Reimplementing the Hierarchical Data System using HDF5

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Abstract

The Starlink Hierarchical Data System has been a very successful niche astronomy file format and library for over 30 years. Development of the library was frozen ten years ago when funding for Starlink was stopped and almost no-one remains who understands the implementation details. To ensure the long-term sustainability of the Starlink application software and to make the extensible N-Dimensional Data Format accessible to a broader range of users, we propose to re-implement the HDS library application interface as a layer on top of the Hierarchical Data Format version 5. We present an overview of the new implementation of version 5 of the HDS file format and describe differences between the expectations of the HDS and HDF5 library interfaces. We finish by comparing the old and new HDS implementations by looking at a comparison of file sizes and by comparing performance benchmarks.

Keywords: data formats, Starlink,

1. Introduction

The Hierarchical Data System (HDS) was created by the Starlink Project in the United Kingdom in the early 1980s (Disney and Wallace, 1982; Lawden, 1991). The requirements were to have a file format that was optimized for data processing applications: allowing for efficient access of data arrays through memory mapping, grouping of related data structures in a hierarchy to make it easy to move data en masse from one location to another, and easy modification of data and structures. At the time FITS (Wells et al., 1981) was mainly thought of as a transport format distributed on tape (Greisen et al., 1980), and the NCSA Hierarchical Data Format would not be developed until the end of the decade (Folk, 2010; Krauskopf and Paulsen, 1988). It was therefore decided to develop a new file format from scratch. Initially called the Starlink Data System before being rebranded as HDS, the first version of the library was written in BLISS-32 before being ported to C on VAX/VMS in the late 1980s (Lupton, 1989).

HDS succeeded in its goal of forming the basis of the Starlink data reduction software packages (ascl:1110.012) and was and is being used at UK observatories for data acquisition and for data reduction pipelines (Bell et al., 2014; Jenness and Economou, 2011; Jenness and Economou, 2015). Its presence was pervasive within the Starlink software stack, being used for parameter storage in the ADAM system (Allan, 1992) and in a graphics database system (Eaton and McIlwrath, 2014) in addition to storing astronomy data and forming the basis of the Starlink V-Dimensional Data Format library (NDF; Jenness et al., 2015, ascl:1411.023). There was very little take up of the format outside the UK community (but see e.g., Meyerdierks, 1993) and as FITS came to be used as a data processing format as well as a transport and archive format, HDS has become a niche product.

HDF5 is a popular file format in other scientific disciplines and is used in fields such as Earth science (e.g., Yang et al., 2005), biology (e.g., Dougherty et al., 2009), nuclear physics (e.g., Pedersen et al., 2013), and molecular simulations (e.g., de Buyl et al., 2014). The astronomy community is currently discussing the wider issues of file formats beyond FITS (Mink et al., 2015; Thomas et al., 2015) and HDF5 is being adopted (e.g., Alexov et al., 2012) or investigated (e.g., Price et al., 2015; Schaaf et al., 2015) in a number of astronomy projects.

Given this context it is therefore worth investigating whether there should be a new version of HDS that is based on HDF5. In this paper we compare the HDS and HDF5 data models, discuss the motivations for such a change, and describe an implementation.

2. Motivation

There are a number of key motivators for migrating from the current HDS format to a more widely-recognized format:

1. Opaque implementation details of the library and format with no resident expert or associated documentation.
2. Lack of support for 64-bit dimensions sizing.
3. HDS has no provision for transparent data compression.
4. HDS has no native support for tables.
5. Sociological impediment to adopting a niche format in the wider astronomy community.

We will discuss each of these in turn.

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2.1. Opaque implementation

The Starlink Project was closed in 2005 after 25 years of operation. The Starlink Software Collection continues to be developed as an open-source project sponsored by the Joint Astronomy Centre to continue support for their data reduction pipelines. Unfortunately none of the remaining developers understand the implementation details and there is no incentive for anyone to learn given other development priorities. The most recent description of the internals of the HDS file format is in Lupton (1989) which documents version 2 of the format. Version 3 (from the port to Unix in 1991) and version 4 (in 2005 to support files larger than 2GB) remain undocumented, outside of extensive comments in the code itself, with an assumption that the design closely matches the original layout. For a data format that is used as an archive format (see e.g., Economou et al., 2015) this lack of documentation and understanding represents a risk for long-term access to the data.

2.2. 64-bit dimension sizes

The HDS library does not currently support 64-bit dimension sizes. This was partially implemented for version 4 of the format but was never completed. It is not clear how much work it would be to finish this work or whether anyone remaining can do so. As data rates increase it is clear that the next generation of heterodyne arrays (e.g., Jenness et al., 2014) will generate data cubes that exceed the capacity of a 32-bit integer counter and these files will render the Starlink software and associated data pipelines unusable without HDS being upgraded. Adding 64-bit support to HDS is a necessary but not sufficient step towards the applications supporting larger datasets, and most libraries and applications in Starlink will need to be updated to support 64-bit counters. HDS is the fundamental building block that has to be converted first, providing new APIs to allow both 32-bit and 64-bit application code to co-exist.

2.3. Data Compression

HDF5 supports transparent data compression of datasets using a number of algorithms in addition to supporting a pluggable architecture. HDS does not support any data compression and relies on the facilities of the NDF library to provide these. NDF can support gzipped data files, requiring a temporary file, as well as FITS-style BSCALE/BZERO and a delta compression scheme natively. Leveraging the HDF5 compression algorithms would be a very easy way to improve the data compression performance in NDF.

2.4. Native Tables

Unlike FITS (Harten et al., 1988) or HDF5, HDS does not have a native table data structure. Tables must be implemented as a collection of independent columns and this can be extremely inefficient for row access. Switching data formats would make it possible to add a native table access API to HDS.

2.5. Sociology

One of the impediments to adoption of the NDF data model is that the reference library implementation uses HDS as the underlying file format. Whilst the NDF data model itself does not require HDS and could be implemented by anyone with sufficient effort available, to adopt NDF currently requires that users adopt HDS. Adopting HDF5 would considerably lower the barrier to entry for people more comfortable in the HDF5 world or who are considering switching from another format, and make data files accessible to tools such as HDFview and h5py. Of course, none of these tools will understand the NDF data model that defines the hierarchical grouping but it makes it easier for other tools to adopt some of the same conventions. Similarly, the Starlink file format conversion tools (Currie et al., 1996) would be able to import formats such as FITS to HDF5 and this infrastructure may prove to be useful for people who are themselves switching to HDF5.

3. Features of HDS

How HDS is used depends on a data model and the data access model. Both of these are important when considering a change in implementation.

3.1. Data Model

HDS is a hierarchical file format where named structures can contain other named structures or named primitive data arrays. It is self-describing in the sense that each layer in the hierarchy can be queried to obtain the number of members below (for structures), their names and their types.

The primitive objects support numerical and string types with up to 7 dimensions. The supported data types are shown in Table 1 and the choice and names reflect the origins of the format as a library designed to be used from Fortran.

All HDS components are typed and this includes structures. Structure typing is important in HDS as it can be used by an application to decide whether a structure can be understood or not. In object-oriented nomenclature the type can be thought of as the object class, whereas the individual named structure is an object instance.

HDS supports the concept of arrays of structures to allow a collection of identical structures to be grouped together. This is used extensively in the lower-levels of the Starlink software stack, for example to support history recording (an array of structures of type HISTORY which is extended each time a new history record is created), or picture definitions in the graphics database.

3.2. Data Access Model

To obtain access to an object within an HDS file the caller must obtain a locator; an opaque C struct containing information about the object needed by the HDS library. These locators mediate all access to the HDS data file.

Component copying. As a consequence of the hierarchical design, it is possible to copy or move arbitrary parts of the tree to other locations within a file or locations in different files.
Table 1: HDS basic data types. The unsigned types did not correspond to standard Fortran 77 data types and were included for compatibility with astronomy instrumentation. HDS supports both VAX and IEEE floating-point formats. The API code indicates the letter appended to function names to indicate the type they support. For compatibility with HDS the _LOGICAL type is a 32-bit bitfield type in memory but stored in an HDF5 file using 8 bits. HDS strings are always stored in Fortran space-padded form and that convention is adopted in the HDF5 HDS implementation.

| Name of type | API Code | Data type       | HDF5 Data type |
|--------------|----------|-----------------|----------------|
| _BYTE        | b        | Signed 8-bit integer | H5T_NATIVE_INT8 |
| _UBYTE       | ub       | Unsigned 8-bit integer | H5T_NATIVE_UINT8 |
| _WORD        | w        | Signed 16-bit integer | H5T_NATIVE_UINT16 |
| _UWORD       | uw       | Unsigned 16-bit integer | H5T_NATIVE_UINT16 |
| _INTEGER     | i        | Signed 32-bit integer | H5T_NATIVE_INT32 |
| _INT64       | k        | Signed 64-bit integer | H5T_NATIVE_INT64 |
| _LOGICAL     | l        | Boolean          | H5T_NATIVE_B8   |
| _REAL        | r        | 32-bit float     | H5T_NATIVE_FLOAT |
| _DOUBLE      | d        | 64-bit float     | H5T_NATIVE_DOUBLE |
| _CHAR[∗n]    | c        | String of 8-bit characters | H5T_STRING     |

Primary and secondary locators. The library has a concept of primary and secondary locators such that when all primary locators associated with a file are freed (or annulled in HDS parlance) all resources associated with that file are also closed and all secondary locators become inactive.

Locator Groups. It is possible to assign locators to a named group. Any child locators are also members of the group. When the group is no longer required it can be flushed with a single command, freeing all the locators that are in the group. This simplifies the management of large numbers of related locators and allows the resources to be freed at one place in the code without having to store them all in user code.

Slicing. Arrays of structures can not be accessed directly but must instead be accessed by requesting a specific cell. Primitive data arrays can also be accessed by individual cells but it is more common to access data arrays by specifying slices. A slice can be requested by specifying upper and lower bounds of each dimension. The Fortran heritage requires that these bounds are indexed starting with a lower bound of 1 rather than 0, and all data arrays are specified in Fortran order; even from the C interface. In some cases the dimensionality is unimportant and the library allows a locator to be vectorized such that subsequent interrogations of the locator will indicate that the object is 1-dimensional regardless of the underlying shape. This can be very useful for such activities as examining every element in turn, or picking the first few elements. Vectorizing works for structures and primitives and does not affect the file itself.

Automatic type conversion. For primitive arrays, the data to be stored or the data to be retrieved do not have to be the same type as the format of the data stored on disk. Floating point data will be converted to integer and vice versa. Also, string and logical/boolean types will be converted to numbers and numbers can be retrieved as strings or logicals. Endianness and floating point representation is also handled transparently, and the native form is used when a file is created.

Memory Mapping. One of the initial requirements for HDS was efficient access to data arrays. This was done using direct mapping of the relevant part of the file into memory¹ and was implemented for read and write operations. The memory mapping facility can be enabled or disabled by use of an environment variable and an in-memory solution is used on systems that do not support memory mapping.

4. Requirements for an Updated Format

The Starlink software collection consists of more than 2.3 million lines of Fortran, C and C++ and a large fraction of that code depends on the HDS library and the HDS API. This includes fundamental infrastructure such as ADAM that is used by all applications. It is therefore imperative that the API for HDS remains the same even with the implementation changing underneath. Any new version of HDS should meet the following requirements:

1. The API should not change.
2. It should be possible to use both old and new format files in the same application.
3. The application should behave in the same way with new files as it does with old files.
4. The application source code should not need to be modified in any way to use the new library.
5. The new format should not impact performance of the application in a negative way or require more computer resources.

These are similar to the requirements described when NetCDF version 4 was implemented on top of HDF5 (Rew and Hartnett, 2004).

¹Using mmap() on POSIX systems
5. HDS Version 5

Given the broad adoption of HDF5 in the scientific community and the close similarity in key parts of the data model between it and HDS, it was decided to write a prototype implementation of the HDS API in terms of HDF5. This would provide information on the feasibility of the approach and also highlight the areas where the data models or access models diverge. The previous version of HDS was version 4 so it was decided this version would be version 5. In the rest of this paper we use the shorthand HDSv5 to refer to the new library implementation and format, and HDSv4 to refer to the current version of the HDS format and library.

5.1. Library Architecture

In order to support both new and old file formats it was necessary for the new library to have access to a complete copy of the existing library. The HDF5-based library and the HDSv4 library are both standalone libraries that are linked into a wrapper library that implements the public interface (see Fig. 1). The versioned libraries can be configured to provide the public API but when used as part of the unified wrapper they are built with names that include the version number to avoid symbol clashes.

The wrapper library is responsible for forwarding the calls to the correct underlying library. There are four major API styles that must be handled: functions that open files and return locators, functions that create files, functions that copy from one locator to another, and functions that work with a single locator.

When a request is made to open a new file, it is first sent to the HDSv4 library to see if it opens. If that fails due to the format being invalid, the HDSv5 library is used to open the file. When migration to the new format is substantially complete the wrapper will be modified to default to using the HDSv5 library first. One caveat is that the library must ensure that HDSv5 files are written to disk immediately on creation such that the HDF5 superblock signature is written. Without this step H5Fis would not correctly determine that a newly created file is an HDF5 file if it has not yet been closed and some Starlink applications and libraries rely on the ability to create an HDS file and then open it in another part of the code without having annulled all previous locators beforehand.

When files are to be created the choice of format is controlled by a tuning parameter. Tuning parameters in HDS can be set programmatically or by reading the environment. By default, files are still created in HDSv4 format using the principle of least surprise. The ability to control this behavior from an environment variable simplifies testing and benchmarking.

When copying one locator to another locator of a different type, tree-walking code had to be written using the HDS public API. The code recursively walks through structures copying primitives and other structures as required.

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3 Somewhat confusingly the library implementing version 4 of the file format is itself version 5.

3 Calling H5Fflush in hdsNew

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Figure 1: Architecture of the HDF5-based implementation of HDS. A wrapper library with the public HDS API forwards calls to the correct version of the library. The Fortran interface is a separate library as it also contains Fortran code that would require a Fortran runtime library.

The bulk of the API takes a single locator as input and does something with it that may or may not result in a new locator being created. We have taken a slightly different approach to that described in Rew and Hartnett (2004). In that paper they registered function table lookups with the newly created data objects, allowing efficient forwarding to the particular library. We decided to take a simpler approach whereby the locator structures in HDSv4 and HDSv5 were adjusted so that they both included a version integer as the first member. The wrapper code then simply checks for the version number in the structure and calls the relevant routine. This approach does simplify the addition of debugging messages and error reporting from each routine at the expense of some calling efficiency.

The wrapper code responsible for this forwarding is generated from the public HDS header file using a simple Python program. This allows the forwarding scheme to be changed rel-
5.2. The Locator Interface

As mentioned previously, a locator is an opaque C struct containing information about a particular object in the HDS file. The size of these structures differs between the two implementations and this required that a change be made to the Fortran interface of the HDS library. For historical reasons an HDS locator is stored in a Fortran character array with a length specified by the HDS constant _SZL0C (currently 16 characters). In HDSv4 the C structure is a proxy for an internal data structure and the Fortran interface copied the contents of the structure to and from the Fortran string. In HDSv5, the C structure is significantly larger and it was unreasonable to increase the Fortran locator size. To support both implementations the Fortran interface was changed such that the structure address was stored in the Fortran string buffer and the size of the string was kept at 16 characters. This allowed the new library to be installed without requiring that any applications be relinked.

5.3. Error handling

HDS uses the Starlink Error Message Service (EMS; Rees et al., 2008) for error handling. EMS uses the concept of inherited status where each function takes a status argument and usually returns immediately if status is non-zero (when resources are to be freed it is usual for the freeing routine to try to execute regardless). If an error condition is to be reported by a function it sets the status to an appropriate value and attaches an error message to the message stack. As the call stack unwinds the error could either be annulled (the calling function may wish to react to the error by trying an alternative) or be augmented with more information.

HDF5 uses a similar error message stack and status code concept internally but uses a function return value to indicate to the external user that a problem has occurred. If the return value is negative the call failed. The error messages and specific status code must then be retrieved separately. In HDSv5 each call to HDF5 is wrapped by a C macro that intercepts the status return value and if necessary queries the HDF5 error message stack and places each of the messages on to the EMS message stack.

In some cases the HDF5 status code is translated to an equivalent HDS error code but in many cases the HDF5 codes are not specific enough and in that case a generic error from HDF5 code is used.

5.4. Data Model

In HDF5, structures are known as groups and primitives are known as datasets. Table 1 shows the mapping of HDS data types to the HDF5 equivalents and the type system is significantly more advanced in HDF5. It was decided that boolean types should be represented in the files as 8-bit bitfields rather than the 32-bit integer type that is used (part of the Fortran legacy). The in-memory datatype is a 32-bit integer for consistency with the public API but the smaller type is used on disk. A bitfield type is used as this allows the HDS type query to be able to distinguish the _BYTE type from _LOGICAL type without requiring the use of HDF5 attributes. Strings in HDS are space-padded fixed size following the Fortran style and this is how strings are stored in HDF5v5. Datasets are stored in HDF5 files in C dimension order with the dimensions being reversed when viewed from HDS. This is the same approach taken by the HDF5 Fortran interface with the variation that the HDS C view of an array must agree with Fortran.

HDF5 has no concept of arrays of structures so this facility is implemented entirely by the HDSv5 library. The containing group is created and within it are placed the number of groups corresponding to the array size. Each of these groups is given a name that contains a root string chosen to deliberately be longer than the maximum allowed length of an HDS component, appended with the coordinates of the structure in the array. For a 2-dimensional array of structures the name of the group could be ARRAY_OF_STRUCTURES_CELL(2,3) for the group at coordinate (2,3). This naming scheme simplifies access to an individual structure (just provide the coordinates) and also simplifies reporting of the full path using HDS nomenclature: to convert the HDF5 path of the structure ROOT/HISTORY/ARRAY_OF_STRUCTURES_CELL(2,3) to the HDS path, just requires the removal of the fixed cell prefix to convert it to ROOT.HISTORY(3)4. The long structure name is hidden by the HDS library and only visible when the file is accessed using HDF5 tools. When an array of structures has been created the dimensionality is stored in an attribute named HDS_STRUCTURE_DIMS. In the future we will consider implementing structure arrays using the HDF5 feature allowing references to arbitrary HDF5 objects to be stored in a dataset, this would have the advantage of reducing the structure complexity and would simplify cell access.

Finally, the data type of a structure is not a fundamental part of HDF5 so this information is stored in an attribute with name CLASS following the convention used in other HDF5 data models such as the Image and Palette classes.

Fig. 2 shows a comparison of the HDS and HDF5 view of the same data file. These traces show that the mapping from HDS structure/primitive to HDF5 group/dataset is being followed with three attributes added to provide the metadata required by HDS.

5.5. Primary locators

In HDF5 the file is kept open until all identifiers associated with a file are closed. HDS distinguishes primary identifiers from secondary identifiers such that a file is closed when the count of active primary locators reaches zero, even if some active secondary locators remain. To implement this in HDSv5 it is necessary to store every locator that is allocated in a global data structure. We use the ut_hash macros (Hanson, 2014) to implement a hash table indexed by the hid_t HDF5 file identifier. Each file identifier key then maps to a utarray dynamic array containing the locators. The individual locators have a

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4HDS uses dot separators rather than directory separators when specifying a path within a data file. This will be familiar to VMS users.
flag indicating whether they are primary or secondary. The uthash macros were chosen since they did not require an additional library, they used a BSD license that was compatible with the HDSv5 library license, and the programming interface was reasonably straightforward.

When each locator is annulled these data structures are scanned to check whether this locator was the final primary locator. If it is, all remaining locators are themselves annulled. One complication is that the file identifier returned will be different for each call to H5Fopen so it is important to determine which file identifiers are associated with the same file. Without accounting for this, critical locators may be annulled at the wrong time. Rather than attempt to guess what the HDF5 library has chosen to do by normalising supplied filenames, the virtual file driver layer is queried to obtain the Unix file descriptor. All file identifiers with a shared file descriptor are queried before deciding whether a file should be closed.

One consequence of this behind-the-scenes freeing of resources is that it is possible for a library user that does not understand the distinction between primary and secondary locators to be left with pointers to structures that have been freed. To prevent unfortunate crashes, when a locator is freed automatically the contents of the structure are reset but the structure itself is not freed. This does result in a small memory leak but is thought to be more acceptable than a core dump.

5.6. Locator groups

Locator groups are not a feature of HDF5 and were implemented natively in the HDSv5 library. The implementation is similar to the primary locator system described previously except that the key for the uthash mapping table is the group name rather than the file identifier. When a group is flushed, all locators in the group are annulled and the group is deleted from the hash table.

5.7. Array slicing

A very powerful feature of HDF5 is the concept of a dataspace. A dataspace determines the rank and dimensions of a dataset and is used to specify the size of the HDS primitives. When a slice or cell request is made a single hyperslab selection is made which adjusts the external view of the dataset. HDS slices and cells are much simpler than what is possible in a hyperslab selection, and are restricted to simple subsets of a region.

When a locator is vectorized the dataspace associated with the locator is reshaped to be 1-dimensional. Subsequent slices of that vectorized dataspace are then handled in the same way as before using a hyperslab.

5.8. Type conversion

HDF5 supports an extremely broad range of data types and automatic conversion of numerical types when storing or retrieving a dataset. Critically, HDF5 does not support type conversion of string and logical types to numeric types (and vice versa) so this facility has been added explicitly in the HDSv5 library to maintain compatibility. This is simplified by HDS having the concept of a “bad” or “magic” value for each datatype that can be used to indicate where a conversion was not possible.

5.9. Memory mapping

An important requirement for any HDS implementation is to support direct memory mapping of files for both read and write operations. This has worked well over the years and helps minimize resource requirements. HDF5 has other priorities and advocates chunked access to minimize resources rather than providing direct access to the bytes on disk. The ability to split a dataset into multiple chunks and to insert arbitrary compression filters and virtual file drivers between the bytes trumps any
perceived advantages of memory mapping. In the HDSv5 implementation memory mapping is only attempted if files are in read only mode, if HDF5 will return the byte offset to the start of the dataset, if the HDF5 type system indicates that the in-memory data type and the on-disk data types are compatible, and if the virtual file driver will provide a file descriptor. In all other cases memory is allocated using standard system calls when a user requests memory mapping, and the data are written back to the file when the data are “ unmapped”. Mapping can also be disabled using a tuning parameter.

As a test a 4 GB dataset was loaded into the GAIA visualization tool (Draper et al., 2009, ascl:1403.024). With memory mapping enabled the image displayed within two seconds and the process only used a few tens of megabytes of memory. With memory mapping disabled it took about ten seconds to load the image and the process took 5 GB of memory.

The ability to memory map at all requires that datasets are created in single chunks and are not resizable. This causes some problems with HDS which assumes that all primitive objects are resizable. The HDSv5 dataset resizing function therefore attempts to use the native HDF5 resizing function but is usually forced to create a new dataset and copy the contents from the existing dataset, before deleting the original and renaming the new dataset. This can result in significant unused space in an HDF5 file.

6. Implementation Issues

The prototype library has largely shown that replacing native HDS with an HDSv5 implementation is feasible. Unfortunately we have found that there are some incompatibilities that have required minor code changes to Starlink applications. So far these have been restricted to applications that open an input file with read access and then open an output file with read/write access. If the input file and output file are the same file (for example when copying a structure within a file), HDS had no issue with this but in HDF5 this is strictly forbidden due to the internal tracking of open files. The changes to Figaro (Shortridge, 1993, ascl:1411.022) and HdStools (Chipperfield, 2002) result in the input being opened to validate it but recording the full path to the requested object. Then the input is closed and the output re-opened in read/write mode. Once this happens the input file can be re-opened and the application can continue as before. The modification also works with HDSv4 so can be adopted at the expense of some more convoluted code.

When designing the mapping of HDS to HDF5 some care was taken to not deliberately restrict the ability of the HDSv5 library to read HDF5 files that were not created by the library. To that end, attributes were chosen that were already in common usage, e.g., CLASS, or were chosen such that the absence of the attribute would result in reasonable behavior (root naming and structure dimensions). However, the implementation can not work miracles in dealing with the mismatch between the HDS and HDF5 data models. In particular, the HDS data model has no concept of attributes in the sense that HDF5 has them. Figure 3 shows the output of an HDS tracing program on a file created from a FITS file as described by Price et al. (2015). HDS is able to read some of the file contents but fails to read groups with names that exceed 16 characters. This limit can be increased by recompiling all Starlink applications but HDS relies on this limit being fixed at compile time. A more complex solution would be for HDF5 to return a shortened form of the name to the HDS API, possibly keeping track of the mapping from long name to short name internally. It is currently unclear how important it will be to handle this situation. What is not obvious from this trace is that the HEADER structure is not empty; all the FITS headers are actually stored as HDF5 attributes and these are invisible to the HDS data model.

7. Metrics

When considering adoption of a new format it is important to consider any performance differences and whether the files use up differing amounts of storage. These tests used HDF5 version 1.8.13 and a late 2014 version of HDSv4.

7.1. File Sizes

Test datasets were generated comparing the new format file sizes with the original file sizes. A comparison is shown in Table 2. The files were generated as follows:

1. The AGI graphics database generated by the SpecDRE demonstration script (Meyerdierks, 1992, ascl:1407.003). The graphics database makes extensive use of arrays of structures and resizing of elements. The HDF5 variant is more than five times larger than the HDSv4 variant with 20 % of that accounted for by empty space.
2. An ADAM parameter file generated from the execution of the ccspix (Taylor, 1998) exercise script. 34 % of the HDF5 file is empty space. Like the graphics database file, this file is updated constantly during program execution.

All these tests were done using the default file access property list settings. Selecting the latest format, via H5Pset:11ver_bounds, results in slightly smaller files for three of the four tests but a larger file in the parameter file test. It has not yet been decided whether HDSv5 should adopt maximal backwards compatibility for files or always be on the cutting edge.
3. A SCUBA-2 acquisition file (Bintley et al., 2014), which contains lots of data as well as table structures and is written in a single operation.
4. Kappa (Currie and Berry, 2013, ascl:1403.022) logo image consisting of a simple NDF with WCS and FITS header.

The numbers indicate that for small files with many structures the HDSv5 files are significantly larger. Some of this may be due to the inability to resize datasets without deleting them but even if the files are repacked they are still larger than HDSv4 versions. For larger data files the situation is less clear cut with the scientific data dominating the file contents the overhead from HDF5 is much lower.

The advantages of HDF5 become obvious once native data compression is used with the SCUBA-2 example file becoming 6% smaller than even the gzipped version of the HDSv4 format.

### 7.2. Benchmarks

The library has been tested on a number of standard Starlink benchmark routines from ccdpack (Draper et al., 2011, ascl:1403.021), ccdbig, and starbench (Rankin et al., 2003). An example data reduction test was also executed using SCUBA-2 data and the orac-dr pipeline (Jenness and Economou, 2015, ascl:1310.001)\(^6\). The results are shown in Table 3 and indicate that for tasks using lots of small files with lots of I/O HDSv4 is much faster. As the tests begin to use more real-world processing tasks with larger datasets the difference disappears and both libraries perform to within a few per cent. The final test involving orac-dr indicates that there may be a small performance advantage to not using memory mapping and this result may inform later decisions on whether to switch to using resizable chunked datasets in the future.

### 8. Conclusion

A new HDF5-based implementation of the HDS programming interface has been written which allows the Starlink software collection to be moved to a more widely-used file format. All but a handful of the approximately 150 HDS API functions have been implemented, with the remaining few being the routines that query low level implementation details. The HDSv5 library consists of approximately 10 000 lines of C with another 5 000 lines of C for the implementation of the wrapper (many of those lines are generated automatically). For comparison, the HDSv4 library consisted of about 18 000 lines of C and HDF5 itself consists of about 120 000 lines of C.

It has been shown that the library performs as well as the HDSv4 implementation in most tests involving reasonably-sized datasets and opens up the possibility for Starlink data products to be more easily consumed by others without requiring a format conversion. A native Python interface to the HDS library does exist but it is far easier to convince prospective consumers of the data files to use something such as h5py (e.g., Collette, 2013) to read the data, albeit with a different view of the data models. Furthermore, these files would be readable by general HDF5 visualization tools.

The Starlink open-source community must now decide whether to pursue this work and integrate it into the Starlink software distribution. It is possible that the project will decide to stick with HDSv4 and attempt to update the library to support 64-bit dimension sizes. This is a reasonable course of action to take, with an uncertain effort requirement, although it does not solve the issues relating to lack of documentation and sociological barrier to adoption of the Starlink software. Furthermore, if the new implementation is adopted, serious consideration must be made as to whether the approximately 4 million HDF5 files in the JCMT Science Archive (Economou et al., 2015) should be converted to HDF5. There is a risk involved for the archive in terms of the cost of keeping the old versions around and whether the conversion has been done correctly. The benefit will be that the raw data archive will immediately become more accessible to the general astronomer.

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\(^6\)These were observations 28, 31, 35, 44 and 51 from 2012 June 11th, reduced using the JCMT Science Archive public processing recipe (Bell et al., 2014).

This work also provides an alternative approach to porting FITS files to HDF5 format (see e.g., Price et al., 2015, for other options). The Starlink convert package (Currie, 1997; Currie et al., 1996) has received significant development effort over the years to map FITS to a hierarchical data model. It will be interesting to see whether the community can agree on a standard model for FITS to HDF5 conversion.

Now that a functioning prototype exists and has been proven to work acceptably, we must consider the possibility of expanding the HDS API to take advantage of HDF5 features. In particular, compound datatypes provide the prospect of native table access (the import of FITS binary tables would benefit significantly from this), an updated slicing API could provide access to hyperslabs, and the ability to specify chunking size and the maximum expected size of a dataset could result in significant efficiency benefits, albeit at the expense of memory mapping. It may be possible to consider allowing the HDS and HDF5 APIs to be used simultaneously on a single file. This has many attractions and provides a simple path to enhancing native applications. It also would mean it would be impossible to switch HDS from HDF5 to another format in the future. If the Advanced Scientific Data Format (ASDF; Droettboom and Bray, 2014; Greenfield et al., 2015) were to suddenly become popular in astronomy it would be conceivable to investigate a port of the HDS API to ASDF. If HDF5 identifiers had been used natively in the code this would be a significantly more complicated task. This is somewhat similar to the problems that are faced in porting NDF to other formats. The NDF standard (Currie et al., 1988) was specifically designed with an “airlock” API that allowed the user to obtain an HDS locator to extensions. This flexibility was important in early adoption and provided an easy way for extensions to be implemented. It also meant that any attempt to switch NDF absolutely required that the HDS API was itself ported, otherwise all the extensions in use would be unreadable. Indeed one key motivation for this work is that it brings NDF along to HDF5 without any NDF code or applications that use extensions having to be modified.

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The source code for the new HDS library and the Starlink software (ascl:1110.012) is open-source and is available on Github at https://github.com/Starlink

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