# Extending HDF5 Datasets: Enhancements to the Chunk Indexing Methods

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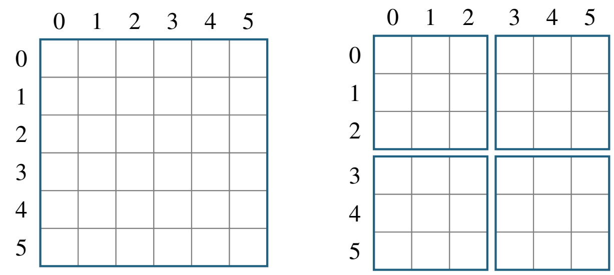
*Abstract*—**The HDF5 library requires the use of chunking when defining extendable datasets. Chunking makes it possible to extend datasets efficiently without having to reorganize contiguous storage excessively. However, to retrieve elements in the datasets that are stored in chunked form, the chunk containing those elements must be located and accessed. Therefore, the library must define and use efficient indexing methods for the retrieval of those chunks. We present in this paper the indexing methods that are being used, as well as some of the enhancements made to improve performance of these methods.**




**(a)** Contiguous. **(b)** Chunked.

Fig. 1: HDF5 dataset storage.

## I. Introduction

The HDF5 library [1] [2] provides users with a high degree of flexibility for data management—users may define and organize data into different groups and datasets and build an hierarchical tree of data. Datasets may be contiguously mapped from the application memory to a file, or stored in more complex patterns to ease further access and analysis of the data. One option that is commonly used is to create and define a dataset as *extendable*, in order to easily append new values to it. An HDF5 dataset is extendable when the maximum dimension sizes of its dataspace are greater than the current dimension sizes, the maximum dimension size being specified as *fixed* size or *unlimited* size.

When defining an extendable dataset, the HDF5 library requires the dataset to be partitioned into fixed-size multi-dimensional chunks—this operation, illustrated in figure 1, is called *chunking*. Chunking makes it possible to extend datasets efficiently without having to reorganize contiguous storage excessively. To retrieve elements in the datasets that are stored in chunked form, the chunk containing those elements must be located and accessed. Several structures can be used to achieve that and the locations of chunks for a dataset have originally been stored in a B-tree data structure, which maps the index of the chunk to the file offset where the chunk's elements are stored. However, depending on the use case and in particular for extendable datasets, the B-tree structure used presents some drawbacks, which are addressed in this paper.

This paper is organized as follows. Section II presents the current indexing method used within the library for chunking as well as modifications that were made to improve performance when a dataset is being extended. Section III presents performance evaluation results. In Section IV we discuss related work before presenting conclusions and future research directions in Section V.

## II. Architecture

Chunking is a technique used in the HDF5 library in various cases: to optimize I/O to disk [3], to compress data [1], to extend datasets. To retrieve elements in the datasets that are stored in chunked form, the chunk containing those elements must be located and accessed. The HDF5 library's default data structure for indexing chunks is based on a B-tree data structure, which maps the index of the chunk to the file offset where the chunk's elements are stored.

### A. B-Trees

B-trees are generally used for indexing data blocks and one of the main components of file systems [4] [5]. Insertion of a new entry and lookup is realized in $O(\log_b n)$, where $n$ is the number of nodes and $b$ the order of the tree. In the case of HDF5 datasets and in the original B-tree structure, referred to as *B-Tree version 1* (BT1), the record for locating the chunk stores the following information:

- The coordinates of the chunk in the dataset's dataspace. This is used as the key for locating chunks in the B-tree.
- The size of the chunk, in bytes.
- The address of the chunk in the file.
- Additional metadata.

As shown in figure 2, each leaf points to the address of a chunk. When a dataset is extended, a new entry is added, which may generate a node split if the node where the record needs to be inserted is full. It is worth noting that most chunked datasets are either fixed dimension or extend in only one dimension. Very few users take advantage of the ability to extend multiple dimensions of a dataset. Because HDF5 datasets only allow their dimensions to be increased or decreased at their upper bound, a B-tree used to index chunks for a 1-D dataset will

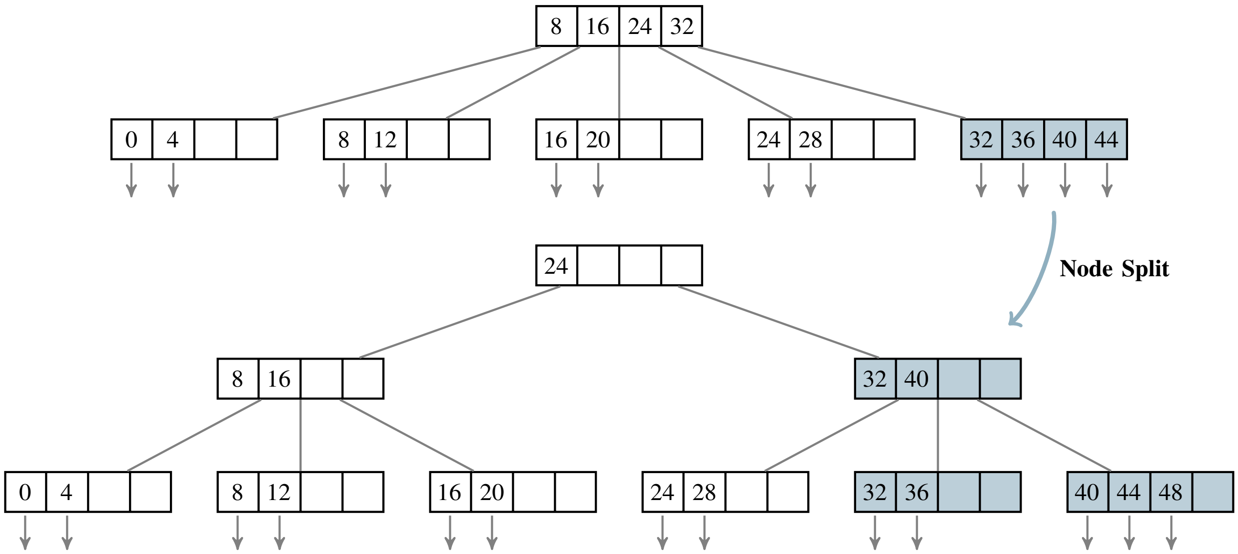



Fig. 2: Simplified version of original B-tree structure used for indexing chunks. In the case of extendable datasets, whenever a new chunk is added to the B-tree, its right-most node, if full, is split and a new half empty node is created.

only ever insert or remove records from its right-most node. One of the problems is that inserting/removing only from the right-most node lets most records half empty, as illustrated in figure 2.

To fix that issue, one of the main improvements made with a new version of the B-tree structure used, referred to as *B-tree version 2* (BT2), is to re-balance the entries so that nodes that were half-empty in version 1 are now full. Additionally, to improve traversal of the tree and easily find the chunks, the B-tree is counted so that alongside every link to a subtree, the number of subtree elements is stored.

Some additional modifications are made to the BT2 to improve performance:

1) When appending to a dataset, the library will insert a new record to the B-tree. To determine that the record to be inserted is not in the tree, the library traverses the corresponding tree nodes and compares the records in each node before the insertion. To accelerate the search, the maximum and minimum records in the tree are determined and stored in the B-tree header. The library can then quickly determine that the new record to be inserted is not in the tree if it is greater than the maximum record or less than the minimum record.
2) The default B-tree node size is $512$, which leads to a greater tree depth than version 1 for the append test scenario. This contributes to a lower performance because the traversal time is increased. The node size for the tree is therefore modified to $2048$, which will flatten the tree with a tree depth that is the same as the BT1.

### *B. Extensible Arrays*

While the version 2 of the B-tree previously mentioned provides a better balancing of the records in the tree, using it in the 1-D case (or for datasets with only one unlimited dimension) still only ever inserts or removes records from the right-most node. This negates most of the advantage of using a complicated data structure like a B-tree to index the chunks. Additionally, for applications, which wish to rapidly append records to the dataset, having to traverse and/or update multiple B-tree nodes for each record insertion imposes an additional performance penalty. This is especially a drawback when splitting one or more B-tree nodes is required to accommodate new record for a chunk.

For this particular case, indexing chunks requires a more appropriate data structure, referred to as *extensible array* (EA), and shown in figure 3. This structure can be seen as a dynamic array structure. Brodnik et al's paper [6] addresses this exact problem, showing how to implement a dynamic array with $O(1)$ append, shrink and lookup operations, along with optimal metadata overhead for indexing the array elements. For indexing chunks in HDF5 datasets, the array elements in the data blocks are pointers to the chunks on disk. As mentioned in [6], the resizable array *super blocks* are not actually constructs in the data structure, they are just shown to conceptually group the data blocks that the index block points to. The super blocks help show the pattern of changes to the data blocks: first the size of the data block doubles, then the number of data blocks of that size doubles, then the size doubles again, then the number of data blocks of that size doubles, etc.

A couple of things should be noted about the data structure in figure 3:

1) The super blocks for the first two data blocks are omitted and the pointers in the index block point directly to the data blocks.
2) Constant time (i.e., $O(1)$) lookup, append and shrink are still in effect. The number of I/O accesses to find any chunk address is always 2 or 3: index block $\rightarrow$ super

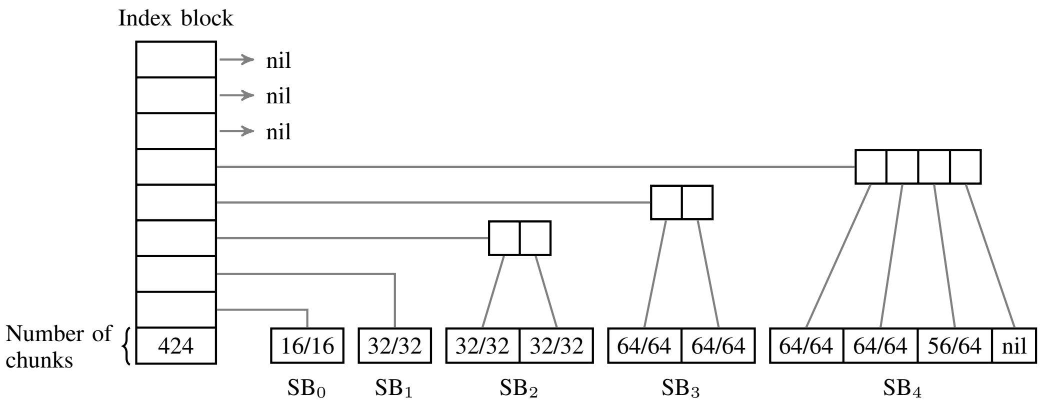



Fig. 3: Simplified version of extensible array structure used for indexing chunks.

block → data block. In actual operation, the index block will certainly be *hot* enough to stay in the HDF5 metadata cache, along with many/most of the super blocks, making the average number of I/O accesses to retrieve a chunk address between 1 and 2, in all likelihood.

3) Super blocks/data blocks, which are not yet needed, are not allocated and have a *nil* pointer in the index block/super block (respectively) that refers to them.
4) The height of the index block is constant and its height can be computed at creation so that resizing it is unnecessary. This can be done by computing the maximum number of chunks possible for the file's address range (typically 64-bits) and deriving the maximum number of data/index blocks needed to index that many blocks. For example, if there are 16 chunks in the initial data block, a chunk size of 2048 (with a single unlimited dimension), and a 4-byte (integer) data element size, the maximum height of the index block needed to store $1.84 \times 10^{19}$ bytes of elements (which is the maximum offset possible in a 64-bit file) is 47.

### C. Additional Optimization

When the dataset is extended and its rank is greater than one, the library scans and updates each entry in the chunk cache, due to the modified dataspace. Each entry is hashed based on a chunk index, which varies according to the dataset dimension sizes. When the dimension sizes are modified, the library re-calculates each entry's chunk index and updates the cache accordingly. The re-calculation is expensive and the update time increases as the number of entries is increased in the cache.

Two modifications are made to the chunk layer to improve performance:

1) Save the component in the chunk index calculation after initial computation so that it can be later used when updating the chunk cache.
2) Use a different formula to hash chunk entries into the cache that do not depend on the chunk index. The new formula is based on the $\log_2$ function for the faster changing dimension sizes, thus reduces the number of chunk cache updates due to consecutive dataset extension operations.

### D. Summary

With these data structures in place, when the chunked dataset has only one unlimited maximum dimension, the extensible array indexing method is used, allowing chunk access in $O(1)$ time. When it has more than one unlimited maximum dimension sizes, the B-tree version 2 indexing method is used, allowing chunk access in $O(\log_b n)$, with $b$ the order of the tree and $n$ the number of nodes.

## III. Evaluation

To evaluate the performance of these new methods, we first consider the extension of datasets so that 1-byte chunks are appended, up to $2,500,000$ bytes. Note that the default storage for chunked datasets is still the default B-tree indexing (BT1). In order to retain as much forward compatibility as possible, all the improvements made are only used when the `H5F_LIBVER_LATEST` value is used as the *high bound* to the call to `H5Pset_libver_bounds`.

### A. Test Scenarios

We consider multiple scenarios, which are defined in settings 1, 2 and 3.

*a) Setting 1:* creates a 1-dimensional chunked dataset with the following dataspace:

```
curr[0] = 0;
max[0] = H5S_UNLIMITED;
sid = H5Screate_simple(1, curr, max);
```

This compares the BT1 and EA indexing methods, when appending to the dataset created with the old and new library format respectively.

*b) Setting 2:* creates a 2-dimensional chunked dataset with the following dataspace, which has one unlimited dimension:

```
curr[0] = 0;
curr[1] = 1;
max[0] = H5S_UNLIMITED;
max[1] = 1;
sid = H5Screate_simple(2, curr, max);
```

TABLE I: Result for all three test settings before optimization.

| Indexing Method | Time (s) | |
|---|---|---|
| *Along the X-direction* | | |
| EA | 149.82 | $\simeq -4\%$ |
| BT1 | 156.15 | |
| BT2 | 166.56 | $\simeq +7\%$ |
| *Along the Y-direction* | | |
| EA | 150.08 | $\simeq -8\%$ |
| BT1 | 163.82 | |
| BT2 | 167.91 | $\simeq +2\%$ |
| *Along the XY-direction* | | |
| EA | – | |
| BT1 | 104.08 | |
| BT2 | 114.39 | $\simeq +10\%$ |

TABLE II: Result for all three test settings after optimization.

| Indexing Method | Time (s) | |
|---|---|---|
| *Along the X-direction* | | |
| EA | 27.54 | $\simeq -19\%$ |
| BT1 | 34.01 | |
| BT2 | 31.59 | $\simeq -7\%$ |
| *Along the Y-direction* | | |
| EA | 29.24 | $\simeq -32\%$ |
| BT1 | 42.97 | |
| BT2 | 33.72 | $\simeq -22\%$ |
| *Along the XY-direction* | | |
| EA | – | |
| BT1 | 35.46 | |
| BT2 | 32.92 | $\simeq -7\%$ |

This compares the BT1 and EA indexing methods when appending to the dataset created with the old and the new library format respectively. Append operations are done along the X or Y directions.

*c) Setting 3:* creates 2-dimensional chunked datasets with the following dataspace, which has two unlimited dimensions:

```
curr[0] = 0;
curr[1] = 1;
max[0] = H5S_UNLIMITED;
max[1] = H5S_UNLIMITED;
sid = H5Screate_simple(2, curr, max);
```

This compares the BT1 and BT2 indexing methods when appending to the datasets created with the old and new library format respectively. Append operations are done along the X and/or Y directions.

### B. Preliminary Results

First, measures are realized on the library before optimization. The quantify tool is used to collect the time in seconds spent in the library code from the test runs. The result listed in table I indicates that the EA indexing method performs better than BT1, while the BT2 indexing method performs worse than BT1. Note also that the library takes a fair amount of time for all three indexing methods.

### C. Results

Measures are realized after optimization. The new results shown in table II indicate that after optimization BT2 performs better than BT1. General chunk index fixes have made a significant improvement for all three indexing methods—almost 80%.

As one can see in figure 4, for significant numbers of chunks, the BT2 and EA indexing methods perform better than BT1. EA shows good scalability and a much better performance than BT1/BT2 as the number of chunks increases. BT2 generally shows better performance than BT1 (it is also worth noting than even if this is not shown in this result, the amount of space taken by BT2 is reduced). Overall these results confirm the optimization made within the library and were what we expected given the complexity of the methods used.

## IV. Related Work

Nimako et al. [7] consider another data structure for indexing chunks, the $O_2$-Tree, which performs query operations (searches) in $O(\log_2 n)$ time, where $n$ is the number of internal nodes. They mention that the conventional arrays and HDF5 incur the cost of reorganizing already allocated array elements. Based on these results and the new optimization made, it would be interesting to make a new comparison. The $O_2$-Tree may perform better than a B-Tree data structure but the re-sizable array data structure will still perform better in the 1-unlimited dimension case, as its complexity is in $O(1)$.

[Other related work?]

## V. Conclusion and Future Work

[Conclusion / need to talk about it]

## Acknowledgments

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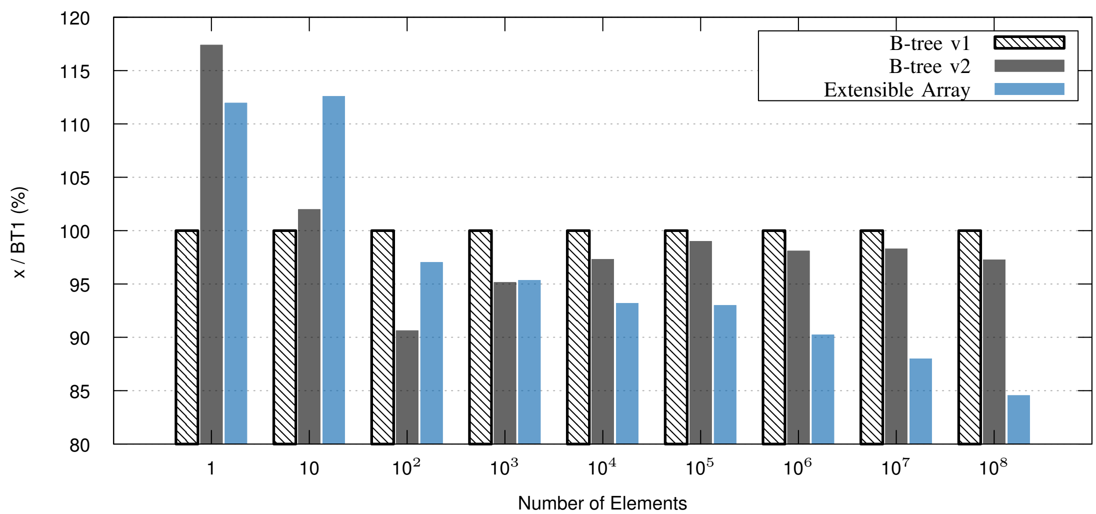

Fig. 4: Performance of BT2 and EA chunk indexing methods compared to BT1. The extensible array method shows good scaling performance, while the B-Tree version 2 shows improved results compared to BT1.