing moldable tasks in OpenMP

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Abstract. This paper introduces a new approach to handle implicit parallelism in library functions. If the library already utilizes a third-party programming model like OpenMP, it may run in parallel. Otherwise, if the library remains sequential, OpenMP directives in client code cannot be used for direct parallelization. To express implicit parallelism and, in the meanwhile, dynamically adjust the parallel degree of a task when its starts, we propose to use moldable tasks. We handle this by introducing a new construct called taskmoldable that generates multiples tasks from a single function call and an iteration space. For the Lapack Cholesky factorization algorithm, our taskmoldable directive allows simple code annotation to express parallelism between tiles and improves programmability. Performance results on a beamforming application indicates that our moldable implementation is slightly faster by 5% in mean, than a parallel execution achieved with Intel MKL.

Keywords: Moldable task · OpenMP Task · Task Dependency

1 Introduction

The task programming model promotes seamless collaboration between application programmers and library developers, ensuring functional composition regardless of their respective choices during development. A work stealing scheduler from Cilk [6] has undergone theoretical analysis to provide guarantees for expected parallel time and space. A provable OpenMP-3.0 task scheduler should inherit these same guarantees. Furthermore, task models with dependencies have been subject to analysis within the same framework [14,30], allowing for the application of similar theoretical results to the OpenMP-4.0 dependent task model.

Although theoretical results have provided satisfactory findings, they are limited to a rigid task model that lacks consideration for the physical parallelism of the target machine during task creation. However, task management, including creation and scheduling, incurs overhead that significantly affects application performance. To mitigate this, researchers have proposed solutions such as lightweight task implementations (e.g., Cilk [6] for independent tasks, Kaapi [15,7]. for data flow dependencies), task throttling [1], high-performance work queue data structures for scalability [3,18], and caching task graph construction for multiple iterations [15,33].

Parallel programs typically involve more arithmetic operations and memory accesses compared to their sequential counterparts. Although these extra overheads don't fundamentally alter the asymptotic number of operations, they do reduce practical efficiency. To mitigate these additional operations, it is crucial to align the parallelism level of the application with the hardware's degree of parallelism. It is important to note that the aforementioned solutions do not address these supplementary costs.

OpenMP efficiently adapts application parallelism to hardware through worksharing constructs. Parallel worksharing loops are automatically distributed among the threads in the current parallel region, ensuring balanced iteration space. The taskloop construct generates the right number of tasks based on the parallel region's size, limiting arithmetic overheads.

This paper proposes a new task generating construct for expressing hidden implicit parallelism in library functions. It allows to define *moldable tasks*, which can adapt their parallel degree to available resources, based on established theoretical scheduling concepts [29,20].

The following section motivates our proposal, focusing on concrete case studies. Section 3 provides detailed information about the taskmoldable directive and its key clauses. We then demonstrate the usage of the new directive in a classical Cholesky factorization and a beamforming application [16,28], concluding the presentation.

2 Motivation

A recently proposed linear algebra API [10] defined batched API to process a set of independent linear algebra subroutine calls on small matrices, with "the aim of providing more efficient, but portable, implementations of algorithms on high-performance manycore architectures [10]." They were present in commonly used APIs such as Nvidia cuBLAS, Magma [17] or Intel MKL.

A call to perform batch_count matrix multiplications on a set of input data is³:

```
1 gemm_batch(m,n,k,A,B,C,bc);
```

where each parameter is an array of size bc, the batch count, of the required parameter to call the BLAS gemm kernel, *i.e.* the call is equivalent to:

```
1 for (int i=0; i < bc; ++i)
2  gemm(m[i],n[i],k[i],A[i],B[i],C[i]);</pre>
```

The gemm_batch operation performs bc independent calls to the gemm BLAS subroutine where each gemm works with different parameters and data provided in the effective array parameters. Because the for loop resides inside the code body of the BLAS batch function it was not accessible to parallelize calls to gemm_batch using any OpenMP worksharing directives or the taskloop

³ For simplicity, we omit some parameters such as the operations on matrices (transposition...), alpha and beta assumed to be 1, the leading dimensions or the info error parameter which are required to pass arguments to each underlying gemm kernel.

generating task construct. Our proposal aims at providing an OpenMP construct to expose the *implicit loop*, and its iterations, as a task generating construct.

The application developer knows that the gemm_batch is equivalent to executing the above implicit iteration loop. Thus the iterations may be partitioned in a disjoint set of N intervals $I_k = [b_k, e_k[$ such that $\bigcup_{k=0}^{N-1} I_k = [0, bc-1],$ such that the batched gemm calls could be rewritten to:

```
1 for (int i=0; i<N; ++i)
2  gemm_batch(m+b_k[i],n+b_k[i],k+b_k[i],A+b_k[i],B+b_k[i],
3  C+b_k[i], e_k[i]-b_k[i]);</pre>
```

Therefore, the gemm_batch operation can be viewed as a list homomorphism [5]. Given a list l, a concatenation operator #, and a function f assumed to be a list homomorphism, we can transform the call f(l1#l2) into calls to $f(l1) \oplus f(l2)$, where \oplus is a reduction operator. In our case, the function f represents the structured block outlined following the OpenMP directive.

Overview of moldable task. The two main issues are defining the implicit loop iteration space (e.g. bc) and passing the effective parameters to the subcalls. We propose annotating the code with a new directive **taskmoldable** used to inform that the following structured block has an implicit loop to partition. The size of the iteration is specified by the clause **batch_count** and the transformation of effective parameters to the parameters of the subsequences calls is specified by the clause **access**.

In this example, the transformation is of kind **linear**, that is a default mapping function, that applies $M_X: i \to X + i$ to any variable X listed in the clause access to pass the parameter on the partition i. We called such transformation a mapping function. It could be defined by the user.

syrk: a list homomorphism with reduction. The proposed clause can be applied to list homomorphisms that involve reduction. Figure 1 illustrates a common call to the syrk subroutine in the left-looking Cholesky factorization [25], as seen in the Lapack netlib potrf. syrk computes $T = T - A \times A^T$ with T symmetric. The moldable task has dependence types in on A and input on T. The computation $T = T - A \times A^T$ is equal to $T = T - \sum_i A_i \times A_i^T$ where A_i is the i-th tile of size $nb \times nb$ (except the last tile) as depicted in Fig. 1.

The moldable task in Fig. 1 expresses the fact that the call to syrk is a list homomorphism with respect to matrix A_i starting at position A+i*nb from A: This is an access strided{nb} with our proposal. Matrix T is fully accessed by all calls to syrk. It was possible to keep the original inout dependence-type, but to keep the possibility to reorder the accumulation depending on the predecessor tasks releasing the matrix bloc A_i the clause specifies that the dependence type on T expressed by generated task is mutexinoutset. Thus by



Fig. 1: Left: SYRK $T = T - A \times A^T$ in left looking version of the Cholesky factorization. Right: annotation with taskmoldable.

accumulating the sequence of syrk calls on each A_i to the matrice T, we obtain the result.

The code that generates the explicit tasks from Fig. 1 is equivalent to the following, where bc is the batch count generated from the clause batch_count.

```
for (int i=0; i < bc; ++i)
    #pragma omp task depend(in: A+i*nb) depend(mutexinoutset: T)
dsyrk(nb,n,-1,A+i*nb,lda,1,T,ldT);</pre>
```

The taskmoldable directive enables the expression of internal parallelism within library functions, including batched or non-BLAS subroutines. By reducing programming efforts, code annotations can result in highly parallel task-based programs. The next section focuses on presenting the taskmoldable directive and its associated clauses, which facilitates the extraction of more parallelism. Section 4 provides detailed accounts of three comprehensive case studies: the application of taskmoldable to matrix-matrix multiplication (gemm), the sequential Lapack left-looking Cholesky factorization [25] and a beamforming application [16,28].

3 A new directive: taskmoldable

As the taskloop directive [31,22], the **taskmoldable** directive is a *task generating* construct. It enhances the functionality of the taskloop directive by allowing the capturing of (implicit) parallel loops within any structured block through user annotations and parameter passing rules to generated tasks.

3.1 General structure

The general structure of the directive is the following:

When a thread encounters a taskmoldable construct, it creates an explicit task that partitions the implicit iterations defined by batch_count into chunks, each of which is assigned to an explicit task for parallel execution. Each chunk has an identifier from 0 to the maximal number of chunks - 1. The size of the chunk is computed before creating the explicit task. The data environment of

each generated task is created according to the data-sharing attribute clauses on the taskmoldable construct, per-data environment ICVs.

The clause access is used to translate the variables to be passed to each explicit task. The effect is as if each variable in the list-item appearing in the structured block is rewritten by applying the data mapping function on the chunk id. The data-mapping is either a predefined identifier: linear, strided{<integer expr>} or full; or a user-defined identifier. Section 3.3 presents the data mapping function. Optionally, the clause access can specify the dependence-type of the generated tasks expressed on the variable.

Clause batch_count accepts a list of integers that are associated to an implicit nested iteration loops. For instance, batch_count($C_0, C_1, ..., C_{k-1}$) is associated with the implicit nested loops generating the tasks as illustrated in the following code. As for the taskloop directive, clauses num_tasks and grainsize limit the number of tasks generated at runtime. For taskmoldable directive, their parameters are a list of values applied on each loop of the nest.

3.2 Compilation

The compiler rewrites the taskmoldable directive to a code equivalent to the following skeleton:

The moldable task is created with dependencies using the weak variant [24,14] of the dependency type used in the depend clauses: e.g. a depend (inout: A) in the taskmoldable definition is translated to depend (weak-inout: A). The objective is to postpone real dependencies on the child tasks (because those are making real memory accesses and computation) rather than to the moldable task which only creates tasks.

Then, the task calls the runtime function $_$ kmpc $_$ omp $_$ taskmoldable $_$ size to compute the size of the tasks in each dimension $S_0, S_1 ..., S_{k-1}$ from the sizes of the batch $_$ count clause (dimension $C_0, C_1, ..., C_{k-1}$) and the values passed in clause num $_$ tasks or grainsize.

3.3 Data mapping functions

A data mapping function is associated with an item using the access clause of the taskmoldable directive:

```
access( mapping_id [{<args>}] [<dependence-type>]: list-item )
```

The optional dependence-type argument is presented in the next section dealing with the expression of dependencies on generated tasks. The runtime defines the subset of the initial workload for each task. It provides a tuple start = $(i_0,i_1,...,i_{k-1})$ that defines the beginning of the sub-iteration space it should process. The access clauses provide information to get the right data for each task. To do so the user provides a function called $mapping_id$ where the declaration is defined as follows:

```
F(item, batch_count, start, args...)
```

which is used to replace items from item-list each time it appear in the structured block.

We propose three basic mappings, strided{args} that take as argument a stride on each dimension, linear that assumes the data are linearly spaced and full that assume all task work on the same data. They are defined as follows:

```
\begin{array}{lll} \texttt{strided}\left(\texttt{A},\texttt{bc},\texttt{start},\texttt{strides}\right) & -> \texttt{A} + \sum_{u=0}^{|bc|-1} i_u \; \star \; \texttt{strides}[\texttt{u}] \\ & \texttt{linear}\left(\texttt{A},\texttt{bc},\texttt{start}\right) & -> \texttt{A} + \sum_{u=0}^{|bc|-1} i_u \; \star \; \prod_{v=0}^{u-1} \; \texttt{bc}[\texttt{v}] \\ & \texttt{full}\left(\texttt{A},\texttt{bc},\texttt{start}\right) & -> \texttt{A} \end{array}
```

Items from list-item are expected to be pointers of types that allow pointer arithmetic.

An implementation of the linear *mapping_id* could be the following:

```
template<T> T* linear(T* A, int* bc, int* starts, int dim_count)
{
  int pos = 0; int size = 1;
  for(int u = 0; u < dim_count; u++)
  {
    pos += starts[u];
    size *= bc[u]
  }
  return A+pos;
}</pre>
```

The runtime tries to decompose the computation into N tasks where N is either provided by the clause num_tasks, or by default, computed automatically: The dimensions of the split are even and computed by the runtime function $_{\tt kmpc_omp_taskmoldable_size}$. Preliminary experimental results reported in section 4.3 show that our proposition of compilation of moldable tasks could be applied to heterogeneous architectures.

3.4 Data dependencies

Task generating constructs often require implicit synchronization to ensure the correctness of parallel executions. However, relaxing these synchronization requirements can enable better utilization of hardware resources. Sharing this goal, a recent proposal to enhance OpenMP, as described in [22], suggests extending the depend clause to include the taskloop construct.

The same issue appears with the taskmoldable directive. The main difference is that iteration loops are hidden from the annotation thus the expression of dependencies on generated task is different. Thanks to the data mapping function we are able to replace the item and the mapped item through the function, as defined in the above section. In that way, the generated task inherits the dependencies from the depend clause in the taskmoldable directive but on items rewritten by the data mapping function.

However, the programmer may optionally refine the way generated tasks declare dependencies through the access clause. This is illustrated in Fig. 1 where the generated tasks declare mutexinoutset dependencies on item T while the moldable task has declared dependency type inout on it. The interest here is to allows commutativity on the reduction operated by syrk in case of faster resolution of dependencies on the A_i .

We assume the availability of the weak-dependencies [24] to postpone real dependencies on the moldable task to the generated tasks. Without them, it is possible to inline the execution of the moldable task creation of the task generating tasks: at runtime, the taskmoldable directive is translated to the code that directly generates the explicit tasks in place of creating the task (that will generate the explicit tasks).

3.5 Implementation

We have created a customized runtime specifically designed to handle moldable tasks, allowing us to validate a prototype before integrating it into the LLVM OpenMP runtime. Thanks to our previous development work in the LLVM runtime, we have taken care to ensure an easier merge process.

The task entry point follows the code outlined in section 3.2. To create a moldable task, we utilize the runtime function __kmpc_omp_task_moldable, which extends __kmpc_omp_task_withdeps to include task dependencies and additional mapping functions. These are stored in supplementary fields of the task data structure kmp_task_t.

We have also incorporated support for partitioning moldable tasks between CPUs and GPUs. If the user provides a GPU version of the list homomorphism function, the runtime divides the implicit iteration between CPUs and GPUs. Initial experiments regarding this feature are reported in section 4.3. We briefly discuss how to integrate moldable tasks with targets in the following perspective.

The runtime should select a granularity for each moldable task, our implementation relies on previous executions of similar functions to compute an expected performance for each worker, then it creates one task for each worker that handles a subset of the moldable task proportional to its performance. Tasks running on GPU targets may be further split by the runtime to fit the memory constraints of the co-processor.

4 Evaluation

The two next sections illustrate our taskmoldable directive with two decompositions of the gemm matrix product, and how to produce a highly parallel



Fig. 2: GEMM block decomposition.

Cholesky factorization from the sequential code of the Lapack netlib library. Then we present a beamforming application with performance evaluation.

4.1 Gemm decomposition

The strided { <pri>optional-args>} mapping function is well-suited when all data are stored in an array by spacing each consecutive partition with a constant stride. As an example, we will show how to generate two classical decomposition of gemm with the taskmoldable directive:

```
1  #pragma omp taskmoldable batch_count(m,n)\
2    access(strided{lda,0}:A)\
3    access(strided{ldc,1}:B)\
4    access(strided{ldc,1}:C)\
5    depend(inout:C) depend(in:A,B)
6    gemm( m, n, k, A, B, C );
```

The result of this decomposition, in case of even split, is presented as figure 2a. It can generate up to $m \times n$ independent tasks. In this case, the block decomposition only works with two dimensions thus the input matrices are split by row or by column but not in blocks. To allows full block decomposition we should handle dependencies between tasks and work on the third dimension of the gemm. The following code result in decomposition 2b. We describe dependency management in 3.4.

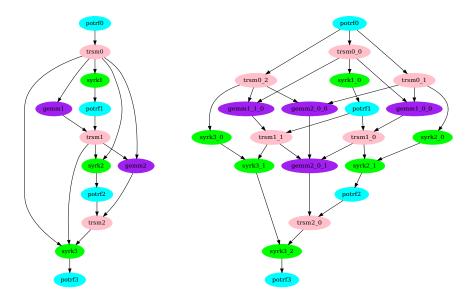
```
1  #pragma omp taskmoldable batch_count(m,n,k)\
2    access(strided{lda,0,1}:A)\
3    access(strided{0,1,ldb}:B)\
4    access(strided{ldc,1,0}:mutexinoutset]:C)\
5    depend(inout:C) depend(in:A,B)
6    gemm( m, n, k, A, B, C );
```

4.2 Lapack Cholesky factorization

The Cholesky factorization algorithm is used in signal processing algorithms such as adaptive beamforming [13], it is also commonly studied in dependency graph generation. We worked on the block left-looking version of the algorithm which is implemented in the subroutine portf in Lapack⁴, the associated code is sketched below⁵:

⁴ https://netlib.org/lapack/

⁵ Code is rewritten in C to follow the guideline of the paper



- (a) Without moldability
- (b) With taskmoldable

Fig. 3: Left looking Cholesky task graph with N/NB = 4

At each iteration, it updates a group of NB columns with their definitive values. A graph of tasks generated with this code is provided as Figure 3a. Whereas the code is elegant and relatively simple, it does not express a lot of parallelism.

By seeing the calls to syrk, gemm and trsm as moldable tasks and adapting the granularity of the split we can achieve the same level of parallelism as a right-looking implementation, the dependency graph is provided as Figure 3b. Furthermore, if we make the granularity finer, as presented in section 4.1, more parallelism can be generated on gemm and trsm function calls. The code is provided below:

```
cholesky ( N, NB, A, lda ):
\frac{1}{3}
      for (j = 0; j < N; j += NB)
4
        #pragma omp taskmoldable batch_count(j) depend(in:A[0][j])
             depend(inout:A[j][j]) access(strided{1}:A[0][j])
5
6
7
8
9
             access(full[mutexinoutset]:A[j][j])
        syrk( NB, j, -1, A[0][j], lda, 1 A[j][j],
#pragma omp task depend( inout: A[j][j] )
        potrf( NB, A[j][j], lda )
10
        if( j + NB < N )
             #pragma omp taskmoldable batch_count((NB,N-j-NB,j)) \
                   depend(in:A,B) depend(inout:C)
                  access(strided{0,1,lda}:A[0][j])\
access(strided{0,1,lda}:A[0][j+NB])\
access(strided{lda,1,0}[mutexinoutset]:A[j][j+NB])
            }
```

The key point here is that original code can be annotated with OpenMP directives⁶ for parallelizing compared to restructuring algorithms to exploit parallelism between tiles [9]. This was possible thanks to advanced features such as dependencies between arrays [8,23].

4.3 Case of study: beamforming

We implement a beamforming algorithm design to work on rectangular arrays of sensors using only moldable tasks, the algorithm is composed of three main parts. First sensor data are converted from the temporal domain to the frequency domain with FFT1D. Then we apply dephasing coefficients to each input to compute the beams, thanks to the shape of the array we can decompose this step in two consecutive matrix multiplications. The final step is to convert complex values to energy by computing the absolute value of each element. Due to data pattern restrictions in the used libraries, we insert a transposition step between the FFT and the matrices multiplications. The pseudo-code is provided below, the values of parameters stride_x are user-defined, constant and depend on the in-memory representation of each array.

```
beamforming():
    #pragma omp taskmoldable batch_count(fft_count) \
    depend(in:Sensor_t) depend(out:Sensor_f)\
    access(strided{fft_stize}:Sensor_t,Sensor_f)
    fft1DExecBatch( fft_stize, Sensor_t, Sensor_f, fft_count )

#pragma omp taskmoldable batch_count( fft_count )\
    depend(in:Sensor_f) depend(out:Sensor_f2)\
    access(strided{fft_size}:Sensor_f)
    access(strided{1}:Sensor_f2)
    transpose( Sensor_f, Sensor_f2 )
```

⁶ Here we have presented C pragma directive - we also assume Fortran compatible directive

```
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```

```
#pragma omp taskmoldable batch_count(gemm_0_count)\
    depend(in:Sensor_f2,Dephase_x) depend(out:Pseudo_beam)\
    access(strided{stride_S},Sensor_f2)\
    access(strided{stride_X},Dephase_x)\
    access(strided{stride_P},Pseudo_beam)
gemmStrideBatch(Sensor_f2,Dephase_x,Pseudo_beam,gemm_0_count)

#pragma omp taskmoldable batch_count(gemm_1_count)\
    depend(in:Pseudo_beam,Dephase_y) depend(Beam)\
    access(strided{stride_P}:Pseudo_beam)\
    access(strided{stride_P}:Pseudo_beam)\
    access(strided{stride_P}:Beam)
gemmStrideBatch(Pseudo_beam,Dephase_y,Beam,gemm_1_count)

#pragma omp taskmoldable batch_count(abs_count)\
    depend(in:Beam) depend(out:Energy)\
    access(strided{1}:Beam,Energy)
abs(Beam,Energy,abs_count)
```

This code was executed on our custom runtime, it ran on a workstation with Intel Xeon 8253, 16 cores processor. It ran about 1M FFT of size 4K, 4K square GEMM of size 1024 and 256M abs values at each iteration. The implementation uses Intel MKL sequential on Intel CPU and OpenBlas on AMD ones, cuBlas and cuFFT are used for Nvidia GPUs.

Overhead of task managements: On this beamforming benchmark, at each iteration of the time step loop, the code generates 40 taskmoldable constructs decomposed into 4062 tasks. The number of dependencies is 103086 between all the tasks. We measure a mean creation cost of 360µs per moldable task; 4µs per task; and 140ns per dependency. Our moldable task runtime does not fit well with the analysis in [27] because the task granularity is not a free execution parameter: It is fixed by the runtime according to available resources and their performances. When more resources are used for the execution, the moldable tasks are decomposed into more finer tasks.

Moreover, we compare the performances of the moldable implementation using MKL sequential and a classical one using MKL parallel library. We find out that the moldable implementation is 5% faster, in mean, than the classical one, thus the overhead implied by the moldability and our runtime is negligible for this workload. Mean execution times over 100 iterations for different core count are provided in table 1.

#core:	1	2	4	8	12	16
MKL parallel: (s)	15.9	8.7	4.4	2.3	1.7	1.3
Moldable (s):	15.3	7.8	4.0	2.0	1.7	1.2
Delta (%):	4	10	9	13	0	8

Table 1: Beamforming execution times

By adding two different RTX GPUs to the workstation, we show that the same code can scale on heterogeneous platforms, it implies to allow a task to execute different code for each target and to handle memory with the runtime. Results of executions speed by adding GPUs are provided in Figure 4 with results on a DGXA100 server. On the RTX platform, CPU-only execution ran in 28s, it was 14.7 times faster than sequential execution and 2.89 times slower than heterogeneous execution. On the DGXA100, CPU-only execution ran in 9s, we reach a speedup of 4.5 by adding GPUs.

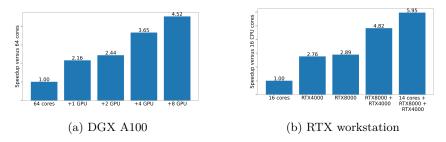


Fig. 4: Beam-forming speedups

5 Related work

Tasks based runtimes are used to schedule tasks on the fly. There are multiple runtimes available as OpenMP [12], StarPU [4], OMPSS [11], Kaapi [15] or PaRSEC [19]. Those runtimes aim to schedule dependent tasks with a lack of knowledge about task computational cost and without knowing tasks that will be scheduled in the future. None of them offer a moldable task concept that allows the expression of functions as a set of tasks. This criterion is absent in the classification of [32]. In [2] the authors theoretically analyze the upper bound on performance using an assumption that tasks are moldable without support in StarPU used by their application. Several moldable task schedulers are proposed and analyzed in scheduling literature [29,20] with ad hoc simulation or experimentation without any runtime support of moldable tasks.

The OpenMP task concept exists and had been extended to provide task creation from loop structures using taskloop [31], moreover, recent contributions open the path to data dependencies between tasks from different taskloops without the need for a global synchronization [22]. Furthermore, [21] provides a structure that allows OpenMP tasks to run inner loops as worksharing constructs, and [26] extensions allow more control over the parallelism generated inside a task that calls library code that uses openMP tasks. OpenMP does not provide a syntax to exploit the implicit parallel structure of library functions.

taskmoldable is a task generating directive. At runtime, it creates an explicit task that postpones real dependencies to its child tasks. Athapascan-1 runtime [14] allows this passing rule with the *postponed access mode*. Similar features are recently proposed under the term *weak-dependencies* in OMPSS [24].

With the absence of weak-dependencies it is always possible to directly create child tasks with an anticipated decision to decompose the moldable task.

6 Conclusion and perspectives

The taskmoldable directive provides a means for users to leverage hidden parallelism in a function without sacrificing the performance of library-specific implementations or requiring an extensive restructuring of the function's internal design. Our evaluation and examples demonstrate how this directive enables the extraction of parallelism from a sequential Cholesky implementation. Furthermore, we achieve minimal overhead when handling moldable tasks in domain-specific workloads like beamforming, allowing us to compete with an MKL implementation.

Our ongoing research aims to expand the scope of our preliminary experimental results, encompassing CPUs and GPUs. This extension will enable users to annotate code, constructing performance models that guide the sizing of partitions. Additionally, we are exploring the integration of target clauses into the directive, facilitating heterogeneous computations based on moldable tasks.

Another future direction involves exploring how to express the moldability of more complex moldable code structures beyond nested loops. For instance, we aim to enable the perception of the entire Cholesky factorization as a moldable task.

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