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Locality-Aware Scheduling of Independent Tasks for Runtime Systems (extended version)

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Abstract. A now-classical way of meeting the increasing demand for computing speed by HPC applications is the use of GPUs and/or other accelerators. Such accelerators have their own memory, which is usually quite limited, and are connected to the main memory through a bus with bounded bandwidth. Thus, a particular care should be devoted to data locality in order to avoid unnecessary data movements. Task-based runtime schedulers have emerged as a convenient and efficient way to use such heterogeneous platforms. When processing an application, the scheduler has the knowledge of all tasks available for processing on a GPU, as well as their input data dependencies. Hence, it is able to order tasks and prefetch their input data in the GPU memory (after possibly evicting some previously-loaded data), while aiming at minimizing data movements, so as to reduce the total processing time. In this paper, we focus on how to schedule tasks that share some of their input data (but are otherwise independent) on a GPU. We provide a formal model of the problem, exhibit an optimal eviction strategy, and show that ordering tasks to minimize data movement is NP-complete. We review and adapt existing ordering strategies to this problem, and propose a new one based on task aggregation. These strategies have been implemented in the STARPU runtime system, which allows to test them on a variety of linear algebra problems. Our experiments demonstrate that using our new strategy together with the optimal eviction policy reduces the amount of data movement as well as the total processing time.

Keywords: Memory-aware scheduling, Eviction policy, Tasks sharing data, Runtime systems.

1 Introduction

High-performance computing applications, such as physical simulations, molecular modeling or weather and climate forecasting, have an increasing demand in computer power to reach better accuracy. Recently, this demand has been met by extensively using GPUs, as they provide large additional performance for a relatively low energy budget. Programming the resulting heterogeneous architecture which merges regular CPUs with GPUs is a very complex task, as one needs to handle load balancing together with data movements and task affinity (tasks have strongly different speedups on GPUs). A deep trend which has emerged to cope with this new complexity is using task-based programming models and task-based runtimes such as PaRSEC [5] or STARPU [3]. These runtimes aim at scheduling scientific applications, described as directed acyclic graphs (DAGs) of tasks, onto distributed heterogeneous platforms, made of several nodes containing different computing cores.

Data movement is an important problem to consider when scheduling tasks on GPUs, as those have a limited memory as well as a limited bandwidth to read/write data from/to the main memory of the system. Thus, it is crucial to carefully order the tasks that have to be processed on GPUs so as to increase data reuse and minimize the amount of data that needs to be transferred. It is also important to schedule the transfers soon enough (prefetch) so that data transfers can be overlapped with computations and all tasks can start without delay. We focus in this paper on the problem of scheduling a set of tasks on one GPU with limited memory, where tasks share some of their input data but are otherwise independent. More precisely, we want to determine the order in which tasks must be processed as well as when their input must be loaded/evicted into/from memory. Our objective is to minimize the total amount of data transferred to the GPUs for the processing of all tasks. We start focusing on independent tasks sharing input data because when using usual dynamic runtime schedulers, the scheduler is exposed at a given time to a subset of tasks, which are independent of each others and the size of this subset is usually quite large. This is in particular the case with linear algebra workflows, such as the matrix multiplication or Cholesky decomposition: except possibly at the very beginning or very end of the computation, a large set of tasks is available for scheduling. Thus, solving the optimization problem for the currently available tasks can lead to a large reduction in data transfers and hence a performance increase.

In this paper, we make the following contributions:

- We provide a formal model of the optimization problem, and prove the problem to be NP-complete. We derive an optimal eviction policy by adapting Belady's rule for cache management (Section 2).
- We review and adapt three heuristic algorithms from the literature for this problem, and propose a new one based on gathering tasks with similar data patterns into packages (Section 3).
- We implement all four heuristics into the STARPU runtime and study the performance (amount of data transfers and total processing time) obtained on various tasks sets coming from linear algebra operations (Section 4). Overall, our evaluation shows that our heuristic generally surpasses previous strategies, in particular in the most constrained situations.

Note that while we focus our experimental validation on GPUs, the optimization problem studied in this paper is not specific to heterogeneous computing: it appears as soon as tasks sharing data must be processed on a system with limited memory and bandwidth. For example, it is also relevant for a computer made of several CPUs with restricted shared memory, and limited bandwidth for the communication between memory and disk.

The problem of fitting a working set in a given amount of memory [9] is a general concern that shows up at various levels such as the processor cache, the operating system page cache (most often solved with only a mere LRU heuristic), or tasks sharing files in a distributed context [12]. By some aspects, our work is for instance close to some studies in cache optimization, which consists in reordering requests to optimize cache reuse [10]. However, contrarily to these studies, we have here complete access to the whole set of tasks, not only a subset, and can completely re-order it. The MST approach [14] is probably closest to our work since it focuses on ordering independent tasks sharing data. They target multicore CPUs, which entails addressing both grouping and ordering tasks. In the experiments presented in this paper, we compare our heuristic to the MST approach.

2 Problem modeling and complexity

We consider the problem of scheduling independent tasks on a GPU with memory size M. As proposed in previous work [12], tasks sharing their input data can be modeled as a bipartite graph $G = (\mathbb{T} \cup \mathbb{D}, E)$. The vertices of this graph are on one side the tasks $\mathbb{T} = \{T_1, \ldots, T_m\}$ and on the other side the data $\mathbb{D} = \{D_1, \ldots, D_n\}$. An edge connects a task T_i and a data D_j iff task T_i requires D_j as input data. For the sake of simplicity, we denote by $\mathcal{D}(T_i) = \{D_j \text{ s.t. } (T_i, D_j) \in E\}$ the set of input data for task T_i . We consider that all data have the same size. The GPU is equipped with a memory of limited size, which may contain no more than M data simultaneously. During the processing of a task T_i , all its inputs $\mathcal{D}(T_i)$ must be in memory.

For the sake of simplicity, we here do not consider the data output of tasks. In the case of linear algebra for instance, the output data is most often much smaller than the input data and can be transferred concurrently with data input. Data output is then not the driving constraint for efficient execution. Our model could however easily be extended to integrate task output.

All tasks must be processed. Our goal is to determine in which order to process them, and when each data must be loaded or evicted, in order to minimize the amount of data movement. More formally, we denote by σ the order in which tasks are processed, and by $\mathcal{V}(t)$ the set of data to be evicted from the memory before the processing of task $T_{\sigma(t)}$. A schedule is made of m steps, each step being composed of the following three stages (in this order):

1. All data in $\mathcal{V}(t)$ are evicted (unloaded) from the memory;

- 2. The input data in $\mathcal{D}(T_{\sigma(t)})$ that are not yet in memory are loaded;
- 3. Task $T_{\sigma(t)}$ is processed.

An example is shown in Figure 1. In this model, input data are loaded in memory as late as possible: loading them earlier would be pointless and possibly trigger more data movements. In real computing systems, a pre-fetch is usually designed to load data a bit earlier so as to avoid waiting for unavailable data, however we



Fig. 1: Example with 5 tasks and 6 data, with a memory holding at most M = 3 data. The graph of input data dependencies is shown on the left. The schedule on the right corresponds to processing the tasks in the natural order with the following eviction policy: $\mathcal{V}(1) = \mathcal{V}(2) = \emptyset$, $\mathcal{V}(3) = \{1\}$, $\mathcal{V}(4) = \{2\}$, $\mathcal{V}(5) = \{3, 4\}$. This results in 7 loads (only D_1 is loaded twice).

do not consider this in our model: we may simply book part of our memory for the pre-fetch mechanism.

Using the previous definition, we define the *live data* L(t) as the data in memory during the computation of $T_{\sigma(t)}$, which can be defined recursively:

$$L(t) = \begin{cases} \mathcal{D}(T_{\sigma(1)}) & \text{if } t = 1\\ L(t) = (L(t-1) \setminus \mathcal{V}(t)) \cup \mathcal{D}(T_{\sigma(t)}) & \text{otherwise} \end{cases}$$

Our memory limitation can then be expressed as $|L(t)| \leq M$ for each step $t = 1, \ldots, m$. Our objective is to minimize the amount of data movement, i.e., to minimize the number of *load* operations: we consider that data are not modified so no *store* operation occurs when evicting a data from the memory. Assuming that no input data used at step t is evicted right before the processing $(\mathcal{V}(t) \cap \mathcal{D}(T_{\sigma(t)}) = \emptyset)$, the number of loads can be computed as follows:

$$#Loads(\sigma, \mathcal{V}) = \sum_{t} \left| \mathcal{D} \left(T_{\sigma(t)} \right) \setminus L(t) \right|$$

There is no reason for a scheduling policy to evict some data from memory if there is still room for new input data. We call *thrifty scheduler* such a strategy, formalized by the following constraints: if $\mathcal{V}(t) \neq \emptyset$, then |L(t)| = M. For this class of schedulers, the number of loads can be computed more easily: as soon as the memory is full, the number of loads is equal to the number of evictions. That is, for the regular case when not all data fit in memory (n > M), we have:

$$\#Loads(\sigma, \mathcal{V}) = M + \sum_{t} |\mathcal{V}(t)|$$

Our optimization problem is stated below:

Definition 1 (MinLoadsForTasksSharingData). For a given set of tasks \mathbb{T} sharing data in \mathbb{D} according to \mathcal{D} , what is the task order σ and the eviction policy \mathcal{V} that minimizes the number of loads #Loads?

A solution to this optimization problem consists in two parts: the order σ of the tasks and the eviction policy \mathcal{V} . An optimal eviction policy has been proposed for cache management policy, which corresponds to the same problem when tasks request a single data [13]: when the memory (or the cache) is full and new data must be loaded, an optimal policy consists in evicting the data whose next use is the furthest in the future. Hence, it requires to know the full series of future requests and is only usable in the offline case. This is the well-known Belady MIN replacement policy [4]. We prove in the following theorem that this rule can be extended to our problem, with tasks requiring multiple data.

Theorem 1. We consider a task schedule σ for a MINLOADSFORTASKS-SHARINGDATA problem. We denote by MIN the thrifty eviction policy that always evicts a data whose next use in σ is the latest (breaking ties arbitrarily). MIN reaches an optimal performance, i.e., for any eviction policy \mathcal{V} ,

$$\#Loads(\sigma, MIN) \leq \#Loads(\sigma, \mathcal{V})$$

Proof. We consider a given task order σ . We transform our problem so that each task depends on a single data (or page). we replace a task T_i depending on data $\mathcal{D}(T_i) = \{D_1, \ldots, D_k\}$ by a series of 2k tasks: $T_i^{(1)}, T_i^{(2k)}$ such that $\mathcal{D}(T_i^{(j)}) = \mathcal{D}(T_i^{(j+k)}) = D_j$ for $j = 1, \ldots, k$. We denote by \mathbb{T}' the modified set of tasks and by σ' the modified task order.

Let \mathcal{V} be an optimal eviction policy for the original problem, i.e. for task set \mathbb{T} and task order σ . We now transform it into an eviction policy for \mathbb{T}' and σ' with the same number of loads and evictions. We group tasks by subsets of 2k tasks (as they were created above) and evict all data in $\mathcal{V}(t)$ before processing tasks $T_{\sigma(t)}^{(1)}, T_{\sigma(t)}^{(2k)}$ (and loading their missing inputs). We denote this strategy by \mathcal{V}' . Clearly, this is a valid strategy (we never exceed the memory if \mathcal{V} did not on the original problem) and it has the same number of loads as \mathcal{V} :

$$#Loads(\sigma, \mathcal{V}) = #Loads(\sigma', \mathcal{V}').$$

Symmetrically, we consider an optimal eviction policy for the transformed problem (\mathbb{T}' and σ') obtained with Belady's MIN replacement policy, denoted by MIN': whenever some data must be evicted, it selects the one whose next use is the furthest in the future. We now prove that it can be transformed into an eviction policy MIN for the original problem with the same performance (loads and evictions), and that MIN also follows Belady's rule. We consider a subset of 2k tasks $T_i^{(1)}, T_i^{(2k)}$ coming from the expansion of task T_i scheduled at time t($\sigma(t) = T_i$) and the set of data V evicted by MIN' right before some task $T_i^{(j)}$. By property of MIN' and as the memory is large enough for the inputs of task T_i ($M \ge k$) no input data of some $T_i^{(j)}$ belongs to V: during the first k tasks, their next occurrence is the closest, and there is no eviction during the processing of the last k tasks. Thus, we can adapt MIN' for the original problem by setting MIN(t) = V. It is easy to verify that MIN reaches the same performance as MIN':

$$#Loads(\sigma, MIN) = #Loads(\sigma', MIN')$$

and that the data evicted at time t are (among the) ones whose next use is the furthest in the future.

As MIN' is known to be optimal for the transformed problem, we have $\#Loads(\sigma', MIN') \leq \#Loads(\sigma', \mathcal{V}')$ and we conclude that $\#Loads(\sigma, MIN) \leq \#Loads(\sigma, \mathcal{V})$, which proves that MIN is optimal on the original problem. \Box

For cache management, Belady's rule has little practical impact, as the stream of future requests is generally unknown; simple online policies such as LRU (Least Recently Used [9]) are generally used. However in our case, the full set of tasks is available at the beginning. Hence, we can greatly take advantage of this optimal offline eviction policy, as our experiments demonstrate below.

Thanks to the previous result, we can restrict our problem to finding the optimal task order σ . Unfortunately, this problem is NP-complete.

Theorem 2. For a given set of tasks \mathbb{T} sharing data in \mathbb{D} according to \mathcal{D} and a given integer B, finding a task order σ such that $\#Loads(\sigma, MIN) \leq B$ is NP-complete.

Proof. We first check that the problem is in NP. Given a schedule σ (and an eviction policy \mathcal{V} , which might be deduced by MIN), it is easy to check in polynomial time that:

- The schedule is valid, that is, no more than M data are loaded in memory at any time step;
- The number of loads is not greater than the prescribed bound B.

The NP-completeness proof consists in a reduction from the cutwidth minimization problem (or CMP), proven NP-complete by Gavril in 1977 [11]. We denote by I_{CMP} an instance of CMP composed of a graph The question is to decide whether there exists a linear arrangement of the vertices such that the cutwidth is at most K. A linear arrangement α is a simple order of the vertices. The cutwidth $CUT_{\alpha}(v)$ of a vertex v under the linear arrangement α is the number of edges that connect vertices ordered before and after v in α , that is, the number of edges $(u, w) \in E$, such as $\alpha(u) < \alpha(v) < \alpha(w)$. The total cutwidth of G is the maximal cutwidth over all vertices : $CUT_{\alpha}(G) = \max_{v \in V} CUT_{\alpha}(v)$.

Given an instance I_{CMP} an instance of CMP, we create an instance $I_{MinLoads}$ of our problem as follows. For each vertex $v_i \in I_{CMP}$, we create a task T_i , and for each edge $e_k = (v_i, v_j)$, we create a data D_k such that D_k is a shared input of T_i and T_j . Then,

 $\mathcal{D}(T_i) = \{D_k, \text{ such that } e_k \text{ is adjacent to } v_i \text{ in } G\}.$

Finally, we set M = K and $B = |\mathbb{D}| = |E|$: we are looking for a solution where each data is loaded exactly once.

We now prove that if I_{CMP} has a solution, then $I_{MinLoads}$ has a solution. Let α be the linear arrangement solution of I_{CMP} . We consider the task order $\sigma = \alpha^{-1}$, and the optimal eviction policy *MIN*. We prove that

(i) A data is evicted only if it is not used anymore;

(ii) Each data is loaded exactly once.

Note that (ii) is a direct consequence of (i). We consider a step t when some data D_j is evicted and some task T_i is processed. We consider the set S of data in memory before starting step t together with the inputs of $T_{\sigma(t)}$ that are loaded in memory during step t. If D_j is evicted, this means that |S| > M (*MIN* is a thrifty policy). We consider S', the subset of S containing the data that are as input for a later step t' > t. By construction of $I_{MinLoads}$, each data $D_k \in S'$ corresponds to an edge $e_k = (v_a, v_b)$ in G such that $\sigma^{-1}(u_a) = \alpha(v_a) < t$ (the data was loaded for a task T_a scheduled before t) and $\sigma^{-1}(v_b) = \alpha(v_b) > t$ (the data is used for a task T_b scheduled after t). Hence, it corresponds to an edge counted in the cutwidth $CUT_{\alpha}(v_i)$. Since this cutwidth is bounded by K = M, there are at most M data in S'. Thus, the evicted data D_j is not used later than t. Since all data are loaded exactly once, the number of loads is not larger than B.

We now prove that if $I_{MinLoads}$ has a solution, then I_{CMP} has a solution. Let σ the task order in the solution of $I_{MinLoads}$. We construct the solution of I_{CMP} such that $\alpha = \sigma^{-1}$. We now prove that its cutwidth is not larger than K. By construction, the cutwidth $CUT_{\alpha}(v_i)$ at some vertex v_i (corresponding to a task T_i scheduled at time t) is the number of data which are used both before t and after t. Given the constraint on the number of loads, each data is loaded once, so such a data must be in memory during the processing of T_i , and there are at most M such data. This proves that $CUT_{\alpha}(v_i) \leq M = B$. Hence α is a solution for I_{CMP} .

3 Algorithms

We present here several heuristics to solve the MINLOADSFORTASKSSHARING-DATA optimization problem. Two of them are adapted from the literature (Reverse-Cuthill-McKee and Maximum Spanning Tree), one of them is the actual dynamic strategy from the STARPU runtime (DMDAR) and we finally propose a new strategy (HFP).

Reverse-Cuthill-McKee (RCM) We have seen above that our problem is close to the cutwidth minimization problem, known to be NP-complete. This motivates the use of the Cuthill-McKee algorithm, which concentrates on a close metric: the bandwidth of a graph. It permutes a sparse matrix into a band matrix so that all elements are close to the diagonal [8]. If the resulting bandwidth is k, it means that vertices sharing an edge are not more than k edges away. We apply this algorithm on the graph of tasks $G^T = (\mathbb{T}, E^T, w^T)$ where there is an edge (T_i, T_j) if tasks T_i and T_j share some data, and where $w^T(T_i, T_j)$ is the number of such shared data. If the bandwidth of the graph is not larger than k, this means in our problem that any task T_i processed at time t has all its "neighbours" tasks (tasks sharing some data with T_i) processed in the time interval [t - k; t + k]. Hence, if k is low, this leads to a very good data locality. Reversing the obtained order is known to improve the performance of the Cuthill-McKee algorithm, which we also notice in our experiments. The adaption of the Reverse-Cuthill–McKee algorithm is described in Algorithm 1.

Algorithm 1 Reverse-Cuthill-McKee heuristic

Build the graph G^T where vertices are tasks and edges are common data between tasks, weighted by the number of such data $\sigma \leftarrow [v]$ where v is the vertex of G^T with smallest weighted degree $i \leftarrow 0$ while $|\sigma| < m$ do Let N be the set of vertices adjacent to $\sigma[i]$ in G^T not yet in σ Sort N by non-decreasing weighted degree Append N at the end of σ $i \leftarrow i + 1$ end while Return σ in the reverse order

Differences CM and RCM

Theorem 3. For a given set of tasks \mathbb{T} sharing data in \mathbb{D} : $\#Loads(\sigma) = \#Loads(\bar{\sigma})$.

Proof. Be σ a schedule. We can deduct from σ and the eviction policy chosen (it can be any eviction policy): \mathbb{S} the order in which data are loaded and \mathbb{V} the order in which the data are evicted from the memory. We add all the evictions for emptying the memory at the end of \mathbb{V} . We create the reverse order of σ : $\bar{\sigma}$. We can deduct from $\bar{\sigma}$: $\bar{\mathbb{S}}$ and $\bar{\mathbb{V}}$. We can say that any loading of \mathbb{S} is an eviction of $\bar{\mathbb{V}}$ and any eviction of \mathbb{V} is a loading of $\bar{\mathbb{S}}$. Thus,

$$NB_I(\mathbb{S}, \mathbb{V}) = NB_I(\bar{\mathbb{S}}, \bar{\mathbb{V}})$$

Let's note $min\#Loads(\sigma)$ the minimal number of loads we can obtain by using an optimal eviction policy. From $min\#Loads(\sigma)$ we can deduct with Belady \mathbb{S}_{min} and \mathbb{V}_{min} . We build a couple $(\bar{\mathbb{S}}, \bar{\mathbb{V}})$ that does at most as much loads as $min\#Loads(\sigma)$. So we have:

$$\#Loads(\mathbb{S}, \mathbb{V}) \leq \#Loads(\mathbb{S}_{min}, \mathbb{V}_{min}) = min \#Loads(\sigma)$$

And:

$$min \#Loads(\bar{\sigma}) \leq \#Loads(\mathbb{S}, \mathbb{V}) \leq min \#Loads(\sigma)$$

So the reverse order does less loads or as much loads than the optimal σ . In the same way we can show that:

 $min \#Loads(\sigma) \le min \#Loads(\bar{\sigma})$

By double inequality:

$$min \# Loads(\sigma) = minNB_I(\bar{\sigma})$$

So the number of loads are the same for σ or $\bar{\sigma}$.

However the performance are not the same. We can see on Figure 2 that RCM is always better than CM. Indeed the total number of load is the same, but the distribution of loads in time is not equal.



(a) On the 2D matrix multiplication.

(b) On the task set of the Cholesky factorization.

Fig. 2: Comparison of Cuthill-McKee and Reverse-Cuthill-McKee.

Maximum Spanning Tree (MST) As outlined in the related work, another heuristic has been proposed to order tasks sharing data to improve data locality [14]. The authors of this study propose to build a Maximum Spanning Tree in the graph G^T using Prim's algorithm [7] and to order the vertices according to their order of inclusion in the spanning tree. By selecting the incident edge with largest weight, we increase the data reuse between the current scheduled tasks and the next one to process. The adaption of the Maximum Spanning Tree algorithm is described in Algorithm 2

Deque Model Data Aware Ready (DMDAR) DMDA or "Deque Model Data Aware" is a dynamic scheduling heuristic designed to schedule tasks on heterogeneous processing units in the STARPU runtime. It takes data transfer time into account and schedules tasks where their completion times is expected to be minimal [2] (also called tmdp). We focus here on a variant, DMDAR, which additionally favors tasks whose data has already been loaded into memory. In our context with a single processing unit, it is reduced to selecting the next task as the one that has the minimum number of inputs not already loaded in memory (see Algorithm 3). DMDAR is a dynamic scheduler that relies on the actual

Algorithm 2 Maximum Spanning Tree heuristic

```
For each vertex v_i set Key\_Value(v_i) to 0

Key\_Value(v_0) \leftarrow 1

while |\sigma| \neq m do

Choose v_i \in \mathbb{T} \notin \sigma such that Key\_Value(v_i) is maximum

Add v_i at the end of the list \sigma

For each couple (v_i, v_j), update Max\_Path\_Length(i, j)

for each v_j adjacent to v_i \cap \notin \sigma do

if Key\_Value(v_j) < Max\_Path\_Length(i, j) then

Key\_Value(v_j) \leftarrow Max\_Path\_Length(i, j)

end if

end for

end while

Return \sigma
```

state of the memory, it thus depends on the eviction policy, which is the LRU policy.

Algorithm 3 DMDAR heuristic

Let T_1 be the first task in \mathbb{T} Add T_1 to σ , $InMem \leftarrow \mathcal{D}(T_1)$ while $|\sigma| \neq m$ do Select a task $T_i \notin \sigma$ such that $|\mathcal{D}(T_i) \setminus InMem|$ is minimal Add T_i to σ $InMem \leftarrow InMem \cup \mathcal{D}(T_i)$ if |InMem| > M then evict data from InMem following LRU's policy end while Return σ

Hierarchical Fair Packing (HFP) HFP builds packages (denoted $P_1, P_2, ...$) of tasks, which are stored as lists of tasks, forming a partition of \mathbb{T} . To do so, it gathers tasks that share the most input data. By extension, we denote by $\mathcal{D}(P_k)$ the set of inputs of all tasks in P_k . We aim at building the smallest number of packages so that for each package, $\mathcal{D}(P_k) \leq M$. The intuition is that once the data $\mathcal{D}(P_k)$ are loaded, all tasks in the package can be processed without any additional data movement. We have proven that building the minimum number of packages is NP-complete(see Theorem 4 and it's proof), hence we rely on a greedy heuristic to build them, described in Algorithm 4.

Theorem 4. For a given set of tasks \mathbb{T} sharing data in \mathbb{D} . Partition tasks into l packages of maximum size M, such as l is minimal, is an NP-complete problem.

Proof. We will restrict this optimization problem to a decision problem noted RP: given a set of tasks \mathbb{T} and an integer L $(1 \leq L \leq m)$, can we partition T in at most L packages such as $\forall iW(P_i) \leq B$? W is the weight or size of a package.

The certificate of our problem RP is: the list of tasks grouped by package. Let's verify our certificate. We need to verify that the number of packages is less than L and that the weight $W(P_i)$ of each package is less than B. To compute the weights, it is necessary, to add the weight of the data while ignoring the duplicates. To detect duplicates it is necessary to browse $|D(P_i)| \times |D(P_i)|$ times the data. We are therefore in polynomial time. Let's check that the size of the certificate is a polynomial. We initially have $|\mathbb{T}|$ lists of data. Browsing the data is done in polynomial time $(\sum_{i=1}^{|\mathbb{T}|} |D(T_i)|)$. We know that $L \leq |\mathbb{T}|$. Thus the size of the data is polynomial in $|\mathbb{T}|$.

Now we can start the polynomial reduction. We note 3P the 3-partition problem. Given an integer M and 3n integer $a_1, a_2, ..., a_n$, the problem is to decide whether we can partition 3n into n triplet whose sum of integers is M. We admit that $\sum_{i=1}^{3n} a_i = nM$ and $\forall i M/4 < a_i < M/2$. So each partition needs exactly three integers to reach M.

We note I_{3P} an instance of 3P and I_{RP} an instance of RP. To convert I_{3P} into I_{RP} , we build tasks that each represent an integer. We note these tasks T_i , and each T_i contains a data d_i that weighs a_i . The numbering is the same, we can use a_i to get the weight of the data d_i and vice versa.

We assume that the weight limit of a package is: B = M. In this reduction we note that L = n. Can we find at most n packages of weight $W(P_i)$ at most M?

 $3P \Rightarrow RP$: If 3P has a solution, then we have n subsets of integers $(S_1, S_2, ..., S_n)$ which verify: $\forall j \sum_{i \in S_j} a_i = M$. We take as a solution for I_{RP} the tasks whose data d_i corresponds to these integers a_i and we group together the tasks in n packages $(P_1, P_2, ..., P_n)$ such that: $\forall i \in S_j \ T_i \in P_j$. We have noted that L = n, we have n packages so we have at most L packages. We know that there are n subsets of integers, each equal to M. Now we know that $\forall j \sum_{i \ inS_j} a_i = M$ therefore the equality $\forall j \sum_{T_i \in P_j} a_i = M$ is also correct. We know that M = B. So each package has a weight of B. We therefore have at most L packages of weight at most B. So RP also has a solution.

 $RP \Rightarrow 3P$: If RP has a solution then there are at most L packages of size at most B. We know that B = M therefore $\forall i \ W(P_i) \leq M$. We know that $\sum_{i=1}^{3n} a_i = nM$ therefore $\sum_{i=1}^{3n} d_i = nM$. B = M, we therefore have L = npackages which must satisfy the following conditions:

$$\begin{cases} \sum_{i=1}^{n} W(P_i) = nM \\ \forall i \ W(P_i) \le M \end{cases}$$

We will use a proof by the absurd. The proposition is assumed to be true: at least one package is not of weight M. Suppose that a package is of weight M' strictly less than M. At most, the other packages can be of weight M, we have in this case:

$$\sum_{i=1}^{n} W(P_i) = (n-1)M + M'$$

M' < M therefore $\sum_{i=1}^{n} W(P_i) < nM$. It contradicts our conditions above. So the *n* packages have the same weight *M*. We take as a solution for I_{3P} the integers a_i whose value corresponds to the data d_i and we group together the integers into n subsets $(S_1, S_2, ..., S_n)$ such that: $\forall d_i \in P_i \ a_i \in S_i$. We thus check the conditions of the problem 3P.

We have proved that $3P \Rightarrow RP$ and that $RP \Rightarrow 3P$ therefore the RP problem is at least as hard as the 3P problem. 3P is strongly NP-complete, so our problem is also strongly NP-complete.

We start with packages containing a single task. Then we consider all packages with fewest tasks and try to merge each of them with another package with whom it shares the most input data. When it is not possible to merge packages without exceeding the M bound, we perform a second step where we gather packages in the same way but ignore the bound M on the input size. The intuition is to create meta-packages that express the data affinity between packages already built. Note that we do not modify the order of tasks within packages when merging them, hence keeping the good data locality inside packages. Eventually, the last remaining package after all merges is the list of tasks for the schedule.

Algorithm 4 Hierarchical Fair Packing heuristic
Let $P_i \leftarrow [T_i]$ for $i = 1 \dots m$ and $\mathbb{P} = \{P_1, \dots, P_m\}$
$SizeLimit \leftarrow true, MaxSizeReached \leftarrow false,$
while $ \mathbb{P} > 1$ do
while (MaxSizeReached = false or SizeLimit = false) and $ \mathbb{P} > 1$ do
$MaxSizeReached \leftarrow true$
for all packages P_i with the smallest number of tasks do
Find a package P_j such that $ \mathcal{D}(P_i) \cap \mathcal{D}(P_j) $ is maximal
if $weight(P_i \cup P_j) \leq M$ or $SizeLimit = false$ then
Merge P_i and P_j : append P_j at then end of P_i and remove P_j from \mathbb{P}
$MaxSizeReached \leftarrow false$
end if
end for
end while
$SizeLimit \leftarrow false$
end while
Return the only package in \mathbb{P}

Complexity of HFP Let's note $\Delta = \max_i |\mathcal{D}(T_i)|$ the maximal number of data for any task. In the best case we merge all the packages two by two at each iteration of the inner while loop. It result in $\log_2 m$ iterations. The number of data of a package is growing at each fusion, it size is at most $\Delta \times 2^i$. At iteration i we have $\frac{m}{2^i}$ packages and $\Delta \times 2^i$ data by package. To find the package with which a package share the most data we must compute $(\frac{m}{2^i})^2$ on the $\Delta \times 2^i$ data of each package. So the cost at iteration i is:

$$(\frac{m}{2^i})^2 \times \Delta \times 2^i = \frac{m^2 \times \Delta}{2^i}$$

If we sum the i iterations we get:

$$\varDelta \times m^2 + \frac{\varDelta \times m^2}{2^1} + \frac{\varDelta \times m^2}{2^2} + \ldots + \frac{\varDelta \times m^2}{2^i} < O(\varDelta \times m^2)$$

So the complexity of Homogeneous packing in the best case is: $O(\Delta \times m^2)$.

In the worst case, the tasks do not have affinities between them, so the total data weight remains the same and the number of packages only decreases by 1 at each iteration of the inner while loop. There are therefore m iterations before having only one package left. We note $a = \sum_i |\mathcal{D}(T_i)|$ the number of access to data on all the tasks, thus, whatever the number of fusion, the number of loads will be less than a. $\sum_i |\mathcal{D}(T_i)| \leq m \times \max_i |\mathcal{D}(T_i)|$, so $a \leq m \times \Delta$. We can rephrase "Find a package P_i such that $|\mathcal{D}(P_i) \cap \mathcal{D}(P_j)|$ is maximal" this way:

- For $P_i \in \mathbb{P}$ we read $\mathcal{D}(P_i)$
- For $P_j \in \mathbb{P}$ we read $\mathcal{D}(P_j)$
- For each of these two loops there are at most a iterations
- Combined this gives a complexity of $O(a^2)$

a is bounded by $m \times \Delta$. So we get a complexity of $O(m^2 \times \Delta^2)$ to find the package P_j . Knowing that there are *m* iterations until getting only one package we have the complexity in the worst case: $O(m^3 \times \Delta^2)$.

In linear algebra in particular, all tasks have a very similar data access pattern and the data shares are regular. Hence, in practice, the complexity is often $O(\Delta * m^2)$.



Fig. 3: Flipping packages to improve HFP. Here we assume that the pair of subpackages (P_i^{end}, P_j^{end}) is the one with the most shared input data, so that only P_j is reversed before merging packages.

Improving HFP with package flipping One problem may appear in the second phase of HFP, when we merge packages without taking care of the M bound: if P_i is merged with P_j , the merged package contains the tasks of P_i followed by the ones of P_j . However, the last tasks of P_i might have very little shared data with the first tasks of P_j , leading to poor data reuse when starting P_j . Hence, for each package P_i , we consider two sub-packages P_i^{start} and P_i^{end} containing the first and last tasks so that the weight of their input data is smaller than M but their cardinal is maximal, as illustrated on Figure 3. Then, we count the common input data of tasks P_i^{start} and P_i^{end} on one side, and P_j^{start} and P_i^{end} on the other side. We identify the pair with most common input data and selectively reverse the packages so that tasks in this pair of sub-packages are scheduled consecutively in the resulting package.

Package flipping requires to go through the set of tasks of two packages. In the worst case, the two packages together contain all of \mathbb{T} , so the complexity is O(m). This complexity is added to the complexity of HFP, it therefore does not add complexity, so it can be neglected.

Here is an example of the tasks processing order of C on a 2D matrix multiplication (0 is the first task to be computed):

16	18	24	$\overline{26}$	68	70	76	78	0	2
17	19	25	27	69	71	77	79	1	3
20	22	28	30	72	74	80	82	4	6
21	23	29	31	73	75	81	83	5	7
32	34	40	42	84	86	92	94	8	10
33	35	41	43	85	87	93	95	9	11
36	38	44	46	88	90	96	98	12	14
37	39	45	47	89	91	97	99	13	15
60	62	64	66	48	50	52	54	56	58
61	63	65	67	49	51	53	55	57	59
						_			

(a) Without flip

(b) With flip

Fig. 4: Tasks computation's order with HFP with or without package flipping on a $10 \mathrm{x} 10$ matrix

4 Experimental evaluation

We present here the results of the experimental evaluation conducted to compare the strategy presented above.³

4.1 Settings

All above strategies have been implemented in the STARPU runtime system [3]. This allows to test them on a variety of applications described as sets of tasks. In order to test the performance of the strategies in different conditions (such as varying GPU memory size), we have used the ability to run STARPU code over the SimGrid simulator [6]. To make simulation times tractable, we have chosen characteristics of the simulated platform which are relatively small, to allow observing locality effects even with a small input matrix: the PCI bandwidth is set to 350MB/s, and the GPU memory size evolves around 500MB. The scheduling algorithms receive the whole set of tasks of the application in a natural order

³ The code used to reproducibly obtain the results in this paper is available at https://gitlab.inria.fr/starpu/locality-aware-scheduling/-/tree/europar2021

(row by row for a matrix multiplication for instance), then outputs this same set of task in a new order, which is used in STARPU to process tasks on the GPU. We measure the obtained performance (in GFlop/s) as well as the total volume of data transferred between CPU and GPU.

We use four set of tasks for these experiments:

- **2D** matrix multiplication To compute $C = A \times B$ in parallel, each task corresponds to the multiplication of one block-row of A per one block-column of B. Input data are thus the rows of A and columns of B.
- **3D** Matrix multiplication All matrices (A, B, C) are tiled, and the computation of each tile of C is decomposed in multiple tasks, each of which requires one tile of A and one tile of B. Tiles of C are also used as input for all tasks on this tiles but the first one.
- Task set from the Cholesky factorization We consider the tasks of the tiled Cholesky decomposition [1], but remove all dependencies, as we are interested only in independent tasks. This allows to have dependencies with some regularity, but more complex than the 2D or 3D matrix multiplication.
- **Randomized 2D matrix operation** We consider the set of tasks and data from the 2D matrix multiplication, but with a random dependency pattern between tasks and data: each task requires one (random) block-row of A and one (random) block-column of B. This allows to test our algorithms on an unstructured dependency graph.

We use the four scheduling heuristics presented above, together with a random task ordering as a baseline. We use the default LRU eviction policy, but also consider the optimal eviction policy, denoted by Belady, presented above. This policy is available only for static heuristics (as it requires complete task order from the beginning), such as RCM, MST and the proposed HFP. For the sake of clarity, we present only the result of the Belady eviction policy on HFP.

4.2 Results on the 2D matrix multiplication

On Figure 5, we plot the performance of each scheduling heuristic when varying either the size of the problem, or the size of the available memory. We also show the quantity of data transfers and the execution time. On these graphs, the dotted horizontal black line represents the maximum GFlop/s (630) that the GPU can achieve when processing elementary matrix product (without I/Os) and is our asymptotic goal. The red dotted vertical line denotes the situation when the GPU memory can fit exactly only one of the two input matrices, and the orange line denotes the situation when it can accommodate both input matrices.

A pathological matrix size for non-data aware algorithms When using a random task order, performance drops right after the orange line. Indeed, when the two input matrices do not fit in memory, the random order keeps triggering data reloads. The DMDAR, MST and RCM heuristics also get pathological behavior



(a) GPU memory size fixed to 500MB, vary- (b) Working set size fixed to 422MB, varying working set size. ing GPU memory size.



Fig. 5: 2D matrix multiplication.

after the red line. Indeed, they tend to process tasks along the rows of C. This allows to reuse the same block-row of matrix A for tasks that compute tiles of the same row of C, but requires reloading the whole matrix B for each new block-row of A, which is a well-known pathological case for the LRU eviction policy.

What happens? First, we have to understand how the LRU works when multiplying matrix. We multiply A by B to get C. Consider that we use the rows of A and the columns of B. So for small matrices we can for example load all of B, a row of A and a piece of C to write the result in it. We compute the first row of C, then we will want to load the second row of A to be able to compute the second row of C. So the LRU will evict the last data used, the first row of A. It goes without problems. On Figure 5a, after 1000MB, neither A nor B fits in memory. The scheduler is therefore forced to load a few columns of B, a row of A and a block of C. It compute the first row of C. Unfortunately it could not load all the columns from B, so when we want to compute a block where all the data are not on memory, it has to evict the first column from B(the oldest therefore) in order to load the column of B it needs. But when we go to the computation of the second row of C, we need the first columns of Bthat we just evicted. It must therefore again evict the last columns of B. This generates many additional data transfers. DMDAR also treat task row by row but when going onto the next row, it choose to compute the tasks that already have data loaded, so using the last columns of B. However once these tasks are done it will treat the first tasks of the row, thus generating a large number of transfers. So all the algorithms treating tasks row by row or column by column will suffer from this is well-known pathological case of LRU. HFP aim to avoid that.

Performances of HFP The HFP heuristic gets performance very close to ideal. Indeed, it tends to gather tasks that compute a square part of C that require parts of A and B that can fit in memory size M. This allows to execute a lot of tasks with very few data to load. The package flipping and Belady variants further improve the results.

Here are the percentage of improvement of HFP with package flipping and Belady over the other heuristics, averaged on the ten points:

Reference algorithm	Random	MST	RCM	DMDAR	HFP	HFP with flip
Improvement	103.6%	42.9%	47.4%	43.8%	1.9%	0.1%

Varying memory size Figure 5b shows the dual view of Figure 5a: the working set is now set to 422MB and we simulate varying amounts of available GPU memory. The measurements at 500MB on Figure 5b are the same as the measurements at 422MB on Figure 5a. We can observe the same results as on 5a but reversed: when the available memory is smaller than the working set, heuristics get pathological behavior. Since we strongly reduce the amount of available memory, we get a more restrictive situation, and package flipping provides a large improvement here (4% versus 1.8% on Figure 5a). Indeed, when memory

is more restricted, the second phase of HFP (without bound on package size) is more important, and it is essential to optimize the transition between packages. Moreover HFP with Belady improve GFlop/s by 7% compared to its variant without it. It is all the more important to evict data correctly when the number of data available in memory is very low.

Belady improvement We can see on Figure 5a that the differences between HFP and HFP with Belady are very slim, HFP with Belady is only 1.5% better. However on Figure 5b, it is 7.7% better. These are situations where the memory is very limited, we cannot fit a whole matrix on the GPU memory. Let's say that we want to process a set of tasks that uses the first 8 rows of A and the first 8 columns of B. We first compute the block of C using the first row and the first column. Let's say that we can compute the first 4 rows of tasks before the memory is full. Then LRU will evict starting from data from the first row of A and the first column of B. But when we need to compute the next tasks that are tasks on the same columns but on the last 4 rows of A, we need data that we just evicted. On the other hand, if we use Belady, in the same situation it would evict data from the first few rows of A, not used again before the last tasks. Thus in this situation Belady saves us a lot of data transfers. For example for the fourth point of Figure 5b, the number of data transfers without Belady is 84, with belady it is 46. We can conclude that if a scheduler knows all the tasks before the start of the execution, using Belady is undoubtedly beneficial.

Data transfers and execution time Figure 5c shows the quantity of data transfers done in MB. It uses the same parameters as the Figure 5a. By looking at these two figures we can see that data transfers increase drastically when GFlop/s decrease.

On Figure 5d we can see that only HFP has a lot of execution time. This happen when there are a lot of tasks. The time it takes to compare each data of each package is exponential with the number of tasks.

4.3 Results on the 3D matrix multiplication

On Figure 6, we plot the performance and amount of data transfers for all heuristics on the 3D matrix multiplication. On this set of tasks, matrix C now plays a role in affinities, which is why we added a vertical green dotted line to denote the situation when all A, B, and C matrices fit in memory.

Performances of MST MST keeps ordering tasks along the rows of C, and thus still gets pathological performance when memory can not fit matrix B. This is confirmed on Figure 6c: the number of loads gets dramatically high.

DMDAR and RCM RCM and DMDAR, however, do not have the same problem. RCM (resp. DMDAR) computes tasks along columns (resp. rows) of C but alternates between tasks of a few consecutive columns (resp. rows). This allows them to improve data reuse: Figure 6c shows that they exhibit a limited number of transfers, even with a large working set.



(a) GPU memory size fixed to 500MB, vary- (b) Working set size fixed to 1250MB, varying working set size. ing GPU memory size.



(c) Data transfers.

Fig. 6: 3D matrix multiplication.

Performances of HFP HFP keeps gathering tasks forming a square part of C, which provides better locality. Here are the percentages of average improvement of HFP with package flipping and Belady over the other heuristics:

Reference algorithm	Random	MST	RCM	DMDAR	HFP	HFP with	flip
Improvement	148.7%	37.9%	13.3%	11.4%	4.3%	0.5%	

As the 3D matrix multiplication already exhibits a better data locality than the 2D multiplication, the differences in performance between heuristics is less pronounced than on Figure 5a, but HFP is still better on average. It is worth noticing that HFP without Belady gets higher performance than MST, RCM and DMDAR, even if it exhibits a similar number of transfers. The latter heuristics indeed tend to periodically require a sudden burst of data loads, while HFP tends to require loads that are nicely distributed over time, and thus well overlapped with computation.

Number of loads We can see on Figure 6c that the number of loads of DMDAR and RCM are consistent with what observe on Figure 6a. However we can see that HFP got better performance than DMDAR but also more data transfers. DMDAR has no long-term visibility. It will compute task that have data already loaded, so more often than not it will compute tasks row by row and insert tasks from other rows in between. So when the working set is too large for the memory size, it can have a lot of loads at once. Hence the distribution of the loads in time is reducing the GFlop/s but does not increase the number of data transfers. On the other hand, HFP groups the tasks in packages of size M which allows to make homogeneous packages that fit on memory. So we have to load data each time we go onto an other packages. Which distribute transfers a lot. So even if there are more data transfers, the GFlop/s are not affected because the data transfers are spread out and we can therefore compute tasks during the transfers. We can also observe that Belady reduce the number of data transfers by 32.5% from HFP without Belady.

Varying the size of the memory On Figure 6b, we can see that DMDAR is better than HFP for the two smallest memory sizes. For very small memory, HFP has a lot of packages, so it cannot build packages sharing a lot of data and can only order packages between them which result in putting one after another tasks that won't share a lot of data.

4.4 Results on the task set of the Cholesky factorization

Random order, RCM and MST Figure 7a present the performance obtained by the heuristics on the set of tasks of the Cholesky decomposition. We notice that these three algorithms get pathological performance once the whole matrix cannot fit the memory. They indeed do not manage to reuse more than one tile between consecutive tasks, thus entailing a lot of tile reloads.



(a) GPU memory size fixed to 500MB, vary- (b) Working set size fixed to 740MB, varying working set size. ing GPU memory size.



(c) Data transfers.

Fig. 7: Task set of the Cholesky factorization.

Favorable natural order for DMDAR DMDAR has better results than HFP (with or without Belady) for a working set inferior to 1.5 times the memory. DMDAR indeed takes advantage of the actual task submission order of the Cholesky algorithm, which starts with tasks which require few input data (POTRF and TRSM kernels). Meanwhile, it can load data for the subsequent tasks with more input dependencies (GEMM kernel). HFP, on the contrary, does not pay attention to the task submission order, and aims for data sharing as much as possible. It will thus introduce a lot of GEMM tasks at the beginning of the execution, and is thus impacted by the loading time. As the working set increases, however, HFP with the Belady eviction achieves good performance.

Performances of HFP The average improvement of HFP with flip and Belady over the other heuristics is as follows:

Reference algorithm	Random	MST	RCM	DMDAR	HFP	HFP with flip
Improvement	127.1%	60.4%	57.1%	6.2%	17.2%	13.2%

Varying the size of the memory As we saw on Figure 7a, we can see on Figure 7b that once all the data fit on memory, DMDAR, MST and RCM are the best algorithms. This is explained by the fact that HFP does not recognize that all the data fits in memory and therefore seeks to make packages which force the loading of certain data several times.

Data transfers Again we can see on Figure 7c that the number of data transfers are equivalent for HFP Belady and DMDAR whereas the number of GFlop/s for HFP with Belady are greater. Again the distribution of loads over time is better for HFP.

4.5 Results on the randomized 2D matrix operation

The randomization of data dependencies of the 2D matrix multiplication, shown on Figure 8a, has an interesting impact on the results previously discussed from Figure 5a. In this randomized setting, MST does not manage to find task affinities any more: it is only able to ensure that a common data is shared between two consecutive tasks, but since it does not benefit from the natural order of task arrival anymore, its performance drops as soon as the two matrices no longer fit into memory. RCM and DMDAR, however, get more sustained performance: the randomization of dependencies actually decreases the effect of the classical LRU pathological case, since they do not tend to execute tasks rows by rows any more. HFP, however, can more nicely find task affinities thanks to its global overview. The addition of the Belady eviction allows to keep excellent performance, thanks to its insight into the ordering of the randomized tasks.

Performances of HFP Its average improvement over the other heuristics is as follows:



(a) GPU memory size fixed to 500MB, vary- (b) Working set size fixed to 422MB, varying working set size. ing GPU memory size.



(c) Data transfers.

Fig. 8: Randomized 2D matrix operation.

Reference algorithm	Random	MST	RCM	DMDAR	HFP	HFP with flip
Improvement	103.2%	70.3%	23.7%	29.4%	10.6%	8.8%

We can also note that when the working set grow, HFP without Belady loses performance. On the other hand, with Belady it stay close to GFlop/s max. Indeed, if the data are random, HFP with LRU can no longer rely on the favorable natural order of tasks in 2D. Belady therefore allows improvements in more general cases as well.

In summary, the simple greedy DMDAR heuristic exhibits robust performance, but HFP, and particularly with the package flipping and Belady improvements, exhibit better performance, including in the case of a tight memory.

5 Conclusion and Future Work

To take the best performance out of GPUs, it is crucial to avoid moving data as much as possible. We provided in this paper a formalization of the problem of ordering independent tasks sharing input data in order to minimize the amount of data transfers, and show that this problem is NP-complete. We also exhibit an optimal eviction scheme, based on Belady's rule. We adapted three heuristics for the ordering problem, based on the state of the art, and compared them with a new algorithm gathering tasks with similar input data into packages of increasing size, called HFP. We also present an improvement of HFP based on package flipping. All four ordering strategies have been implemented in the STARPU runtime and extensively tested on various set of tasks. In all cases, the proposed HFP heuristic provides significant speedups. For instance, it allows on average a 43% (resp. 11%) improvement for 2D (resp. 3D) matrix multiplication. HFP is very relevant and obtains important speedups particularly in the case when the memory is very constrained compared to the size of the total working set. We also notice that in some situations, HFP ends up with as many data transfers than another heuristic, but with better performance, which shows that HFP is also good in distributing data transfer over time to increase transfer/computation overlap. Studying this final problem (minimizing computation time with overlap) is one for our future directions. We also plan to focus on the very beginning of the execution, where it is crucial to first schedule tasks with few input data. On a longer term, we want to tackle the general case with tasks sharing not only input data, but with inter-task dependencies, as well as targeting multi-GPU platforms, for which our approach with packages seems particularly well suited.

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