




1 pyfive: A pure-Python HDF5 reader

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DOI: [10.xxxxxx/draft](https://doi.org/10.xxxxxx/draft)

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Submitted: 01 January 1970

Published: unpublished

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10 Summary

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

24 Statement of need

25 HDF5¹(Folk et al., 2011) is probably the most important data format in physical science, used
26 across the piste. It is particularly important in environmental science, particularly given the
27 fact that netCDF4²(Rew et al., 2006) is HDF5 under the hood. From satellite missions, to
28 climate models and radar systems, the default binary format has been HDF5 for decades. While
29 newer formats are starting to get mindshare, there are petabytes, if not exabytes, of existing
30 HDF5, and there are still many good use-cases for creating new data in HDF5. However,
31 despite the history, there are few libraries for reading HDF5 file data that do not depend on
32 the official HDF5 library maintained by the HDF Group, and in particular, apart from pyfive,
33 in Python there are none that cover the needs of environmental science. While the HDF5
34 c-library is reliable and performant, and battle-tested over decades, there are some caveats to
35 depending upon it: Firstly, it is not thread-safe, secondly, the code is large and complex, and
36 should anything happen to the financial stability of the HDF5 Group, it is not obvious the
37 C-code could be maintained. Finally, the code complexity also meant that it is not suitable
38 for developing bespoke code for data recovery in the case of partially corrupt data. From a
39 long-term curation perspective both of these last two constraints are a concern.

40 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 Dask³ 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 data⁴. 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/>

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

98 Examples

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

101 Remote Access

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

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

```
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"]
```

108 for an HTTPS data server, the usage is similar:

```
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]
```

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

111 Lazy Loading

112 A key tenet of efficient remote access is that variable inspection is quick and involves the
 113 minimum of network traffic between storage and the client application.

114 However when this is coupled with the common pattern of using Dask, some flexibility in what
 115 is loaded when is beneficial.

116 By default when one inspects the contents of a file using pyfive nothing more is read from
117 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]
```

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

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

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

127 However, there are situations where loading the b-tree at variable instantiation is not wanted,
128 and all is wanted is to be able to view all the variable attributes. To support this option pyfive
129 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())
```

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

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

136 Cloud Optimisation

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

142 HDF5 data files direct from simulations and instruments are often not in this state as information
143 about the number of variables, the number of chunks per variable, and the compressed size of
144 those variables is not known as the data is being produced.

145 In such cases the data is also often not chunked along the dimensions being added to as the
146 file is written (since it would have to be buffered first).

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

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

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

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

```
159 float64 time(time) ;
160         time:standard_name = "time" ;
161         time:_n_chunks = 292192 ;
162         time:_chunk_shape = (1,) ;
163         time:_btree_range = (31808, 19854095942) ;
164         time:_first_chunk = 9094 ;
165
166 float32 uas(time, lat, lon) ;
167         uas:_Storage = "Chunked" ;
168         uas:_n_chunks = 292192 ;
169         uas:_chunk_shape = (1, 143, 144) ;
170         uas:_btree_range = (28672, 19854809382) ;
171         uas:_first_chunk = 36520 ;
```

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

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

```
180 float64 time(time) ;
181         time:_Storage = "Chunked" ;
182         time:_n_chunks = 1 ;
183         time:_chunk_shape = (292192,) ;
184         time:_btree_range = (11861, 11861) ;
185         time:_first_chunk = 40989128 ;
186         time:_compression = "gzip(4)" ;
187 float32 uas(time, lat, lon) ;
188         uas:_Storage = "Chunked" ;
189         uas:_n_chunks = 5844 ;
190         uas:_chunk_shape = (50, 143, 144) ;
191         uas:_btree_range = (18663, 347943) ;
192         uas:_first_chunk = 41041196 ;
193         uas:_compression = "gzip(4)" ;
```

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

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

203 **Author contributions**

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

210 **Acknowledgements**

211 Most of the recent developments outlined have been supported by the UK Met Office and
212 UKRI via 1) UK Excalibur Exascale programme (project ExcaliWork), 2) the UKRI Digital
213 Research Infrastructure programme (project WacaSoft), and 3) the national capability funding
214 of the UK National Center for Atmospheric Science (NCAS). Ongoing maintenance of pyfive
215 is expected to continue under the auspices of NCAS national capability funding.

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