HDF5.jl: Hierarchical Data Storage for Julia

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What is HDF5?

HDF5 stands for Hierarchial Data Format version 5 and is maintained by The HDF Group, formerly part of the National Center for Supercomputing Appplications (NCSA).

- HDF5 is a file format with an open specification.
- HDF5 is a C Library and API.
- HDF5 is a data model.

When to use HDF5

- Store numeric array and attributes in nested groups.
- Use it when you want to compactly store binary data.

When not to use HDF5

- You have arrays of variable-length strings. Used fixed lengths strings instead.
- You have tables of heterogeneous data. Consider using columnar layouts. Other formats are more optimized for tables.

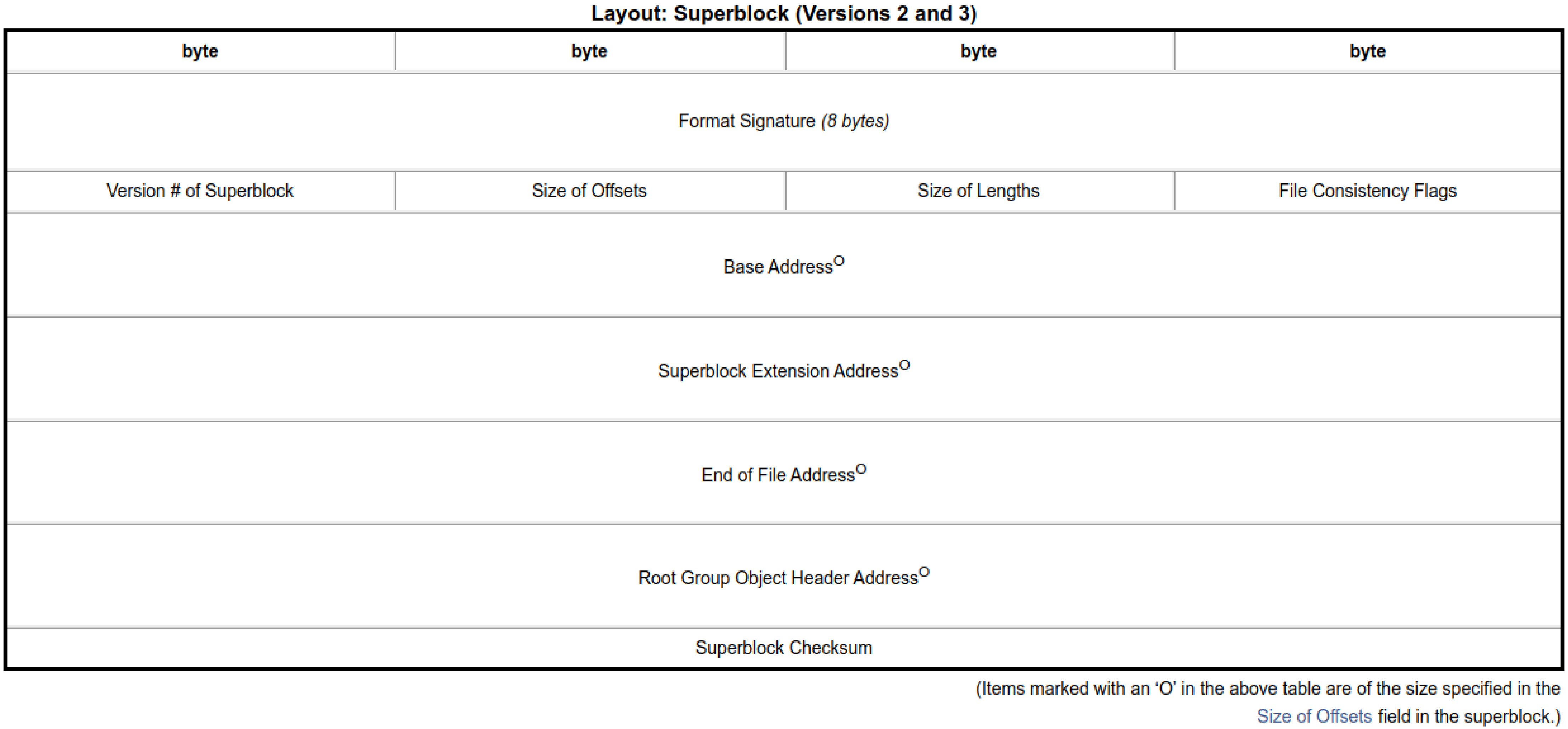
Related formats

HDF5 is used as a base for other formats

- NetCDF - Network Common Data Form v4 (Unidata, UCAR)
- MAT - MATLAB data files v7.3+
- PyTables - Pandas

HDF5 Specification: Superblock

HDF5 structures are variably sized and use Bob Jenkin's Lookup3 checksum for metadata integrity.



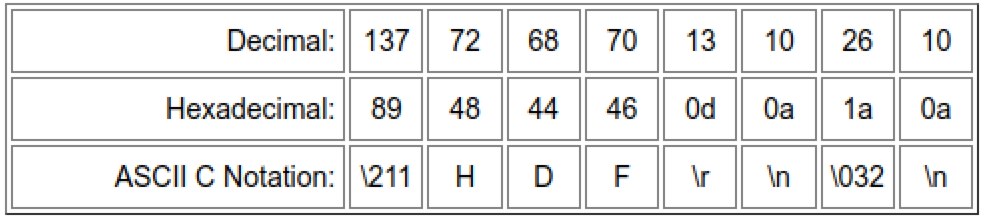
Layout: Superblock (Versions 2 and 3)

byte	byte	byte	byte
Format Signature *(8 bytes)*			
Version # of Superblock	Size of Offsets	Size of Lengths	File Consistency Flags
Base Address^{O}			
Superblock Extension Address^{O}			
End of File Address^{O}			
Root Group Object Header Address^{O}			
Superblock Checksum			

(Items marked with an 'O' in the above table are of the size specified in the Size of Offsets field in the superblock.)

A HDF5 Hex Dump

```
00000000  89 48 44 46 0d 0a 1a 0a  03 08 08 00 00 00 00 00  |.HDF............|
00000010  00 00 00 00 ff ff ff ff  ff ff ff ff 82 08 01 00  |................|
00000020  00 00 00 00 30 00 00 00  00 00 00 00 92 3c c0 2c  |....0........<.,|
00000030  4f 48 44 52 02 20 a3 5c  ae 64 a3 5c ae 64 a3 5c  |OHDR. .\.d.\.d.\|
00000040  ae 64 a3 5c ae 64 78 02  12 00 00 00 00 ff ff ff  |.d.\.dx.........|
00000050  ff ff ff ff ff ff ff ff  ff ff ff ff ff 0a 02 00  |................|
00000060  01 00 00 06 14 00 00 01  00 09 7a 61 72 72 73 68  |..........zarrsh|
00000070  61 72 64 c3 00 00 00 00  00 00 00 00 40 00 00 00  |ard.........@...|
00000080  00 00 00 00 00 00 00 00  00 00 00 00 00 00 00 00  |................|
```



Decimal:	137	72	68	70	13	10	26	10
Hexadecimal:	89	48	44	46	0d	0a	1a	0a
ASCII C Notation:	\211	H	D	F	\r	\n	\032	\n

What is HDF5.jl?

HDF5.jl is a wrapper around the HDF5 C Library.

It consists of

- A low level interface, a direct mapping to the C API
- A mid level interface, lightweight helpers
- A high level interface, a Julia API

HDF5.jl Early Contributors

- There are many contributors
- Konrad Hisen initiated Julia's support for HDF5
- Tim Holy and Simon Kornblith were the initial primary authors
- Tom Short, Blake Johnson, Isaih Norton, Elliot Saba, Steven Johnson, Mike Nolta, Jameson Nash
- Justin Willmert improved many aspects C to Julia API interface

HDF5.jl Current Developers

- Mustafa Mohamad, Mark Kittisopikul, and Simon Byrne are the current maintainers
- Mark Kittisopikul has been expanding API coverage, especially with chunking
- Simon Byrne has been working on package organization, filter interface, virtual datasets, and parallelization
- Other recent contributors: t-bltg, Henrik Ranocha, Nathan Zimmerberg, Joshua Lampert, Tamas Gal, David MacMahon, Juan Ignacio Polanco, Michale Schlottke-Lakemper, linwaytin, Dmitri Iouchtchenko, Lorenzo Van Munoz, Jared Wahlstrand, Julian Samaroo, machakann, James Hester, Ralph Kube, Kristoffer Carlsson

What advantages does Julia bring to HDF5.jl?

- HDF5.jl wraps the C library directly in Julia via `@ccall`.
  - This is partially automated via Clang.jl and https://github.com/mkitti/LibHDF5.jl .
- HDF5.jl dynamically create types to match the stored HDF5 types.
- HDF5.jl can use Julia's reflection capabilities to create corresponding HDF5 types.
- HDF5.jl is easily extensible using multiple dispatch.
- HDF5.jl can create callbacks for C for efficient iteration.

Basic HDF5.jl Usage

```julia
using HDF5

# Write a HDF5 file
h5open("mydata.h5", "w") do h5f
    # Store an array
    h5f["group_A/group_B/array_C"] = rand(1024,1024)
    # Store an attribute
    attrs(h5f["group_A"])["access_date"] = "2023_07_21"
end

# Read a HDF5 file
C = h5open("mydata.h5") do h5f
    # Access an attribute
    println(attrs(h5f["group_A"])["access_date"])
    # Load an array and return it as C
    h5f["group_A/group_B/array_C"][:,:]
end
```

Exploring a HDF5 file with HDF5.jl

```
julia> h5f = h5open("mydata.h5")
🗂️ HDF5.File: (read-only) mydata.h5
└─ 📂 group_A
   ├─ 🏷️ access_date
   └─ 📂 group_B
      └─ 🔢 array_C

julia> C  = h5f["group_A"]["group_B"]["array_C"][1:16,1:16]
16×16 Matrix{Float64}:
...

julia> close(h5f)
```

Structs and HDF5 Types

```
julia> struct Foo
           x::Int64
           y::Float64
       end

julia> HDF5.datatype(Foo)
HDF5.Datatype: H5T_COMPOUND {
      H5T_STD_I64LE "x" : 0;
      H5T_IEEE_F64LE "y" : 8;
   }
```

Reading and writing structs

```
julia> h5open("mystruct.h5", "w") do h5f
           h5f["Foo"] = [Foo(1, 3.0)]
       end
1-element Vector{Foo}:
 Foo(1, 3.0)

julia> h5open("mystruct.h5", "r") do h5f
           h5f["Foo"][]
       end
1-element Vector{NamedTuple{(:x, :y), Tuple{Int64, Float64}}}:
 (x = 1, y = 3.0)

julia> h5open("mystruct.h5", "r") do h5f
           read(h5f["Foo"], Foo)
       end
1-element Vector{Foo}:
 Foo(1, 3.0)
```

Compression Filter Plugin Packages

Glue code written in Julia.

- H5Zblosc.jl - Blosc.jl (Thank you, Steven G. Johnson)
- H5Zzstd.jl - CodecZstd.jl
- H5Zlz4.jl - CodecLZ4.jl
- H5Zbzip2.jl - CodecBzip2.jl
- H5Zbitshuffle.jl

Chunking and Built-in Gzip Compression Usage

```
using HDF5

h5open("simple_chunked.h5", "w", libver_bounds=v"1.12") do h5f
    h5ds = create_dataset(h5f, "gzipped_data", UInt8, (16,16),
        chunk=(4,4),
        filters=[HDF5.Filters.Deflate()],
        alloc_time = :early
    )
end
```

Chunking and Filter Plugin Usage

```julia
using HDF5, H5Zzstd

h5open("zstd_chunked.h5", "w", libver_bounds=v"1.12") do h5f
    h5ds = create_dataset(h5f, "zstd_data", UInt8, (16,16),
        chunk=(4,4),
        filters=[ZstdFilter(3)]
    )
end
```

Future: Loading CodecZstd.jl will trigger a package extension

Using External Native Plugin Filters

The HDF5 C library has a filter plugin mechanism. Plugins are shared libraries located in `/usr/local/hdf5/lib/plugin` or as specified by `$HDF5_PLUGIN_DIR`.

```
using HDF5.Filters

bitshuf = ExternalFilter(32008, Cuint[0, 0])
bitshuf_comp = ExternalFilter(32008, Cuint[0, 2])

data_A = rand(0:31, 1024)
data_B = rand(32:63, 1024)

filename, _ = mktemp()
h5open(filename, "w") do h5f
    # Indexing style
    h5f["ex_data_A", chunk=(32,), filters=bitshuf] = data_A
    # Procedural style
    d, dt = create_dataset(h5f, "ex_data_B", data_B, chunk=(32,), filters=[bitshuf_comp])
    write(d, data_B)
end
```

Iteration

For accessing data has two kinds of interfaces for accessing enumerated data:

1. `h5a_get_name_by_idx(loc_id, obj_name, index_type, order, idx, name, size, lapl_id)`
2. `h5a_iterate(obj_id::hid_t, idx_type::Cint, order::Cint, n::Ptr{hsize_t}, op::Ptr{Cvoid}, op_data::Any)`, `op` is function pointer

The `_by_idx` calls are easy to use via a simple `for` loop but are very inefficient for iterating over many items.

The `_iterate` calls require a C callback, `op`, and can be challenging to use but are efficient.

Multithreading

- The HDF5 C library is not directly compatible with multithreading for parallel I/O. The preferred parallelization is via MPI.
- There is a `H5_HAVE_THREADSAFE` compile time option that uses a recursive lock.
- In HDF5.jl we have applied a `ReentrantLock` on all API calls.

Parallelization via Message Passing Interface (MPI)

Other Related Julia Packages

- HDF5_jll.jl, C Library from HDF Group
- MAT.jl, MATLAB files
- JLD.jl, Julia Data Format
- JLD2.jl, Julia Data Format 2, Pure Julia implementation of a subset of HDF5