Unified Sparse Formats for Tensor Algebra Compilers

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This paper shows how to build a sparse tensor algebra compiler that is agnostic to tensor formats (data layouts). We develop an interface that describes formats in terms of their capabilities and properties, and show how to build a modular code generator where new formats can be added as plugins. We then describe six implementations of the interface that compose to form the dense, CSR/CSF, COO, DIA, ELL, and HASH tensor formats and countless variants thereof. With these implementations at hand, our code generator can generate code for any tensor algebra expression on any combination of the aforementioned formats.

To demonstrate our modular code generator design, we have implemented it in the open-source taco tensor algebra compiler. Our evaluation shows that we get better performance by supporting more formats specialized to different tensor structures, and our plugins makes it easy to add new formats. For example, when data is provided in the COO format, computing a single matrix-vector multiplication with COO is up to 3.6× faster than with CSR. Furthermore, DIA is specialized to tensor convolutions and stencil operations and therefore performs up to 22% faster than CSR for such operations. To further demonstrate the importance of support for many formats, we show that the best vector format for matrix-vector multiplication varies with input sparsities, from hash maps to sparse vectors to dense vectors. Finally, we show that the performance of generated code for these formats is competitive with hand-optimized implementations.

Additional Key Words and Phrases: sparse tensor algebra compilation, tensor formats, modular code generation.

1 INTRODUCTION

Tensor algebra is a powerful tool to compute on multidimensional data with applications in machine learning [Abadi et al. 2016], data analytics [Anandkumar et al. 2014], physical sciences [Feynman et al. 1963], and engineering [Kolecki 2002]. Tensors generalize matrices to any number of dimensions and are often large and sparse, meaning most components are zeros. To efficiently compute with sparse tensors requires exploiting their sparsity in order to avoid unnecessary computations.

Recently, Kjolstad et al. [2017] proposed a compiler for sparse tensor algebra called taco. Their compiler technique generates efficient code for computing with any number of tensors, where each tensor can be described as dense or sparse along each dimension. This includes tensors stored in dense arrays as well as variants of the compressed sparse row (CSR) format.

These are, however, only some of the tensor formats that are used in practice. Important formats that are not supported by taco include the coordinate (COO) format, the diagonal (DIA) format, the ELLPACK (ELL) format, and hash maps (HASH), along with countless blocked and high-dimensional variants and compositions of these. Each format is important for different reasons. COO is the natural way to enumerate sparse tensors and is often the format in which users provide data [Smith et al. 2017a]. It is not the most performant format, but when a tensor will only be used once it is often more efficient to compute directly with COO than to convert the data to another format. ELL exposes vectorization opportunities for SpMV and is useful for matrices that contain a bounded number of nonzeros per row, such as matrices from well-formed meshes. DIA has the added benefit of being very compact and is suited to matrices that compute stencils on Eulerian grids and images. Hash maps support random access without having to explicitly store zeros and can be useful for...
multiplications involving very sparse operands. An application may need any, or even several, of these formats, making it important to support computing with all and any combination of them.

The approach of Kjolstad et al. [2017] was hard-coded for sparse dimensions that are compressed using the same arrays as CSR. By contrast, COO matrices store full coordinates, while DIA implicitly encodes coordinates of nonzeros using very different data structures. To enable efficiently computing with any format, a tensor algebra compiler must emit distinct code to cheaply iterate over each format. COO, for instance, needs a single loop that iterates over row and column dimensions together (Figure 1a), whereas CSR needs two nested loops that each iterate a dimension (Figure 1b). To efficiently compute with operands in multiple formats, a compiler must emit code that concurrently iterates over the operands. Figure 1c shows, however, that this is not a straightforward combination of code that individually iterate over the operand formats. Instead, a compiler must emit distinct code for each combination of formats to get good performance. Because the number of combinations is exponential in the number of formats though, a compiler must be modular with respect to formats.

We generalize the recent work on tensor algebra compilation to support a much wider range of disparate tensor formats. We describe a level-based abstraction that captures how to efficiently access data structures for encoding tensor dimensions, but that hides the specifics behind a fixed interface. We develop six per-dimension formats, all of which expose this common interface, that compose to express all the tensor formats mentioned above. Two of these per-dimension formats—dense and compressed—were hard-coded into taco. The other four—singleton, range, offset, and hashed—are new to this work and compose to express variants of COO, DIA, ELL, HASH, and countless other tensor formats. We then present a code generation algorithm that, guided by our abstraction, generates efficient tensor algebra kernels that are optimized for operands stored in any mix of formats. The result is a powerful system that lets users mix and match formats to suit their application and data, and which can be readily extended to support new tensor formats without modifying the code generation algorithm. We make the following contributions:

**Levelization** We survey many known tensor formats (Section 2) and show that they can be represented as hierarchical compositions of just six per-dimension level formats (Figure 4).

**Level abstraction** We describe an abstraction for level formats that hides the details of how a level format encodes a tensor dimension behind a common interface, which describes how to access the tensor dimension and exposes its properties (Section 3).
Modular code generation We present a code generation technique that emits code to efficiently compute on tensors stored in any combination of formats, which reasons only about capabilities and properties of level formats and is not hard-coded for any specific format (Section 4).

To evaluate our technique, we implemented it as an extension, called fmttaco, to the open-source tensor algebra compiler taco. We find that our technique generates code that have performance competitive with existing sparse linear and tensor algebra libraries. fmttaco’s support for more disparate formats lets it achieve better end-to-end performance than taco. Computing a single matrix-vector multiplication with a COO matrix using fmttaco, for instance, is up to 3.6× faster than with CSR using taco when starting out with data stored in COO (Section 5).

2 TENSOR STORAGE FORMATS

There exists many formats for storing sparse tensors that are used in practice. Each format is ideal under specific circumstances, but none is universally superior. The ideal format depends on the structure and sparsity of the data, the computation, and the hardware. It is thus desirable to support computing with as many formats as possible. This is, however, made difficult by the need for specialized code for every combination of operand tensor formats, even for the same computation.

Several examples of tensor storage formats from the literature are shown in Figure 2. A straightforward way to store an $n$th-order tensor (i.e., a tensor with $n$ dimensions) is to use an $n$-dimensional dense array, which explicitly stores all tensor components including zeros. Figure 2b shows dense storage for an 1st-order tensor (a vector). A desirable feature of dense arrays is that the value at any coordinate can be accessed in constant time. Storing a sparse tensor in a dense array, however, is inefficient as a lot of memory is wasted to store zeros. Furthermore, performance is lost computing with these zeros even though they do not meaningfully contribute to the result. For tensors with many large dimensions, it may even be impossible to use a dense array due to lack of memory.

The simplest way to efficiently store a sparse tensor is to keep a list of its nonzero coordinates and values (Figures 2c, 2f, and 2n). This is typically known as the coordinate (COO) format [Bader and Kolda 2007]. In contrast to dense arrays, COO consumes only $O(\text{nnz})$ memory. The COO format also closely resembles common file formats for storing tensors, such as the Matrix Marketplace exchange format [National Institute of Standards and Technology 2013] and the FROSTT sparse tensor format [Smith et al. 2017a]. This minimizes preprocessing cost as inserting nonzero values and their coordinates only requires appending them to the $\text{idx}$ and $\text{vals}$ arrays.

Unlike dense arrays, COO does not provide efficient random access, which is useful for multiplications. Hash maps resolve this by storing tensor coordinates in a hash table (Figure 2d). However, hash maps do not support cheaply iterating nonzeros in order, which would be useful for additions.

COO also redundantly stores row coordinates, which the compressed sparse row (CSR) format for sparse matrices (2nd-order tensors) compress out (Figure 2g). This increases performance for memory bandwidth-bound computations, such as sparse matrix-vector multiplication (SpMV). In Figure 2f, for instance, the row coordinate is repeated for the first three nonzeros in the same row. CSR removes the redundant row coordinates, using an auxiliary array (pos in Figure 2g) to keep track of which nonzeros belong to each row. The doubly compressed sparse row (DCSR) format achieves additional compression for hypersparse matrices by only storing the rows that contain nonzeros (Figure 2b) [Buluç and Gilbert 2008]. For higher-order tensors, Smith and Karypis [2015] describe a generalization of CSR, called compressed sparse fiber (CSF), that compresses every dimension (Figure 2o). All these compressed formats, however, can be costly to assemble or modify.

Many important applications work with tensors whose nonzero components form a regular pattern. Matrices that encode vertex-edge connectivity of well-formed unstructured meshes, for instance, have a bounded number of nonzero components per row. This is exploited by the ELLPACK
The block compressed sparse row (BCSR) format generalizes CSR by storing a dense block of nonzeros in the vals array for every nonzero coordinate (Figure 2k). This reduces storage and exposes opportunities for vectorization, and is ideal for inherently blocked matrices from FEM applications. The mode-generic sparse tensor storage format, proposed by Baskaran et al. [2012],

Fig. 2. Identical tensors stored in various formats. Array elements shaded blue encode the same nonzero.

(ELL) format, which stores the same number of components for each row (Figure 2i) [Kincaid et al. 1989]. Thus, it only has to store the column coordinates and values of the rows, which are stored contiguously in memory making it possible to efficiently vectorize SpMV [D’Azevedo et al. 2005]. If the nonzeros are further restricted to a few dense diagonals, then their coordinates can be computed from the offsets of the diagonals. This pattern is common in grid and image applications, and allows the nonzeros to be further restricted to a few dense diagonals, then their coordinates can be computed from the offsets of the diagonals. This pattern is common in grid and image applications, and allows.

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generalizes the idea of BCSR to higher-order tensors (Figure 2p). It stores a tensor as a sparse collection of any-order dense blocks and uses the COO format (the idx arrays) to represent the sparse collection of blocks. By contrast, the compressed sparse block (CSB) format, proposed by Buluç et al. [2009], represents a matrix as a dense collection of sparse blocks stored in COO (Figure 2l).

The existence of so many disparate tensor formats makes it challenging to support efficiently computing with all of them. As we have seen, different formats may use vastly dissimilar data structures to encode tensor coordinates and thus need very different code to iterate over them. Iterating over a dense matrix’s column dimension, for instance, simply entails looping over all possible coordinates along the dimension. Efficiently iterating over a CSR matrix’s column dimension, by contrast, requires looping over its idx array and dereferencing it at each position to access the column coordinates (Figure 1b, lines 2–5). Furthermore, to efficiently compute with tensors stored in different combinations of formats can require completely different strategies for simultaneously iterating over multiple formats. For example, code to compute the component-wise product of CSR matrix $B$ with dense matrix $C$ simply has to iterate over $B$ and pick out corresponding nonzeros from $C$ (Figure 1b, line 6). Computing the same operation with COO matrix $C$, however, requires vastly different code as neither CSR nor COO supports efficient random access into the column dimension. Instead, code to compute the component-wise product has to simultaneously co-iterate over and merge the idx arrays that encode $B$ and $C$’s column coordinates (Figure 1c, lines 8–20). Thus, to get good performance with all tensor formats, a code generator needs to be able to emit specialized code for any combination of distinct formats. Since the number of such combinations grows exponentially with the number of supported formats though, it is infeasible to hard-code optimized code generation strategies for each combination individually.

3 TENSOR STORAGE ABSTRACTION

As we have seen, a tensor algebra compiler must generate specialized code for every possible combination of supported formats in order to get good performance. Since the number of combinations grows exponentially with the number of formats though, it is infeasible to exhaustively hard-code support for every possible format. In this section, we will show how common variants of all the tensor formats examined in Section 2 can be expressed as compositions of just six per-dimension formats. We will also present an abstraction that captures shared capabilities and properties of per-dimension formats. The abstraction generalizes common patterns of accessing tensor storage and guides a format-agnostic code generation algorithm that we will describe in Section 4.
3.1 Coordinate Hierarchies

The per-dimension formats can be understood by viewing tensor storage as a hierarchy of coordinates, where each hierarchy level encodes the coordinates along one tensor dimension. Each path from the root to a leaf in this hierarchy encodes the coordinates in each dimension of one tensor component. Figure 3 shows examples of coordinate hierarchies for a matrix stored in different formats. The matrix component values are shown at the bottom of each hierarchy. In Figure 3b, for instance, the rightmost path represents the tensor component $B(3, 4)$ with the value 9. As we will see in Section 4, representing tensor storage hierarchically lets a code generator decompose any computation into the simpler problem of merging coordinate hierarchy levels.

The structure of a coordinate hierarchy reflects the encoding of nonzeros in memory and lets the code generator reason about how to iterate over tensors without knowing the specific tensor format. For example, the coordinate hierarchy of a COO tensor in Figure 3a consists of coordinate chains that encode each nonzero. This chain-structure reflects that the COO format stores every coordinates of each nonzero. By contrast, the coordinate hierarchy of a CSR matrix in Figure 3b is tree-structured and components on the same row share a row coordinate parent. This tree-structure reflects that the CSR format removes redundant row coordinates using the auxiliary pos array.

A coordinate hierarchy has one level—shaded light gray in Figure 3—for every tensor dimension, and per-dimension level formats describe how to store the hierarchy levels. Each position (a node) in a level may encode some coordinate (the number in the node) along the corresponding tensor dimension. Alternatively, a position may contain an unlabeled node, which encodes no coordinate. Each position may also be connected to a parent in the previous level. Coordinates that share the same parent are referred to as siblings. The coordinates highlighted in dark gray in Figure 3b, for instance, are siblings that share the parent row coordinate 3. A coordinate’s ancestors refer to the set of coordinates that are encoded by the path from its parent to the root.

We propose six level formats that are sufficient to represent all the tensor formats described in Section 2, though many more are possible within our framework. Some of these level formats implicitly encode coordinates (e.g., as a range), while others explicitly store them (e.g., in a segmented vector). Given a parent coordinate, the six level formats encode its children coordinates as follows:

**Dense** levels store the size of the corresponding dimension ($N$) and encode the coordinates in the range $[0, N)$. The array on the right encodes the dense row dimension of the CSR matrix in Figure 3b.

**Compressed** levels store coordinates in a segment of the $\text{idx}$ array, with segment bounds stored in the pos array. The arrays on the right encode the compressed column dimension of the CSR matrix in Figure 3b. Given a parent coordinate 1, for instance, the level encodes two child coordinates 0 and 1, stored in $\text{idx}$ between positions $\text{pos}[1] = 2$ and $\text{pos}[2] = 4$.

**Singleton** levels store one coordinate in the $\text{idx}$ array. The array on the right encodes the singleton column dimension of the COO matrix in Figure 3a.

**Range** levels encode the coordinates in a range with bounds computed from an offset and from the dimension sizes $N$ and $M$. The arrays on the right encode the range row dimension of the DIA matrix in Figure 3c. Given a parent coordinate 1, for instance, the level encodes coordinates between $\max(0, -\text{offset}[1]) = 1$ and $\min(4, 6 - \text{offset}[1]) = 4$.

**Offset** levels encode a coordinate, shifted from the parent coordinate by a value in $\text{offset}$. The array on the right encodes the offset column dimension of the DIA matrix in Figure 3c. Given a parent coordinate 3 and offset index 1, for instance, the level encodes the coordinate $3 + \text{offset}[1] = 3$. 

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(a) Vector storage formats

(b) Matrix storage formats

(c) Order-3 tensor storage formats

Fig. 4. Common tensor formats composed from per-dimension level formats. We cast structured matrix formats as higher-order tensor formats. The label beside a level identifies the tensor dimension it represents. Unless otherwise stated, all levels other than hashed are ordered and unique (see Section 3.3); hashed levels are unordered and unique. (¬O) denotes an unordered level and (¬U) denotes a non-unique level.

Table 1. Supported capabilities and properties of each level type described above. V, P, I, and A indicate that a level type supports coordinate value iteration, coordinate position iteration, insert, and append respectively. A (✓) indicates that a level type can be configured to either possess or not possess a particular property.

<table>
<thead>
<tr>
<th>Level Type</th>
<th>Capabilities</th>
<th>Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Iteration</td>
<td>Locate</td>
</tr>
<tr>
<td>Dense</td>
<td>V</td>
<td>✓</td>
</tr>
<tr>
<td>Range</td>
<td>V</td>
<td>✓</td>
</tr>
<tr>
<td>Compressed</td>
<td>P</td>
<td>A</td>
</tr>
<tr>
<td>Singleton</td>
<td>P</td>
<td>A</td>
</tr>
<tr>
<td>Offset</td>
<td>P</td>
<td></td>
</tr>
<tr>
<td>Hashed</td>
<td>P</td>
<td>✓</td>
</tr>
</tbody>
</table>

Hashed levels store coordinates in a segment, of size $W$, of a hash map ($\text{idx}$).

The arrays on the right, with empty buckets marked by $-1$, encode the hashed dimension of a hash map vector.

Table 2 provides the precise semantics of the level formats, and Figure 4 shows how they can be composed to express the tensor formats described in Section 2. We cast structured matrix formats, like BCSR, as formats for higher-order tensors; the added dimensions expose tensor structure.

The code generator in Section 4 emits code that accesses and modifies coordinate hierarchy levels through an abstract level interface, which ensures the code generator is not tied to specific formats. This makes it extensible and maintainable as adding support for new formats does not require any
Table 2. Level functions defined for each of the six level types listed in Section 3.1. Section 3.2 describes how these level functions implement the access capabilities supported by each level type, as identified in Table 1.

<table>
<thead>
<tr>
<th>Level Type</th>
<th>Level Function Definitions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dense</td>
<td><code>coordinateiter(i_1, ..., i_k-1)</code>:&lt;br&gt; <code>locate(p_k-1, i_1, ..., i_k)</code>:&lt;br&gt; <code>coordinateaccess(p_k-1, i_1, ..., i_k)</code>:&lt;br&gt; <code>return &lt;p_k-1 * N_k + i_k, true&gt;</code></td>
</tr>
<tr>
<td>Range</td>
<td><code>coordinateiter(i_1, ..., i_k-1)</code>:&lt;br&gt; <code>locate(p_k-1, i_1, ..., i_k)</code>:&lt;br&gt; <code>coordinateaccess(p_k-1, i_1, ..., i_k)</code>:&lt;br&gt; <code>return &lt;p_k-1 * N_k + i_k, true&gt;</code></td>
</tr>
<tr>
<td>Compressed</td>
<td><code>pos_iter(p_k-1)</code>:&lt;br&gt; <code>return &lt;pos[p_k-1], pos[p_k-1] + 1&gt;</code>&lt;br&gt; <code>pos_access(p_k, i_1, ..., i_k-1)</code>:&lt;br&gt; <code>return &lt;idx[p_k], true&gt;</code></td>
</tr>
<tr>
<td>Singleton</td>
<td><code>pos_iter(p_k-1)</code>:&lt;br&gt; <code>return &lt;pos[p_k-1], p_k-1 + 1&gt;</code>&lt;br&gt; <code>pos_access(p_k, i_1, ..., i_k-1)</code>:&lt;br&gt; <code>return &lt;idx[p_k], true&gt;</code></td>
</tr>
<tr>
<td>Offset</td>
<td><code>pos_iter(p_k-1)</code>:&lt;br&gt; <code>return &lt;pos[p_k-1], p_k-1 + 1&gt;</code>&lt;br&gt; <code>pos_access(p_k, i_1, ..., i_k-1)</code>:&lt;br&gt; <code>return &lt;idx[p_k], true&gt;</code></td>
</tr>
<tr>
<td>Hashed</td>
<td><code>locate(p_k-1, i_1, ..., i_k)</code>:&lt;br&gt; <code>int p_k = i_k % W_k + p_k-1 * W_k</code>&lt;br&gt; <code>if (idx[p_k] != i_k &amp;&amp; idx[p_k] != -1) {</code>&lt;br&gt; <code>int end = p_k</code>&lt;br&gt; <code>do {</code>&lt;br&gt; <code>p_k = (p_k + 1) % W_k + p_k-1 * W_k</code>&lt;br&gt; <code>}</code>&lt;br&gt; <code>while (idx[p_k] != i_k &amp;&amp; idx[p_k] != -1 &amp;&amp; p_k != end) {</code>&lt;br&gt; <code>}</code>&lt;br&gt; <code>return &lt;p_k, idx[p_k] == i_k&gt;</code></td>
</tr>
</tbody>
</table>

Table 2. Level functions defined for each of the six level types listed in Section 3.1. Section 3.2 describes how these level functions implement the access capabilities supported by each level type, as identified in Table 1.

changes to the code generation algorithm. The abstract interface to a coordinate hierarchy level consists of level capabilities and properties. Level capabilities instruct the code generator on how to iterate over and index into levels, as well as on how to add coordinates to a level. Properties of a level let the compiler emit optimized loops that exploit tensor attributes to increase computational performance. Table 1 identifies the capabilities and properties of each level type.

### 3.2 Level Access Capabilities

Every coordinate hierarchy level provides a set of capabilities that can be used to access or modify its coordinates. Each capability consists of level functions that a level must implement to support it and that provide an abstraction for manipulating physical indices in a format-agnostic manner.

Table 1 lists supported level capabilities and Table 2 shows the level functions that implement them for each of the six level formats. As an example, the column dimension of a CSR matrix is a compressed level, which provides the coordinate position iteration capability. This capability is exposed as two level functions, `pos_iter` and `pos_access`, as shown in Table 2. To access the column coordinates in dark gray in Figure 3b, we first determine their range by calling `pos_iter` with the position of row coordinate 3 as input. We then call `pos_access` for each position in this range to get the column coordinate values. Under the hood, `pos_iter` indexes the `pos` array to locate the `idx` array segment that stores the column coordinates, while `pos_access` retrieves each of the coordinates from `idx`. These level functions fully describe how to access CSR indices efficiently, while hiding details such as the existence of the `pos` and `idx` arrays from the caller.
Iterating over a sparse vector

```cpp
for (int i = 0; i < size; ++i) {
    // coords and values dominated by i at pos
    // p_k encode subtensor B(i_1, ..., i_k, i_{k+1}, ...)
}
```

(c) Coordinate value iteration.

```cpp
coord_iter(i_1, ..., i_{k-1}) -> <ibegin_k, iend_k>
coord_access(p_{k-1}, i_1, ..., i_k) -> <p_k, found>
```

More precisely, given a list of ancestor coordinates \((i_1, ..., i_{k-1})\), the function `coord_iter` returns the bounds of an iterator over coordinates that may have those ancestors. For each coordinate \(i_k\) within those bounds, the function `coord_access` returns the position of a child of \(p_{k-1}\) that encodes \(i_k\), or returns `found` as false if the coordinate does not actually exist. These functions can be used to iterete tensor coordinates in the general case as demonstrated in Figure 5c. In practice though, the code in Figure 5c can be optimized by removing the conditional if we know that an implementation of `coord_access` always returns `found` as true.

Coordinate Position Iteration. The coordinate position iteration capability, on the other hand, iterates over coordinate positions. It generalizes the method in Figure 5b for iterating over a sparse vector and is also exposed as two level functions. The first returns an iterator over positions in a level (`pos_iter`) and the second accesses the coordinate encoded at each position (`pos_access`):

```cpp
pos_iter(p_{k-1}) -> <pbegin_k, pend_k>
```

The abstract interface to a coordinate hierarchy level exposes three different access capabilities: coordinate value iteration, coordinate position iteration, and locate. Every level must provide coordinate value iteration or coordinate position iteration and may optionally also provide the locate capability. Table 1 identifies the access capabilities supported by each level type. Our code generation algorithm will emit code that calls level functions to access physical indices, which ensures the algorithm is not tied to any specific type of physical index.

Coordinate Value Iteration. The coordinate value iteration capability directly iterates over coordinates. It generalizes the method in Figure 5a for iterating over a dense vector and is exposed as two level functions. The first returns an iterator over coordinates of a coordinate hierarchy level (`coord_iter`) and the second accesses the position of each coordinate (`coord_access`):

```cpp
ibegin_k, iend_k = coord_iter(i_1, ..., i_{k-1});
for (i_k = ibegin_k; i_k < iend_k; ++i_k) {
    p_k, found = coord_access(p_{k-1}, i_1, ..., i_k);
    if (found) {
        // coords and values dominated by i_k at pos
        // p_k encode subtensor B(i_1, ..., i_k, i_{k+1}, ...)
    }
}
```

(d) Coordinate position iteration.
More precisely, given a coordinate at position $p_{k-1}$, the function `pos_iter` returns the bounds of an iterator over positions that may have $p_{k-1}$ as their parent. For each position $p_k$ within those bounds, the function `pos_access` returns the coordinate encoded at that position, or returns `found` as false if $p_k$ is not actually a child of $p_{k-1}$ or does not encode a coordinate. These functions can be used to iterate tensor coordinates with code like that shown in Figure 5d. This code is very similar in structure to that for coordinate value iteration, but with the roles of $i_k$ and $p_k$ reversed.

**Locate.** The locate capability provides random access into a coordinate hierarchy level through a function that computes the position of a coordinate:

\[
\text{locate}(p_{k-1}, i_1, \ldots, i_k) \rightarrow (p_k, \text{found})
\]

The function `locate` has similar semantics as `coord_access`. Given a coordinate $i_{k-1}$ at position $p_{k-1}$, `locate` attempts to locate among its children the coordinate $i_k$. If `locate` finds $i_k$, then it returns $i_k$’s position $p_k$ and `found` as true; otherwise it returns `found` as false. Traversing a path in a coordinate hierarchy to access a single tensor component can be done by successively calling `locate` at every level. As we will see in Section 4, having operands with efficient implementations of the locate capability leads to code that avoids iterating over every nonzero in those operands.

### 3.3 Level Properties

A coordinate hierarchy level may also declare up to five properties: full, ordered, unique, branchless, and compact. These properties describe characteristics of a level, such as whether coordinates are arranged in order, and are invariants that are explicitly enforced or implicitly assumed by the underlying physical index. The column dimension of a CSR matrix, for instance, is both ordered and unique (Figure 4), which means it stores every coordinate just once and in increasing order. Our code generation technique relies on these level properties to emit optimized code.

Table 1 identifies the properties of each level type. Some coordinate hierarchy levels may be configured with a property, depending on the application. Configurable properties reflect invariants that are not tied to how a physical index encodes coordinates. For example, the `idx` array in compressed levels typically store coordinates in order when used in the CSR format, but the same data structure can also store coordinates out of order. Figure 4 shows how level types with configurable properties can be configured to represent tensor formats.

**Full.** A level is full if every collection of coordinates that have the same ancestors includes all valid coordinates along the corresponding tensor dimension. For instance, a level representing a CSR matrix’s row dimension (Figure 3b) encodes every row coordinate and is thus full. By contrast, a level representing the column dimension is not full as it only stores coordinates of nonzeros.

**Unique.** A level is unique if no collection of coordinates that have the same ancestors contains duplicates. For example, a level representing a CSR matrix’s row dimension necessarily encodes every coordinate just once and is thus unique. By contrast, a level representing a COO matrix’s row dimension (Figure 3a) can store a coordinate more than once and is thus not unique.

**Ordered.** A level is ordered if coordinates that have the same ancestors are ordered in increasing value, coordinates with different ancestors are ordered lexicographically by their ancestors, and duplicates are ordered by their parents’ positions. For example, a level representing a standard CSR matrix’s column dimension stores coordinates in increasing order and is thus ordered. A level representing a hash map vector, however, is not as coordinates are stored in hash order instead.
Branchless. A level is branchless if no coordinate has a sibling and each coordinate in the previous level has a child. For example, the coordinate hierarchy for a COO matrix consists strictly of chains of coordinates, making the lower level branchless. By contrast, a level that represents a CSR matrix’s column dimension can have multiple coordinates with the same parent and is thus not branchless.

Compact. A level is compact if no two coordinates are separated by an unlabeled node that does not encode a coordinate. For instance, a level that represents a CSR matrix’s column dimension encodes coordinates in one contiguous range of positions and is thus compact. A level representing a hash map vector, however, is not as it can have unlabeled positions that reflect empty buckets.

3.4 Level Output Assembly Capabilities

The capabilities described in Section 3.2 iterate over and access coordinate hierarchy levels. A level may also provide insert and append capabilities for adding new coordinates. These capabilities let us assemble, in a format-agnostic manner, the data structures that store the result of a computation. Table 1 identifies the assembly capabilities that are supported by various level types, and Appendix A provides definitions of level functions that implement those capabilities.

Insert Capability. Inserts coordinates at any position and is exposed as four level functions:

- `insert_coord(p_k, i_k) -> void`
- `insert_init(sz_{k-1}, sz_k) -> void`
- `size(sz_{k-1}) -> sz_k`
- `insert_finalize(sz_{k-1}, sz_k) -> void`

The level function `insert_coord` inserts a coordinate `i_k` into an output level at position `p_k` given by locate, and requires that the level provide the locate capability. The level function `insert_init` initializes an output level, `insert_finalize` does any post-processing a level requires after all coordinates have been inserted, and `nonzeros` returns the number of nodes in a level (its size). The `size` function takes as input the size of the parent, `sz_{k-1}`, and returns size of this level, while `insert_init` and `insert_finalize` take as inputs the size of this level and the previous level.

Append Capability. Appends coordinates to a level and is also exposed as four level functions:

- `append_coord(p_k, i_k) -> void`
- `append_init(sz_{k-1}, sz_k) -> void`
- `append_edges(p_{begin_k}, p_{begin_k+1}) -> void`
- `append_finalize(sz_{k-1}, sz_k) -> void`

The level function `append_coord` appends a coordinate `i_k` to the end of an output level (`p_k`). The function `append_edges` inserts edges that connect all coordinates between positions `p_{begin_k}` and `p_{begin_k+1}` to the coordinate at position `p_{k-1}` in the previous level. This enables attaching appended coordinates to the rest of the coordinate hierarchy. In contrast to the insert capability, the append capability requires result coordinates to be appended in order. `append_init` and `append_finalize` serve identical purposes as `insert_init` and `insert_finalize` and take the same arguments.

As an example, the following implements the append capability for a compressed level:

```
append_coord(p_k, i_k):
    idx[p_k] = i_k

append_init(sz_{k-1}, sz_k):
    for (int p_{k-1} = 0; p_{k-1} <= sz_{k-1}; ++p_{k-1}) {
        pos[p_{k-1}] = 0
    }

append_edges(p_{begin_k}, p_{begin_k+1}):
    pos[p_{k-1} + 1] = p_{begin_k} - p_{begin_k}

append_finalize(sz_{k-1}, sz_k):
    int cumsum = pos[0]
    for (int p_{k-1} = 1; p_{k-1} <= sz_{k-1}; ++p_{k-1}) {
        cumsum += pos[p_{k-1}]
        pos[p_{k-1}] = cumsum
    }
```

Following the semantics of the append capability, we can, for instance, assemble the `idx` array of a CSR matrix by calling `append_coord` with the coordinates of every nonzero in a computation’s result as inputs. Similarly, the `pos` array can be assembled with calls to `append_init`, `append_edges` after the nonzeros of each row have been computed, and `append_finalize`.

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4 CODE GENERATION

This section describes a code generation algorithm that emits efficient code to compute on tensors stored in any combination of formats. The algorithm supports any tensor format expressible as compositions of level formats, which includes all those described in Section 2 and many others. Our algorithm extends the code generation technique proposed by Kjolstad et al. [2017] to handle many more disparate formats by only reasoning about capabilities and properties of level formats. This approach makes the complexity of our algorithm independent from the number of formats supported. Thus, support for new formats can be added without modifying the code generator.

4.1 Background

The code generation algorithm of Kjolstad et al. [2017] takes as input a tensor algebra expression in tensor index notation. Matrix addition, for example, is expressed in this notation as $A_{ij} = B_{ij} + C_{ij}$, while matrix multiplication is $A_{ij} = \sum_k B_{ik} C_{kj}$. Computing an expression requires iterating over the joint iteration space of the operands, dimension by dimension. For instance, code to add sparse matrices must iterate over only rows that have nonzeros in either matrix and, for each row, iterate over components that are nonzero in either matrix. Additive computations iterate over the union of the operand nonzeros, while multiplicative ones iterate over the intersection of the operands.

The proper order in which to iterate over tensor dimensions is determined from an iteration graph. The iteration graph for a tensor algebra expression consists of a set of index variables that appear in the expression and a set of directed tensor paths that represent accesses into input and output tensors. Each tensor path connects index variables that are used in a corresponding tensor access and is ordered based on the order of index variables in the access expression and the order of dimensions in the accessed tensor. Determining the order in which to merge dimensions reduces to ordering index variables into a hierarchy, such that every tensor path edge goes from an index variable higher up to one lower down. Figure 6a shows the iteration graph for matrix addition with a CSR matrix and a COO matrix as inputs and a row-major dense matrix as output.

For each dimension in the merged iteration space, its corresponding merge lattice describes what loops are needed to compute the combination of intersection and union merges involving the input tensor dimensions. Each point in the ordered lattice encodes a set of tensor dimensions containing nonzero coordinates that must be co-iterated in one loop, while lattice points dominated by the lattice point encode the cases that the aforementioned loop must consider when computing the merge. Every path from the top lattice point to the bottom lattice point represents a sequence of loops that may be executed at runtime to merge the inputs’ iteration spaces. Figures 6b and 6c show merge lattices for matrix addition with a CSR matrix and a COO matrix that has no empty row.
4.2 Property-Based Merge Lattice Optimizations

Optimizations on merge lattices that simplify them to yield optimized code were described by Kjolstad et al. [2017]. Those were, however, all hard-coded to dense and compressed level formats. We reformulate the optimizations with respect to properties and capabilities of coordinate hierarchy levels, so that they can be applied to other level types. In particular, our algorithm optimizes merging of any number of full dimensions (i.e., those represented by full coordinate hierarchy levels) by emitting code to iterate just one of them. This optimization is valid as long as the other full levels to be merged all support the locate capability. Our algorithm also remove all lattice points below the top point that do not co-iterate with a full dimension, since full dimensions are supersets of any sparse dimension. These optimizations give us the optimized merge lattice shown in Figure 6b, which contains a single lattice point even though the computed operation requires a union merge.

4.3 Level Iterator Conversion

As we will see in Section 4.4, efficient algorithms exist for merging coordinate hierarchy levels that are ordered and unique, as well as for intersection merges where unordered levels provide the locate capability. Level iterator conversion turns iterators over unordered and non-unique levels without the locate capability into iterators with any desired properties. The aforementioned algorithms can then be used in conjunction to merge any coordinate hierarchy levels.

In the rest of this subsection, we describe two types of iterator conversion, deduplication and reordering, that can be composed to extend support to any combination of coordinate hierarchy levels. The flowchart on the right in Figure 8 identifies, for each operand in an intersection merge, the iterator conversions that are needed to merge the operands. Our code generation algorithm emits code to perform these necessary iterator conversions on the fly at runtime.

**Deduplication.** Duplicate coordinates complicate merging because it results in code that repeatedly visit points in the iteration space. Deduplication removes duplicates from iterators over ordered and non-unique levels using a deduplication loop. Lines 5–7 in Figure 1c shows an example that scans ahead and aggregates duplicate coordinates, resulting in an iterator without duplicates.

When non-unique levels are at the bottom of coordinate hierarchies, our technique emits deduplication loops that sum the values of duplicate coordinates. Otherwise, the emitted deduplication loop combines the iterators over the duplicate coordinates’ children into a single iterator. In general, this requires a scratch array to store the child coordinates. Figure 7 shows how to avoid the scratch array by chaining together the iterators over the children. This, however, requires that the child level support position iteration and that the child and parent levels be both ordered and compact. With iterator chaining, the starting bound of the first set of children and the ending bound of the last set of children become the bounds of the chained iterator. The resulting iterator provides the same interface as a regular coordinate position iterator and can thus participate in merging without a scratch array. Figure 1c shows iterator chaining used to iterate over columns of a COO matrix.
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4.4 Level Merge Code

As a direct result of how we defined coordinate hierarchies in Section 3, merging tensor dimensions is equivalent to merging the coordinate hierarchy levels that represent those dimensions. The most efficient method for merging levels depends on the properties of the levels and the capabilities that the levels support. Consider, for instance, the component-wise multiplication of two vectors \( x \) and \( y \), which requires iterating over the intersection of the coordinate hierarchy levels that encode their nonzero coordinates. Figure 8 shows asymptotically most efficient strategies for computing the intersection merge depending on whether the inputs are ordered or unique and whether they support the locate capability; these are the same strategies our code generation algorithm selects.

If neither input vector supports the locate capability, we can co-iterate the coordinate hierarchy levels that represent those vectors and compute a new output component whenever we encounter nonzero components in both inputs that share the same coordinate. Another example of this method, applied to merge the column dimensions of a CSR matrix and a COO matrix, is shown on lines 8–20 in Figure 1c. This method generalizes the two-way merge algorithm used in merge sort [Knuth 1973, Chapter 5.2.4] to merge any number of inputs, but still requires being able to enumerate input coordinates uniquely and in order. Nonetheless, this method can still be used in conjunction with the level iterator conversions described in Section 4.3 to merge any levels.

If one of the input vectors, \( y \), supports the locate capability (e.g., a dense array), then we can instead just iterate over the nonzero coordinates of \( x \) and, for each coordinate, locate the corresponding coordinate in \( y \). Another example of this method, applied to merge the column dimensions of a CSR matrix and a dense matrix, is shown on lines 2–9 in Figure 1b. This alternative method reduces the merge complexity from \( O(\text{nnz}(x) + \text{nnz}(y)) \) to \( O(\text{nnz}(x)) \) assuming locate runs in constant time. Moreover, this method does not require enumerating the coordinates of \( y \) in order. We do not even need to enumerate the coordinates of \( x \) in order, as long as there are no duplicates and we do not

**Reordering.** A precondition for code to co-iterate levels is that coordinates are enumerated in order. Reordering uses a scratch array to store an ordered copy of an unordered level and replaces iterators over the unordered level with iterators over the ordered copy. The code generation algorithm can then emit code that merges unordered levels by co-iterating over the ordered copies.
need to compute output components in order (e.g., if the output supports the insert capability). This method is thus ideal for computing intersection merges of unordered coordinate hierarchy levels.

We can generalize and combine the two methods described above to, with the aid of merge lattices, compute arbitrarily complex merges involving unions and intersections of any number of tensor dimensions. If a merge lattice contains multiple lattice points, then each lattice point can be converted to a loop that co-iterates over all the corresponding coordinate hierarchy levels that need to be merged. However, if a merge lattice contains just one non-bottom lattice point, then it can be converted to a loop that co-iterates over only levels that do not support the locate capability. Within that loop, the emitted code can locate into the remaining levels that also need to be merged.

4.5 Code Generation Algorithm

Figure 9a shows our code generation algorithm, which incorporates all of the concepts we presented in the previous subsections. Each part of the algorithm is labeled from 1 to 11; throughout the discussion of the algorithm in the rest of this section, we will identify relevant parts using these labels. The algorithm emits code that iterates over the proper intersections and unions of the input tensors by calling relevant access capability level functions. At points in the merged iteration space, the emitted code computes result values and assembles the output tensor by calling relevant assembly capability level functions. The emitted code is then specialized to compute with specific tensor formats by mechanically inlining all level function calls. This approach bounds the complexity of the code generation mechanism, since it only needs to account for a finite and fixed set of level capabilities and properties. The result is an algorithm that supports many disparate tensor formats and that does not need modification to add support for more level types and tensor formats. Figure 9b shows an example of code that our algorithm generates, with level function calls inlined.

Our algorithm takes, as input, a tensor algebra expression and recursively calls itself on index variables in the expression, in the order given by the corresponding iteration graph. At each recursion level, it generates code for one index variable $i_v$ in the input index expression. The algorithm begins by emitting code that initializes iterators over input coordinate hierarchy levels, which entails calling their appropriate coordinate value or position iteration level functions (1). It also emits code to perform any necessary iterator conversion described in Section 4.3 (1, 2).

The algorithm also constructs a merge lattice, simplified with optimizations described in Section 4.2, at every recursion level for the corresponding input expression and index variable $i_v$. For every point $L_p$ in this merge lattice, the algorithm emits a loop that merges the coordinate hierarchy levels that represent input tensor dimensions associated with $L_p$ (4). Within each loop, the generated code dereferences (potentially converted) iterators over the levels to be co-iterated (5, 7, 10), making sure to not process coordinates that are not actually encoded in the levels (6). Each merged coordinate is then computed (8) and, if the merge is an intersection, used to index into levels that can be accessed with the locate capability (9). At the very end, the algorithm emits appropriate code to advance the iterators that referenced merged coordinates (11).

The algorithm also emits code within each loop to compute output values and to assemble output indices (3). The latter entails emitting code to track where to insert or append new result coordinates in the output, as well as emitting code that calls the appropriate assembly level functions to assemble the physical indices. The algorithm emits specialized compute and assembly code for each merge lattice point that is dominated by $L_p$, which handles the case where the corresponding subset of inputs contain nonzeros at the same coordinate.

Fusing Iterators. By default, at every recursion level, the algorithm emits loops that iterate over a single coordinate hierarchy level of each input tensor. However, an optimization that improves performance when computing with formats like COO entails emitting code that simultaneously
code-gen(index-expr, iv):
  let L := merge-lattice(index-expr, iv)
  for Dj in coord-value-iteration-dims(L):
    emit "int ivDj, int Dj_end = pos_iter_Dj(pDj-1);"
  for Dj in coord-pos-iteration-dims(L):
    if Dj-1 is unique:
      emit "int pDj, int Dj_end = pos_iter_Dj(pDj-1);"
      else:
        emit "int pDj, int Dj_end = pos_iter_Dj(pDj);"
        emit "_Dj_end = pos_iter_Dj(_Dj_end - 1);"
    for Dj in noncanonical-dims(L):
      emit-sort(Dj, scratch, 0, Dj_end);
      emit "int nDj = 0;"
      if result dimension Dj indexed by iv, supports append, is branching:
        emit "int pbeginDj = pDj;"
        for lp in L:
          if iterator for each Dj in coiter-dims(lp) is unfused:
            emit "while(\!(pDj-1 < Dj_end) for Dj in cdims) {\"
              for Dj in coord-value-iteration-dims(lp):
                emit "int pDj, bool fDj = coord_access_Dj(pDj-1, ..., ivDj);"
                emit "while(\!(fDj && ivDj < Dj_end) {\"
                  emit "pDj = coord_access_Dj(pDj-1, ..., ivDj);"
                }
              }
              emit "for Dj in noncanonical-dims(lp):
                emit "int ivDj = Dj_scratch[ivDj];"
                emit "int pDj = Dj_scratch[ivDj];;\"
                emit "int iv = min(\!(ivDj) for Dj in canonical-coiter-dims(lp));\"
                emit "for Dj in locate-capable-dims(lp) \&\& \!
                emit "int pDj, bool fDj = locate_access_Dj(pDj-1, ..., ivDj);"
                emit "while(\!(fDj && ivDj < Dj_end) {\"
                  emit "pDj = locate_access_Dj(pDj, ..., ivDj-1);"
                }
              }
              emit "else if(\!(fDj) {\"
                emit "if\((\!)Dj supports append\) {\"
                  emit "append_edges_Dj(pDj-1, pbeginDj, pDj);\"
                }
              }
            }
          }
        }
      emit-available-expressions(index-expr, iv)
      if result dimension Dj indexed by iv, supports insert:
        emit "int available-expressions(index-expr, iv)
        emit all(\!(ivDj == iv) for Dj in cdims) && \!
        emit "int pDj = locate_access_Dj(pDj-1, ..., ivDj);"
        for child-iv in children-in-iteration-graph(iv):
          emit "code-gen(index-expr, child-iv)
          emit code-expressions(index-Lq, child-iv)
          emit compute-statements()\"
        if result dimension Dj indexed by iv and Dj-1 not branchless:
          emit "if Dj supports append: \"
            emit "append_edges_Dj(pDj-1, pDj - 1, pDj);"
          D1 := Dj-1 \# parent dimension in output hierarchy
          emit "insert[append].coord_Dj(pDj-1, ...);";
        if Dj supports append:
          emit "pDj++;"
        while Dj is branchless:
          if Dj supports append:
            emit "append_edges_Dj(pDj-1, pDj - 1, pDj);"
          D1 := Dj-1 \# parent dimension in output hierarchy
          emit "insert[append].coord_Dj(pDj-1, ...);";
          emit "pDj++;"
        emit \});\"
      for Dj in coiter-dims(lp):
        if Dj is not full:
          emit "if ivDj == iv \"
          if Dj in coord-value-iteration-dims(lp):
            emit "ivDj++;"
          else:
            emit "pDjDj = Dj_end;"
          emit \});\"
        if iterator for each Dj in coiter-dims(lp) is unfused:
          emit \});\"
        if result dimension Dj indexed by iv, supports append, is branching:
          emit "append_edges_Dj(pDj-1, pbeginDj, pDj);\"
      (a) Algorithm to generate tensor algebra code.
iterates over multiple coordinate hierarchy levels of one tensor. The algorithm implements this optimization by fusing iterators over branchless levels with iterators over their preceding levels. This is legal as long as the associated merges are intersections and the other merged levels can be accessed with the locate capability. The algorithm then avoids emitting loops for levels accessed by fused iterators (4), which eliminates unnecessary branching overhead. For some computations, however, this optimization transforms the emitted kernel from a gather code that enumerates each output nonzero once to a scatter code that accumulates into the output. In such cases, the algorithm ensures the output coordinate hierarchy levels can also be accessed with the locate capability.

5 EVALUATION

To evaluate our contributions, we compare code that our technique generates to five state-of-the-art sparse linear and tensor algebra libraries. We find that the sparse tensor algebra kernels our technique emits for many disparate formats have performance competitive with hand-implemented kernels, which shows we can get both performance and generality. We further find that generality in supported formats is crucial for achieving performance in real-world tensor algebra applications.

5.1 Experimental Setup

We implement our technique as an extension, called fmtaco, to the open-source taco tensor algebra compiler [Kjolstad et al. 2017]. We do not compare fmtaco directly to taco as our technique generates identical code for the tensor formats that taco supports. To evaluate formats not supported by taco, we compare fmtaco-generated code to five existing sparse linear and tensor algebra libraries: Intel MKL [Intel 2012], SciPy [Jones et al. 2001], MTL4 [Gottschling et al. 2007], the MATLAB Tensor Toolbox [Bader and Kolda 2007], and TensorFlow [Abadi et al. 2016]. Intel MKL is a C and Fortran math processing library that is heavily optimized for Intel processors. SciPy is a popular scientific computing library for Python. MTL4 is a C++ library that specializes linear algebra operations for fast execution using template metaprogramming. The Tensor Toolbox is a MATLAB library that implements many kernels and factorization algorithms for dense and sparse tensors of any order. TensorFlow is a machine learning library that supports some basic sparse tensor operations.

All experiments were run on a two-socket, 12-core/24-thread 2.4 GHz Intel Xeon E5-2695 v2 machine with 30 MB of L3 cache per socket and 128 GB of main memory, using GCC 5.4.0 and MATLAB 2016b. We ran each experiment multiple times with the cache cleared of input data before each run and report average execution times. All results are for single-threaded execution.

We ran our experiments with an array of real-world and synthetic tensors as input. Appendix B describes these tensors in more detail. The real-world tensors were obtained from the SuiteSparse Matrix Collection [Davis and Hu 2011] and the FROSTT Tensor Collection [Smith et al. 2017b]. We store tensor coordinates as integers and component values as double-precision floats, except for the Tensor Toolbox’s TTM and INNERPROD kernels. Those two kernels do not support integer coordinates, so we used double-precision floating-point coordinates.

5.2 Sparse Matrix Computations

Our technique generates high-performing tensor algebra kernels specialized to the layouts and attributes (e.g., sortedness) of the tensor operands. In this section, we compare the performance of fmtaco-generated kernels, which compute various operations on COO, CSR, DIA, and ELL matrices, with implementations in MKL, SciPy, MTL4, and TensorFlow.

Figure 10 shows results for sparse matrix-vector multiplication (SpMV). fmtaco is the only system that supports all the formats we examine; MTL4 does not support DIA, neither MKL nor SciPy supports ELL, and TensorFlow only supports COO. MKL and SciPy also only support struct of arrays (SoA) COO, shown in Figure 2f. TensorFlow, on the other hand, only supports array of
Fig. 10. Normalized execution time of SpMV ($y = Ax$) with matrix $A$ stored in several formats, using fmtaco and other libraries. Results are normalized to the fastest library for each matrix and format. COO-S and COO-A are the struct-of-arrays and array-of-structs COO variants. Unlabeled cells in gray indicate a library does not support that format. fmtaco is the only library that supports every tensor format.

Structs (AoS) COO, where a single idx array interleaves coordinates along different dimensions. By contrast, fmtaco supports both variants; supporting AoS COO requires a slight variant of the compressed and singleton level formats with modified pos_access functions.

Figures 11 and 12 show results for sparse matrix-dense matrix multiplication (SpDM) and matrix addition with sparse COO matrices. Figure 13 shows results for CSR matrix addition. The fmtaco system is again the only one that supports all operations. SciPy does not support COO SpDM, while MTL4 only supports SpDM with sorted COO matrices. Furthermore, only TensorFlow and fmtaco support computing COO matrix addition with a COO output, and TensorFlow does not support CSR matrix addition. These omissions highlight the advantage of a compiler approach such as ours that does not require every operation to be manually implemented.

Overall, the results show that our technique generates code that have performance competitive with existing libraries. For SpDM and sparse matrix addition, fmtaco-emitted code consistently have performance equal to or better than other libraries. For SpMV, fmtaco-emitted code outperform TensorFlow, perform similar to SciPy and MTL4, and is competitive with MKL on the whole. Even for DIA, fmtaco is only about 21% slower than MKL on average. These results are explained below.

5.2.1 COO Kernels. The code fmtaco generates to compute COO SpMV implements the same algorithm as SciPy and MKL, and they therefore have the same performance. MTL4 also implements this algorithm, but stores the result of the computation in a temporary that is subsequently copied to the output. This incurs additional cache misses for matrices with larger dimensions, such as webbase. TensorFlow, on the other hand, does not implement a COO SpMV kernel and the operation must be cast as an SpDM with a single-column matrix. It therefore incurs overhead because every input vector access requires a loop over its trivial column dimension.

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Fig. 11. Normalized execution time of COO SpDM ($A = BC$, where $B$ is in COO and $A$ and $C$ are dense matrices) with fmtaco and other libraries that support the operation, relative to fmtaco for each matrix.

Fig. 12. Normalized execution time of COO matrix addition ($A = B + C$, where all matrices are stored in the AoS COO format) with fmtaco and TensorFlow, relative to fmtaco for each matrix.

The COO matrix addition code that fmtaco emits is specialized to the order of the tensor operands. By contrast, TensorFlow has loops that iterate over the coordinates of each component. These loops let TensorFlow support tensors of any order but again introduces unnecessary overhead. TensorFlow’s sparse addition kernel is also hard-coded to work with 64-bit coordinates, whereas fmtaco can emit code with narrower-width coordinates. This reduces memory traffic.

5.2.2 CSR Kernels. fmtaco-generated code for CSR SpMV iterates over the rows of the input matrix and, for each row, computes its dot product with the input vector. SciPy and MTL4 implement the same algorithm and thus have similar performance as fmtaco, while MKL vectorizes the dot product. This, however, requires vectorizing the input vector gathers, which most SIMD architectures cannot handle very efficiently. Thus, while this optimization is beneficial with many of our test matrices (e.g., rma10), it is not always so (e.g., mac_econ).

The generated code for CSR matrix addition also uses the same algorithm as SciPy and MKL and thus has similar performance. The emitted code exploits the sortedness of the input matrices to enumerate result nonzeros in order. This lets it cheaply assemble the output idx array with appends. By contrast, MTL4 assigns one operand to a sparse temporary and then increments it by the other operand. This latter step can require significant data shuffling to keep coordinates stored in order within the sparse temporary. Finally, converting the temporary back to CSR incurs yet more overhead, leading to MTL4’s poor performance.

5.2.3 DIA and ELL SpMV. The code that fmtaco generates for DIA SpMV iterates over each matrix diagonal and, for each diagonal, accumulates the component-wise product of the diagonal and the input vector into the result. SciPy implements the same algorithm that fmtaco emits and has the same performance. MKL, by contrast, tiles the computation to maximize cache utilization and thus outperform both fmtaco and SciPy, particularly for large matrices with many diagonals. Future work includes generalizing our technique to support iteration space tiling.

Similarly, fmtaco generates code for ELL SpMV that iterates over matrix components in the order they are laid out in memory. MTL4, on the other hand, iterates over components row by row.
Table 3 shows the results of this experiment, with Intel MKL, SciPy, and MTL4 omitted as they do not support sparse higher-order tensor algebra. The Tensor Toolbox and TensorFlow are on different sides of the trade-off space for hand-written sparse tensor algebra libraries. The Tensor Toolbox supports all the operations we evaluate but has poor performances, while TensorFlow supports only one operation but has better performance. Our technique, on the other hand, generates efficient code for all five operations, demonstrating that generality and performance are not mutually exclusive.

As with sparse matrix addition, the code fmtaco generates for adding 3rd-order COO tensors has better performance than TensorFlow’s generic sparse tensor addition kernel. Furthermore, fmtaco generates code that significantly outperforms the Tensor Toolbox kernels, often by more than an order of magnitude. This is because the Tensor Toolbox relies on MATLAB functionalities that cannot directly operate on tensor indices or exploit tensor properties to optimize the computation. To add two sparse tensors, for instance, the Tensor Toolbox computes the set of nonzero output coordinates by calling a MATLAB built-in function that computes the union of the sets of input nonzero coordinates. MATLAB’s implementation of set union, however, cannot exploit the fact that the inputs are already individually sorted and must sort the concatenation of the two input indices. By contrast, fmtaco emits code that directly iterates over and merges the two input indices without first re-sorting them, which reduces the asymptotic complexity of the computation. Additionally, fmtaco emits code that directly assembles sparse output indices, whereas for computations such as TTM the Tensor Toolbox stores the results in intermediate dense structures.

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5.4 Benefits of Supporting Disparate Formats

taco’s support for tensor formats is limited to dense arrays and variants of CSR. For computations that work solely with those formats, fmtaco generates identical code as taco. However, depending on characteristics of the computation and the sparsity structure of the tensor operands, fmtaco’s support for more disparate formats enables it to outperform taco in practical applications.

The COO format, for instance, is the intuitive way to represent sparse tensors and is used by many file formats to encode sparse tensors. Thus, it is a natural format for importing and exporting sparse tensors into and out of an application. As the blue bars in Figure 14 show, however, computing matrix-vector products directly on COO matrices can take up to twice as much time as with CSR matrices due to increased memory traffic. If a matrix is imported into the application in COO though, then it must be converted to a CSR matrix before the more efficient CSR SpMV kernel can be used. This preprocessing step incurs significant overhead that, as the red bars in Figure 14 show, exceeds the cost of computing on the original COO matrix. The overhead can be amortized for iterative applications that repeatedly compute with the same matrix, making CSR SpMV important from a performance standpoint. For non-iterative applications, on the other hand, fmtaco’s COO SpMV offer better end-to-end performance than taco by eliminating format conversion overheads.

Which format is most performant also depends on the tensor’s sparsity structure. To show this, we compare the performance of SpMV computed on CSR and DIA matrices using fmtaco-generated kernels. For matrices like Lin and synth1 whose nonzeros are confined to a few densely-filled diagonals, storing them in DIA exposes opportunities for vectorization. As Figure 15 shows, fmtaco can exploit them to improve SpMV performance by up to 22% relative to taco, which only supports CSR SpMV. However, DIA SpMV performs significantly worse for matrices like rma10 whose nonzeros are spread amongst many sparsely-filled diagonals. This is because DIA SpMV has to compute with all the zeros in the nonempty diagonals, even though they do not affect the result.

We further compare the performance of CSR SpMV with input vectors stored as dense arrays, sparse vectors, and hash maps, for operands of varying density. Figure 16 shows the results. When the input vector contains mostly nonzeros, dense arrays are suitable for SpMV as they provide efficient random access without needing to explicitly store coordinates of nonzeros. Conversely, when the input vector contains mostly zeros and the matrix is much denser, sparse vectors offer better performance for SpMV as it can be computed without accessing all matrix nonzeros. However,
Fig. 16. Normalized execution time of fmtaco’s CSR SpMV with inputs of varying density and input vectors stored in different formats, relative to the most performant format for each configuration. Each cell shows results for dense arrays (top), sparse vectors (middle), and hash maps (bottom). Cells are highlighted based on which vector format is most performant (blue for dense arrays, green for sparse vectors, red for hash maps).

when the input vector is large and sparse but still denser than the matrix, computing SpMV with hash map vectors reduces the number of accesses that go out of cache. At the same time, the hash map format’s random access capability makes it possible to compute SpMV without accessing the full input vector. This would enable fmtaco, with its support for hash maps, to outperform taco, which only supports the dense array and sparse vector formats.

6 RELATED WORKS

Related work in this area can be roughly categorized into explorations of different sparse tensor formats (including sparse matrix and vector formats) and prior work on abstractions for sparse tensor storage and code generation for sparse tensor computations.

6.1 Sparse Tensor Formats

There is a large body of work on sparse matrix and higher-order tensor formats. Sparse matrix data structures were first introduced by Tinney and Walker [1967], who appear to have implemented the CSR data structure. McNamee [1971] described an early library that supports computations on sparse matrices stored in a compressed variant of CSR. The analogous CSC format is also commonly used partly because it is convenient for direct solves [Davis 2006]. Many other formats for storing sparse matrices and higher-order tensors have since been proposed; Section 2 describes them in detail. This work shows that all these tensor formats can be represented within the same framework with just six composable level formats that share a common interface.

Other proposed sparse tensor formats include BICRS [Yzelman and Bisseling 2012], which extends the CSR format to efficiently store nonzeros of a sparse matrix in Hilbert order. For efficiently computing SpMV on GPUs, Monakov et al. [2010] proposed sliced ELLPACK, which generalizes ELL by partitioning the matrix into strips of a fixed number of adjacent rows, with each strip possibly storing a different number of nonzeros per row so as to minimize the number of stored zeros. Liu et al. [2017] also proposed F-COO, which extends COO for enabling efficient computation of sparse higher-order tensor kernels on GPUs. Bell and Garland [2008] described the HYB format, which stores most components of a matrix in an ELL submatrix and the remaining components in another COO submatrix. The HYB format is useful for computing SpMV on vector architectures with matrices that contain similar numbers of nonzeros in most rows but have a few rows that
contain many more nonzeros. The Cocktail Format in clSpMV [Su and Keutzer 2012], generalizes HYB to support any number of submatrices stored in one of nine fixed sparse matrix formats.

### 6.2 Tensor Storage Abstractions and Code Generation

Researchers have also explored approaches to describing sparse vector and matrix storage for sparse linear algebra. Thibault et al. [1994] proposed a technique that describes regular geometric partitions in arrays and automatically generates corresponding indexing functions. The technique compresses matrices with regular structure, but does not generalize to unstructured matrices.

In the context of compilers for sparse linear and tensor algebra, Kjolstad et al. [2017] proposed a formulation for tensor formats that designates each dimension as either dense or sparse, which are stored using the same physical indices as dense and compressed level types in our abstraction. However, their formulation can only describe formats that are composed strictly of those two specific types of indices, which precludes their technique from generating tensor algebra kernels that compute on many other common formats like COO and DIA. The Bernoulli project [Kotlyar 1999; Kotlyar et al. 1997; Stodghill 1997], which adopted a relational database approach to sparse linear algebra compilation, proposed a black-box protocol with access paths that describe how matrices map to physical storage. The black-box protocol is similar to our level format interface, but they only address linear algebra and only computations involving multiplications and not additions. The black-box protocol also does not support on-the-fly assembly of sparse indices, which is often essential for applications with sparse high-order outputs. SIPR [Pugh and Shpeisman 1999], a framework that transforms dense linear algebra code to sparse code, represents sparse vectors and matrices with hard-coded element stores that provide enumerators and accessors that are analogous to level capabilities. The framework provides just two types of element store and cannot be readily extended to support new types of element store for representing other formats. Arnold et al. [2011; 2010] proposed LL, a verifiable functional language for sparse matrix programs in which a sparse matrix format is defined as some nesting of lists and pairs that encode components of a dense matrix. How an LL format should be interpreted is described as part of the computation in LL, so the same computation with different matrix formats can require completely different definitions.

Bik and Wijshoff [1993; 1994] developed an early compiler that transforms dense linear algebra code to equivalent sparse code by moving nonzero guards into sparse data structures. More recently, Venkat et al. [2015] proposed a technique for generating inspector/executor code that may, at runtime, transform input matrices from one format to another. Both techniques support a fixed set of standard sparse matrix formats and only generate code that work with matrices stored in those formats. Finally, Rong et al. [2016] proposed a technique that discovers and exploits invariant properties of matrices in a sparse linear algebra program to optimize the program as a whole.

Much work has also been done on compilers [Nelson et al. 2015; Spampinato and Püschel 2014] and loop transformation techniques [McKinley et al. 1996; Wolf and Lam 1991; Wolfe 1982] for dense linear algebra. An early effort for dense higher-order tensor algebra was the Tensor Contraction Engine [Auer et al. 2006]. libtensor [Epifanovsky et al. 2013], CTF [Solomonik et al. 2014], and GETT [Springer and Bientinesi 2016] are examples of systems and techniques that transform tensor contractions into dense matrix multiplications by transposing tensor operands. TBLIS [Matthews 2017] and InTensLi [Li et al. 2015] avoid explicit transpositions by computing tensor contractions in-place. All of these systems and techniques deal exclusively with tensors stored as dense arrays.

### 7 CONCLUSION

We have described and implemented a new technique for generating tensor algebra kernels that efficiently compute on tensors stored in disparate formats. Our technique’s modularity enables it to support a wide range of formats and to be readily extended to new formats without modifying the...
code generator. Such extensibility makes our technique practical for disparate domains that need to efficiently perform very different types of computations with very dissimilar data. Large-scale applications that need performance may also require multiple formats for different subcomputations, with each format optimized for characteristics of a subcomputation and its data. A technique like ours that shapes computation to data makes it possible to work with different formats without having to incur excessive data translation costs, thus optimizing whole-program performance.

Future work includes implementing new level formats that can be composed to support even more tensor formats. This can include custom formats designed to take advantage of power-law structures in social graphs for graph analytics or specialized hardware accelerator capabilities for deep learning architectures [Chen et al. 2017]. The code generation algorithm can also be extended to perform additional optimizations like iteration space tiling, as well as to specifically target accelerators (e.g., GPUs) and distributed memory systems. Our modular approach, which separates tensor formats from code generation, enables these lines of research to be pursued independently.

REFERENCES


Timothy A Davis. 2006. Direct methods for sparse linear systems. SIAM.


## IMPLEMENTATIONS OF ASSEMBLY CAPABILITIES

Table 4. Definitions of level functions that implement assembly capabilities for various level types.

<table>
<thead>
<tr>
<th>Level Type</th>
<th>Level Function Definitions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dense</td>
<td><strong>insert_coord(p_k, i_k):</strong> // do nothing</td>
</tr>
<tr>
<td></td>
<td><strong>insert_init(sz_k−1, sz_k):</strong> // do nothing</td>
</tr>
<tr>
<td></td>
<td><strong>size(sz_k−1):</strong></td>
</tr>
<tr>
<td></td>
<td>size(sz_k−1_max * N_k)</td>
</tr>
<tr>
<td></td>
<td><strong>insert_finalize(sz_k−1, sz_k):</strong> // do nothing</td>
</tr>
<tr>
<td>Compressed</td>
<td><strong>append_coord(p_k, i_k):</strong></td>
</tr>
<tr>
<td></td>
<td>idx[p_k] = i_k</td>
</tr>
<tr>
<td></td>
<td><strong>append_init(sz_k−1, sz_k):</strong></td>
</tr>
<tr>
<td></td>
<td>for (int p_k−1 = 0; p_k−1 &lt;= sz_k−1; ++p_k−1) { pos[p_k−1] = 0 }</td>
</tr>
<tr>
<td></td>
<td><strong>append_edges(p_k−1, pbegin_k, pend_k):</strong></td>
</tr>
<tr>
<td></td>
<td>pos[p_k−1 + 1] = pend_k - pbegin_k</td>
</tr>
<tr>
<td></td>
<td><strong>append_finalize(sz_k−1, sz_k):</strong></td>
</tr>
<tr>
<td></td>
<td>int cumsum = pos[0]</td>
</tr>
<tr>
<td></td>
<td>for (int p_k−1 = 1; p_k−1 &lt;= sz_k−1; ++p_k−1) {</td>
</tr>
<tr>
<td></td>
<td>cumsum += pos[p_k−1]</td>
</tr>
<tr>
<td></td>
<td>pos[p_k−1] = cumsum</td>
</tr>
<tr>
<td>Singleton</td>
<td><strong>append_coord(p_k, i_k):</strong></td>
</tr>
<tr>
<td></td>
<td>idx[p_k] = i_k</td>
</tr>
<tr>
<td></td>
<td><strong>append_init(sz_k−1, sz_k):</strong></td>
</tr>
<tr>
<td></td>
<td>// do nothing</td>
</tr>
<tr>
<td></td>
<td><strong>append_edges(p_k−1, pbegin_k, pend_k):</strong></td>
</tr>
<tr>
<td></td>
<td>// do nothing</td>
</tr>
<tr>
<td></td>
<td><strong>append_finalize(sz_k−1, sz_k):</strong></td>
</tr>
<tr>
<td></td>
<td>// do nothing</td>
</tr>
<tr>
<td>Hashed</td>
<td><strong>insert_coord(p_k, i_k):</strong></td>
</tr>
<tr>
<td></td>
<td>idx[p_k] = i_k</td>
</tr>
<tr>
<td></td>
<td><strong>insert_init(sz_k−1, sz_k):</strong></td>
</tr>
<tr>
<td></td>
<td>for (int p_k = 0; p_k &lt; sz_k; ++p_k) {</td>
</tr>
<tr>
<td></td>
<td>idx[p_k] = -1</td>
</tr>
<tr>
<td></td>
<td><strong>size(sz_k−1):</strong></td>
</tr>
<tr>
<td></td>
<td>return sz_k−1_max * W_k</td>
</tr>
<tr>
<td></td>
<td><strong>insert_finalize(sz_k−1, sz_k):</strong></td>
</tr>
<tr>
<td></td>
<td>// do nothing</td>
</tr>
</tbody>
</table>
## SUMMARY OF TEST TENSORS

Table 5. Summary of matrices and tensors used in experiments.

<table>
<thead>
<tr>
<th>Tensor</th>
<th>Domain</th>
<th>Dimensions</th>
<th>Nonzeros</th>
<th>Diagonals</th>
</tr>
</thead>
<tbody>
<tr>
<td>pdb1HYS</td>
<td>Protein database</td>
<td>36K × 36K</td>
<td>4,344,765</td>
<td>25,577</td>
</tr>
<tr>
<td>jnlbrng1</td>
<td>Optimization</td>
<td>40K × 40K</td>
<td>199,200</td>
<td>5</td>
</tr>
<tr>
<td>obstclae</td>
<td>Optimization</td>
<td>40K × 40K</td>
<td>197,608</td>
<td>5</td>
</tr>
<tr>
<td>chem</td>
<td>Chemical master equation</td>
<td>40K × 40K</td>
<td>201,201</td>
<td>5</td>
</tr>
<tr>
<td>rma10</td>
<td>3D CFD</td>
<td>46K × 46K</td>
<td>2,329,092</td>
<td>17,367</td>
</tr>
<tr>
<td>dixmaanl</td>
<td>Optimization</td>
<td>60K × 60K</td>
<td>299,998</td>
<td>7</td>
</tr>
<tr>
<td>cant</td>
<td>FEM/Cantilever</td>
<td>62K × 62K</td>
<td>4,007,383</td>
<td>99</td>
</tr>
<tr>
<td>consph</td>
<td>FEM/Spheres</td>
<td>83K × 83K</td>
<td>6,010,480</td>
<td>13,497</td>
</tr>
<tr>
<td>denormal</td>
<td>Counter-example problem</td>
<td>89K × 89K</td>
<td>1,156,224</td>
<td>13</td>
</tr>
<tr>
<td>Baumann</td>
<td>Chemical master equation</td>
<td>112K × 112K</td>
<td>748,331</td>
<td>7</td>
</tr>
<tr>
<td>cop20k_A</td>
<td>FEM/Accelerator</td>
<td>121K × 121K</td>
<td>2,624,331</td>
<td>221,205</td>
</tr>
<tr>
<td>shipsec1</td>
<td>FEM</td>
<td>141K × 141K</td>
<td>3,568,176</td>
<td>10,475</td>
</tr>
<tr>
<td>scircuit</td>
<td>Circuit</td>
<td>171K × 171K</td>
<td>958,936</td>
<td>159,419</td>
</tr>
<tr>
<td>mac_econ</td>
<td>Economics</td>
<td>207K × 207K</td>
<td>1,273,389</td>
<td>511</td>
</tr>
<tr>
<td>pwtk</td>
<td>Wind tunnel</td>
<td>218K × 218K</td>
<td>11,524,432</td>
<td>19,929</td>
</tr>
<tr>
<td>Lin</td>
<td>Structural problem</td>
<td>256K × 256K</td>
<td>1,766,400</td>
<td>7</td>
</tr>
<tr>
<td>synth1</td>
<td>Synthetic matrix</td>
<td>500K × 500K</td>
<td>1,999,996</td>
<td>4</td>
</tr>
<tr>
<td>synth2</td>
<td>Synthetic matrix</td>
<td>1M × 1M</td>
<td>1,999,999</td>
<td>2</td>
</tr>
<tr>
<td>ecology1</td>
<td>Animal movement</td>
<td>1M × 1M</td>
<td>4,996,000</td>
<td>5</td>
</tr>
<tr>
<td>webbase</td>
<td>Web connectivity</td>
<td>1M × 1M</td>
<td>3,105,536</td>
<td>564,259</td>
</tr>
<tr>
<td>atmosmodd</td>
<td>Atmospheric model</td>
<td>1.3M × 1.3M</td>
<td>8,814,880</td>
<td>7</td>
</tr>
<tr>
<td>Facebook</td>
<td>Social media</td>
<td>1.6K × 64K × 64K</td>
<td>737,934</td>
<td></td>
</tr>
<tr>
<td>NELL-2</td>
<td>Machine learning</td>
<td>12K × 9.2K × 29K</td>
<td>76,879,419</td>
<td></td>
</tr>
<tr>
<td>NELL-1</td>
<td>Machine learning</td>
<td>2.9M × 2.1M × 25M</td>
<td>143,599,552</td>
<td></td>
</tr>
</tbody>
</table>