Zarr vs. HDF5

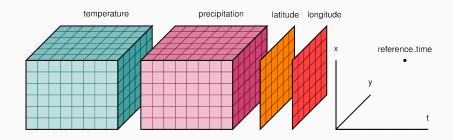
Joe Jevnik

November 4th, 2019

PyData NYC 2019

Core Concepts

Multidimensional Data



Compression

same information in less space

Compression

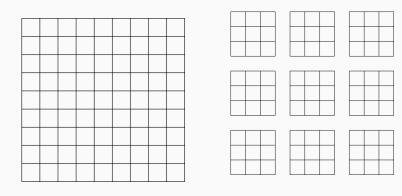
same information in less space lossless

Compression

same information in less space

lossless

lossy



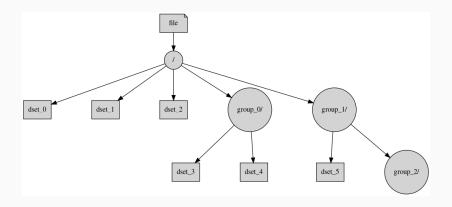
 $compression/random\ access\ trade\ off$

compression/random access trade off throughput/latency access trade off

compression/random access trade off throughput/latency access trade off reduce io

compression/random access trade off throughput/latency access trade off reduce io facilitate caching

Hierarchy



Nodes

Definition (Dataset)

a multidimensional array

leaves of a Zarr or HDF5 tree

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Definition (Dataset)

a multidimensional array leaves of a Zarr or HDF5 tree

Definition (Group)

collection of datasets or groups

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Definition (Dataset)

a multidimensional array leaves of a Zarr or HDF5 tree

Definition (Group)

collection of datasets or groups

Definition (Node)

either a dataset or group

Attributes

Definition (Attributes)

key-value data

Attributes

Definition (Attributes)

key-value data property of each **node**

Python Interface

nested dictionaries

nested dictionaries leaves are *array-like*

nested dictionaries leaves are *array-like* supports numpy-style indexing

nested dictionaries leaves are *array-like* supports numpy-style indexing NOTE: describes h5py, not pytables

zarr

```
>>> import zarr
>>> f = zarr.open('file.zarr')
>>> f
<zarr.hierarchy.Group '/'>
```

zarr

```
>>> import zarr
>>> f = zarr.open('file.zarr')
>>> f
<zarr.hierarchy.Group '/'>
>>> f['dset'] = np.arange(20 * 5).reshape(20, 5)
>>> f['dset']
>>> <zarr.core.Array '/dset' (20, 5) int64>
```

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<zarr.hierarchy.Group '/'>
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>>> f['dset']
>>> <zarr.core.Array '/dset' (20, 5) int64>
>>> f['dset'][10, 3]
53
>>> f['dset'][:]
array([...]])
```

```
>>> import h5py
>>> f = h5py.File('file.h5', 'r+')
>>> f
<HDF5 file "file.h5" (mode r+)>
>>> f['dset'] = np.arange(20 * 5).reshape(20, 5)
>>> f['dset']
<HDF5 dataset "dset": shape (20, 5), type "<i8">
>>> f['dset'][10, 3]
53
>>> f['dset'][:]
array([...]])
```

Node.attrs to get access to attributes as dict-like object

Node.attrs to get access to attributes as dict-like object Group.create_dataset to set chunk shape and compression

Node.attrs to get access to attributes as dict-like object Group.create_dataset to set chunk shape and compression Group.create_group to create sub-groups

Node.attrs to get access to attributes as dict-like object
Group.create_dataset to set chunk shape and compression
Group.create_group to create sub-groups
Dataset.read_direct to read into existing buffers

Making a Decision

• over 20 years old

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- excellent cross language support

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HDF5

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- lots of existing software
- written in (very clean) C
- can be made thread safe, not thread optimal
- extensible in C

• first release in 2015, 1.0 on May 17, 2016

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- extensible in Python

filters and compressors

filters and compressors storage backends

filters and compressors storage backends which extensions come as part of the library itself?

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filters and compressors
storage backends
which extensions come as part of the library itself?
how to extend the libraries for non-default use cases?
ease of distributing extensions

Definition (Filter)

a function that sits between the raw data and the storage

Definition (Filter)

a function that sits between the raw data and the storage compressors

Definition (Filter)

- a function that sits between the raw data and the storage
- compressors
- checksumming

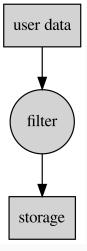
Definition (Filter)

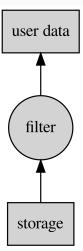
- a function that sits between the raw data and the storage
- compressors
- checksumming
- composable

Definition (Filter)

- a function that sits between the raw data and the storage
- compressors
- checksumming
- composable
- act on one chunk at a time

write read





Filter Pipelines

write read





Default Filters in HDF5

- lzf
- gzip
- szip (patent issues)
- scale-offset (lossy)
- shuffle
- fletcher32 (checksum)

Default Filters in Zarr

- blosc
- 1z4
- zstd
- zlib
- gzip
- bz2
- lzma

- delta
- fixed_scale_offset
- quantize (lossy)
- pack_bits (boolean packing)
- ullet categorical (str o int)
- json, msgpack, pickle
- vlen_string

Writing an HDF5 Filter

```
static size_t
f(unsigned int flags,
    size_t cd_nelmts, const unsigned cd_values[],
    size_t nbytes, size_t *buf_size, void **buf) {
```

Writing an HDF5 Filter

```
static size_t
f(unsigned int flags,
  size_t cd_nelmts, const unsigned cd_values[],
  size_t nbytes, size_t *buf_size, void **buf) {
    if (!(flags & H5Z_FLAG_REVERSE)) {
        /* encode data */
    else {
        /* decode data */
```

Writing an HDF5 Filter

```
static size_t
f(unsigned int flags,
  size_t cd_nelmts, const unsigned cd_values[],
  size_t nbytes, size_t *buf_size, void **buf) {
    if (!(flags & H5Z_FLAG_REVERSE)) {
        /* encode data */
    else {
        /* decode data */
    }
    return /* number of bytes in new buffer
              or 0 on failure */;
```

Writing an HDF5 Filter Cont.

```
static htri_t
can_apply(hid_t dcpl_id, hid_t type_id, hid_t space_id) {
    /* return -1 for error, 0 for false, or 1 for true */
}
```

Writing an HDF5 Filter Cont.

```
const int my_filter_id = /* ... */;
static H5Z_class2_t filter = {
    .version = H5Z_CLASS_T_VERS,
    .id = my_filter_id,
    .encoder_present = 1,
    .decoder_present = 1,
    .name = "my_filter",
    .can_apply = can_apply,
    .set_local = NULL,
    .filter = f,
};
int my_filter_register() { return H5Zregister(&filter); }
```

Using a Custom HDF5 Filter

```
import ctypes
dll = ctypes.CDLL('filter.so')
assert dll.my_filter_register() == 0
filter_id = ctypes.c_int.in_dll(
         dll, 'my_filter_id',
).value
```

Using a Custom HDF5 Filter

```
import ctypes
dll = ctypes.CDLL('filter.so')
assert dll.my_filter_register() == 0
filter_id = ctypes.c_int.in_dll(
    dll, 'my_filter_id',
).value
f = h5py.File('a.h5', 'r+')
dset = f.create_dataset(
    'dset',
    compression=filter_id,
    dtype='i8',
    shape=(100,),
```

h5py statically links to hdf5 by default

h5py statically links to hdf5 by default h5py doesn't re-export H5Zregister

```
h5py statically links to hdf5 by default
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$ HDF5_VERSION=1.10 pip install --no-binary :all:
h5py
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can't use custom pipelines in h5py yet (I think)
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h5py
hard to thread parameters
hard to manage state
must use malloc/free
can't use custom pipelines in h5py yet (I think)
doesn't trigger until flush
```

Good Points with Custom HDF5 Filters

filter ids use central authority

Good Points with Custom HDF5 Filters

filter ids use central authority can be used in different languages

Good Points with Custom HDF5 Filters

filter ids use central authority can be used in different languages plugin directory to find extension

Writing a Zarr Filter

```
import numcodecs
from numcodecs.abc import Codec
class MyFilter(Codec):
    codec_id = 'my_filter'
    def encode(self, buf):
        . . .
    def decode(self, buf, out=None):
numcodecs.register_codec(MyFilter)
```

Using a Custom Zarr Filter

```
import numpy as np
import zarr
from my_filter import MyFilter
f = zarr.open('a.zarr', 'w')
dset = f.create_dataset(
    'dset'.
    compressor=MyFilter(),
    #filters=[..., MyFilter(), ...],
    dtype='i8',
    shape=(100,),
```

Problems with Custom Zarr Filters

no central authority, names can collide

Problems with Custom Zarr Filters

no central authority, names can collide require Python code or an alternative implementation

Problems with Custom Zarr Filters

no central authority, names can collide require Python code or an alternative implementation probably want to be written in native code anyways

written in Python

written in Python easy distribution (Python package)

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written in Python
easy distribution (Python package)
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easy to manage state

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easy to pass parameters to filter
easy to manage state
split API is more clear

written in Python
easy distribution (Python package)
easy to pass parameters to filter
easy to manage state
split API is more clear
easily works in filter pipelines

Delta of Deltas Example

```
https://github.com/llllllllllllzarr-vs-hdf5-talk/blob/master/examples/delta_of_delta_filter
```

Storage

 $abstract\ storage\ of\ structures$

abstract storage of structures no single file type

abstract storage of structures no single file type configurable

abstract storage of structures no single file type configurable two kinds of data

abstract storage of structures no single file type configurable two kinds of data user data

```
abstract storage of structures
no single file type
configurable
two kinds of data
user data
metadata (tree structure, extra driver info)
```

virtual contiguous memory space

virtual contiguous memory space allocator-like

virtual contiguous memory space allocator-like no information about semantic data

virtual contiguous memory space allocator-like no information about semantic data library handles caching/locking

virtual contiguous memory space allocator-like no information about semantic data library handles caching/locking single threaded

based on dict from str to bytes

based on dict from str to bytes Python mapping protocol

based on dict from str to bytes Python mapping protocol key contains semantic information

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based on dict from str to bytes
Python mapping protocol
key contains semantic information
group/dset/0.3
can manage locking, not required

based on dict from str to bytes Python mapping protocol key contains semantic information group/dset/0.3 can manage locking, not required composable

Default Storage Backends in HDF5

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Default Storage Backends in HDF5

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- windows (Windows file API)
- stdio (buffered, C stdio.h)
- core (in memory)
- family (directory of blocks)

Default Storage Backends in HDF5

- sec2 (posix API)
- windows (Windows file API)
- stdio (buffered, C stdio.h)
- core (in memory)
- family (directory of blocks)
- fileobj (h5py only)

Default Storage Backends in Zarr

- MemoryStore
- DirectoryStore
- TempStore
- NestedDirectoryStore
- ZipStore (single file)
- DBMStore
- LMDBStore

- SQLiteStore
- MongoDBStore
- RedisStore
- ABSStore (Azure Blob Storage)
- LRUStoreCache
- ConsolidatedMetadataStore
- S3Map (third party)

```
struct H5FD_class_t;
```

```
struct H5FD class t:
herr_t (*write)(H5FD_t* file, H5FD_mem_t type,
                hid_t dxpl, haddr_t addr,
                size_t size, const void* buffer);
herr_t (*read)(H5FD_t* file, H5FD_mem_t type,
               hid_t dxpl, haddr_t addr,
               size_t size, void* buffer);
/* 28 more member functions and
   static member variables */
```

```
import h5py
from my_driver_as_extension_module import set_fapl
h5py.register_driver('my_driver', set_fapl)
```

```
import h5py
from my_driver_as_extension_module import set_fapl
h5py.register_driver('my_driver', set_fapl)
file = h5py.File(
    'path/to/pass/to/driver/open'
    'w',
    driver='my_driver',
    **extra_driver_kwargs,
```

huge API

huge API no semantic information

huge API no semantic information hard to optimize

huge API no semantic information hard to optimize not composable

huge API
no semantic information
hard to optimize
not composable
need to rely on HDF5 to do a lot of things for you

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small ABI incompatibility between 1.8 and 1.10

huge API
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need to rely on HDF5 to do a lot of things for you
small ABI incompatibility between 1.8 and 1.10
single threaded

huge API no semantic information hard to optimize not composable need to rely on HDF5 to do a lot of things for you small ABI incompatibility between 1.8 and 1.10 single threaded not many people have published file drivers

set_fapl makes it easy to thread arguments

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reasonable state management

set_fap1 makes it easy to thread arguments
reasonable state management
source code of built in drivers is very clear

set_fapl makes it easy to thread arguments reasonable state management source code of built in drivers is very clear can be built to minimize copies

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source code of built in drivers is very clear
can be built to minimize copies
can flatten or cut up the data to use different drivers
64 bit memory space always

Writing a Custom Zarr Storage Backend

```
from collections.abc import MutableMapping
class MyStorageBackend(MutableMapping):
    def __getitem__(self, key):
    def __setitem__(self, key, data):
    def __delitem__(self, key):
    # ... __iter__, __len__
```

Problems with Custom Zarr Storage Backends

always need to copy on read

composable

composable

user defined caching, consolidation, etc.

composable user defined caching, consolidation, etc. semantic information available

composable user defined caching, consolidation, etc. semantic information available written in Python

Conclusion

Takeaways

Zarr

- lots of modern features
- actively developed
- responsive and helpful devs
- Python focused/specific*
- easier to prototype extensions

HDF5

- stable mature code
- cross language support
- very single threaded
- harder to write extensions

Thank You

- https://github.com/llllllllll (10 lowercase L's)
- Example delta of deltas filter for both HDF5 and Zarr: https://github.com/lllllllllll/zarr-vs-hdf5-talk/ blob/master/examples/delta_of_delta_filter
- S3 file driver for HDF5: https://github.com/h5s3/h5s3
- @__qualname__