Abstract—We address the problem of fusing array operations based on criteria such as shape compatibility, data reusability, and communication. We formulate the problem as a graph partition problem that is general enough to handle loop fusion, combinator fusion, and other types of subroutines.

I. INTRODUCTION

Array operation fusion is a program transformation that combines, or fuses, multiple array operations into a kernel of operations. When it is applicable, the technique can drastically improve cache utilization through temporal data locality and enables other program transformations such as streaming and array contraction [1]. In scalar programming languages, such as C, array operation fusion typically corresponds to loop fusion where multiple computation loops are combined into a single loop. The effect is a reduction of array traversals (Fig. 1a). Similarly, in functional programming languages it typically corresponds to fusing individual combinators. In array programming languages, such as HPF [2] and ZPL [3], fusing array operations are crucial, since a program written in these languages will consist almost exclusively of array operations. Lewis et al. demonstrates a runtime improvement of up to 400% when optimizing for array contraction at the array rather than the loop level [4].

However, not all fusions of operations are allowed. Consider the two loops in Fig. 1b; since the second loop traverses the result from the first loop in reverse, we must compute the complete result of the first loop before continuing to the second loop, preventing fusion. Clever analysis sometimes allows transforming the program into a form that is amenable to fusion, but such analysis is outside the scope of the present work. Throughout the remainder of this paper, we assume that any such optimizations have already been performed.

Deciding which operations to fuse together is the same as finding a partition of the set of operations in which the blocks obey the same execution dependency order as the individual operations, and in which no block contains two operations that may not be fused. Out of all such partitions, we want to find one that enables us to save the most computation or memory. It is not an easy problem, in part because fusibility is not transitive. That is, even when it is legal to fuse subroutines \( x, y \) and \( y, z \), it may be illegal for all three of \( x, y, z \) to be executed together. Thus, one local decision can have global consequences on future possible partitions.

The problem can be stated in a quite general way: “Given a mixed graph, find a legal partition of vertices that cuts all non-

directed edges and minimizes the cost of the partition.”\(^1\). We call this problem the Weighted Subroutine Partition problem, abbreviated WSP.

The general formulation is applicable to a broad range of optimization objectives. The cost function can penalize any aspect of the partitions, e.g., data accesses, memory use, communication bandwidth, and/or communication latency. The only requirement to the cost function is monotonicity:

- Everything else equal, it must be cost neutral or a cost advantage to place two subroutines within the same partition block.

Similarly, the definition of partition legality is flexible.

- Any aspect of a pair of subroutines can make them illegal to have in the same partition block, such as preventing mixing of sequential and parallel loops, different array shapes, or access patterns.

- Subroutines may have dependencies that impose a partial order. Then a legal partition must observe this order, i.e., must not introduce cycles.

The remainder of the paper is structured as follows: In Section 3, we formally define the Weighted Subroutine Partition problem, which unifies array operation-, loop-, and combinator fusion, and prove that it is NP-hard. Section 4 shows how WSP is used to solve array operation fusion for the Bohrium automatic parallelization framework, and gives a correctness proof. In Section 5, we describe a branch-and-bound algorithm.

\(^1\)See Sec. II for the definition of a legal partition and legal cost function.
that computes an optimal solution, as well as two approximation algorithms that compute good results rapidly enough to use in JIT-compilation. All the algorithms are implemented in Bohrium, and work for any choice of monotonic cost function, which allows us to compare directly with other fusion schemes from the literature. Section 6 shows measurements performed on 15 benchmark programs, comparing both the optimal to the approximation schemes, and to three other fusion schemes.

II. THE WEIGHTED SUBROUTINE PARTITION PROBLEM

The Weighted Subroutine Partition (WSP) problem is an extension of the The Weighted Loop Fusion Problem [5] where we include the weight function in the problem formulation. In this section, we will formally define the WSP problem and show that it is NP-hard.

Definition 1 (WSP graph). A WSP graph is a triplet \( G = (V, E, d) \) such that \( (V, E_d) \) is a directed acyclic graph describing dependency order, and \( (V, E_f) \) is an undirected graph of forbidden edges.

Definition 2 (WSP order). A WSP graph, \( G = (V, E_d, E_f) \), induces a partial order \( \preceq \) on \( V \) as follows: \( v \preceq v' \) iff there exists a path from \( v \) to \( v' \) in \( (V, E_d) \). Since \( (V, E_d) \) is acyclic, this partial order is strict.

Definition 3 (Partitions). A partition of a set \( V \) is a set \( P = \{B_1, B_2, \ldots, B_k\} \) such that \( V \) is the disjoint union of the blocks \( B_1, \ldots, B_k \). The set \( \Pi_V \) of all partitions of \( V \) is partially ordered as \( P \preceq P' \) iff \( \forall B \in P \exists B' \in P' : B \subseteq B' \), i.e. if each block in \( P \) is a subset of a block in \( P' \).

The set of partitions \( \Pi_V \) is a lattice with bottom and top elements \( \bot = \{V\} \) and \( \top = \{\{V\}\} \). The successors to a partition \( P \) in the partition order are those partitions that are identical to \( P \) except for merging two of the blocks. Conversely, splitting a result in a predecessor. We write \( P \prec P' \) if \( P' \) is a successor to \( P \). This defines a binary merge operator:

Definition 4 (Block merge operator). Given a partition \( P = \{B_1, B_2, \ldots, B_k\} \), define \( P/(\{B_1, B_2\} = \{B_1 \cup B_2, B_3, \ldots, B_k\} \) to be the successor to \( P \) in which \( B_1 \) and \( B_2 \) are merged and all other blocks are left the same.

Definition 5 (Legal partition). Given a WSP graph, \( G = (V, E_d, E_f) \), we say that the partition \( P \in \Pi_V \) is legal when the following holds for every block \( B \in P \):

1) \( \forall v_1, v_2 \in B : (v_1, v_2) \in E_f \), i.e. no block contains both endpoints of a forbidden edge.

2) If \( v_1 \preceq v_2 \preceq v_3 \) and \( v_1, v_3 \in B \) then \( v_2 \in B \), i.e. the directed edges between blocks must not form cycles.

Definition 6 (WSP cost). Given a partition, \( P \), of vertices in a WSP graph, a cost function \( \text{cost}(P) \) returns the cost of the partition and respects the following conditions:

1) \( \text{cost}(P) \geq 0 \)

2) \( P \preceq P' \implies \text{cost}(P) \geq \text{cost}(P') \)

Definition 7 (WSP problem). Given a WSP graph, \( G = (V, E_d, E_f) \), and a cost function, \( \text{cost}(P) \), the WSP problem is the problem of finding a legal partition, \( P^* \), of \( V \) with minimal cost:

\[
P^* \in \arg \min_{P \in \Pi_V} \text{cost}(P)
\]

where \( \Pi_V \) denotes the set of legal partitions of \( V \).

A. Complexity

In order to prove that the WSP problem is NP-hard, we perform a reduction from the Multiway Cut Problem [6], which Dahlhaus et al. has shown is NP-hard for fixed \( k \geq 3 \).

Definition 8 (Multiway Cut). Given a tuple \( (V, E, S, w) \) consisting of a graph \( (V, E) \), a terminal set \( S = \{s_1, \ldots, s_k\} \) of vertices, and a non-negative weight \( w(u, v) \) for each edge \( (u, v) \in E \), a multiway cut is an edge set \( E' \) the removal of which leaves each terminal in separate components. The solutions to the MWC problem are the multiway cuts of minimal total weight.

Theorem 1. The WSP problem is NP-hard for graphs \( G = (V, E_d, E_f) \) that have a chain of three or more edges in \( E_f \).

Proof. We prove NP-hardness through a reduction from multiway cut. Given an MWC-instance, \( (V, E, S, w) \), we build a WSP-instance as follows. Let \( G = (V, E_d, E_f) \), \( E_f = \{(s_i, s_j) : 1 \leq i < j \leq k\} \), and \( E_d = \emptyset \). Define the cut of a partition as the set of edges that connect the blocks:

\[
cut(P) = \{(u, v) \in E_f : \exists B \in P : (u, v) \in B\}
\]

The cuts of the legal WSP partitions \( \Pi_V \) are exactly the set of multiway cuts:

- The set of directed edges in \( E_d \) is empty, which makes Def. 2 and Def. 5(2) trivially satisfied.
- The fuse-preventing edges \( E_f \) connect each terminal in \( S \) and no other vertices. Hence, by Def. 5(1), \( \Pi_V \) are exactly those partitions for which no block contains two terminals.

Let now the cost function be the total weight of the cut:

\[
\text{cost}(P) = \sum_{(u, v) \in \cut(P)} w(u, v)
\]

This is a valid WSP cost function (by Def. 6): it is non-negative, and if \( P \preceq P' \) in the partition order, then \( \cut(P) \supseteq \cut(P') \), whereby \( \text{cost}(P) \geq \text{cost}(P') \). Since \( \text{cost}(P) \) is the MWC total weight, Eq. (1) gives the multiway cuts of minimal total weight. \( \square \)

III. WSP USED TO OPTIMIZE ARRAY OPERATION FUSION IN BOHRUM

Stating the WSP problem formulation in a general way allows a great deal of flexibility, as long as the cost function is monotonic. In this section, we use WSP to solve a concrete optimization problem, demonstrating its real world use. The concrete problem is an optimization phase within the Bohrium runtime system [7] in which a set of array operations are
In order to demonstrate various challenges and trade-offs, the application Fig. 2a shows a Python application that uses Bohrium as a computation backend for array programming languages and libraries that supports a range of languages, such as Python, C++, and .NET, and a range of computer architectures, such as CPU, GPU, and clusters of these. The idea is to decouple the domain specific frontend implementation from the hardware specific backend implementation in order to provide a high-productivity and high-performance framework.

Similar to NumPy [8], a Bohrium array operation operates on a set of inputs and produces a set of outputs [7]. Both input and output operands are views of arrays. An array view is a structured way to observe the whole or parts of an underlying base array. A base array is always a contiguous one-dimensional array whereas views can have any shape, stride, and dimensionality [7]. In the following, when we refer to an array, we mean an array view; when we refer to identical arrays, we mean identical array views that point to the same base array; and when we refer to overlapping arrays, we mean array views that points to some of the same elements in a common base array.

Fig. 2a shows a Python application that uses Bohrium as a drop-in replacement for NumPy. The application allocates and initiates four arrays (line 4-7), manipulates those arrays through array operations (line 8-14), and prints the content of one of the arrays (line 16).

As Bohrium is language agnostic, it translates the Python array operations into bytecode (Fig. 2b) that the Bohrium backend can execute\(^2\). In the case of Python, the Python array operations and the Bohrium array bytecode is almost in one-to-one mapping. The first bytecode operand is the output array and the remaining operands are either input arrays or input literals. Since there is no scope in the bytecode, Bohrium uses `DEL` to destroy arrays and `SYNC` to move array data into the address space of the frontend language – in this case triggered by the Python `print` statement (Fig. 2a, line 16). There is no explicit bytecode for constructing arrays; on first encounter, Bohrium constructs them implicitly.

In the next phase, Bohrium partitions the list of array operations into blocks that consists of fusible array operations – the FAO problem. As long as the preceding constraints between the array operations are preserved, Bohrium is free to reorder them as it sees fit, making code optimizations based on data locality, array contraction, and streaming possible.

In the final phase, the hardware specific backend implementation JIT-compiles each block of array operations and executes them.

1) Fusibility: In order to utilize data-parallelism, Bohrium and most other array programming languages and libraries require data-parallelism of array operations that are to be executed together. The property ensures that the runtime system can calculate each output element independently without any communication between threads or processors. In Bohrium, all array operation must have this property.

We first introduce some operations that keep track of memory allocation, deallocation, reads, and writes:

**Definition 10.** Given an array operation \( f \), the notation \([f]\) denotes the set of arrays that \(f \) reads; \([f]\) denotes the set of arrays that \( f \) writes; \([f]\) denotes the set of new arrays that \( f \) allocates; and \([f]\) denotes the set of arrays that \( f \) deletes (or de-allocates).

**Furthermore, given a set of array operations, \( B \), we define the following:**

\[
\text{out} [B] \equiv \bigcup_{f \in B} \text{out}[f]
\]

\[
\text{in} [B] \equiv \bigcup_{f \in B} \text{in}[f]
\]

\[
\text{new} [B] \equiv \bigcup_{f \in B} \text{new}[f]
\]

\[
\text{del} [B] \equiv \bigcup_{f \in B} \text{del}[f]
\]

\[
\text{ext} [B] \equiv (\text{in}[B] \setminus \text{new}[B]) \cup (\text{out}[B] \setminus \text{del}[B])
\]

Here, \(\text{ext}[B]\) gives the set of external data accesses. “\(\setminus\)” is disjoint union: arrays that are both read and written are counted twice. \(\text{DEL}\) and \(\text{SYNC}\) are counted as having no input or output.

\(^2\)For a detailed description of this Python-to-bytecode translation we refer to previous work [9], [10].
This allows us to formulate the data-parallelism property that determines when array operation fusion is allowed:

**Definition 11.** A Bohrium array operation, \( f \), is data parallel, i.e., each output element can be calculated independently, when the following holds:

\[
\forall i \in \text{in}[f], \forall o, o' \in \text{out}[f] : \\
(i \cap o = \emptyset \lor i = o) \land (o \cap o' = \emptyset \lor o = o')
\]  

(2)

In other words, if an input and an output or two output arrays overlaps, they must be identical.

Fusing array operation must preserve data-parallelism:

**Definition 12.** In Bohrium, two array operations, \( f \) and \( f' \), are said to be fusible when the following holds:

\[
\forall i' \in \text{in}[f'], \forall o \in \text{out}[f] : \\
i' \cap o = \emptyset \lor i' = o
\]

(1)

\[
\forall o' \in \text{out}[f'], \forall o \in \text{out}[f] : \\
o' \cap o = \emptyset \lor o' = o
\]

(2)

\[
\forall o' \in \text{out}[f'], \forall i \in \text{in}[f] : \\
o' \cap i = \emptyset \lor o' = i
\]

(3)

It follows from Definition 11 that fusible operations are those that can be executed together without losing independent data-parallelism.

In addition to the data-parallelism property, the current implementation of Bohrium also requires that the length and dimensionality of the fusible array operations are the same.

1) **Cost Model:** The motivation of fusing array operations is to improve the overall runtime performance. To accomplish this, Bohrium implements two techniques:

**Data Locality** When a kernel accesses an array multiple times, Bohrium will only read and/or write to that array once, avoiding access to main memory. Consider the two for-loops in Fig. 1a that each traverse \( \mathcal{A} \) and \( \mathcal{T} \). Fusing the loops avoids one traversal of \( \mathcal{A} \) and one traversal of \( \mathcal{T} \) (Fig. 1c). Furthermore, the compiler can reduce the access to the main memory by \( 2N \) elements since it can keep the last read element of \( \mathcal{A} \) and \( \mathcal{T} \) in register.

**Array Contraction** When an array is created and destroyed within a single partition block, Bohrium will not allocate the array memory, but calculate the result in-place in one single temporary register variable per parallel computing thread. Consider the program transformation from Fig. 1a to 1d, in which, beside loop fusion, the temporary array \( T \) is replaced by the scalar variable \( t \). In this case, the transformation reduces the accessed elements with \( 3N \) and memory requirement by \( N \) elements.

In order to utilize these optimization techniques, we introduce a WSP cost function that penalizes memory accesses from different partition blocks. For simplicity, we will not differentiate between reads and writes, and we will not count access to literals or register variables.

**Definition 13.** In bohrum, the cost of a partition, \( P = \{B_1, B_2, ..., B_k\} \), of array operations is given by:

\[
\text{cost}(P) = \sum_{B \in P} \|\text{ext}[B]\|
\]

where the length \( \|x\| \) is the total number of bytes accessed by the set of arrays in \( x \).

The Bohrium cost-savings when merging two partition blocks depends only on the blocks:

**Proposition 1 (Merge-savings).** Let \( P \) be a partition and \( P' = P/(B_1, B_2) \) be its successor derived by merging \( B_1 \) and \( B_2 \). Using the cost function of Def. 13, the difference in cost between the two partitions is:

\[
\text{cost}(P) - \text{cost}(P') = \|\text{ext}[B_1] \cap \text{ext}[B_2]\|
\]

\[
+ \|\text{new}[B_1] \cap \text{new}[B_2]\|
\]

\[
+ \|\text{out}[B_1] \cap \text{del}[B_2]\|
\]

(4)

Since this cost reduction depends only on \( B_1 \) and \( B_2 \), we define a function, saving\((B_1, B_2)\), that counts the savings from merging \( B_1 \) and \( B_2 \), which is independent of the rest of the partitions.

Proof. If \( P = \{B_1, B_2, \ldots\} \) and \( P' = \{B_1 \cup B_2, \ldots\} \), then the reduction in cost is:

\[
\text{cost}(P) - \text{cost}(P') = \|\text{ext}[B_1]\| + \|\text{ext}[B_2]\| - \|\text{ext}[B_1 \cup B_2]\|
\]

since all other blocks are the same. By using the fact that \( B_1 \) must be executed before \( B_2 \), whereby \( \text{in}[B_1] \cap \text{new}[B_2] = \emptyset \) and \( \text{del}[B_1] \cap \text{out}[B_2] = \emptyset \), as well as the new’s and del’s being disjoint, direct calculation yields Eq. 4.

Note that Prop. 1 directly implies that the cost function of Def. 13 is positive and monotonically decreasing, as required by Def. 6. We next show how the problem can be formulated as a WSP instance.

**3) Constructing a WSP-problem from Bohrium bytecode:** Given a list \( A \) of Bohrium array operations, a WSP problem \( G = (V, E_d, E_f) \) is constructed as follows.

1) The data dependencies between array operations define a partial order: \( a \prec a' \) iff \( a' \) must be executed before \( a \).
2) Each array operation \( a \in A \) defines a vertex \( (v(a), v(a')) \) for each pair \( a, a' \in A \) with \( a \prec a' \).
3) The dependency graph \( E_d \) has an edge \((v(a), v(a'))\) for each non-fusible pair \( a, a' \in A \).
4) The fuse-prevention graph \( E_f \) has an edge \((v(a), v(a'))\) for each non-fusible pair \( a, a' \in A \).

The cost function is as in Def. 13, but note that it can be calculated incrementally using Prop. 1.

The complexity of this transformation is \( O(V^2) \) since we may have to check all pairs of array operations for dependencies, fusibility, and cost-saving, all of which is \( O(1) \). Fig. 3 shows the trivial partition, \( \perp \), of the Python example, where every array operation has its own block. The cost is 94.

**4) WSP solves Fusion of Array Operations:** Finally, we can show that a solution to the WSP problem also is a solution to the FAO problem.

**Theorem 2.** WSP solves Fusion of Array Operations.

Proof. It is clear from Def. 5 and the construction above that the legal partitions \( \Pi_V \) are exactly all those that fulfill
Total Partition Cost: 94

Fig. 3. A partition graph of the Python application in Fig. 2. For illustrative proposes, the graph does not include ignored weight edges (cf. Fig. 4).

Properties (1) and (2) of Def. 9. Thus, Def. 7 yields a global minimum for all such partitions, fulfilling also Def. 9(3). □

IV. ALGORITHMS

In this section, we present an exact algorithm for finding an optimal solution to WSP (with exponential worst-case runtime), and two fast algorithms that find approximate solutions. We use the Python application shown in Fig. 2 to demonstrate the results of each partition algorithm.

A. Partition graphs and chains of block merges

All three algorithms work on data structures called partition graphs, defined as follows:

**Definition 14** (Partition graph). Given a graph $G = (V, E)$ and a partition $P$ of $V$, the corresponding partition graph is the graph $G(P) = (P, E(P))$ that has an edge $(B, B')$ if there is an edge $(u, v) \in E$ with $u \in B$ and $v \in B'$. That is, the vertices are the blocks, connected by the edges that cross block boundaries.

From this we build the state needed in WSP computations:

**Definition 15** (WSP state). Given a WSP-instance $G = (V, E_d, E_f, \text{cost})$ and a partition $P$, the WSP state is the partition graph $G(P) = (P, E_d(P), E_f(P))$ together with a complete weighted graph $\hat{E}_w(P)$ with weights $w(B_1, B_2) = \text{cost}(P) - \text{cost}(P/(B_1, B_2))$.

Notice that $w(B_1, B_2) = \text{saving}(B_1, B_2)$ for the Bohrium cost function, as shown in Prop. 1, and does not require a full cost calculation.

**Definition 16** (Merge operator on partition graphs). We extend the merge operator of Def. 4 to partition graphs as $G(P)/(B_1, B_2) = G(P/(B_1, B_2))$. This acts exactly as a vertex contraction on the partition graph.

The merge operator is commutative in the sense that the order in a sequence of successive vertex contractions doesn’t affect the result [11]. An auxiliary function, MERGE, is used in each algorithm to update the state.

**Definition 17.** Let $S = (\hat{G}, \hat{E}_w)$ be a WSP state. We define

$$\text{MERGE}((S, u, v)) = (\hat{G}/(u, v), \hat{E}_w')$$

where $\hat{E}_w'$ is the updated weight graph on the edges incident to the new vertex $z = u \cup v$.

The complexity of MERGE is dominated by the weight update, which requires a saving computations per edge incident to the merged vertex, and is bounded by $O(V^2)$. We next need a local condition for when a merge is allowed:

**Lemma 1** (Legal merge). Let $P_{1,2} = P/(B_1, B_2)$ be the successor to a legal partition $P \in \Pi_V$, derived by merging blocks $B_1$ and $B_2$. Then $P_{1,2} \in \Pi_V$ if and only if

1. $(B_1, B_2) \notin \hat{E}_f(P)$, and
2. there is no path of length $\geq 2$ from $B_1$ to $B_2$ in the partition graph $\hat{E}_d(P)$.

**Proof.** Recall that $\Pi_V$ is the subset of partitions in $\Pi_V$ that satisfy Def. 5. Because $P$ is legal, no block contains an edge in $E_f$. Hence $P_{1,2}$ obeys Def. 5(1) if and only if no two vertices $u \in B_1$ and $v \in B_2$ are connected in $E_f$, or equivalently, $(B_1, B_2) \notin \hat{E}_f(P)$.

Similarly, by assumption, there are no cycles in $\hat{E}_d(P)$. Thus, $P_{1,2}$ violates Def. 5(2) if and only if $\hat{E}_d(P)$ contains a path $B_1 \to B' \to \cdots \to B_2$, forming the cycle $B_1 \to B' \to \cdots \to B_1$ in $\hat{E}_d(P_{1,2})$ (where $B_{1,2} = B_1 \cup B_2$). □

**Proposition 2** (Reachability through legal merges). Given two legal partitions $P < P'$, there exists a successor chain $P < P_1 < P_2 < \cdots < P'_n$ entirely contained in $\Pi_V$, i.e. corresponding only to legal block merges.

**Proof.** A successor chain $P < P_1 < P_2 < \cdots < P'_n$ always exists in the total set of partitions $\Pi_V$, and all such chains are of the same length $n$. Any such chain contains no partition that violates Def. 5(1): each step is a merge, so once a fuse-preventing edge is placed inside a block, it would be included also in a block from $P'$. Hence we only need to worry about Def. 5(2).

We now show by induction that a successor chain consisting of only legal partitions exists. First, if $P < P'$, it is trivially so. Assume now that the statement is true for all $n \leq N$, and consider $P < P'$ of distance $N + 1.$


No cycles, because the path is in the transitive reduction. Now $P$ satisfies Def. 5(2), by induction.

Theorem 3. A path containing a non-fusible edge.

A block (Definition 18), non-fusible set)

In order to reduce the size of the partition graph to be formalized this property using the non-fusible sets unintrusively fusible impose any restriction to future possible vertex merges in the merged vertex in $\hat{G}$, whenever:

1. $\theta[u] = \theta[v] = \theta[z]$, i.e. the non-fusibles are unchanged.
2. Either $u$ or $v$ is a pendant vertex in $E_{\hat{L}}$, i.e. the degree of either $u$ or $v$ must be 1.

Proof. If Condition 1 is satisfied, any merge that is disallowed at a further stage due to Def. 5(1) would be disallowed also without the merge. Similarly, merging a pendant vertex with its parent does not affect the possibility of introducing cycles through future merges (Def. 5(1)). Finally, since the cost function is monotonic, the merge cannot adversely affect a future cost.

Fig. 4. A help function that determines whether the weight edge, $e \in E_w[\hat{G}]$

Pick any successor chain from $P$ to $P'$. If any step violates Def. 5(2), then let $P_{i+1} = P_i/(B_1, B_2)$ be the first partition in the chain that does so. Then there is a path $B_1 \to B \to \cdots \to B_2$ in the transitive reduction of $E_{\hat{L}}(P_i)$. Because $P'$ satisfies Def. 5(2), $B_1 \cup B \cup B_2$ is contained in a block from $P'$, whereby $P'_{i+1} = P_i/(B_1, B) < P'$. This merge introduces no cycles, because the path is in the transitive reduction. Now let $P_{i+1} \prec P'_{i+1} \prec P'_{i+2} \prec \cdots \prec P'_{i+k} \prec \cdots \prec P'$ be a legal successor chain of length $N - i$, known to exist by hypothesis. Then $P \prec P_1 \prec \cdots \prec P_{i+1} \prec \cdots \prec P'$ is a length-$N + 1$ successor chain consisting of only legal partitions, concluding the proof by induction.

In particular, the optimal solutions can be reached in this way from the bottom partition $\bot = \{(v_1), (v_2), \ldots, (v_n)\}$, which we will use in the design of the algorithms.

B. Unintrusive Partition Algorithm

In order to reduce the size of the partition graph to be analyzed, we apply an unintrusive strategy where we merge vertices that are guaranteed to be part of an optimal solution. Consider the two vertices, $a, e$, in Fig. 3. The only beneficial merge possibility $a$ has is with $e$, so if $a$ is merged in the optimal solution, it is with $e$. Now, since fusing $a, e$ will not impose any restriction to future possible vertex merges in the graph, the two vertices are said to be unintrusively fusible. We formalize this property using the non-fusible sets:

Definition 18 ($\theta$, non-fusible set). The non-fusible set, $\theta[b]$ for a block $b$ is the set of blocks connected with $b$ in $E_{\hat{L}}$ through a path containing a non-fusible edge.

Theorem 3. Given a partition graph $\hat{G}$, let $z = u \cup v$ be the merged vertex in $\hat{G}/(u, v)$. The vertices $u$ and $v$ are unintrusively fusible whenever:

1. $\theta[u] = \theta[v] = \theta[z]$, i.e. the non-fusibles are unchanged.
2. Either $u$ or $v$ is a pendant vertex in $E_{\hat{L}}$, i.e. the degree of either $u$ or $v$ must be 1.

Proof. If Condition 1 is satisfied, any merge that is disallowed at a further stage due to Def. 5(1) would be disallowed also without the merge. Similarly, merging a pendant vertex with its parent does not affect the possibility of introducing cycles through future merges (Def. 5(1)). Finally, since the cost function is monotonic, the merge cannot adversely affect a future cost.

Fig. 5. The unintrusive merge algorithm that only merge unintrusively fusible vertices.

Fig. 5 shows the unintrusive partitioning algorithm. It uses a helper function, FINDCANDIDATE, to find two vertices that are unintrusively fusible. The complexity of FINDCANDIDATE is $O(E(E + V))$, which dominates the while-loop in UNINTRUSIVE, whereby the overall complexity of the unintrusive merge algorithm is $O(E^2 (E + V))$. Note that there is little need to further optimize UNINTRUSIVE since we will only use it as a preconditioner for the optimal solution, which will dominate the computation time.

Fig. 8 shows an unintrusive partition of the Python example with a partition cost of 70. However, the significant improvement is the reduction of the number of weight edges in the graph. As we shall see next, in order to find an optimal graph partition in practical time, the number of weight edges in the graph must be modest.

C. Greedy Partition Algorithm

Fig. 6 shows a greedy merge algorithm. It uses the function FIND-HEAVIEST to find the edge in $E_w$ with the greatest weight and either remove it or merge over it. Note that FIND-HEAVIEST must search through $E_w$ in each iteration since MERGE might change the weights.

The number of iterations in the while loop (line 2) is $O(E)$ since at least one weight edge is removed in each iteration either explicitly (line 7) or implicitly by MERGE (line 5). The complexity of finding the heaviest (line 3) is $O(E)$, calling LEGAL is $O(E + V)$, and calling MERGE is $O(V^2)$ thus the overall complexity is $O(V^2 E)$.

Fig. 7 shows a greedy partition of the Python example. The partition cost is 58, which is a significant improvement over no merge. However, it is not the optimal partitioning, as we shall see later.

Fig. 4. A help function that determines whether the weight edge, $e \in E_w[\hat{G}]$.
1: function \textsc{Greedy}(G)
2: while $E_w(G) \neq \emptyset$ do
3: \hspace{1em} $(u, v) \leftarrow \textsc{Find-Heaviest}(E_w(G))$
4: \hspace{1em} if \textsc{Legal}(G, (u, v)) then
5: \hspace{2em} $G \leftarrow \textsc{Merge}(G, u, v)$
6: \hspace{1em} else
7: \hspace{2em} Remove edge $(u, v)$ from $E_w$
8: \hspace{1em} end if
9: end while
10: return $G$
11: end function

Fig. 6. The greedy merge algorithm that greedily merges the vertices connected with the heaviest weight edge in $G$.

Because the WSP problem is NP-hard, we cannot in general hope to solve it exactly in polynomial time. However, we may be able to solve the problems within reasonable time in common cases given a carefully chosen search strategy through the $2^k$ possible partitions. For this purpose, we have implemented a branch-and-bound algorithm, exploiting the monotonicity of the partition cost (Def. 6(2)). It is shown in Fig. 10, and proceeds as follows:

Before starting, the largest unintrusive partition is found. This is the largest partition that we can ensure is included in an optimal partition. The blocks of the unintrusive partition will be the vertices in our initial partition graph. Second, a good suboptimal solution is computed. We use the greedy algorithm for this purpose, but any scheme will do. We now start a search rooted in the $\top$-partition where everything is one block. This has the lowest cost, but will in general be illegal. Each recursion step cuts a weight edge that has not been considered before, if it yields a cost that is strictly lower than the currently best partition $G_{\text{min}}$ (if the cost is higher than for $G_{\text{min}}$, no further splitting will yield a better partition, and its search subtree can be ignored). If we reach a legal partition, this will be the new best candidate, and no further splitting will yield a better one. When the work queue is empty, $G_{\text{min}}$ holds an optimal solution to WSP.

Fig. 10 shows the implementation, Fig. 9 shows an example of a branch-and-bound search tree, and Fig. 11 shows an optimal partition of the Python example with a partition cost of 38.

E. Linear Merge

For completeness, we also implement a partition algorithm that does not use a graph representation. In this naïve approach, we simply go through the array operation list and add each array operation to the current partition block unless the array operations makes the current block illegal, in which case we add the array operation to a new partition block, which then becomes the current one. The asymptotic complexity of this algorithm is $O(n^2)$ where $n$ is the number of array operations.
Fig. 10. The optimal merge algorithm that optimally merges the vertices in $G$. The function, $cost(G)$, returns the partition cost of the partition graph $G$.

```python
1: function MERGEBYMASK($G, M$)  # Flag that indicates fusibility
2:  $f$ ← $true$
3:  for $i$ ← 0 to $|E_u[G]| - 1$ do
4:      if $M_i = 1$ then
5:          $(u, v) ←$ the $i$'th edge in $E_u[G]$
6:          if not FUSIBLE$(G, u, v)$ then
7:              $f ← false$
8:          end if
9:          $G ←$ MERGE$(G, u, v)$
10:    end for
11:    return $(G, f)$
12: end function
```

Fig. 11. A partition graph of the optimal merge of the graph in Fig. 3.

```
1: function OPTIMAL(G)
2:  $G ←$ UNINTRUSIVE(G)
3:  for $(v, u)$ ← $|E_u[G]|$ do
4:      if not LEGAL$(G, (u, v))$ then
5:          Remove edge $(u, v)$ from $E_u$
6:      end if
7:  end for
8:  $G_{min} ←$ GREEDY$(G)$  # Good guess
9:  $M_{0}, |E_u[G]| ← 1$  # Fill array $M$
10: $o ← 0$  # The mask offset
11: $Q ← ∅$
12: ENQUEUE$(Q, (M, o))$
13: while $Q ≠ ∅$ do
14:     $(M, o) ←$ DEQUEUE$(Q)$
15:     $(G', f) ←$ MERGEBYMASK$(G, M)$
16:     if $cost(G') < cost(G_{min})$ then
17:         if $f$ and $G'$ is acyclic then
18:             $G_{min} ← G'$  # New best partitioning
19:         end if
20:     end if
21:     for $i$ ← $o$ to $|M| - 1$ do
22:         $M_i' ← M_i$
23:         $o ← 0$
24:         ENQUEUE$(Q, (M', i + 1))$
25:     end for
26: end while
27: return $G_{min}$
28: end function
```

Fig. 12. A partition graph of a Linear partition of the Python example (Fig. 2).

Fig. 12 show that result of partitioning the Python example with a cost of 58.

F. Merge Cache

In order to amortize the runtime of applying the merge algorithms, Bohrium implements a merge cache of previously found partitions of array operation lists. It is often the case that scientific applications use large calculation loops such that an iteration in the loop corresponds to a list of array operations. Since the loop contains many iterations, the cache can amortize the overall runtime time.

V. Evaluation

In this section, we will evaluate the different partition algorithm both theoretically and practically. We execute a range of scientific Python benchmarks, which are part of an open source benchmark tool and suite named Benchpress

Table I shows the specific benchmarks that we uses and Table II specifies the host machine. When reporting runtime results, we use the results of the mean of 10 identical executions as well as error bars that shows two standard deviations from the mean.

We would like to point out that even though we are using benchmarks implemented in pure Python/NumPy, the performance is comparable to traditional high-performance languages such as C and Fortran. This is because Bohrium overloads NumPy array operations in order to JIT compile and execute them in parallel seamlessly.

Theoretical Partition Cost: Fig. 13 shows that theoretical partition cost (Def. 13) of the four different partition algorithms previously presented. Please note that the last five benchmarks do not show an optimal solution. This is because

3Available at [link removed for double blind review]. For reproducibility, the exact version can be obtained from the source code repository at [link removed for double blind review].
Benchmark | Input size (in 64-bit floats) | Iterations
--- | --- | ---
Black Scholes | $1.5 \times 10^8$ | 20
Game of Life | $10^8$ | 20
Heat Equation | $1.44 \times 10^8$ | 20
Leibnitz PI | $10^8$ | 20
Gauss Elimination | 2800 | 2799
LU Factorization | 2800 | 2799
Monte Carlo PI | $10^8$ | 20
27 Point Stencil | $4.2875 \times 10^7$ | 20
Shallow Water | $1.024 \times 10^7$ | 20
Rosenbrock | $2 \times 10^8$ | 20
Successive over-relaxation | $1.44 \times 10^8$ | 20
NBody | 6000 | 20
NBody Nice | 40 plants, $2 \times 10^9$ asteroids | 20
Lattice Boltzmann D3Q19 | $3.375 \times 10^9$ | 20
Water-Ice Simulation | $6.4 \times 10^9$ | 20

TABLE I

<table>
<thead>
<tr>
<th>Benchmark</th>
<th>Processor: Intel Core i7-3770</th>
<th>Clock: 3.4 GHz</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>#Cores: 4</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Peak performance: 108.8 GFLOPS</td>
<td></td>
</tr>
<tr>
<td></td>
<td>L3 Cache: 16MB</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Memory: 128GB DDR3</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Operating system: Ubuntu Linux 14.04.2 LTS</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Software: GCC v4.8.4, Python v2.7.6, NumPy 1.8.2</td>
<td></td>
</tr>
</tbody>
</table>

TABLE II

SYSTEM SPECIFICATIONS

the associated search trees are too large for our branch-and-bound algorithm to solve. For example, the search tree of the Lattice Boltzmann is $2^{664}$, which is simply too large even if the bound can cut 99.999% of the search tree away.

As expected, we observe that the three algorithms that do fusion, Linear, Greedy, and Optimal, have a significant smaller cost than the non-fusing algorithm Singleton. The difference between Linear and Greedy is significant in some of the benchmarks but the difference between greedy and optimal does almost not exist.

![Fig. 13. Theoretical cost of the different partition algorithms. NB: the last five benchmarks, Lattice Boltzmann, NBody, NBody Nice, SOR, Water-Ice Simulation, do not show an optimal solution.](image)

![Fig. 14. Runtime of the different partition algorithms using a warm cache.](image)

**Practical Runtime Cost:** In order to evaluate the full picture, we do three runtime measurements: one with a warm fuse cache, one with a cold fuse cache, and one with no fuse cache. Fig. 14 shows the runtime when using a warm fuse cache thus we can compare the theoretical partition cost with the practical runtime without the overhead of running the partition algorithm. Looking at Fig. 13 and Fig. 14, it is evident that our cost model, which is a measurement of unique array accesses (Def. 13), compares well to the practical runtime result in this specific benchmark setup. However, there are some outliers – the Monte Carlo PI benchmark has a theoretical partition cost of 1 when using the Greedy and Optimal algorithm but has a significantly greater practical runtime. This is because the execution becomes computation bound rather than memory bound thus a further reduction in memory accesses does not improve performance. Similarly, in the 27 Point Stencil benchmark the theoretical partition cost is identical for Linear, Greedy, and Optimal, but in practice Optimal is marginally better. This is an artifact of our cost model, which define the cost of reads and writes identically.

With the cold fuse cache, the partition algorithm runs once in the first iteration of the computation. The results show that 20 iterations, which most of the benchmarks uses, is enough to amortize the partition overhead (Fig. 15). Whereas, if we run with no fuse cache, i.e. we execute the partition algorithm in each iteration (Fig. 16), the Linear partition algorithm outperforms both the Greedy and Optimal algorithm because of its smaller time complexity.

**A. Alternative Cost Model**

With the theoretical and practical framework we are presenting in this paper, it is straightforward to explore the impact of alternative cost models. In this section, we will do exactly that – replace our cost model with alternative cost models and evaluate the effect on the runtime of the generated code.

Let us define and evaluate three alternative cost models, *Max Contract, Max Locality,* and *Robinson,* which are used in related literature [13], [14], [15]:
Definition 19. The cost model Max Contract defines the cost of a partition, \( P \), of array operations, \( A \), as follows:

\[
\text{MaxContract}(A, P) = |\text{new}[A]| - \sum_{B \in P} |\text{new}[B] \cap \text{del}[B]|
\]

(5)

where \(|\text{new}[A]|\) is the total number of allocated arrays. Thus, in this cost model, all arrays that are not contracted add 1 to the cost.

Definition 20. The cost model Max Locality defines the cost of a partition, \( P \), of array operations, \( A \), as follows:

\[
\text{MaxLocality}(A, P) = \sum_{B \in P} \sum_{f \in B} \sum_{f' \in (A \setminus B)} |\text{ext}[f] \cap \text{io}[f']|
\]

(6)

In other words, this cost model penalizes each pair of array accesses not fused with a cost of 1. NB: the cost is a pair-wise sum of all identical array accesses. Thus, fusing four identical array accesses achieves a cost saving of 6 rather than 4.

Fig. 15.Runtime of the different partition algorithms using a cold cache.

Fig. 16. Runtime of the different partition algorithms using no cache.

Fig. 17. Runtime of the different cost models using the Linear partition algorithm and a warm cache.

Fig. 18. Runtime of the different cost models using the Greedy partition algorithm and a warm cache.

Definition 21. The cost model Robinson defines the cost of a partition, \( P \), of array operations, \( A \), as follows:

\[
\text{Robinson}(A, P) = |P| + N \cdot \text{MaxContract}(A, P) + N^2 \cdot \text{MaxLocality}(A, P)
\]

(7)

where \( N \) is the total number of accessed arrays. In other words, this cost model combines Max Locality, Max Contract, and penalizes the number of partition blocks (in that priority). Furthermore, the size of \( N \) guarantees that Max Locality always attach more importance than Max Contract which in turn always attach more importance than the number of partition blocks.

Fig. 17, 18, and 19 compares the runtime of the cost models using the Linear, Greedy, and Optimal partition algorithms.
represent data dependencies between loops, and undirected edges represent data sharing between loops. Edges that connect fusible loops have a non-negative weight that represents the cost saving associated with fusion of the two loops. Edges that connect non-fusible loops are marked as fuse-preventing. Now, the objective is to find a partition of the vertices into blocks such that no block has vertices connected with fuse-preventing edges and that minimize the weight sum of edges that connects vertices in different blocks.

Megiddo et al. have shown that it is possible to formulate the WLF problem as integer linear programming (ILP) [14]. Based on the WLF graph, the idea is to transform the edges into linear constraints that implement the dependency and fusibility between the vertices and transform weights into ILP objective variables. The values of the objective variables are either the values of the weights when the associated vertices are in different partitions or zero when in the same partition. The objective of the ILP is then to minimize the value of the objective variables. The problem is NP-hard, but the hope is that with an efficient ILP solver, such as lp-solve [16], and a modest problem size it might be practical as a compile time optimization. Darie et al. [13] proved that the WLF problem is NP-hard through a reduction from multiway cut [6]. Furthermore, since maximizing data locality may not maximize the number of array contractions (Fig. 20), they introduce an ILP formulation with the sole objective of maximizing the number of array contractions (the Max Contract cost model in Section V-A).

Robinson et al. [15] describe an ILP scheme that combines the objectives of Megiddo and Darie: both maximizing data locality and array contractions while giving priority to data locality (corresponds to our Robinson cost model). However, optimization using WLF has a significant limitation: it only allows static edge weights. That is, when building
Thus, it is perfectly legal to have cost models that reward fusion of specific operation types e.g. rewarding fusion of multiply and addition instructions to utilize the FMA instruction set available on recent Intel and AMD microprocessors.

VIII. Conclusion

In this paper, we introduce the Weighted Subroutine Partition Problem (WSP), which unifies program transformations for fusion of loops, array operations, and combinators. Contrary to previous formulations of this problem, WSP incorporates the cost function into the formulation, which makes WSP able to handle a wide range of optimization objects. Furthermore, we show that the cost function must be part of the formulation to enable optimization objects that minimize data locality correctly.

We prove that WSP is NP-hard and implement a branch-and-bound algorithm that finds an optimal solution. Out of 15 application benchmarks, this branch-and-bound algorithm finds a solution for ten benchmarks within reasonable runtime.

We implement a greedy algorithm that finds a good solution to the WSP problem, works with any cost function, and is fast enough for Just-In-Time compilation (20 iterations is typically enough to amortize overhead).

To evaluate various WSP algorithms, we have incorporated the algorithms into Bohrium. The optimization objective is then to minimize data accesses through array contractions and data reuses within Just-In-Time compiled computation kernels.

As expected, our evaluation shows that minimizing data accesses have a significant performance impact. The 15 application benchmarks we evaluate in this paper experience a speedup ranging between 2 and 30, compared to no optimization.

However, our evaluation also shows that the various approaches to approximate or solve the WSP have only a marginal impact on the overall runtime performance of the benchmarks. Out of 15, only one benchmark performs significantly better using the optimal algorithm – approximately a speedup of 1.3 compared to the greedy algorithm. Similarly, the impact of various optimization objects is also minimal. This tells us that approximation algorithms will give us most of the savings, so more is won by making them faster than closer to optimal.

REFERENCES


