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pyfive: A pure-Python HDF5 reader

Bryan N. Lawrence [1,2], **Ezequiel Cimadevilla** [3], **Wout De Nolf** [4], **David Hassell** [1,2], **Jonathan Helmus** [7], **Brian Maranville** [5], **Benjamin Hodel** [7], **Kai Mühlbauer** [6], and **Valeriu Predoi** [1,2]

1 National Center for Atmospheric Science (NCAS), United Kingdom. **2** Department of Meteorology, University of Reading, Reading, United Kingdom. **3** Instituto de Física de Cantabria (IFCA), CSIC-Universidad de Cantabria, Santander, Spain. **4** European Synchrotron Radiation Facility (ESRF), Grenoble, France. **5** NIST Center for Neutron Research **6** Institute of Geosciences, Meteorology Section, University of Bonn, Germany. **7** No affiliation.

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Summary

`pyfive` (https://pyfive.readthedocs.io/en/latest/) is an open-source thread-safe pure Python package for reading data stored in HDF5. While it is not a complete implementation of all the specifications and capabilities of HDF5, it includes all the core functionality necessary to read gridded datasets, whether stored contiguously or with chunks, and to carry out the necessary decompression for the standard options. All data access is fully lazy, the data is only read from storage when the numpy data arrays are manipulated. Originally developed some years ago, the package has recently been upgraded to support lazy access, and to add missing features necessary for handling all the environmental data known to the authors. It is now a realistic option for production data access in environmental science and more widely. The API is based on that of `h5py` (which is a Python shimmy over the HDF5 C-library, and hence is not thread-safe), with some API extensions to help optimise remote access. With these extensions, coupled with thread safety, many of the limitations precluding the efficient use of HDF5 (and netCDF4) on cloud storage have been removed.

Statement of need

HDF5[1](Folk et al., 2011) is probably the most important data format in physical science, used across the piste. It is particularly important in environmental science, particularly given the fact that netCDF4[2](Rew et al., 2006) is HDF5 under the hood. From satellite missions, to climate models and radar systems, the default binary format has been HDF5 for decades. While newer formats are starting to get mindshare, there are petabytes, if not exabytes, of existing HDF5, and there are still many good use-cases for creating new data in HDF5. However, despite the history, there are few libraries for reading HDF5 file data that do not depend on the official HDF5 library maintained by the HDF Group, and in particular, apart from `pyfive`, in Python there are none that cover the needs of environmental science. While the HDF5 c-library is reliable and performant, and battle-tested over decades, there are some caveats to depending upon it: Firstly, it is not thread-safe, secondly, the code is large and complex, and should anything happen to the financial stability of the HDF5 Group, it is not obvious the C-code could be maintained. Finally, the code complexity also meant that it is not suitable for developing bespoke code for data recovery in the case of partially corrupt data. From a long-term curation perspective both of these last two constraints are a concern.

The original implementation of `pyfive` (by JH), which included all the low-level functionality

[1] https://www.hdfgroup.org/solutions/hdf5/
[2] https://www.unidata.ucar.edu/software/netcdf

to deal with the internals of an HDF5 file was developed with POSIX access in mind. The recent upgrades were developed with the use-case of performant remote access to curated data as the primary motivation, but with additional motivations of having a lightweight HDF5 reader capable of deploying in resource or operating-system constrained environments (such as mobile), and one that could be maintained long-term as a reference reader for curation purposes. The lightweight deployment consequences of a pure-Python HDF5 reader needs no further introduction, but as additional motivation we now expand on the issues around remote access and curation.

Thread safety has become a concern given the wide use of Dask[3] in Python based analysis workflows, and this, coupled with a lack of user knowledge about how to efficiently use HDF5, has led to a community perception that HDF5 is not fit for remote access (especially on cloud storage). Issues with thread safety arise from the underlying HDF5 c-library, and cannot be resolved in any solution depending on that library, hence the desire for a pure Python solution. Remote access has been bedevilled by the widespread need to access remotely data which has been chunked and compressed, combined with the use of HDF5 data which was left in the state it was when the data was produced - often with default unsuitable chunking (Rew, 2013) and with interleaved chunk indexes and data. Solutions have mainly consisted of reformatting the data (and rechunking it at the same time) or utilising kerchunk mediated direct access to chunked HDF5 data[4]. However, in practice using kerchunk requires the data provider to generate kerchunk indices to support remote users, and it leads to issues of synchronicity between indices and changing datasets.

This version of `pyfive` was developed with these use-cases in mind. There is now full support for lazy loading of chunked data, and methods are provided to give users all the benefits of using kerchunk, but without the need for a priori generation. Because `pyfive` can access and cache (in the client) the b-tree (index) on a variable-by-variable basis, most of the benefits of kerchunk are gained without any of the constraints. However, the kerchunk index is always a contiguous object accessible with one get transaction, this is not necessarily the case with the b-tree, unless the source data has been repacked to ensure contiguous metadata using a tool like h5repack. Much of the community is unaware of the possibility of repacking the index metadata, and this together with relatively opaque information about the internal structure of files (and hence the necessity or other wise of such repacking), means that repacking is rarely done. To help with this process, `pyfive` also includes extensions to expose information about how data and indexes are distributed in the files. With these tools, index extraction with `pyfive` can be comparable in performance to obtaining a kerchunk index, and completely opaque to the user.

With the use of `pyfive`, suitably repacked and rechunked HDF5 data can now be considered "cloud-optimised", insofar as with lazy loading, improved index handling, and thread-safety, there are no "format-induced" constraints on performance during remote access. To aid in discovering whether or not a given HDF5 dataset is cloud-optimised, `pyfive` also now provides simple methods to expose information about file layout - both in API extensions, and in a new `p5dump` utility packaged with the `pyfive` library, which provides (in the default view) functionality similar to ncdump, and when used with `p5dump -s`, information about storage characteristics.

The issues of the dependency on a complex code maintained by one private company in the context of maintaining data access (over decades, and potentially centuries), can only be mitigated by ensuring that the data format is well documented, that data writers use only the documented features, and that public code exists which can be relatively easily maintained. The HDF5group have provided good documentation for the core features of HDF5 which include all those of interest to the weather and climate community who motivated this reboot of `pyfive`, and while there is a community of developers beyond the HDF5 group (including

[3] https://www.dask.org/
[4] https://fsspec.github.io/kerchunk/

some at the publicly funded Unidata institution), recent events suggest that given most of those developers and their existing funding are US based, some spreading of risk would be desirable. To that end, a pure Python code, which is relatively small and maintained by an international constituency, alongside the existing C-code, provides some assurance that the community can maintain HDF5 access for the foreseeable future. A pure Python code also makes it easier to develop scripts which can work around data and metadata damage should they occur.

Examples

We now introduce three aspects of the new functionality that `pyfive` now provides: remote access, configurable lazy loading, and determining whether files are cloud optimised.

Remote Access

A notable feature of the recent `pyfive` upgrade is that it was carried out with thread-safety and remote access using fsspec (https://filesystem-spec.readthedocs.io) in mind. We provide two examples of using `pyfive` to access remote data, one in S3, and one behind a modern http web server:

For accessing the data on S3 storage, we will have to set up an `s3fs` virtual file system, then pass it to `pyfive`:

```python
import pyfive
import s3fs
# storage options for an anon S3 bucket
# there are also caching options for the s3 middleware, not shown here
storage_options = {
    "anon": True,
    "client_kwargs": {"endpoint_url": "https://s3server.ac.uk"}
}
fs = s3fs.S3FileSystem(**storage_options)
file_uri = "s3-bucket/myfile.nc"
with fs.open(file_uri, "rb") as s3_file:
    nc = pyfive.File(s3_file)
    dataset = nc["var"]
```

for an HTTPS data server, the usage is similar:

```python
import fsspec
import pyfive
# there are also caching options for the fsspec middleware, not shown here
fs = fsspec.filesystem("http")
with fs.open("https://site.com/myfile.nc", "rb") as http_file:
    nc = pyfive.File(http_file)
    dataset = nc[var]
```

This is of course exactly the same pattern as remote access using `h5py`, and that is by design - to make moving to `pyfive` easy for users!

Lazy Loading

A key tenet of efficient remote access is that variable inspection is quick and involves the minimimum of network traffic between storage and the client application.
However when this is coupled with the common pattern of using Dask, some flexibility in what is loaded when is beneficial.

By default when one inspects the contents of a file using `pyfive` nothing more is read from the file than the names of the variables ("datasets" in the language of HDF5): for example:

```
with pyfive.File("myfile.h5","r") as f:
  variables_in_file = [v for v in f]
```

involves nothing more than getting a set of variable names. When one wishes to inspect these variables:

```
with pyfive.File("myfile.h5","r") as f:
  temp = f["temp"]
print(temp[1:10])
```

the default in `pyfive` is to get only the metadata associated with each variable - but crucially at this point the b-tree index is also loaded and the variable can now be accessed outside the context manager. Data loading is now completely lazy and the variable instance (`temp`) has all the information needed to extract data as needed. This is done so that in Dask applications, when one passes each Dask computational chunk a portion of the variable, each such Dask chunk has already got the index, and when it does want to load data, it can be as efficient as possible.

However, there are situations where loading the b-tree at variable instantation is not wanted, and all is wanted is to be able to view all the variable attributes. To support this option `pyfive` also offers the `get_lazy_view` file method, so one can do:

```
with pyfive.File("myfile.h5","r") as f:
  temp = f.get_lazy_view("temp")
print(temp.attrs())
```

It is still possible to access the data and the b-tree index is loaded when data access is first attempted.

This extra lazy view is new functionality. It would obviously have been possible to make the default not load the b-tree, but in the opinion of the current `pyfive` maintainers loading the b-tree at variable instantiation is likely more consistent with user expectations as it is more equivalent to the behaviour of other packages like `h5py`.

Cloud Optimisation

To be fully cloud optimised - as defined by Stern et al. (2022) - an HDF5 file needs to have a contiguous index for each variable, and the chunks for each variable need to be sensibly chosen and broadly contiguous within the file. When these criteria are met, indexes can be read efficiently, and middleware such as fsspec can make sensible use of readahead caching strategies.

HDF5 data files direct from simulations and instruments are often not in this state as information about the number of variables, the number of chunks per variable, and the compressed size of those variables is not known as the data is being produced.
In such cases the data is also often not chunked along the dimensions being added to as the file is written (since it would have to be buffered first).

Of course, once the file is produced, such information is available. Metadata can be repacked to the front of the file and variables can be rechunked and made contiguous - which is effectively the same process undertaken when HDF5 data is reformatted to other cloud optimised formats.

The HDF5 library provides a tool "h5repack" which can do this, provided it is driven with suitable information about required chunk shape and the expected size of metadata fields. `pyfive` supports both a method to query whether such repacking is necessary, and to extract necessary parameters.

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In the following example we compare and contrast the unpacked and repacked version of a particularly pathological file, and in doing so showcase some of the `pyfive` API extensions which help us understand why it is pathological, and how to address those issues for repacking.

If we extract just a piece of the output of `p5dump -s` on this file (which has surface wind velocity at three hour intervals for one hundred years):

```
float64 time(time) ;
                time:standard_name = "time" ;
                time:_n_chunks = 292192 ;
                time:_chunk_shape = (1,) ;
                time:_btree_range = (31808, 19854095942) ;
                time:_first_chunk = 9094 ;

float32 uas(time, lat, lon) ;
                uas:_Storage = "Chunked" ;
                uas:_n_chunks = 292192 ;
                uas:_chunk_shape = (1, 143, 144) ;
                uas:_btree_range = (28672, 19854809382) ;
                uas:_first_chunk = 36520 ;
```

we can immediately see that this will be a problematic file! The b-tree index is clearly interleaved with the data (compare the first chunk address with last index addresses of the two variables), and with a chunk dimension of (1,), any effort to use the time-dimension to locate data of interest will involve a ludicrous number of 1 number reads (all underlying libraries read the data one chunk at a time). It would feel like waiting for the heat death of the universe if one was to attempt to manipulate this data stored on an object store!

It is relatively easy (albeit slow) to use h5repack to fix this - e.g see Hassell & Cimadevilla Alvarez (2025) - after which we see:

```
float64 time(time) ;
                time:_Storage = "Chunked" ;
                time:_n_chunks = 1 ;
                time:_chunk_shape = (292192,) ;
                time:_btree_range = (11861, 11861) ;
                time:_first_chunk = 40989128 ;
                time:_compression = "gzip(4)" ;
float32 uas(time, lat, lon) ;
                uas:_Storage = "Chunked" ;
                uas:_n_chunks = 5844 ;
                uas:_chunk_shape = (50, 143, 144) ;
                uas:_btree_range = (18663, 347943) ;
                uas:_first_chunk = 41041196 ;
                uas:_compression = "gzip(4)" ;
```

Now data follows indexes, the time dimension is one chunk, and there is a more sensible number of actual data chunks. While this file would probably benefit from splitting, with a contiguous set of indexes, it is now possible to exploit this data via S3.

All the metadata shown in this dump output arises from `pyfive` extensions to the `pyfive.h5t.DatasetID` class. `pyfive` also provides a simple flag: `consolidated_metadata` for a `File` instance, which can take values of `True` or `False` for any given file, which simplifies at least the "is the index packed at the front of the file?" part of the optimisation question - though inspection of chunking is a key part of the workflow necessary to determine whether or not a file really is optimised for cloud usage.

DRAFT

Author contributions

JH designed and implemented the original software library, including all the fundamental infrastructure for working with low-level HDF artifacts. BM, WDN and BH made contributions to earlier versions of the library. BNL led the overall refresh of the library, designed and implemented the support for lazy loading of chunked data, cloud and other optimisations, and wrote the paper (with input from the other authors). EC, DH, BM, KM and VP made contributions to the recent versions of the library.

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