# Memory-aware Adaptive Scheduling of Scientific Workflows On Heterogeneous Architectures

***Abstract*—Scientific workflows are often represented as directed acyclic graphs (DAGs), where vertices correspond to tasks and edges represent the dependencies between them. Typically, each task requires a certain amount of memory to be executed and needs to communicate data to its successor tasks. The goal is generally to execute the workflow as fast as possible (i.e., to minimize its makespan), while satisfying the memory constraints. Hence, we investigate the memory-aware scheduling of DAG-shaped workflows on heterogeneous platforms, where each processor can have a different speed and a different memory size. We propose a variant of HEFT (Heterogeneous Earliest Finish Time) that (in contrast to the original) accounts for memory and includes eviction strategies for cases when it might be beneficial to remove some data from memory in order to have enough memory to execute other tasks. Furthermore, while HEFT assumes perfect knowledge of the execution time and memory usage of each task, the actual values might differ upon execution. Thus, we propose an adaptive scheduling strategy, where a schedule is recomputed when there has been a significant variation in terms of execution time or memory. The scheduler has been closely integrated with a runtime system, allowing us to perform a thorough experimental evaluation on real-world workflows. The runtime system warns the scheduler when the task parameters have changed, and a schedule can be recomputed on the fly. The memory-aware strategy allows us to schedule task graphs that would run out of memory with a state-of-the-art scheduler, and the adaptive setting allows us to significantly reduce the makespan.**

## I. Introduction

The analysis of massive datasets, originating from fields such as genomics, remote sensing, or biomedical imaging – to name just a few – has become ubiquitous in science; this often takes the form of workflows, i.e., separate software components chained together in some kind of complex pipeline [21]. These workflows are usually represented as directed acyclic graphs (DAGs). The DAG vertices represent the software components (or, more generally, the workflow *tasks*), while the edges model I/O dependencies between the tasks [1], [23]. Large workflows with resource-intensive tasks can easily exceed the capabilities of a single computer and are therefore executed on a parallel or distributed platform. An efficient execution of the workflows on such platforms requires mapping tasks to specific processors; to increase utilization by reusing finished processors, one also needs a task schedule (i.e., a valid execution order that respects the dependencies) and possibly also starting times for the tasks.

Modern computing platforms are often heterogeneous, meaning they feature varying CPU speeds and memory sizes. In general, having different memory sizes per CPUs makes it more challenging to compute a schedule that respects all memory constraints – meaning that no task is executed on a processor with less memory than needed for the task. This is, however, very important to avoid (possibly expensive) runtime failures and to provide a satisfactory user experience. Hence, building on previous related work [15], [16], [20], we consider a scheduling problem formulation that takes memory sizes as explicit constraints into account. Its objective is the very common *makespan* [23], which acts as proxy for the total execution time of a workflow. However, to the best of our knowledge, the only memory-aware heuristics that would account for memory constraints are partitioning the DAG and not reusing processors once they have processed a part of the graph, leading to high values of makespan compared to a finer grain solution that reuses processors.

While previous work with memory constraints has been focusing on partitioning the graph, and not reusing processors during execution, a seminal list scheduling heuristic for workflows on heterogeneous platforms, without accounting for the memory constraint, is HEFT (heterogeneous earliest finish time) [33]. It has two phases: (i) each task is assigned a priority; and (ii) the tasks in a priority-ordered list are assigned to processors, where the "ready" task with the highest priority is scheduled next on the processor where it would complete its execution first. HEFT has been extended (e.g., by Shi and Dongarra [30]) and adjusted for a variety of different scheduling problem formulations. Yet, none of them adhere to memory constraints as we propose – see discussion of related work in Section II.

Another limitation in practice of HEFT (and many other scheduling strategies) is their assumption that the task running times provided to them are accurate. In practice, this is not the case and deviations from user estimates or historical measurements are very common [18]. As a consequence, one should adapt the schedule when *major* deviations occur. However, the original list-based schedulers, such as HEFT, are only defined in a static setting with accurate task parameters.

The main contributions of this paper are both algorithmic and experimental:

- We formalize the problem with memory constraints, where communication buffers are used to evict data from memory if it will be later used by another processor.
- We design three HEFT-based heuristics that adhere to memory size constraints: HEFTM-BL, HEFTM-BLC, and HEFTM-MM (M behind HEFT for memory, BL for bottom level, BLC for bottom level with communication, and MM for minimum memory traversal). The difference

between the new heuristics is the way they prioritize tasks (for processor assignment).
- We implement a runtime system able to provide some feedback to the scheduler when task requirements (in terms of execution time and memory) differ from the initial predictions, and we recompute a schedule, based on the reported deviations.
- We perform extensive simulations, first in the static case by comparing the schedules produced by these heuristics with the classical HEFT as baseline, which however does not take memory sizes into account; while HEFT returns invalid schedules that exceed the processor memories and cannot execute correctly, the new heuristics are able to successfully schedule large workflows, with reasonable makespans.
- In the dynamic setting, we use a runtime system that allows us to simulate workflow executions, introducing deviations in running times and memory requirements of tasks that are communicated back to the scheduler; the scheduler can then recompute a schedule. Without these recomputations, most schedules become invalid after deviations, since the memory constraint is exceeded for most workflows, hence demonstrating the necessity of a dynamic adjustment of the schedule.

We first review related work in Section II. Then, we formalize the model in Section III and the algorithms in Section IV. The adaptation of the heuristics in a dynamic setting is discussed in Section V, and experiment results are presented in Section VI. Finally, we conclude and provide future working directions in Section VII.

## II. Related work

First, we focus on HEFT-like scheduling heuristics from the literature that do not necessarily consider memory constraints. Then, we discuss memory-aware scheduling algorithms. Finally, we move to related work on dynamic or adaptive algorithms.

### A. Static list schedulers, especially HEFT-based algorithms

Introduced in 2002, HEFT [33] is a list-based heuristic. It and all its successors consist of two phases: task prioritization/ordering and task assignment. In the first phase, the algorithms compute bottom levels of the tasks based on some priorities (create the list), and then schedule tasks in the order of these priorities. The modifications of HEFT revolve around the way the priorities of the tasks are computed and the logic of the processor assignment. All such algorithms assume a heterogeneous execution environment.

Hence, during the task prioritization phase in [32], the standard deviation of the computation cost (between processors) is computed, and added to the mean value to account for the differences between processor speeds. In the processor choice phase, the entry task and the longest parent tasks are duplicated during idle times on the processor.

PEFT (Predict earliest finish time) [4] is a HEFT variant that computes an Optimistic Cost Table (OCT). The OCT is computed per task-processor pair and stores the longest shortest path from this task to the target task if this processor is chosen for this task. Ranking is based on OCT values. The processor choice stage minimizes the optimistic EFT, which is EFT plus the longest path to the exit node for each task.

The HSIP (Heterogeneous Scheduling with Improved task Priorities) [34] has an improved first step in comparison to HEFT. It combines the standard deviation with the communication cost weight on the tasks. In the second stage, the algorithm duplicates the entry task if there is a need for it.

The TSHCS (Task Scheduling for Heterogeneous Computing Systems) algorithm [2] improves on HEFT by adding randomized decisions to the second phase. The decision is whether the task be assigned to the processor with the lowest execution time or to the processor that produces the lowest finish time.

The SDC algorithm [30] considers the percentage of feasible processors in addition to task's average execution cost in its weight. The selected task is then assigned to a processor which minimizes its Adjusted Earliest Finish Time (AEFT) that additionally notes how large the communication between current node and its children will be on the average provided that it is scheduled on the current processor.

HEFT can also be adapted in cloud-oriented environments [28] and even combined with reinforcement learning techniques [37].

### B. Memory-aware scheduling algorithms

Respecting processor memories adds a constraint to a scheduling problem. Therefore, only specifically memory-targeted algorithms address this issue. Moreover, the way processor memories are represented in the model has a decisive impact on the way the constraint is formulated and addressed in the algorithm. Different models of memory available on processors and memory requirements of tasks have been presented.

Marchal et al. [25] assume a memory model where each processor has an individual memory available. Workflow tasks have no memory requirements, but they have input and output files that need to be stored in the memory. A polynomial-time algorithm for computing the peak memory needed for a parallel execution of such a DAG is provided, as well as an ILP solution to the scheduling problem. The memory model requires deleting all input data upon starting of the task and adding all output files there.

In an assumed dual-memory systems [17], a processor can have access to a memory of two different kinds (red or blue), and each task can be executed on only one sort of memory. The communications happen only between these two kinds of processors (communications within each group are ignored). The authors then formulate an ILP solution for this problem formulation.

Yao et al. [38] consider that each processor has an own internal memory and all processors share a common external one. The internal (local) memory is used to store the task files. The external memory is used to store evicted files to

make room for the execution of a task on a processor. All processors, including the original one, can access these files. Each edge has two weights – the size of the files transferred along it, and the time of communication along this edge. The tasks themselves have no memory requirements, but need to hold all their incoming and outgoing files.

In [12], there are connected processors with individual limited memories. The collective set of memories forms the global memory, to which each processor has access, however the access time to global memory is different. Each memory access in the graph is modeled as a memory access token on the task, while the edges have no weights. The solved problem is how to allocate initial input data in processor memories so that the overall execution is minimized and the memories are not exceeded. The authors propose an integer linear programming model.

In [27], the authors assume memory requirement on tasks represented as tiles. Each processor has individual memories to process the task, but only the shared memories store the tiles containing memory tiles occupied by memory tiles.

Finally, there are some cloud-oriented models that include costs associated with memory usage [22].

Overall, there are a variety of memory models, but, to the best of our knowledge, the only study on a multiprocessor platform that is fully heterogeneous, with individual memories, is the one from [20], but where a partition of the workflow is proposed, hence preventing processor reuse. Hence, in [20], there is no need of communication buffers to store data that should be communicated between two processors when tasks are ready to execute.

### C. Dynamic/adaptive algorithms

We now review related work in a dynamic setting. With no variation in task parameters, DVR HEFT [29] rather considers that new tasks arrive in the system. They use an almost unchanged HEFT algorithm in the static step, executing three slightly varying variants of task weighting and choosing the variant that gives the best overall makespan. In the dynamic phase, they receive new tasks and schedule them on either idle processors or those processors that give them the earliest finish time.

Rahman *et al.* [26]'s dynamic critical path (DCP) algorithm for grids maps tasks to machines by calculating the critical path in the graph dynamically at every step. They schedule the first task on the critical path to the best suitable processor and recompute the critical path. The heuristic also uses the same processor to schedule parent and children tasks, as to avoid data transfer between processors. The approach is evaluated on random workflows of the size up to 300 tasks.

Garg *et al.* [14] propose a dynamic scheduling algorithm for heterogeneous grids based on rescheduling. The procedure involves building a first (static) schedule, periodic resource monitoring and rescheduling the remaining tasks. The resource model contains resource groups (small tightly-connected sub-clusters), connected between each other. For each resource group, there is an own scheduler, and an overall global scheduler responsible for distributing tasks to groups. The static heuristic is HEFT with earliest start time as priority. Upon rescheduling, a new mapping is calculated from scratch, and this mapping is accepted if the resulting makespan is smaller than the previous one. The experiments were conducted on a single workflow with 10 tasks.

Most dynamic or adaptive algorithms are formulated for clouds, where the execution environment is not fixed, but constrained by cost.

Wang et al. [35] propose a dynamic particle swarm optimization algorithm to schedule workflows in a cloud. Particles are possible solution in the solution space. However, the dynamic is only in the choice of generation sizes, not in the changes in the execution environment. Similarly, Singh et al. [31] addresses dynamic provisioning of resources with a constraint deadline.

De Olivera *et al.* [11] propose a tri-criteria (makespan, reliability, cost) adaptive scheduling algorithm for clouds. They solve a set of linear equations that represent the cost of an execution based on the criteria. The authors test out 4 scenarios - one preferring each criteria, and a balanced one. The algorithm chooses the best virtual machine for each next task based on the cost given by the model. The authors used workflows with less than 10 tasks, but repeated them so that the execution had up to 200 tasks.

Daniels et al. [10] formalize the concept of robust scheduling with variable processing times on a single machine. The changes in runtimes of tasks are not due to changing machine properties, but are rather task-related (that means that these runtime changes are unrelated to each other). The authors formulate a decision space of all permutations of $n$ jobs, and the optimal schedule in relation to a performance measure $\phi$. Then they proceed to formulate the Absolute Deviation Robust Scheduling Problem as a set of linear constraints.

While several related work consider building a new schedule once some variation has been observed, we are not aware of work implementing a real runtime system that interacts with the scheduler, and tested on workflows with thousands of tasks, as we propose in this paper. Furthermore, we are not aware of any previous work discussing dynamic algorithms combined with memory constraints.

## III. Model

We first describe the model for our target applications, which are (large scientific) workflows for which we do not have perfect a priori knowledge, in Section III-A. Next, we define the execution environment, a heterogeneous system (in terms of processor speed and memory size), in Section III-B. Finally, we present the optimization problem in Section III-C. The key notation is summarized in Table I.

### A. Workflow

A workflow is modeled as a directed acyclic graph $G = (V, E)$, where $V$ is the set of vertices (tasks), and $E$ is a set of directed edges of the form $e = (u, v)$, with $u, v \in$

$V$, expressing precedence constraints between tasks. Each task $u \in V$ is performing $w_u$ operations, and it also requires some amount of memory to be executed, denoted as $m_u$. Each edge $e = (u, v) \in E$ has a cost $c_{u,v}$ that corresponds to the size of the output file written by task $u$ and used as input by task $v$. Note that $m_u$ is the total memory usage of a task during its execution, including input and output files currently being read and written, and hence the total memory requirement for the execution of task $u$ consists of the maximum between the input files (total size of the files to be received from the parents), the output files (total size of the files to be sent to the children), and the total memory size $m_u$ (usually achieving the maximum):

$$r_u = \max \left\{ m_u, \sum_{v:(v,u)\in E} c_{v,u}, \sum_{v:(u,v)\in E} c_{u,v} \right\}.$$

The parents of a task $u \in V$ are the directly preceding tasks that must be completed before $u$ can be started, i.e., the set of parents is $\Pi_u = \{v \in V : (v, u) \in E\}$. A task without parents is called a *source task*. The children tasks of $u$ are the tasks following $u$ directly according to the precedence constraints, i.e., $C_u = \{v \in V : (u, v) \in E\}$. A task without children is called a *target task*. Each task may have multiple parents and children.

Furthermore, we place ourselves in a context where we do not have perfect knowledge of the task parameters ($w_u$ and $m_u$) before the tasks start their execution, but only estimates [14], [26]. Hence, scheduling decisions are made on these estimated parameters, and may be reconsidered at runtime when a task starts its execution and we know its exact parameters.

### B. Execution environment

The goal is to execute the workflow on a heterogeneous system, denoted as $\mathcal{S}$, which consists of $k$ processors $p_1, \ldots, p_k$. Each processor $p_j$ ($1 \leq j \leq k$) has an individual memory of size $M_j$, a communication buffer of size $MC_j$ and a speed $s_j$. We can decide to evict some data from the main memory if we are sending the data to another processor; it then stays in the communication buffer until it has been sent. The execution time of a single task $u \in V$ on a processor $p_j$ is expressed as $\frac{w_u}{s_j}$. We assume that all processors are connected with the same bandwidth $\beta$.

We keep track of the current ready time of each processor and each communication channel, $rt_j$ and $rt_{j,j'}$, for each processor $j$ and all pairs $(j, j')$. Initially, all the ready times are set to 0. We also keep track of the currently available memory, $availM_j$ and $availC_j$, on the processor memory and communication buffer, respectively. Furthermore, $PD_j$ is a priority queue with the *pending data* that are in the memory of size $M_j$ but may be evicted to be communicated if more memory is needed on $p_j$. They are ordered by non-decreasing size and correspond to some $c_{u,v}$.

We use the MEMDAG algorithm developed by Kayaaslan *et al.* [19] to compute the memory requirement; it transforms the workflow into a series-parallel graph and then finds the traversal that leads to the minimum memory consumption.

| Symbol | Meaning |
|---|---|
| $G = (V, E)$ | Workflow graph, set of vertices (tasks) and edges |
| $\Pi_u$, $C_u$ | Parents of a task $u$, children of a task $u$ |
| $m_u$ | Memory weight of task $u$ |
| $w_u$ | Workload of task $u$ (normalized execution time) |
| $c_{u,v}$ | Communication volume along the edge $(u, v) \in E$ |
| $F$, $\mathcal{F}$ | A partitioning function and the partition it creates |
| $V_i$ | Block number $i$ |
| $\mathcal{S}$, $k$ | Computing system and its number of processors |
| $p_j$, proc($V_i$) | Processor number $j$, processor of block $V_i$ |
| $M_j$, $MC_j$, $s_j$ | Memory size, comm. buffer size, and speed of proc. $p_j$ |
| $\beta$ | Bandwidth in the compute system |
| $\underline{l}_u$ | Bottom weight of task $u$ |
| $\mu_G$, $\mu_i$ | Makespan of the entire workflow $G$ and of a block $V_i$ |
| $\Gamma = (\mathcal{V}, \mathcal{E})$ | Quotient graph, its vertices and its edges |
| $r_u$, $r_{V_i}$ | Memory requirement of task $u$ and of block $V_i$ |

TABLE I
NOTATION

### C. Optimization problem

The goal is to find a schedule of the DAG $G$ for the $k$ processors, so that the makespan (total execution time) is minimized while respecting memory constraints. If a processor runs out of memory to execute a task mapped on it, the schedule is said to be *invalid*.

Since tasks are subject to variability, we aim at minimizing the actual makespan achieved at the end of the execution, while decisions may be taken building on the estimated task parameters.

Note that the problem is already NP-hard even in the homogeneous case and without memory constraints, because of the DAG structure of the application. Hence, we focus on the design of efficient scheduling heuristics.

## IV. SCHEDULING HEURISTICS

We design variants of HEFT that account for memory usage and aim at minimizing the makespan. First, we present in Section IV-A the baseline HEFT heuristic that does not account for the memory (and hence, may return invalid schedules that will not be able to run on the platform by running out of memory). Then, Section IV-B focuses on the presentation of the novel heuristics, including eviction strategies to move some data in communication buffers in case there is not enough memory available on some processors.

### A. Baseline: original HEFT without memories

Original HEFT does not consider memory sizes. The solutions it provides can be invalid if it schedules tasks to processors without sufficient memories. However, these solutions can be viewed as a "lower bound" for an actual solution that considers memory sizes.

HEFT works in two stages. In the first stage, it computes the ranks of tasks by computing their non-increasing bottom levels. The bottom level of a task is defined as

$$bl(u) = w_u + \max_{(u,v)\in E} \{c_{u,v} + bl(v)\}$$

(the max is 0 if there is no outgoing edge). The tasks are sorted by non-decreasing ranks.

In the second stage, the algorithm iterates over the ranks and tries to assign the task to the processor where it has the earliest finish time. We tentatively assign each task $v$ to each processor $j$. The task's starting time $st_v$ is dictated by the maximum between the ready time of the processor $rt_j$, and all communications that must be orchestrated from predecessor tasks $u \notin T(p_j)$. The starting time is then:

$$ST(v, p_j) = \max\{rt_j, \max_{u \in \Pi(v)}\{FT(u) + c_{u,v}/\beta, rt_{proc(u),p_j} + c_{u,v}/\beta\}\}$$

Finally, its finish time on $p_j$ is $FT(v, p_j) = st_v + \frac{w_v}{s_j}$.

Once we have computed all finish times for task $v$, we keep the minimum $FT(v, p_j)$ and assign task $v$ to processor $p_j$.

*Assignment to processor.* When assigning the task, we set the ready time $rt_j$ of processor $j$ to be the finish time of the task. For every predecessor of $v$ that has been assigned to another processor, we adjust ready times on communication buffers $rt_{j',j}$ for every predecessor $u$'s processor $j'$: we increase them by the communication time $c(u, v)/\beta$.

### B. Memory-aware heuristics

Like the original HEFT, the memory-aware versions of HEFT consist of two stages: first, they compute the task ranks, and second, they assign tasks to processors in the order defined in the first stage. We consider three variants of HEFT accounting for memory usage (HEFTM), which only differ in the order they consider tasks to be scheduled in the first stage.

**Compute task ranks.**

We design three variants of memory-aware HEFT:

- HEFTM-BL orders tasks by non-increasing bottom levels, where the bottom level is defined as
$$bl(u) = w_u + \max_{(u,v)\in E}\{c_{u,v} + bl(v)\}$$
(the max is 0 if there is no outgoing edge).
- HEFTM-BLC is giving more priority at tasks with potential large incoming communications, hence aiming at clearing the memory used by files as soon as possible, to have more free memory for remaining tasks to be executed on the processor. Therefore, for each task, we compute a modified bottom level accounting for communications:
$$blc(u) = w_u + \max_{(u,w)\in E}\{c_{u,w} + blc(w)\} + \max_{(v,u)\in E} c_{v,u}.$$
- Finally, HEFTM-MM orders tasks in the order returned by the MEMDAG algorithm [19], which corresponds to a traversal of the graph that minimizes the peak memory usage.

**Task assignment.**

Then, the idea is to pick the next free task in the given order, and greedily assign it to a processor, by trying all possible options and keeping the most promising one. We first detail how a task is tentatively assigned on a processor, by carefully accounting for the memory usage. Next, we explain the steps to be taken to effectively assign a task on a given processor.

*Tentative assignment of task $v$ on $p_j$.*

**Step 1.** First, we need to check that for all predecessors $u$ of $v$ that are mapped on $p_j$, the data $c_{u,v}$ is still in the memory of $p_j$, i.e., $c_{u,v} \in PD_j$. Otherwise, the finish time is set to $+\infty$ (invalid choice).

**Step 2.** Next, we check the memory constraint on $p_j$, by computing

$$Res = availM_j - m_v - \sum_{u\in\Pi(v), u\notin T(p_j)}\{c_{u,v}\} - \sum_{w\in Succ(v)}\{c_{v,w}\}.$$

$T(p_j)$ is the set of tasks already scheduled on $p_j$; by step 1, their files are already in the memory of $p_j$. However, the files from the other predecessor tasks must be loaded in memory before executing task $v$, as well as $m_v$ and the data generated for all successor tasks. $Res$ is then checking whether there was enough memory; if it is negative, it means that we have exceeded the memory of $p_j$ with this tentative assignment.

In this case ($Res < 0$), we try evicting some data from memory so that we have enough memory to execute task $v$. We need to evict at least $Res$ data. We propose a greedy approach, evicting the largest files of $PD_j$ until $Res$ data has been evicted. A variant where the smallest files are evicted first has been tested, and it led to comparable results. While tentatively evicting files, we remove them from the list of pending memories and move them into a list of memories pending in the communication buffer. We keep track of the available buffer size, too – each time a file gets moved into the pending in buffer, the available buffer size is reduced by its weight.

If we still do not have enough memory after having tentatively evicted all files from $PD_j$, or if while doing so we exceeded the size of the available buffer, we set the finish time to $+\infty$ (invalid choice).

**Step 3.** We tentatively assign task $v$ on $p_j$. Its starting time $st_v$ is dictated by the maximum between $rt_j$, and all communications that must be orchestrated from predecessor tasks $u \notin T(p_j)$. The starting time is therefore:

$$ST(v, p_j) = \max\{rt_j, \max_{u\in\Pi(v), u\notin T(p_j)}\{FT(u), rt_{proc(u),p_j}\} + c_{u,v}/\beta\}.$$

Finally, its finish time on $p_j$ is $FT(v, p_j) = ST(v, p_j) + \frac{w_v}{s_j}$.

*Assignment of task $v$.*

Once we have computed all finish times for task $v$, we keep the minimum $FT(v, p_j)$ and assign task $v$ to processor $p_j$. In detail, we:

- Evict the file memories that correspond to edge weights that need to be evicted to free the memory. We remove these files from pending memories $PD_j$, add them to pending data in the communication buffer, and reduce the available buffer size accordingly.
- Calculate the new $availM_j$ on the processor. We subtract the weights of all incoming files from predecessors

assigned to the same processor, and add the weights of outgoing files generated by the currently assigned task.
- For every predecessor of $v$ that has been assigned to another processor, we adjust ready times on communication buffers $rt_{j',j}$ for the processor $j'$that the predecessor $u$ has been assigned to: we increase them by the communication time $c(u,v)/\beta$. We also remove the incoming files from either the pending memories or pending data in buffers of these other processors, and increase the available memories or available buffer sizes on these processors.
- We compute the correct amount of available memory for $p_j$ (for when the task is done). Then, for each predecessor that is mapped to the same processor, we remove the pending memory corresponding to the weight of the incoming edge, also freeing the same amount of available memory (increasing $availM_j$). For each successor, we rather add the edge weights to pending memories and reduce $availM_j$ by the corresponding amount.

## V. Dynamic scenario

In a workflow execution environment, the scheduling method interacts with the runtime environment, which provides information such as resource estimates. This information may include memory usage, runtime, graph structures, or the status of the underlying infrastructure. In order to ensure that the information is up to date, a monitoring system observes the workflow execution and collects metrics for tasks and the underlying infrastructure. By incorporating dynamic monitoring values, e.g., the resources a task consumed, the runtime environment can incorporate the data into the prediction model to provide more accurate resource predictions. Also the underlying infrastructure can change during the workflow execution. Examples are processor failures, node recoveries, or acquisition of new nodes. However, also when the hardware of the infrastructure does not change, the set of nodes provided as a scheduling target might change due to release or occupation in shared cluster infrastructures. As infrastructure information and resource predictions are dynamically updated and provided to the scheduler during the workflow runtime, the previous schedule becomes invalid and a new one must be calculated.

For state-of-the-art memory prediction methods, a cold-start median prediction error for heterogeneous infrastructures of approximately 15% is shown [24]. Online prediction methods were able to significantly reduce the error during runtime, with the reduction reaching up to one-third of the cold-start error [5], [36]. Such a dynamic execution environment requires a dynamic scheduling method where the schedule can be recomputed during the workflow execution.

### *Retracing the effects of change on an existing schedule*

After the monitoring system has reported changes, we need to assess their impact on the existing schedule. These changes can invalidate the schedule (*e. g.* if there is not enough memory for some tasks to execute anymore), they can lead to a later finishing time (*e. g.* if some tasks are longer and they delay other tasks), or they can have no effect (*e. g.* if new processors joined the cluster, but the old schedule did not account for them). To assess the impact, we need to retrace the schedule.

First, we find out if at least one processor that had assigned tasks has exited - this instantly invalidates the entire schedule.

We then iterate over all tasks of the workflow in a topological order - any of the orderings given by rankings BL, BLC or MM is a topological ordering. We then repeat steps similar to those we did during tentative assignment in the heuristics, except that we do not choose a processor anymore, but rather we check whether the current processor assigned to the task still fits.

For each task $v$, we first assess its current memory constraint $Res$ using Step 2 from the heuristic. The factors that affect $Res$ are possible changes in $m_v$, in $c_{u,v}$ from predecessors $u$ or $c_{v,w}$ from successors $w$, available memory $availM_j$ on the processor (due to either changed $M_j$ or changed memory requirements from other tasks). If originally, $Res$ was positive (no files were evicted from memory into the communication buffer), then it has to stay this way – otherwise, evicted files can invalidate next tasks. If original $Res$ was negative, then we need to make sure that evicted files still fit into the communication buffer. If either $Res$ is newly negative, or the communication buffer is not large enough, this invalidates the schedule. We update the $availM_j$ and $availMC_j$ values according to the new memory constraints.

Then, we can re-calculate the finish time of the task on its processor like in Step 3. The factors that affect it are changes in own execution time $w_v$ of the tasks, changed ready time of the processor (after delayed previous tasks), and changed communication buffer availability.

Finally, after having updated the processor's values, we move on to the next task.

## VI. Experimental evaluation

We first describe the experimental setup in Section VI-A. Then, we report results on static experiments to assess the performance of the memory-aware heuristics in Section VI-B, before discussing the heuristics behavior in a dynamic setting in Section VI-C. Finally, we report running times of the heuristics in Section VI-D.

### *A. Experimental setup*

All algorithms are implemented in C++ and compiled with g++ (v.8.5.0). The experiments are managed by simexpal [3] and executed on workstations with 192 GB RAM and 2x 12-Core Intel Xeon 6126 @3.2 GHz and CentOS 8 as OS. Code, input data, and experiment scripts are available to allow reproducibility of results, at https://zenodo.org/records/13919214 and https://zenodo.org/records/13919302.

We first describe the set of workflows used for the evaluation, and then the clusters on which the workflows are scheduled.

*1) Workflow instances:* We run experiments on a dataset that consists of real-world workflows: we use workflows coming from [6] (atacseq, bacass, chipseq, eager and methylseq), and also we increase their size using the WFGen generator [7].

*a) Workflow graphs:* For the five real-world workflows, their nextflow definition (see [13]) was downloaded from the respective repository and transformed into .dot format using the nextflow option "-with-dag". The resulting DAG contains many pseudo-tasks that are only internal representations in nextflow (and not actual tasks); that is why we removed them.

For the size-increased workflows, the graph is produced by the WFGen generator, based on a *model workflow* and the desired number of tasks. We used the real-world workflows as models, except for bacass that lead to errors in the generator. As number of tasks, we use: 200, 1 000, 2 000, 4 000, 8 000, 10 000, 15 000, 18 000, 20 000, 25 000, 30 000. We divide the workflows into four groups by size: tiny ones with up to 200 tasks, small ones with 1 000 to 8 000 tasks, middle ones with 10 000 to 18 000 tasks, and big ones with 20 000 to 30 000 tasks.

*b) Task and edge weights:* For the real-world workflows, we use historical data files provided by Bader *et al.* [6]. The columns in these files are measured Linux PS stats, acquired during an execution of a nextflow workflow. Each row corresponds to an execution of one task on one cluster node. Since the operating system cannot distinguish between (a) the RAM the task uses for itself and (b) the RAM it uses to store files that were sent or received from other tasks, the values in the historical data are total memory requirements (input/output files plus memory consumption of the computation). In a similar manner, the historical data provided by [6] do not store the actual weights of edges between tasks, but only the overall size of files that the task sends to all its children.

For each task, historical data can contain multiple values, obtained from the runs with different input sizes. The same workflow can require different memory capacity and take different time to execute depending on the size of its input. We simulate these various runs by obtaining values corresponding to each input size. For each of the four families, there are five input sizes, so we run each workflow in five variants corresponding to these inputs

Not all tasks have historical runtime data stored in the tables. In fact, for two workflows, Bader *et al.* do not provide data for more than 50% of the tasks. For two more, around 40% of tasks have no historical runtime data stored. Hence, in the absence of historical data about a task, we give it fixed weights. We give it an execution time of 1, a memory requirement of $50MB$, and files written and received of $1KB$. These values align with the findings of [6] about small tasks.

*2) Target computing systems:* To fully benefit from the historical data, the *default* experimental environment that we consider is a cluster based on the same six kinds of real-world machines that were used in the experimental evaluation in [6]. We set the number of each kind of node to 12, thus having 72 processors in total. Each machine has a (normalized) CPU speed and a memory size (in GB), and we list them as (name, speed, memory): ($local$, 4, 16) – very slow machines; ($A1$, 32, 32), ($A2$, 6, 64), ($N1$, 12, 16) – average machines; ($N2$, 8, 8) – machine with very small memory; and ($C2$, 32, 192) – *luxury* machine with high speed and large memory (see Table II).

| Processor name | CPU speed (GHz) | Memory size (GB) *default* | Memory size (GB) *mem-constrained* |
|---|---|---|---|
| local | 4 | 16 | 1.6 |
| A1 | 32 | 32 | 3.2 |
| A2 | 6 | 64 | 6.4 |
| N1 | 12 | 16 | 1.6 |
| N2 | 8 | 8 | 0.8 |
| C2 | 32 | 192 | 19.2 |

TABLE II
CLUSTER CONFIGURATION.

We also consider a more constrained setting, by varying the cluster configuration. The *memory-constrained cluster* is consisting of 72 nodes (12 of each kind) as the default cluster, but each node has 10 times less memory. Hence, the *luxury* machine $C2$ has 19.2 GB memory in this setting instead of 192 GB, $A2$ has 6.4 GB instead, of 64 GB etc. The processor speeds and their relations stay unchanged (see Table II).

Note that in both clusters, we set the size of the communication buffer to be equal to ten times the the memory size.

*3) Runtime system:* To simulate the execution of a workflow, we implemented a runtime system. It reads the historical data and builds weights for tasks, as explained above. In the static case, these values are being sent to the scheduler, which builds a schedule according to these weights. However, in the dynamic setting, the runtime system applies a deviation function to the values. The deviation function computes a normally distributed deviated value, where the initial value is the mean and the deviation is 10%. This scenario corresponds to the real-life scenarios identified in [6] and other works dedicated to predicting runtimes of tasks [8], [9].

Hence, the scheduler receives deviated values and makes decision based on them. This leads to several types of possible issues:

- A processor is blocked by another task. If the scheduler underestimated the execution time of a task, it will block another one from starting.
- A predecessor has not yet finished. The scheduler may request a task to start on its processor, while some of the predecessors of the tasks have in fact not yet completed their execution, and the task is therefore not yet ready.
- Not enough memory. If the scheduler underestimated the amount of memory a task requires, this task might not be able to execute on a chosen processor.
- A task took less time than expected. We only consider this case if a task took more than 10% less time than expected. In this case, we want to exploit the newly acquired free time by possibly starting other tasks earlier.

### B. Results in a static setting

We first study the heuristics behavior when the weights do not change upon runtime, hence the scheduler has a perfect knowledge of task memory requirements and execution times. We have compared two eviction strategies, starting with large files first or small files first, and did not report any significant

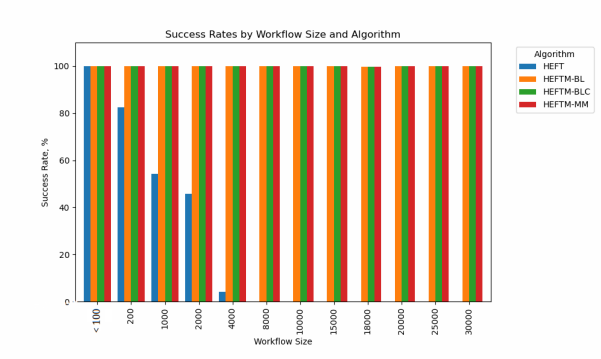


Fig. 1. Success rates on the default cluster. Higher is better.

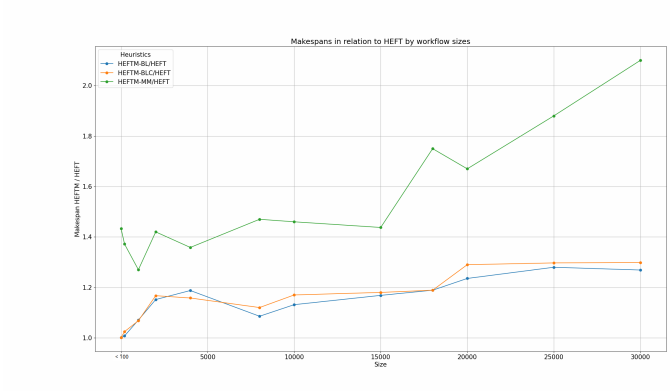


Fig. 2. Relative makespans of heuristics normalized by HEFT makespan, by workflow size, on default cluster. Smaller is better.

changes in terms of validity of schedule or makespan. Hence, we only present results with the eviction of largest files first.

*1) Scheduling on the default cluster:* On the default cluster, the three memory-aware heuristics are able to schedule all workflows (see Figure 1), while the baseline HEFT has 24.2% success rate (75.7% failure rate). Indeed, HEFT is only able to schedule small workflows, but no workflow over the size of 4000 tasks can be scheduled correctly; some tasks run out of memory. As soon as we are not in a setting with abundant processing resources for small workflows, it is hence necessary to adopt a memory-aware strategy in order to produce valid schedules.

We also report in Figure 2 the relative makespan found by the memory-aware heuristics, normalized to the makespan achieved by HEFT, often through an invalid over-optimistic schedule that exceeds the bound on memory. On average, the makespans found by HEFTM-BL are 7.8% worse than those found by the baseline, the makespans of HEFTM-BLC are 8% worse, and those found by HEFTM-MM are 82.6% worse. These are still very encouraging results, in particular for HEFTM-BL and HEFTM-BLC, since the makespans of HEFT correspond to invalid schedules.

Finally, we study the percentage of memory occupied by the schedule, which is another good indicator of the memory usage of the heuristic and its ability to produce valid schedules. Figures 3 and 4 show the percentage of memory occupied on

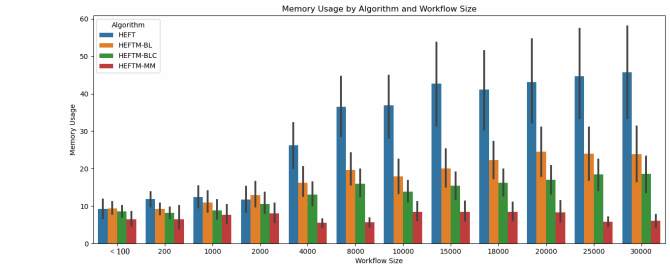


Fig. 3. Memory usage on default cluster, including invalid HEFT schedules.

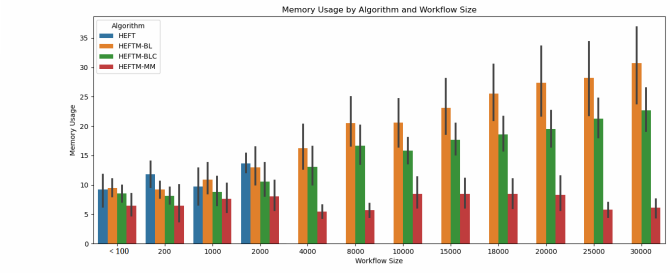


Fig. 4. Memory usage on default cluster, including only valid HEFT schedules.

average by the schedule produced by the different heuristics, for different workflow sizes, first on all schedules (hence including HEFT schedules that were not valid), and then only on valid schedules (hence, no results for HEFT on large workflow sizes).

HEFTM-MM continuously outperforms other heuristics in terms of memory usage, using from 46% less memory on the smallest workflows to 4 times less memory on the largest 30 000-task workflows. If we consider the invalid HEFT schedules, too, we see that they would require more and more memory on average, which explains why these schedules rapidly become invalid. This is because some assignments require more that 100% of memory (which makes them invalid). We can assess the degree of invalidity by comparing HEFT memory usage with the memory usage of HEFTM-BL. HEFTM-BL differs from the baseline only in the sense that it respects available memory on the processors. For the largest workflows, HEFT schedules require almost twice the memory of HEFTM-BL.

*2) Scheduling on the memory-constrained cluster:* On the memory-constrained cluster, HEFT could produce valid assignments in only 14 experiments out of 290 (4.8% success rate). The successful schedules were achieved exclusively on the tiny workflows (with only two 200-task size-increased workflow among them). HEFTM-BL could successfully schedule 38% of workflows, HEFTM-BLC could schedule 49% of them, while HEFTM-MM could still schedule all the workflows, including even the largest ones, see Figure 5. As also observed on the normal cluster, HEFTM-MM seems to be less affected by the size of the workflow when scheduling it than the other heuristics.

Similarly to the default cluster, we observe that relative

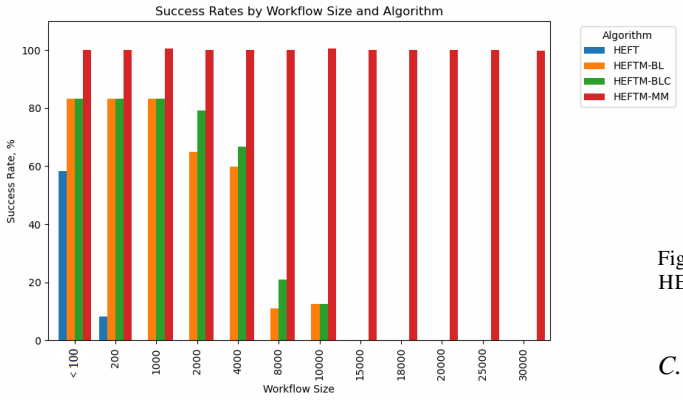


Fig. 5. Success rates on the memory-constrained cluster. Higher is better.

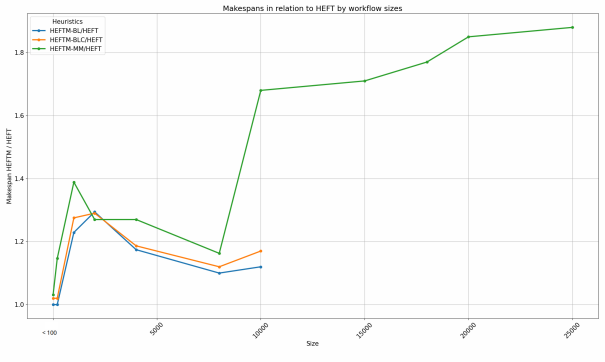


Fig. 6. Relative makespans on the memory-constrained cluster. Smaller is better.

makespan of HEFTM-MM is usually greater than those of HEFT (see Fig. 6), but HEFT schedules are almost all invalid. It is therefore very interesting to resort to HEFTM-MM for large workflows in a constrained cluster, since tasks are processed in an order that minimizes the memory usage of schedule.

Memory usages on the constrained cluster are depicted in Fig. 7, and we observe that the memory footprint of HEFTM-MM remains constant with workflow size.

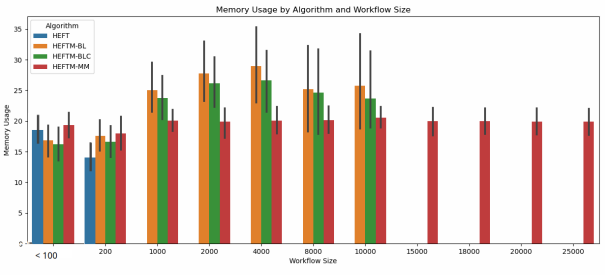


Fig. 7. Memory usage on the memory-constrained cluster.

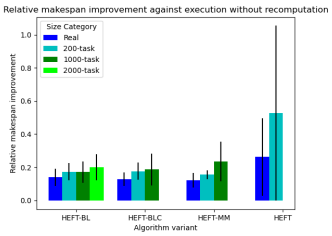


Fig. 8. Relative (excess) makespan of HEFTM-BL, HEFTM-BLC and HEFTM-MM for different . Smaller is better.

### C. Dynamic experiments

*a) Memory-constrained cluster:* The makespan in case of no recomputation becomes invalid as soon as at least one task finds itself in an invalid memory size situation - that is, if the scheduler assumed its memory to be smaller than it actually was and assigned it to a processor with not enough memory capacity. Due to an extremely constrained memory in the tiny cluster, only 134 experiments out of 1160 for all algorithm variants ended with a valid makespan without recomputation. In case of HEFT, 14 valid initial makespans were computed. Out of them, 13 managed to stay valid until the end, after all the update requests. The same 13 experiments ended with a valid makespan in case of no recomputation. So, these workflows required so few resources that there was no point in re-scheduling them. In case of HEFTM-MM, all 290 workflows could be scheduled initially and all the schedules remained valid until the end. 16 experiments ended with a successful makespan without recomputation. The rate of successful schedules without recomputation is therefore 5.5% HEFTM-BLC could produce 142 valid initial schedules and kept 141 of them valid until the end. 50 experiments were successful without recomputation, too, making it 35% out of all successful final schedules. HEFTM-BL kept 105 schedules valid until the end out of 110 initial valid schedules. 55 were able to be kept valid until the end even without recomputation, roughly 50% of all succeses.

HEFTM-BL and HEFTM-BLC were successful on smaller workflows and failed on larger ones, the success of the strategy without recomputation was limited to even the smallest of these smaller workflows. So, the strategy without recomputation dfelivered valid makespans (independently of the algorithm) on 56 original workflows with $< 100$ tasks, 47 200-task ones, 25 1000-task ones and 6 2000-task ones.

Figure 8 shows the increase in makespan in case of no recomputation for these experiments. With growing size of the workflow, the excess makespan of not recomputing grows - from 13.9% to 20% for HEFTM-BL, from 12.7% to 18.7% on HEFTM-BLC (but there is no data for the 2000-task workflows in this case), 12.1% to 23.5% for HEFTM-MM. The larger variations for HEFT can be explained by the small amount of data - for example, there were only 2 200-task workflows for this case.

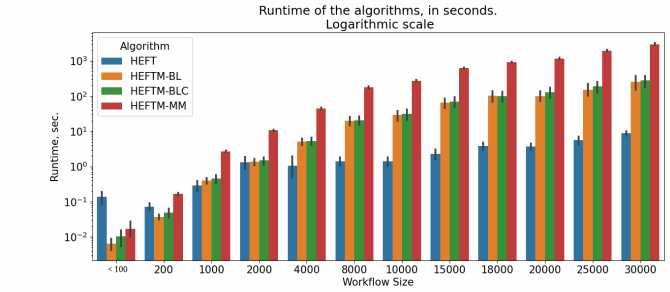


Fig. 9. Running times of the heuristics. The y axis is logarithmic.

### D. Running times of the heuristics

To be able to answer the runtime system without holding it up for too long, the scheduler needs to be able to compute a schedule rapidly. The bottom-level-based heuristics HEFTM-BL and HEFTM-BLC provide smaller running times than HEFTM-MM, and also scale better with growing workflow sizes (see Fig. 9). Their running times are similar and grow from tens of milliseconds for the smallest workflows to $25-27$ seconds for the largest workflows. HEFTM-MM, however, needs to compute a memory-optimal traversal of the entire workflow to compute the ranks of the tasks, so its running time scales from also tens of milliseconds for the smallest workflows, to thousands of seconds - $1172.7$ for $20\,000$-task workflows and $2994.9$ seconds for the largest, $30\,000$-task workflows. This increased running time is, though, offset by the unique $100\%$ success rate this algorithm obtained when scheduling large workflows in difficult (memory-constrained) setups.

## VII. Conclusion

We have formalized a scheduling problem in memory-constrained environments, where tasks may exceed the memory available on a processor and resort to communication buffers to store and communicate data between processors. In this context, we have designed three memory-aware HEFT-based heuristics, which account for memory constraints while scheduling tasks.

Two heuristics rely on an ordering of tasks based on the bottom level of tasks, with the objective of minimizing the makespan and hence scheduling critical tasks first. The third one, HEFTM-MM, goes one step further and handles tasks in an order dictated by an efficient traversal of the graph in terms of memory requirements, hence reducing the memory used by the schedule. Experimental results on a large set of workflows coming from real-life applications demonstrate that the memory-aware heuristics are successfully producing valid schedules. In the most memory-constrained setting, HEFTM-MM succeeds to schedule even the largest workflows, while other heuristics return invalid schedules exceeding the memory capacity of processors. It comes at a price of a makespan that is not quite as good as the one obtained by HEFTM-BL and HEFTM-BLC, which focus on makespan by ordering tasks by bottom level. As expected, the baseline HEFT that is not memory aware returns invalid schedules in almost all settings, except for very small workflows.

Another key contribution is that we have adapted these heuristics for a dynamic setting, where exact task parameters (execution times and memory requirements) are not know in advance. We have implemented a runtime system that interacts with the scheduler, returning exact parameter values once a task arrives in the system, while only estimates are known for future tasks. Some preliminary experiments have been conducted in this setting, and demonstrated that it is necessary to adapt the schedule on the fly in order to avoid an execution failure because of a shortage in memory. To the best of our knowledge, this is the first study of adaptive algorithms accounting for memory constraints.

This work could be extended in several directions. First, the model could be refined to include heterogeneous bandwidths, while we consider a homogeneous communication network. More importantly, it would be interesting to consider other types of variability, for instance if new tasks appear in the graph (or disappear), or if there is variability in the platform, with processors arriving and departing. We believe that we could adapt the current approach by recomputing schedules on the fly, and we plan to perform a new set of experiments to further assess the impact of dynamic scheduling.

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