

Task-Graph Scheduling Extensions for Efficient Synchronization and Communication

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Abstract

Task graphs have been studied for decades as a foundation for scheduling irregular parallel applications and incorporated in programming models such as OpenMP. While many high-performance parallel libraries are based on task graphs, they also have additional scheduling requirements, such as synchronization from inner levels of data parallelism and internal blocking communications.

In this paper, we extend task-graph scheduling to support efficient synchronization and communication within tasks. Our scheduler avoids deadlock and oversubscription of worker threads, and refines victim selection to increase the overlap of sibling tasks. To the best of our knowledge, our approach is the first to combine gang-scheduling and work-stealing in a single runtime. Our approach has been evaluated on the SLATE high-performance linear algebra library. Relative to the LLVM OMP runtime, our runtime demonstrates performance improvements of up to 13.82%, 15.2%, and 36.94% for LU, QR, and Cholesky, respectively, evaluated across different configurations.

Keywords: Gang Scheduling, OpenMP, Runtime System, Task Graph, Work Stealing

1 Introduction

On-node parallelism in high-performance computing systems has increased significantly over the past years. This massive amount of parallelism has the potential to deliver significant speedups, but there is a concomitant burden on application developers to exploit this parallelism in the presence of inherent load imbalances and communication/synchronization requirements. One popular approach to reduce the complexity of application development for modern processors is to introduce high-performance libraries. High-performance linear algebra libraries have pioneered the use of task graphs to deal with load imbalances in parallel kernels such as LU, QR,

and Cholesky factorizations while also exploiting data locality across dependent blocks.

At the same time, there is now increased support for task-parallel execution models with task dependencies in modern parallel programming models, such as OpenMP. Many task graphs in real-world applications include library calls or nested parallel regions that involve blocking operations such as barriers. They often include mixed sequences of communication and computation operations for latency hiding. The tasks also often create groups of child tasks to exploit potential available resources. However, current task-based programming models are unable to support these real-world application requirements, which motivates the work presented in this paper.

Further, tasks often spawn nested parallel regions through calls to library functions or user code with internal parallelism. These nested parallel regions lead to execution by additional pools of threads, which in turn causes oversubscription of cores. This oversubscription can delay intra/inter-node communication or synchronization operations, which often occur in periodic time steps. Scheduling these operations without interference from other parallel regions helps reduce the overall critical path of the application. On the other hand, delaying the execution of communication operations can lead to overall degraded performance. One approach to addressing the challenge of oversubscription in nested parallel regions is to adopt the use of user-level threads (ULTs)[4, 17]. However, ULTs cannot support general nested parallel regions involving blocking synchronization and communication operations. In general, adopting ULTs can lead to deadlock because all of the ULTs are not guaranteed to be scheduled onto worker threads when a blocking operation occurs. Figure 1a(a) shows how adopting ULTs can lead to deadlock when a nested parallel region contains blocking synchronization operations.

In this work, we show how a standard task scheduling runtime system can be extended to support the real-world constraints discussed above by (1) combining gang-scheduling and work-stealing and (2) supporting hybrid victim selection. Our approach provides deadlock-avoidance in the scenario where multiple user-level contexts are synchronized with blocking operations. The integration of gang-scheduling with work-stealing helps nested parallel regions run efficiently without oversubscription and deadlock.

The parallel regions to be gang-scheduled are created as ULTs and scheduled onto a consecutive set of cores that are close to the worker that executed the task that initiated the parallel region, as shown in Figure 1a(b). Workers can schedule other tasks in work-stealing mode while they are gang-scheduling ULTs from specified parallel regions. ULTs that are gang-scheduled on reserved workers can steal tasks from their parallel region when they reach a join barrier. When multiple gangs are created within the same node, they're ordered globally to prevent a deadlock across ULTs that are scheduled on workers. This hybrid scheduling of gang-scheduling and work-stealing reduces interference and increases data locality for data parallel tasks that involve synchronization and communication in each time step.

In addition to gang-scheduling, our runtime system adopts a hybrid victim selection policy in work-stealing to increase communication-computation overlap as well as data locality. Figure 2 shows the performance difference from different victim selection policies. The existing OpenMP runtime systems schedule tasks as in the *Locality* case, while our approach pursues both the *Locality* and the *Overlapping* cases. To the best of our knowledge, ours is the first work to propose and implement a

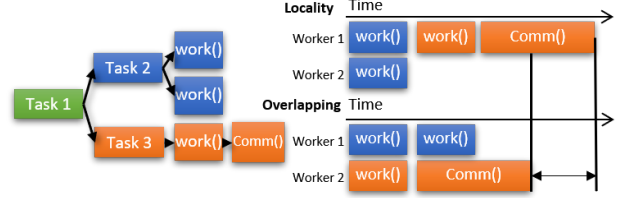


Figure 2. Difference in critical path of mixed sequences of communication and computations

hybrid scheduling of gang-scheduling and work-stealing as well as hybrid victim selection in a production-level runtime system and to demonstrate the implementation on real-world examples.

The contributions of this paper are as follows:

- Extension of task-based runtime systems to integrate gang-scheduling with work-stealing in an efficient manner.
- Introduction of hybrid victim selection to increase the overlap of tasks in task graphs while still preserving data locality.
- Evaluation of our approach on real-world linear algebra kernels in the SLATE library: LU, QR, and Cholesky factorizations. Relative to the LLVM OMP runtime, our runtime demonstrates performance improvements of up to 13.82%, 15.2%, and 36.94% for LU, QR, and Cholesky, respectively, evaluated across different configurations.

2 Background

2.1 Task graphs in Task-Level Programming Models

Many task-level parallel programming models have introduced task graphs in different ways to extract parallelism from irregular parallel applications. The first type of interface for task graphs is *explicit task dependency* through objects such as promises and futures in C++ [18] and Go [11]. Tasks wait on objects until the predecessors of the objects put data on the objects, which resolve the dependencies of the successors. The other type is *implicit task dependency*, which automates the management of objects to improve programmability with the help of compiler and runtime systems that form dependencies through directives as *depend* in OpenMP 4.0 [24] or data flow of variables. After dependencies of tasks are resolved, they become *ready tasks* and are treated as normal tasks. Most task-based runtime systems including OpenMP use per-thread stealing queues so threads where the tasks become ready push tasks to their local work-stealing queue.

2.2 User-level threads for Task-Level Programming Models

In parallel programming models, user-level threads (ULTs) have been used to resolve oversubscription issues by scheduling user-level threads onto kernel-level threads

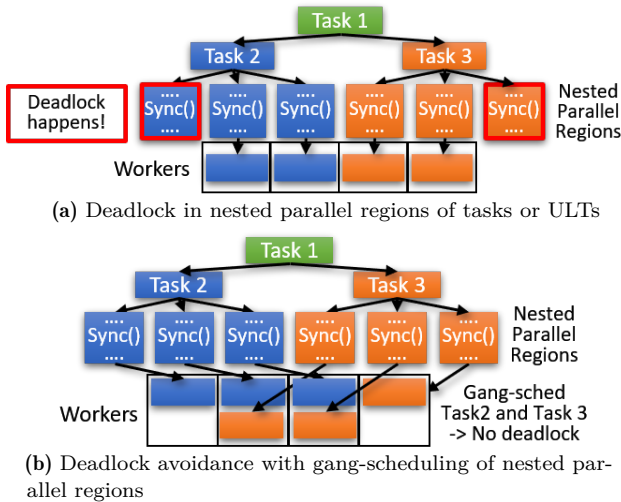


Figure 1. Deadlock issues in nested parallel regions from a group of tasks or User-level Threads(ULT)

(KLTs) when multiple parallel regions are running on the same cores. The mapping of ULT to KLT enables lightweight context switching through storing necessary data for context switching in a user space rather than in a kernel space. There have been several implementation of user-level threads to benefit from its lightweight context switching in different contexts [20, 31, 32]. In spite of the benefits of ULT, they have deadlock issues because of a lack of coordination with kernels as described in Figure 1a(a). The OS kernel cannot identify the status of each ULT, which can lead to deadlock if user-level threads encounter blocking operations such as barriers and locks. There have been several efforts where runtime systems share ULT information with the OS kernel, such as scheduler activations [3]. However, the previous works require significant changes in both the ULT runtime and OS kernel, which has inhibited the adoption of their APIs in operating systems.

2.3 Gang-scheduling and Work-stealing

Gang-scheduling [13, 26] was initially proposed to reduce the interference of a group of threads by other threads or processes. Gang-scheduling, as first introduced, uses a matrix to pack thread requests from processes in which each row is scheduled one at a time. Thus, context switching occurs when it moves from one row to the next row, which reduces the delay in communication across threads incurred by unnecessary context switching. However, a waste of resources results when the threads in each gang have a load imbalance or insufficient cores are available to meet their requests. Different packing policies have been proposed to address these inefficiencies [12, 13, 33], but they did not solve the issue completely. Also, gang-scheduling introduces significant overhead through its use of global data structures. In contrast, work-stealing is a distributed scheduling policy in which each worker schedules tasks independently. Each worker creates tasks and pushes them into their work-stealing queues. Then, other workers steal tasks from the worker by running a work-stealing algorithm independently. Work-stealing maximizes load balancing but incurs overheads due to reduced locality through context switching as well as communication delays, since locality and communication are not part of the task-parallel models that work-stealing schedulers were designed to support. Extended work-stealing algorithms have been introduced to alleviate the cost of work-stealing by considering the locality of participating processing elements [1, 15, 23]. Some of the previous works also extended work-stealing to distributed systems [10, 22, 29].

3 Design

This section describes the algorithm and interface we designed to address the limitations of current task-parallel runtimes mentioned in Section 1. We propose the use of *gang-scheduling* to schedule ULTs of a parallel region without oversubscription and deadlock. Our design supports the use of gang-scheduling for specific parallel regions or globally, while other parallel regions and tasks are scheduled with work-stealing. In addition to gang-scheduling, we also discuss how the victim selection policy, which impacts how a task graph is traversed, affects the overlapping of communication and computation tasks, and we propose a *hybrid victim selection policy* to improve the overlapping supported by the task scheduler.

3.1 Gang-Scheduling of Data-Parallel Tasks

3.1.1 Integrating gang-scheduling with work-stealing. Gang-scheduling and work-stealing have been thought of as oil and water in task scheduling. Each has its advantages and disadvantages as compared to the other. Integrating them so that each can be used in cases when it is beneficial can help improve the overall performance of task-parallel applications. We propose extending the *omp parallel* construct to schedule threads of selected parallel regions in gang-scheduling mode. Users can apply gang-scheduling to upcoming or all parallel regions through our proposed API in Listing 1. By default, all top-level parallel regions are scheduled in gang-scheduling mode. Other parallel regions that are not set by the proposed API are scheduled in work-stealing mode by putting all their ULTs into the calling worker’s local work-stealing queue. For the rest of this paper, we refer to ULTs to be scheduled in gang-scheduling mode as *gang* ULTs, while other ULTs and tasks are referred to as *normal* ULTs and tasks.

```
export OMP_GANG_SCHED=1; //Apply gang-scheduling to
all parallel regions
void ompx_set_gang_sched(); // All following parallel
regions are gang-scheduled after this call
void ompx_reset_gang_sched(); // Parallel regions
after this call are scheduled in default
scheduling policy
```

Listing 1. API to apply gang-scheduling to parallel regions

3.1.2 Gang-scheduling of user-level threads without deadlock. When multiple gang-scheduled parallel regions are running simultaneously, it is important they be scheduled without the possibility of deadlock. To prevent deadlock as described in Figure 1a, we assign a monotonically increasing *gang id* to each parallel region, which is incremented atomically across all workers. We use this *gang id* to restrict the scheduling order of gangs so as to guarantee that deadlock does not occur. Algorithm

1 describes how the *gang* ULTs from a parallel region are assigned the *gang_id* and *nest_level* of the current worker; the runtime system then gang-schedules *gang* ULTs of each parallel region. **gang_sched()** is synchronized by a shared lock in the *fork* stage of a region in the OpenMP runtime. The *fork* phase involves access to global data structures which are synchronized by a global lock for the *fork* and *join* phases in the runtime system. Thus, parallel regions have an inevitable serialization in the *fork* phase, and *gang_sched* contributes a marginal additional waiting time to the *fork* phase of each region.

When each gang is assigned a set of workers (“reserved” workers), the number of gang ULTs and the distance of each worker from the master thread are considered. We assume that all the worker threads are pinned to avoid any migration cost and uncertainty that may be caused by the OS thread scheduler. The workers that are closer to the current worker and less loaded with gang-scheduled ULTs have higher priority in **get_workers()**. Workers are selected to be as close to each other (preferably, consecutive) as possible.

Gang ULTs become stealable after they are scheduled onto the reserved workers. Other workers can steal the *gang* ULTs from the reserved workers, which enables an earlier start of *gang* ULTs if the reserved workers for the gang are busy executing other *normal* ULTs

Algorithm 1 Gang-scheduling with Load Balancing and Deadlock Avoidance

```

1: function GANG_SCHED(n_request, threads)
2:   ▷ Gang-schedule threads to n_request workers
3:   gang_id ← monotonic_gang_id
4:   workers ← get_workers(n_request)
5:   n_gang_threads ← n_gang_threads + n_request
6:   for i = 0 to n_request − 1 do
7:     threadi.gang_id ← gang_id
8:     threadi.nest_level ← cur_worker.nest_level
9:     push threadi to workeri.gang_deq
10: function GET_WORKERS(n_request)
11:   ▷ Retrieve a list of least loaded n_request workers
12:   avg_load ← n_gang_threads / n_workers
13:   if cur_worker_id − n_request ≥ n_workers then
14:     start_worker ← cur_worker_id − n_request + 2
15:   else
16:     start_worker ← cur_worker_id − 1
17:   idx ← start_worker, i ← 0
18:   while i < n_request do
19:     if workeridx.n_gang_threads ≤ avg_load then
20:       reserved_workersi ← workeridx
21:       idx ← idx + 1 % n_workers
22:   return reserved_workers
23: function IS_ELIGIBLE_TO_SCHED(thread)
24:   ▷ Check if worker can steal thread
25:   if worker.cur_gang_id < 0 then return true
26:   if thread.nest_level > worker.nest_level then return true
27:   else if thread.nest_level = worker.nest_level
28:     and thread.gang_id < worker.gang_id then return true
29:   return false

```

and tasks. This is because we only consider the number of *gang* ULTs on each worker. This additional work-stealing resolves unidentified load imbalance without tracking all *normal* ULTs and tasks. The work-stealing of *gang* ULTs happens at every scheduling point, such as barriers, along with *normal* tasks and ULTs. *Gang* ULTs have the highest priority in work-stealing and go through an additional function to check if each *gang* ULT from a victim worker can be scheduled on the caller through **is_eligible_to_sched**. This function compares the *nest_level* and *gang_id* of the current worker with the corresponding variables in the victim *gang* ULT which are assigned in **gang_sched**. This function guarantees parallel regions are scheduled in a certain partial order where gangs, which are started earlier or in lower nested levels, have precedence over those that started later or are in upper levels. In this way, our gang-scheduling approach prevents deadlock of multiple parallel regions contending on the same pool of workers as described in Figure 1a, allowing us to benefit from work-stealing for load balancing.

When *gang* ULTs reach a join-barrier at the end of a parallel region, they can steal *normal* ULTs and tasks from workers in parallel regions of the upper nest level even when they’re not reserved for the gang. When any stolen task spawns a parallel region, the task is suspended to prevent a waiting time incurred by the new nested parallel region. Each suspended task is pushed back to a separate work-stealing queue for suspended tasks. These tasks have higher priority than other tasks.

3.1.3 Comparison with previous work. With the algorithms and heuristics described in this section, only selected parallel regions are guaranteed to be scheduled in gang-scheduling mode. The gang-scheduling we proposed is relatively relaxed compared with previous work because our algorithm guarantees a parallel region to run simultaneously at some point in runtime. Some of the threads in the region can run earlier than others, which may lose the locality of stronger approaches to gang-scheduling. However, this relaxed gang-scheduling algorithm can also result in less waiting time and more efficient use of workers. Our scheme doesn’t require a global table to keep track of threads and reduces waiting time by allowing each region to start immediately and to make ULTs stealable after being gang-scheduled.

3.2 Hybrid Victim Selection for Overlapping and Data Locality

Task graphs involving communication and computation tasks are commonly used to exploit parallelism by overlapping tasks in different iterations of iterative applications. In linear algebra kernels, block-based algorithms have similar task graphs to overlap the waiting time of

current tasks by doing some computation for the next tasks. As mentioned in Section 1, many task-level runtime systems use heuristics to schedule tasks in task graphs to maximize data locality. One of the common heuristics is to use a history of previous successful steals. This heuristic is intuitively helpful for data locality by making workers steal the same loaded victim threads until their task queue becomes empty. However, this heuristic may prevent the overlapping of communication and computation across sibling tasks. When one task becomes ready earlier than another and both of them have nested child tasks to exploit potential available parallelism, the history-based heuristic makes all workers first steal the child tasks from the first task, before moving on to the next task—even though the next task becomes ready while the first and its child tasks are being executed. This prevents overlapping of communication on the next task with computation on the first task. To resolve these unintended anomalies, we tested random work-stealing, which just chooses a victim thread randomly without the use of history. This random stealing, however, suffers from a loss of data locality. Thus, we combined history-based and random work-stealing so that each worker alternatively steals tasks from its history of successful steals and from random victims. This simple heuristic can make use of data locality and overlapping of communication and computation tasks.

Algorithm 2 is a combined algorithm that chooses victim workers for stealing. Each worker calls *do_workstealing* when their local-task queue is empty and waiting for other threads on any synchronization point. First, each worker tries to retrieve the victim thread from its local history of steals. If this steal turns out to be successful, then it moves to the next slot in the local steal history

Algorithm 2 Work-Stealing with hybrid of history and random victim selection

```

1: function DO_WORKSTEALING
2:   ▷ Steal a task from other workers, record the steal for the
   next steal
3:    $cur\_idx \leftarrow cur\_worker\_history\_idx$ 
4:    $victim \leftarrow select\_victim, task \leftarrow steal\_task(victim)$ 
5:   if  $task$  is valid then
6:      $cur\_worker\_prev\_victim\_id, cur\_idx \leftarrow victim$ 
7:      $increment\ cur\_worker\_history\_idx$ 
8:   else
9:      $cur\_worker\_prev\_victim\_id, cur\_idx \leftarrow -1$ 
10:     $decrement\ cur\_worker\_history\_idx$ 
11:   return  $task$ 
12: function SELECT_VICTIM
13:   ▷ Retrieve a worker id from previous steals or rand()
14:    $cur\_idx \leftarrow cur\_worker\_history\_idx$ 
15:   if  $cur\_worker\_prev\_victim\_id, cur\_idx \geq 0$  then
16:      $victim\_id \leftarrow cur\_worker\_prev\_victim\_id, cur\_idx$ 
17:   else
18:      $victim\_id \leftarrow rand \% n\_workers$ 
19:   return  $victim\_id$ 

```

array. This makes the worker try random-stealing after a successful steal. If the current steal fails, regardless of whether it uses history or a randomly chosen victim, it moves back to its previous slot in the history array. If the entry has a valid victim thread id, this worker will try to steal from the victim where the latest successful steal occurred. If not, it keeps stealing from randomly chosen victims. This combined selection of victim from history and random method prevents workers from repeatedly stealing from the same victim, which would result in a serialized sequence of communication and computation without overlapping.

4 Implementation

In this section, we introduce our integrated runtime system of Habanero-C library and LLVM OpenMP runtime to implement the proposed gang-scheduling algorithm and victim selection policy.

4.1 Overview of Our Implementation

We integrated LLVM OpenMP runtime and Habanero-C library (HCLib) to use HCLib’s user-level threading routines. This integrated runtime creates OpenMP threads as user-level threads that run on HCLib workers. This runtime can run pure C++ codes using HCLib APIs, OpenMP codes, and HCLib with OpenMP codes. In this work, we use pure OpenMP codes to focus on the task dependency graph issues in production-level applications. The user needs to load this library to their application binary using OpenMP through *LD_PRELOAD*. The LLVM OpenMP runtime supports gcc, icc, and clang, so any OpenMP binary built with the compilers can run on our integrated runtime without any change to their codes.

Figure 3 shows how OpenMP instances are scheduled onto HCLib workers when gang-scheduling is enabled through the interface in Algorithm 1. User-level threads in each gang can be stolen by idle workers. When idle workers try to steal a ULT from any gang, they check with *IS_ELIGIBLE_SCHED* function if it is fine to schedule the ULT by comparing their active *gang_id* and *nest_level* with the ULT. Within each gang, OpenMP

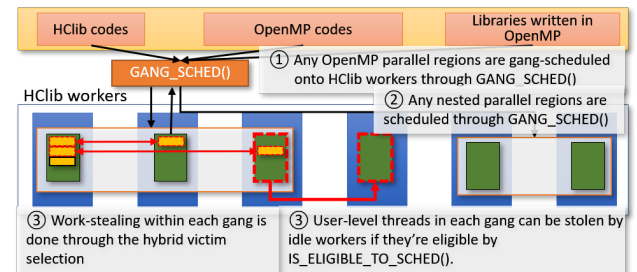


Figure 3. Implementation of Integrated HCLib and OpenMP runtime

threads steal tasks through the hybrid victim selection. In the following sections, we will describe how we implement gang-scheduling and work-stealing for nested-parallel regions in this integrated runtime system.

4.2 Scheduling of Parallel Regions on the shared pool of workers

Multiple OpenMP instances can run on this integrated runtime system by gang-scheduling and work-stealing, so workers may have different nest-levels. User-level threads from each OpenMP instance running on the workers should be able to get access to each other. So, we implemented that each worker has arrays for its active *gang_id*, *nest_level* and *thread_array*. These arrays are indexed by *internal_nest_level* of each worker to point to an active entry for the current running parallel region.

Figure 4 shows how our implementation schedules multiple parallel regions onto the shared workers. When any ULT on each worker tries to schedule a new OpenMP instance onto workers, it creates a new *thread_array* which is assigned an atomically incremented *gang_id*. Each ULT also contains a copy of *gang_id*, *nest_level* and pointer to *thread_array*. When each ULT is eligible on a worker by *IS_ELIGIBLE_SCHED*, it is stolen by the worker, which copies the information of the ULT to its local entries indexed by *internal_nest_level* for *gang_id*, *nest_level* and *thread_array*. The worker store its *worker_id* and *internal_nest_level* in the *thread_array[internal_nest_level][the ULT's thread id]* where other ULTs can find the ULT and its work-stealing queue on this worker. So, other workers scheduling ULTs in the same OpenMP instance steal a task through this

shared *thread_array*. Each worker keeps a separate array of queues for *normal* ULTs and tasks indexed by *internal_nest_level*, which are reused without being re-allocated for each new instance. For *gang* ULTs, each worker has a local *gang_deq* where a master thread initiating a parallel region pushes a *gang* ULT through *gang_sched* function in Algorithm 1, which has highest priority over other queues. Each worker gets a ULT by atomically popping from this *gang_deq*. On any scheduling point, each worker checks this queue first before they schedule tasks in *queues[internal_nest_level]*.

4.3 Work-stealing across different Parallel Regions

Each gang has reserved workers. Any synchronizations, such as barriers and locks, are handled without deadlock within each gang. Each worker does work-stealing among workers where ULTs in the same gang are running. As mentioned above, each worker finds a work-stealing queue of a victim ULT through recorded info in the shared *thread_array*. Work-stealing across different parallel regions is not allowed in the middle of each parallel region. When each ULT reaches its join barrier at the end of its parallel region, it can steal tasks from other parallel regions. This work-stealing out of parallel regions is allowed because we assume there is no work left until the end of this parallel regions, and this cross-region work-stealing has been proven to help reduce the idle time of unbalanced parallel regions in previous works [4]. If any stolen task leads to a nested parallel region, the task is suspended and pushed to the worker's local work-stealing queue for suspended tasks, which has the highest priority over other queues. To prevent any possibility that the work-stealing can lead to a deadlock by creating a cycle, we restrict this out-of-region work-stealing to happen from lower nested parallel regions to upper parallel regions on each worker. In other words, each worker can do this out-of-region stealing at *thread_array[internal_nest_level:0]*.

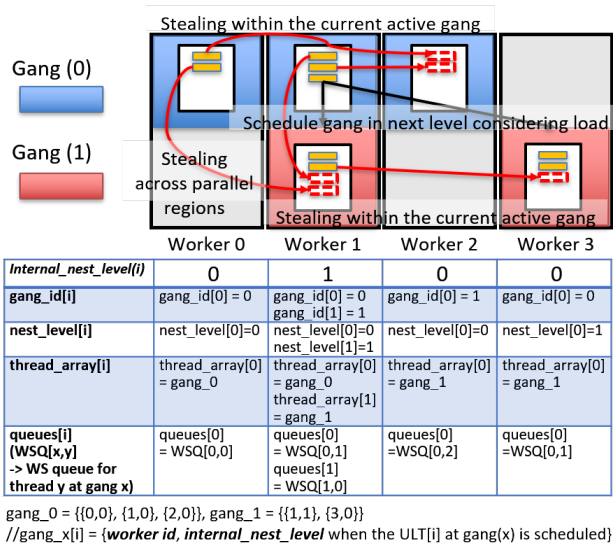


Figure 4. Gang-scheduling for nest-parallel regions and Work-stealing within and across gangs

5 Application Study

We use three linear algebra kernels from the SLATE library [14] to showcase the benefits of our work: LU, QR, and Cholesky. SLATE is a state-of-the-art library developed by the University of Tennessee that is designed to make efficient use of the latest multicore CPUs and GPUs in large-scale computing with common parallel computing techniques such as wavefront parallelism for latency hiding and heterogeneous use of CPU and GPU in distributed environments. SLATE outperforms existing vendor-provided libraries and its predecessor, ScaLAPACK [9]. For our evaluation, we used the NERSC

Cori GPU cluster and built SLATE from its main repository¹ with the configuration in Table 1. For the baseline OpenMP runtime system, we used the LLVM OpenMP runtime, which was forked from the LLVM github repository on 06/29/2020.

Hardware Configuration (per node)		Software Configuration	
Cluster	NERSC Cori GPU	SLATE	06/22/2020 Commit
CPU	2 x Intel Skylake 6148 (20C, 40SMT)	Compiler	GCC 8.3
GPU	8 x Nvidia V100	MKL	2020.0.166
NIC	4 x dual-port Mellanox EDR	CUDA/MPI	10.2.89, OpenMPI 4.0.3

Table 1. Hardware/Software Configuration for Experiments

We tested different configurations of ranks-per-node and cores-per-rank using the LLVM OMP baseline, and selected the best configurations for all our experiments as follows. For LU and QR, we ran each kernel with 4 MPI ranks on each node with 10 OpenMP threads per rank, while for Cholesky, we used 2 MPI ranks per node with 20 OpenMP threads per rank. For GPU runs, we used 4 GPUs per node which showed the best baseline performance. The OpenMP threads and HCLib workers are pinned in the same fashion, using the best affinity setting among those tested.

We ran SLATE’s performance test suite to measure the performance of each kernel in GFlops with different configurations. Each performance measure is a mean of 6 runs after the first run as warm-up. We ran the kernels with small and large matrices to cover common sizes of input matrices on single and multi-node runs. For GPU runs, we used only large matrices where the GPU version starts to outperform the CPU-only runs. For Cholesky, we ran the CPU-only version because the GPU version of Cholesky offloads the trailing matrix update to the GPU, without offering an opportunity to overlap the trailing task and panel task (since no prior runtime was able to exploit this overlap using the victim selection approach in our runtime).

For comparison, we ran the test suite with the ScaLAPACK reference implementation using sequential MKL (denoted by *ScaLAPACK (MKL)*), the SLATE default implementation using *omp task depend* on LLVM OpenMP runtime (denoted by *LLVM OMP*), and the same SLATE implementation on our integrated runtime (denoted by *HCLib OMP*).

5.1 Overview of Task Graphs for LU, QR, and Cholesky in SLATE

Figure 5 shows the general form of task graphs for factorization kernels in SLATE. SLATE uses lookahead tasks and panel factorization for overlapping of computation and communication as well as data locality. Factorization kernels factor panels (each panel is a block column)

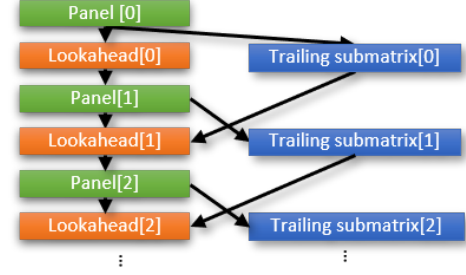


Figure 5. Simplified task graph of factorization kernels in SLATE

and then send tiles in the factored panel to other ranks so that they can update their next block column and trailing submatrix. Lookahead tasks update the next block column for the next panel factorization, and the trailing submatrix task updates the rest of the trailing submatrix. Panel and lookahead tasks are assigned a higher priority than trailing submatrix computation with a *priority* clause to accelerate the critical path of the task graph, which is supported by only a few OpenMP runtime systems such as GNU OpenMP. Regardless of the support of *priority*, it doesn’t guarantee that the scheduling of higher priority tasks will precede lower priority tasks even when it is supported because a *priority* clause simply gives precedence to only *ready tasks* specified with higher priority. The *trailing submatrix[i-1]* task and its child tasks become ready earlier than the *panel task[i]* and its child tasks. For this sequence of tasks, the common history-based work-stealing can prevent the expected overlapping of computation in *trailing submatrix* and communication in *panel task*. Cholesky factorization has significant degradation from this anomaly.

Each factorization kernel has a different series of computations and communication routines in the panel, lookahead, and trailing submatrix tasks depending on its algorithm. Each of the tasks consists of a block of columns. In the following sections, we’ll discuss in detail how our suggested approaches improve the performance of these kernels.

5.2 LU, QR Factorization: Gang-Scheduling of Parallel Panel Factorization

LU factorization is a basic factorization kernel for solving linear systems of equations in which the coefficient matrices are non-symmetric. Several optimizations for LU factorization have been suggested. SLATE adopts a multi-threaded panel algorithm to achieve a best-performing LU implementation [21]. Figure 6 shows what each task in the task graph in Figure 5 does in the LU and QR factorization of SLATE. First, the LU factorization in SLATE does a panel factorization on a block of columns in panel tasks. The panel factorization is parallelized in a nested-parallel region.

¹<https://bitbucket.org/icl/slate>

Each panel is internally decomposed into tiles. Each thread is persistently assigned tiles in a round-robin manner, which helps cache reuse and load balancing. Each

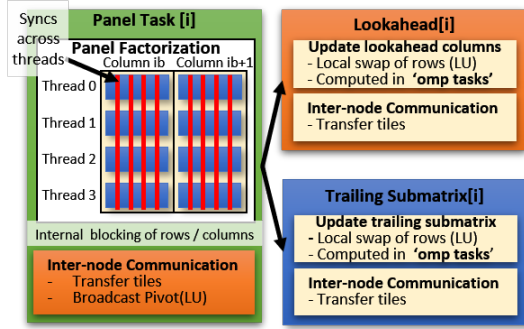


Figure 6. Panel, lookahead, and submatrix tasks of LU and QR in SLATE

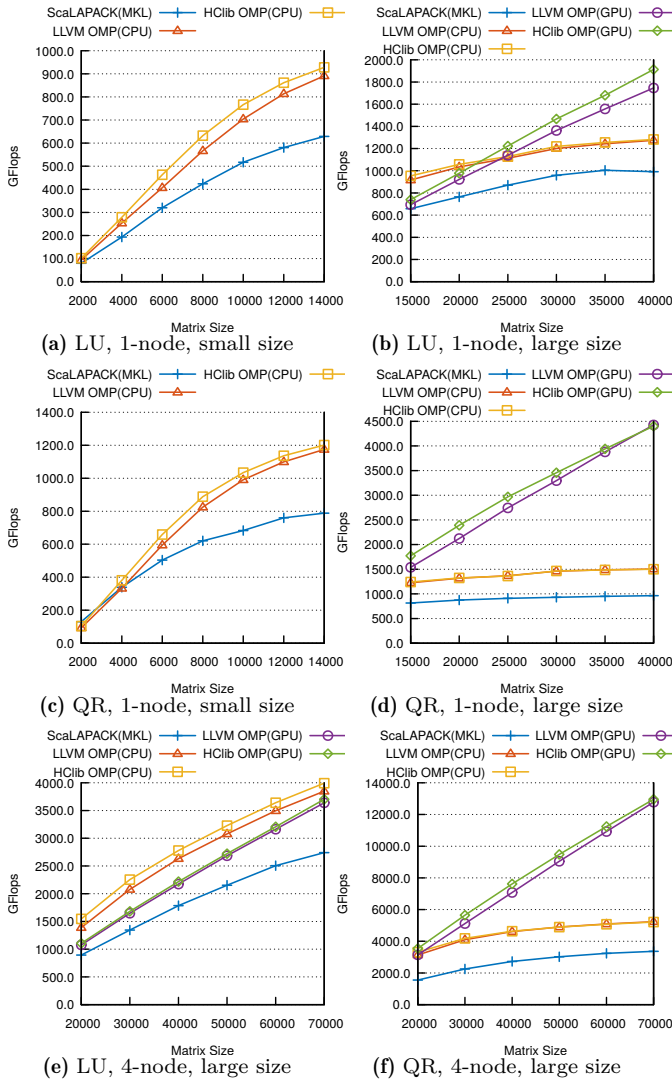


Figure 7. Performance of LU / QR factorization on single / 4-node of Cori-GPU (Skylake + V100) with double precision (CPU: CPU-Only, GPU: CPU+GPU)

thread factors a column, and an updated trailing matrix in the assigned blocks is synchronized at the end of each step (using a custom barrier operation in the library), until a master thread does partial pivoting across threads and other ranks. Because of these synchronizations, a user-level threaded runtime without coordination can lead to deadlock. After the panel factorization, all ranks exchange the rows to be swapped for partial pivoting; the first rank broadcasts the top row down the matrix. The default implementation in SLATE uses a nested parallel region for the parallel panel factorization. However, this nested parallel region interrupts the communication and synchronization by oversubscription of threads on the same cores. Our gang-scheduling makes sure the nested parallel region runs on reserved workers without interference from OpenMP threads in the upper level while other workers can schedule trailing submatrix tasks for overlapping. As Figure 5 implies, *trailing submatrix task[i-1]* can run concurrently with *panel task[i]*. The workers, which are scheduled for gang-scheduling, help to execute the trailing submatrix tasks by work-stealing when they reach the join barrier of the nested parallel region.

Figures 7a, 7b, 7e show the performance of LU factorization on single- and multi-node runs on Cori GPU in double precision. The LU implementation of SLATE includes the sequential global pivoting phase after the OpenMP region, so the overall improvement is relatively small compared with other kernels, which is up to 13.82% on CPU-only runs. Our gang-scheduling has diminishing improvement in CPU-only runs with bigger matrices. However, with bigger matrices, the GPU version of LU outperforms CPU-only runs and the reduction in synchronization and communication leads to noticeable improvement in GPU runs. We'll explain this performance trend in CPU-only and GPU runs in the following section.

Similarly, QR factorization does parallel panel factorization. Unlike LU, QR doesn't include partial pivoting, so panel tasks in QR do not involve global communication for pivoting and QR doesn't have sequential global pivoting after the parallel region. Thus, QR factorization shows relatively more significant speed-up with our runtime over the baseline LLVM OpenMP runtime with oversubscription compared with LU factorization. SLATE uses a communication-avoiding QR algorithm for QR factorization. It doesn't include any communication in the panel factorization, while each panel task transfers the tiles factored after the panel factorization to other ranks before it proceeds with lookahead and trailing submatrix tasks. The panel factorization is also the most critical task to the task graph of QR factorization in SLATE. Thus, gang-scheduling helps minimize

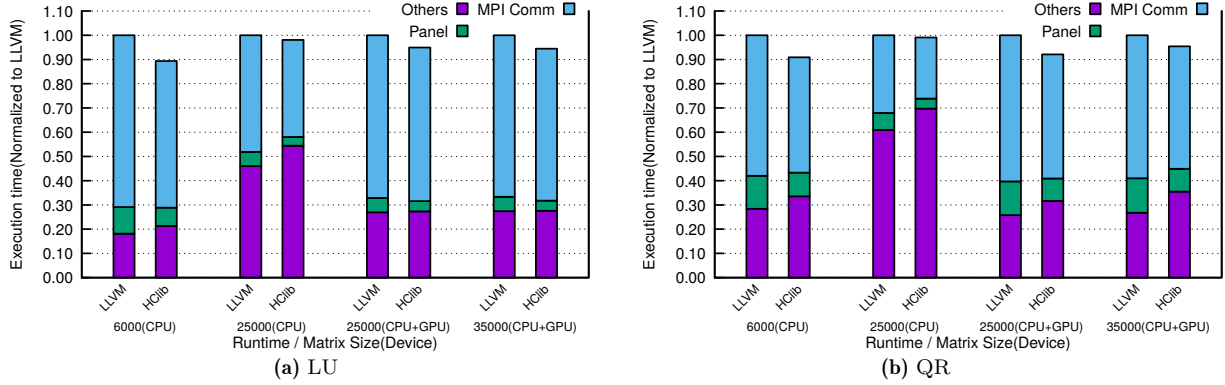


Figure 8. Detailed Critical Path of LU and QR factorization on a single node with LLVM and HCLib OMP

the interference of the nested parallel regions as it does for LU.

Figures 7c, 7d, 7f show the performance of QR factorization on single- and multi-node runs. Our work improves the QR factorization up to 14.7% at CPU-only runs and 15.2% at GPU runs on a single node over CPU-only and GPU runs with LLVM OpenMP runtime. Gang-scheduling shows considerable improvement in 4-node runs up to 12.8%. QR factorization also has diminishing returns of improvement with bigger matrices, as explained in the following section.

5.3 Detailed Analysis of Improvement in LU and QR

Figure 8 represents how much MPI routines, panel task and other routines consist of the overall execution time in terms of critical path. The tasks transfer tiles between ranks in the beginning and end of panel, lookahead, and submatrix tasks. So, MPI communication and panel factorization determines the length of the critical path of LU and QR task graphs. Child tasks from lookahead and trailing submatrix tasks run in parallel with these routines to overlap the critical routines, which consists of most portion of *Others*. Each bar is normalized to the total execution time of LLVM with the corresponding input matrix.

The benefits of gang-scheduling in our integrated runtime for single- and multi-node runs diminish for both LU and QR factorization. Gang-scheduling helps remove the delayed synchronization by oversubscription with deadlock avoidance, which leads to reduction in *Panel*. The reduction makes the tile transfer happen earlier, at the end of the panel task, which shortens the waiting time in other MPI ranks that need the tiles to proceed. This is shown on the reduction of *MPI Comm* in Figure 8. This improvement is diluted with the combined effect of oversubscription. The degree of degradation incurred by oversubscription depends on the inter-barrier time of an application [16]. The bigger input matrix has longer inter-barrier time, which leads to less significant degradation from context switching by oversubscription. Rather,

oversubscription hides waiting time from OS and hardware events monitored at the kernel-level, which makes our runtime shows increase in *Others* consisting of single-threaded BLAS kernels. It is because the latency hiding of oversubscription is removed. The decreasing degradation of oversubscription on bigger matrices leads to diminishing returns of gang-scheduling over oversubscription.

However, the benefit of gang-scheduling becomes more significant on the GPU offloaded version because a significant portion of computation in *others* is offloaded to GPUs where oversubscription helps on the large matrices. A larger portion of the single-threaded BLAS kernels is offloaded in LU than in QR. So, QR has diminishing returns on the GPU version as the size of the input matrix becomes bigger. If more computation in QR is offloaded, our gang-scheduling can bring more improvement in QR.

5.4 Cholesky Factorization: Maximized Overlap of Communication and Computation

Cholesky factorization is a decomposition of a Hermitian positive definite matrix into a lower triangular matrix and its conjugate transpose. Cholesky is used for standard scientific computations such as linear least squares and Monte Carlo simulations. It has proven to be twice

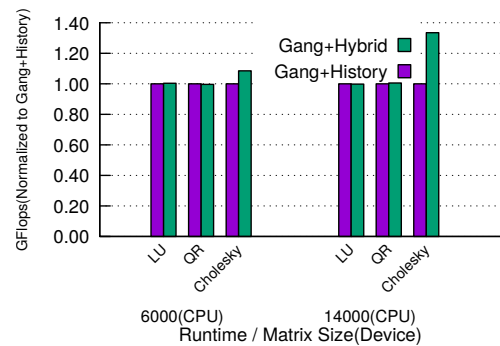


Figure 9. Performance Difference of LU, QR, and Cholesky with history and hybrid victim Selection on HCLib OMP

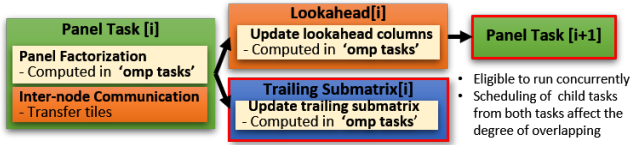


Figure 10. Panel, Lookahead, and Submatrix Tasks of Cholesky in SLATE

as efficient as LU when it is applicable. The panel factorization is much lighter, so lookahead and trailing submatrix tasks are critical to improving the performance of Cholesky. As we mentioned above, *trailing submatrix tasks* $[i-1]$ and *panel task* $[i]$ can run concurrently. LU and QR factorization have heavy *panel tasks* which are parallelized in a nested-parallel region, so any workers that finish lookahead tasks will push dependent panel tasks into ready queues. Most often, they’re pushed to the worker’s work-stealing queue, so panel tasks are likely to be scheduled just after lookahead tasks. Also, the panel tasks are heavy and take a large portion of execution time, so the degree of overlapping of the panel tasks and trailing submatrix tasks have limited impact on the performance. In Figure 9, the victim selection policies don’t affect LU and QR significantly while Cholesky is highly influenced by the victim policies which affect the overlapping of the two tasks. As described in Figure 10, its panel factorization is done in a bunch of independent tasks and takes less time than trailing submatrix tasks, so when the panel task becomes available after its preceding lookahead task is done, child tasks from the preceding trailing submatrix task are already being scheduled. The timing for the child tasks from the panel tasks is determined by how each worker chooses a victim for work-stealing. If they use the typical history-based victim selection, every worker will keep stealing from the worker in which the trailing submatrix is running and create its child tasks. This work-stealing from the same victim leads to a delay in the scheduling of the panel task and less overlapping of inter-node communication on the panel task with the child tasks from the trailing submatrix task.

Figures 11a, 11b, 11c show the performance of Cholesky factorization. As we expected, the improved overlapping of computation in trailing submatrix tasks and communication in panel tasks enhances the performance of Cholesky factorization significantly. The improvement is more significant with bigger matrices because it takes more time to transfer tiles to other ranks and update the trailing submatrix, which gives more opportunity for overlapping. On a single node, the improvement is up to 36.94% with double-precision. On 4-node runs, the kernel is improved up to 28.83%.

We analyze Cholesky in detail to clarify where the improvement comes from. We profile each OpenMP worker

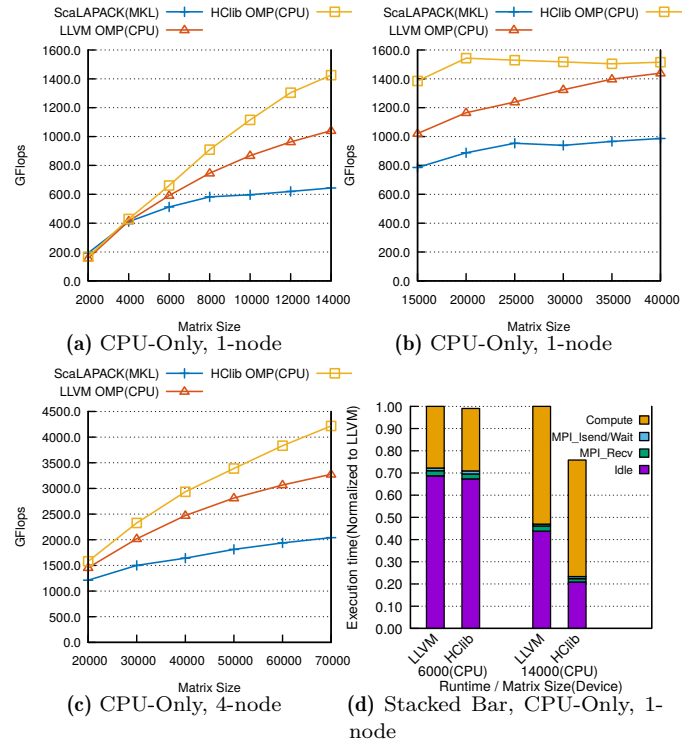


Figure 11. Performance of Cholesky factorization on single/4-node of Cori-GPU (Skylake + V100) with double precision (CPU: CPU-Only)

in different MPI ranks and compute the average of each event such as *Idle*, *MPI_Recv*, *MPI_Isend/Wait*, and *Compute* which includes all computations from panel, lookahead, and trailing submatrix tasks. The largest portion of *Idle* consists of waiting time until the updated tiles are received through *MPI_Recv* from other MPI ranks. Figure 11d shows the detailed analysis of Cholesky factorization on a single node with two matrix sizes on LLVM and HClb OMP. In the small matrix, the amount of computation is relatively small, which doesn’t affect the degree of overlapping significantly regardless of when MPI routines are called. However, on the large matrix, the computation from the trailing submatrix takes longer time, which can overlap MPI routines. So, our victim selection successfully hides the latency of MPI routines, which leads to significant reduction in the overall idle time.

6 Related Work

6.1 Task Graphs in Task-Based Parallel Programming Models

Task graphs have been adopted in most industry and academic works. As mentioned in earlier sections, languages supporting task graphs provide constructs for explicit task dependency through objects such as promise and futures in C++11 [18], Habanero [5], Go [11]. A recent

work, Legate-Numpy [6], shows that implicit parallelism can be extracted from the data flow of library calls. These task-based parallel programming models supporting task graphs haven't paid much attention to data-parallel tasks or overlapping of tasks on the graphs. Hence, we have focused our attention on these tasks, which are highly crucial for performance.

6.2 Runtime Systems Based on User-level Threads

User-level threads have been adopted to benefit from their lightweight context switching cost. One of the most common uses of ULTs is to remove the oversubscription by multiple parallel regions. Lithe [27] resolved the composability of different OpenMP instances by providing a dedicated partition of cores to each instance through user-level contexts. However, this partitioning can lead to less resource utilization because of imbalanced loads across instances. Several runtime systems [4, 17, 25, 28] share the underlying kernel-level threads through work-stealing or their own scheduling algorithm with ULTs. They tried to make use of the lightweight context switching cost of ULTs in different contexts but couldn't resolve the deadlock issue completely. Shenango [25] tried to provide a bypass for blocking kernel calls, but other blocking operations used in library calls or written by users can lead to a deadlock. Our work benefits from the advantages of ULTs without deadlock or inefficient resource utilization due to coarse-grained partitioning.

6.3 Communication and Computation Overlap

Asynchronous parallel programming models [2, 7, 8, 19] have been suggested for overlapping by making all of the function calls asynchronous, which directs the runtime system to interleave communication and computation inherently. However, asynchronous parallel programming models require significant effort on the part of users to write their applications without deadlock, and tracking control flow of functions calls is not intuitive. J. Richard et al. [30] studied the overlapping of OpenMP tasks with asynchronous MPI routines in which the application uses the *priority* clause and task loops. As previously mentioned, the examples we used cannot benefit from the *priority* clause because it works only for *ready* tasks. Our victim selection helps the overlapping of child tasks from multiple ready tasks even when *priority* doesn't help or is not supported.

7 Conclusion

In this work, we proposed gang-scheduling and hybrid victim selection in our runtime system to improve the performance of task graphs involving inter/intra-node

communication and computation. Our approach schedules nested parallel regions involving blocking synchronizations and global communications with minimal interference as well as with desirable data locality. It is implemented efficiently using a monotonic identifier and an eligibility function to enforce an ordering of gangs so as to ensure the absence of deadlock. Also, it interoperates with work-stealing to minimize unused resources within and across gangs. Our suggested victim selection resolved the problem of the common heuristic based on a history of previously successful steals by applying random-stealing and history-based alternatives within a fixed window size to overlap communication and computation.

We evaluated our work on three commonly used linear algebra kernels, LU, QR, and Cholesky factorizations, from the state of the art SLATE library. Our approach showed an improvement for LU of 13.82% on a single node in double precision and of 11.36% on multiple nodes. The improvements for QR went up to 15.21% on a single node and 12.78% on four nodes with double precision. Cholesky factorization was improved by our hybrid victim selection, with an improvement of up to 36.94% on a single node and 28.83% on multiple nodes with double precision. Further, unlike current runtimes, our approach guarantees the absence of deadlock in these kernels for all inputs. Finally, our approach is applicable to any application written using task graphs that also needs to perform additional synchronization and communication operations as in the SLATE library.

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