Memo: UVH5 file format

Paul La Plante, and the pyuvdata team

November 28, 2018 Revised March 29, 2021

Contents

1 Introduction

This memo introduces a new HDF5¹-based file format of a UVData object in $pyuvdata^2$, a python package that provides an interface to interferometric data. Here, we describe the required and optional elements and the structure of this file format, called UVH5.

Note that this file format is specifically designed to represent UVData objects. Other HDF5-based datasets for radio interferometers, such as katdal³ or HDFITS⁴ are not compatible with the standard as defined here. We refer the reader to the documentation of those other formats to find out more about them.

We assume that the user has a working knowledge of HDF5 and the associated python bindings in the package h5py⁵, as well as UVData objects in pyuvdata. For more information about HDF5, please visit https://portal.hdfgroup.org/display/HDF5/HDF5. For more information about the parameters present in a UVData object, please visit http://pyuvdata.readthedocs.io/en/latest/uvdata_parameters.html. An example for how to interact with UVData objects in pyuvdata is available at http://pyuvdata.readthedocs.io/en/latest/tutorial.html.

Note that throughout the documentation, we assume a row-major convention (i.e., C-ordering) for the dimension specification of multi-dimensional arrays. For example, for a two-dimensional array with shape (N, M), the M-dimension is varying fastest, and is contiguous in memory. This convention is the same as Python and the underlying C-based HDF5 library. Users of languages with the opposite column-major convention (i.e., Fortran-ordering, seen also in MATLAB and Julia) must transpose these axes.

¹https://www.hdfgroup.org/

²https://github.com/HERA-Team/pyuvdata

³https://github.com/ska-sa/katdal

⁴https://github.com/telegraphic/fits2hdf

⁵https://www.h5py.org/

2 Overview

A UVH5 object contains the interferometric data from a radio telescope, as well as the associated metadata necessary to interpret it. A UVH5 file contains two primary HDF5 groups: the Header group, which contains the metadata, and the Data group, which contains the data itself, the flags, and information about the number of samples corresponding to the data. Datasets in the Data group are also typically passed through HDF5's compression pipeline, to reduce the amount of on-disk space required to store the data. However, because HDF5 is aware of any compression applied to a dataset, there is little that the user has to explicitly do when reading data. For users interested in creating new files, the use of compression is not strictly required by the UVH5 format, again because the HDF5 file is self-documenting in this regard. However, be warned that most UVH5 files "in the wild" typically feature compression of datasets in the Data group.

In the discussion below, we discuss required and optional datasets in the various groups. We note in parenthesis the corresponding attribute of a UVData object. Note that in nearly all cases, the names are coincident, to make things as transparent as possible to the user.

3 Header

The Header group of the file contains the metadata necessary to interpret the data. We begin with the required parameters, then continue to optional ones. Unless otherwise noted, all datasets are scalars (i.e., not arrays). The precision of the data type is also not specified as part of the format, because in general the user is free to set it according to the desired use case (and HDF5 records the precision and endianness when generating datasets). When using the standard h5py-based implementation in pyuvdata, this typically results in 32-bit integers and double precision floating point numbers. Each entry in the list contains (1) the exact name of the dataset in the HDF5 file, in boldface, (2) the expected datatype of the dataset, in italics, (3) a brief description of the data, and (4) the name of the corresponding attribute on a UVData object. Note that unlike in other formats, names of HDF5 datasets can be quite long, and so in most cases the name of the dataset corresponds to the name of the UVData attribute.

Note that string datatypes should be handled with care. See Appendix ?? for appropriately defining them for interoperability between different HDF5 implementations.

3.1 Required Parameters

- latitude: float The latitude of the telescope site, in degrees. (latitude)
- longitude: float The longitude of the telescope site, in degrees. (longitude)
- altitude: float The altitude of the telescope site, in meters. (altitude)

- **telescope_name**: *string* The name of the telescope used to take the data. The value is used to check that metadata is self-consistent for known telescopes in pyuvdata. (*telescope_name*)
- **instrument**: *string* The name of the instrument, typically the telescope name. (*instrument*)
- **object_name**: *string* The name of the object tracked by the telescope. For a drift-scan antenna, this is typically "zenith". (*object_name*)
- **history**: string The history of the data file. (history)
- **phase_type**: *string* The phase type of the observation. Should be "phased" or "drift". Note that "drift" in this context more accurately means "unphased", in that baselines are computing using ENU coordinates, without any w-projection. Any other value is treated as an unrecognized type. (*phase_type*)
- Nants_data: int The number of antennas that data in the file corresponds to. May be smaller than the number of antennas in the array. (Nants_data)
- Nants_telescope: int The number of antennas in the array. May be larger than the number of antennas with data corresponding to them. (Nants_telescope)
- ant_1_array: int An array of the first antenna numbers corresponding to baselines present in the data. All entries in this array must exist in the antenna_numbers array. This is a one-dimensional array of size Nblts. (ant_1_array)
- ant_2_array: int An array of the second antenna numbers corresponding to baselines present in the data. All entries in this array must exist in the antenna_numbers array. This is a one-dimensional array of size Nblts. (ant_2_array)
- antenna_numbers: int An array of the numbers of the antennas present in the radio telescope (note that these are not indices, they do not need to start at zero or be continuous). This is a one-dimensional array of size Nants_telescope. Note there must be one entry for every unique antenna in ant_1_array and ant_2_array, but there may be additional entries. (antenna_names)
- antenna_names: string An array of the names of antennas present in the radio telescope. This is a one-dimensional array of size Nants_telescope. Note there must be one entry for every unique antenna in ant_1_array and ant_2_array, but there may be additional entries. (antenna_names)
- **Nbls**: *int* the number of baselines present in the data. For full cross-correlation data (including auto-correlations), this should be Nants_data×(Nants_data+1)/2. (Nbls)

- **Nblts**: *int* The number of baseline-times (i.e., the number of spectra) present in the data. Note that this value need not be equal to Nbls × Ntimes. (Nblts)
- Nspws: int The number of spectral windows present in the data. (Nspws)
- Nfreqs: int The total number of frequency channels in the data across all spectral windows. (Nfreqs)
- **Npols**: int The number of polarization products in the data. (Npols)
- Ntimes: int The number of time samples present in the data. (Ntimes)
- uvw_array: float An array of the uvw-coordinates corresponding to each observation in the data. This is a two-dimensional array of size (Nblts, 3). Units are in meters. (uvw_array)
- **time_array**: *float* An array of the Julian Date corresponding to the center of an integration. This is a one-dimensional array of size Nblts. (*time_array*)
- **integration_time**: *float* An array of the length of time in seconds of an integration. This is a one-dimensional array of size Nblts. (*time_array*)
- **freq_array**: *float* An array of the frequencies stored in the file in Hertz. This is a one-dimensional array of size (Nfreqs). (*freq_array*)
- **channel_width**: *float* The width of frequency channels in the file in Hertz. This is a one-dimensional array of size (Nfreqs). (*channel_width*)
- spw_array : int An array of the spectral windows in the file. This is a one-dimensional array of size Nspws. (spw_array)
- flex_spw_id_array: int The mapping of individual channels along the frequency axis to individual spectral windows, as listed in the spw_array. This is a one-dimensional array of size (Nfreqs). (flex_spw_id_array)
- polarization_array: int An array of the polarizations contained in the file. This is a one-dimensional array of size Npols. Note that the polarizations should be stored as an integer, and use the convention defined in AIPS Memo 117. (polarization_array)
- antenna_positions: float An array of the antenna coordinates relative to the telescope location (in the ITRF frame), which is implicitly defined by the latitude, longitude, and altitude (LLA) parameters. The conversion between LLA and ECEF is given by WGS84. This is a two-dimensional array of size (Nants_telescope, 3). (antenna_positions)

- flex_spw: bool Whether the data are saved using flexible spectral windows. Following the convention above, this should always be True. See Sec. 5.2.2 for a discussion of historical files for which this was not true. (flex_spw)
- version: string The version of the HDF5 file. The latest version (and the one described in this memo) is Version 1.0. Note it should be a string, such as `1.0'. See Sec. 5 for the version history of the HDF5 specification. (version)

3.2 Optional Parameters

- dut1: float DUT1 (google it), in seconds. AIPS 117 calls it UT1UTC. (dut1)
- earth_omega: float Earth's rotation rate in degrees per day. Note the difference in units, which is inherited from the way this quantity is handled in UVFITS datasets (AIPS 117 calls it DEGPDY). (earth_omega)
- **gst0**: *float* Greenwich sidereal time at midnight on reference date, in degrees. AIPS 117 calls it GSTIAO (qst0)
- rdate: string Date for which GST0 (or whichever time saved in that field) applies. Note this is different from how UVFITS handles this quantity, which is saved as a float rather than a string. The user is encouraged to ensure it is being handled self-consistently for their desired application. (rdate)
- timesys: string Time system. pyuvdata currently only supports UTC. (timesys)
- **x_orientation**: *string* The orientation of the x-arm of a dipole antenna. It is assumed to be the same for all antennas in the dataset. For instance, "E" or "East" may be used. (*x_orientation*).
- antenna_diameters: float An array of the diameters of the antennas in meters. This is a one-dimensional array of size (Nants_telescope). (Nants_telescope)
- uvplane_reference_time: int The time at which the phase center is normal to the chosen UV plane for phasing. Used for interoperability with the FHD package⁶.
- **phase_center_ra**: *float* The right ascension of the phase center of the observation in radians. Required if phase_type is "phased". (*phase_center_ra*)
- **phase_center_dec**: *float* The declination of the phase center of the observation in radians. Required if phase_type is "phased". (*phase_center_dec*).
- **phase_center_epoch**: *float* The epoch year of the phase applied to the data (*e.g.*, 2000.). Required if phase_type is "phased". (*phase_center_epoch*)

⁶https://github.com/EoRImaging/FHD

- phase_center_frame: string The frame the data and uvw_array are phased to. Options are "gcrs" and "icrs", with default "icrs". These frames are defined as coordinate systems in astropy. (phase_center_frame)
- lst_array: float An array corresponding to the local sidereal time of the center of each observation in the data in units of radians. If it is not specified, it is calculated from the latitude/longitude and the time_array. Saving it in the file can be useful for files with many values in the time_array, which would expensive to recompute. (lst_array)

3.3 Extra Keywords

UVData objects support "extra keywords", which are additional bits of arbitrary metadata useful to carry around with the data but which are not formally supported as a reserved keyword in the Header. In a UVH5 file, extra keywords are handled by creating a datagroup called extra_keywords inside the Header datagroup. In a UVData object, extra keywords are expected to be scalars, but UVH5 makes no formal restriction on this. Also, when possible, these quantities should be HDF5 datatypes, to support interoperability between UVH5 readers. Inside of the extra_keywords datagroup, each extra keyword is saved as a key-value pair using a dataset, where the name of the extra keyword is the name of the dataset and its corresponding value is saved in the dataset. Though the use of HDF5 attributes can also be used to save additional metadata, it is not recommended, due to the lack of support inside of pyuvdata for ensuring the attributes are properly saved when writing out.

4 Data

In addition to the Header datagroup in the root namespace, there must be one called Data. This datagroup saves the visibility data, flags, and number of samples corresponding to each entry. All three datasets must be present in a valid UVH5 file. They are also all expected to be the same shape: (Nblts, Nfreqs, Npols). Note that due to the intermixing of the baseline and time axes, it is *not* required for data to exist for every baseline and time in the file. This behavior is similar to UVFITS and MIRIAD file formats. Also note that there is no explicit ordering required for the baseline-time axis. A common ordering is to write the data in "correlator order", and have all baselines for a single time t_i , followed by all baselines for the next time t_{i+1} , etc. However, this is merely a convention, and is not explicitly required for the UVH5 format.

4.1 Visdata Dataset

The visibility data is saved as a dataset named visdata. It should be a 3-dimensional, complex-type dataset with shape (Nblts, Nfreqs, Npols). Most commonly this is saved

as an 8-byte complex number (a 4-byte float for the real and imaginary parts), though some flexibility is possible. 16-byte complex floating point numbers (composed of two 8-byte floats), as well as 8-byte complex integers (two 4-byte signed integers), are also common. In all cases, a compound datatype is defined, with an `r' field and an `i' field, corresponding to the real and imaginary parts, respectively. The real and imaginary types must also be the same datatype. For instance, they should both be 8-byte floating point numbers, or 32-bit (4-byte) integers. Mixing datatypes between the real and imaginary parts is not allowed.

Using h5py, the datatype for visdata can be specified as `c8' (8-byte complex numbers, corresponding to the np.complex64 datatype) or `c16' (16-byte complex numbers, corresponding to the np.complex128 datatype) out-of-the-box, with no special handling by the user. h5py transparently handles the definition of the compound datatype. For examples of how to handle complex integer datatypes in h5py, see Appendix ??.

4.1.1 Conjugation Convention

A cross-correlation between two antennas is defined by the baseline connecting them, and the conjugation of one of the input data streams. Accordingly, the uvw coordinates and the conjugation of the visibility data are interconnected, based on the definition of one's coordinate system. For UVH5 files, it is assumed that the convention for the Radio Interferometer Measurement Equation (RIME) of a visibility \mathcal{V} for antennas i and j is as follows:

$$\mathcal{V}(u_j - u_i, v_j - v_i) = \int dl \, dm \, I(l, m) g_i(l, m) e^{-2\pi i (u_i l + v_i m)} g_j^*(l, m) e^{2\pi i (u_j l + v_j m)}.$$
(1)

That is, the baseline vector defined by the uvw coordinates is directed from antenna i to antenna j (so the baseline vector can be computed as $\mathbf{r_j} - \mathbf{r_i}$, where \mathbf{r} is the position vector of a given antennas), and the data corresponding to antenna j is conjugated. Note that if a file is generated with the opposite convention, it is usually sufficient to multiply uvw coordinates by -1 to generate a self-consistent dataset.

4.2 Flags Dataset

The flags corresponding to the data are saved as a dataset named flags. It is a 3-dimensional, boolean-type dataset with shape (Nblts, Nfreqs, Npols). Values of True correspond to instances of flagged data, and False is non-flagged. Note that the boolean type of the data is not the HDF5-provided H5T_NATIVE_HB00L, and instead is defined to conform to the h5py implementation of the numpy boolean type. When creating this dataset from h5py, one can specify the datatype as np.bool. Behind the scenes, this defines an HDF5 enum datatype. See Appendix ?? for an example of how to write a compatible dataset from C.

As with the nsamples dataset discussed below, compression is typically applied to the flags dataset. The LZF filter (included in all HDF5 libraries) provides a good compromise between speed and compression. In the special cases of single-valued arrays, the dataset occupies virtually no disk space.

4.3 Nsamples Dataset

The number of data points averaged into each data entry is saved as a dataset named nsamples. It is a 3-dimensional, floating-point type dataset with shape (Nblts, Nfreqs, Npols). Note that it is not required to be an integer, and should not be saved as an integer type. The product of the integration_time array and the data in the nsample array reflects the total amount of time that went into a visibility. The best practice is for the nsamples dataset to track flagging within an integration time (leading to a decrease of the nsamples array value to be less than 1) and LST averaging (leading to an increase in the nsamples array value). Datasets that have not been LST averaged should have values in nsamples that are less than or equal to 1. Although this convention is not adhered to by all data formats serviced by pyuvdata, it is recommended to follow it as closely as possible in UVH5 files. What should be true is the product of the integration_time array and nsamples array corresponding to the total amount of time included in a visibility.

5 Version History

The UVH5 specification has been through several minor version updates, and in the interest of maximizing interoperability between different readers and writers external to pyuvdata, it is useful to define a version history. This is not a strict semantic versioning scheme, but instead intended to capture some of the important changes that the specification has gone through. Note that, as much as possible, pyuvdata intends to be fully compatible, and be able to read any valid UVH5 file written. Those interested in writing fully compatible readers/writers may look there for further details.

5.1 version dataset

When present, the version information is stored in the Header as a string-based dataset with the key version. Note that files have not always contained this dataset, but as much as possible, new files written should contain this dataset to clarify.

5.2 Version 0.x/0.1

Historically, UVH5 files written by pyuvdata and the HERA correlator did not include the version dataset as part of the header. Implicitly, these files are v0.x. More recently, pyuvdata has begun writing the version information to files, and so the version dataset is present in these files. Below, we discuss some of the changes that occurred within the Version 0.1 generation, to make users aware of the different flavors of UVH5 files they may encounter "in the wild."

5.2.1 integration_time dataset

Initially, UVH5 files were written with a single value for integration_time. It has since been modified to its current length of Nblts to allow for data with varying integration time between time samples or baselines.

5.2.2 Flexible Spectral Windows

A significant update to how the frequency axis was handled in UVData objects was implemented to allow for a more flexible handling of data from different spectral windows. Initially, inspired by the handling of multiple spectral windows in UVFITS files, the spectral window (spw) axis was treated as a separate axis in metadata and data arrays. However, this approach is relatively inflexible, because it requires all spectral windows to have the same number of frequency channels to efficiently store the data (the alternatives being to use ragged-length arrays, which are inefficient for storing or accessing the data, or padded arrays which can contain a large amount of wasted storage to ensure arrays are regularly spaced).

To overcome these limitations, taking inspiration from how frequency data are stored in MIRIAD, the idea of "flexible spectral windows" was adopted to save the frequency information. Analogously to how baselines and times are collapsed to a "baseline-time axis", frequencies and spectral windows are collapsed to a "frequency-spectral window" axis. This allows for more versatility in how data from different spectral windows are stored inside of a single file, but it requires the change of several important components of metadata. We summarize these changes here.

- The value for Nfreqs is the total number of frequency channels saved in the data across all spectral windows.
- Where required, the number of spectral windows Nspws is required to be 1.
- The channel_width dataset was changed from a single number to a 1-d array of length Nfreqs.
- The flex_spw_id_array dataset was added to identify which spectral window a given channel belongs.
- The flex_spw dataset was added to identify whether the file in question supports flexible spectral windows (if True) or not (if False).

Although both kinds of datasets (with or without flexible spectral windows) are supported by the UVH5 specification, it is preferred that they be saved with flexible spectral windows, even in the case where there is a single spectral window. This helps standardize the UVH5 format going forward, while being backwards compatible with legacy files.

5.3 Version 1.0

5.3.1 Rank-3 Array Convention

Version 1.0 of UVH5 represents a significant change in the way that the data arrays (visdata, flags, and nsamples) and metadata arrays are stored. The previously vestigial spectral-window axis is removed, meaning that data arrays are rank-3 instead of rank-4. Explicitly, these arrays have shape (Nblts, Nfreqs, Npols), where Nfreqs includes the number of channels across all spectral windows. The description of data and metadata in the body of this memo assumes the Version 1.0 specification. Although pyuvdata plans to indefinitely support files written with the previous convention (i.e., having an explicit spectral window-axis), UVH5 files should be written such that they conform to Version 1.0.

Appendix A Writing Strings from h5py

String datatypes are finicky, and require special handling to ensure that they are compatible with the HDF5 bindings in various languages. This is especially true for files written from h5py, which handles strings differently between python2 and python3. Though python2 is nearing its end-of-life, UVH5 should be backwards compatible with older versions of h5py as much as possible. To help service this, all string-type metadata in UVH5 files must be fixed-length ASCII type. Not only does this allow for interoperability between different h5py versions, but it also ensures that strings can be round-tripped through other HDF5 bindings, such as those in C, MATLAB, IDL, Fortran⁷, etc. Note that the string should use one byte per character, and be null-terminated. This corresponds to the numpy S datatype in both versions of python2 and python3.

When writing a string-like dataset from h5py, scalar data should be written by casting a string to a numpy.string_ object. Array data should be written as a S<n> dataset, where <n> represents the length of the strings to be saved. Upon reading, strings can be cast to bytes using the tostring() method, at which point the data is <str>-type (python2) or can be decoded as UTF-8 to become <str>-type (python3).

Below is an example for how to read and write string scalar and array-type datasets using h5py in python2 and python3.

A.1 python2

```
import numpy as np
import h5py
# open file and write string datasets
with h5py.File('test_file.uvh5', 'w') as f:
    header = f.create_group('Header')
    # scalar dataset
    header['scalar_string'] = np.string_('Hello world!')
    # array dataset
    str_array = np.array(['hello', 'world'])
    n_words = len(str_array)
    max_len_words = np.amax([len(n) for n in str_array])
    dtype = "S{:d}".format(max_len_words)
    header.create_dataset('array_string', (n_words,), dtype=dtype,
                          data=str_array)
# read the data back in again
with h5py.File('test_file.uvh5', 'r') as f:
```

⁷Strings in Fortran are not null-terminated, so these require special handling.

```
header = f['Header']
    # read scalar dataset
   scalar_string = header['scalar_string'].value.tostring()
   assert scalar_string == 'Hello world!'
   # read array dataset
   str_array_file = [n.tostring() for n in header['array_string'].value]
   assert np.all(str_array_file == str_array)
A.2 python3
import numpy as np
import h5py
# open file and write string datasets
with h5py.File('test_file.uvh5', 'w') as f:
   header = f.create_group('Header')
   # scalar dataset
   header['scalar_string'] = np.string_('Hello world!')
   # array dataset
   str_array = ['hello', 'world']
   header['array_string'] = np.string_(str_array)
# read the data back in again
with h5py.File('test_file.uvh5', 'r') as f:
   header = f['Header']
    # read scalar dataset
   scalar_string = header['scalar_string'].value.tostring().decode('UTF-8')
   assert scalar_string == 'Hello world!'
   # read array dataset
   str_array_file = [n.tostring().decode('UTF-8')
                      for n in header['array_string'].value]
   assert np.all(str_array_file == str_array)
```

Appendix B Integer Datatype Support for Visibility Data

The HERA correlator writes datasets which have 32-bit integer real and imaginary components. Due to the self-describing nature of HDF5 datasets, this information is captured by the file format. Nevertheless, special handling must be used to interpret these datasets

as complex numbers. The astype context manager in h5py is used to convert the datatype on the fly from integers to complex numbers. Below is an example of how to do this.

```
import numpy as np
import h5py
# define integer datatype
int_dtype = np.dtype([('r', '<i4'), ('i', '<i4')])
# open file and read in the dataset
with h5py.File('test_file.uvh5', 'r') as f:
    visdata = f['Data/visdata']
    dshape = visdata.shape
    data = np.empty(dshape, dtype=np.complex128)
    with visdata.astype(int_dtype):
        data.real = visdata['r'][:, :, :]
        data.imag = visdata['i'][:, :, :]</pre>
```

Appendix C Defining numpy Boolean Arrays in C

As mentioned in Sec. 4.2, the flags array in a UVH5 file uses an HDF5 enum datatype to encode the numpy boolean type. When creating such a datatype using h5py, the user simply needs to ensure the datatype is np.bool. The building of the enum is transparent. When building the enum from a different language, the precise specification is necessary to ensure compatibility. The following code is a template for how to build the appropriate datatype using C. The construction in other languages, such as Fortran, should follow analogously.

```
#include <hdf5.h>
#define CPTR(VAR,CONST) ((VAR)=(CONST),&(VAR))

typedef enum {
   FALSE,
   TRUE
} bool_t;

int main() {
   bool_t val;
   static hid_t boolenumtype;
   hid_t file_id, dspace_id, flags_id;
   herr_t status;
```

```
/* define enum type */
boolenumtype = H5Tcreate(H5T_ENUM, sizeof(bool_t));
H5Tenum_insert(boolenumtype, "FALSE", CPTR(val, FALSE));
H5Tenum_insert(boolenumtype, "TRUE" , CPTR(val, TRUE ));
/* open a new file */
file_id = H5Fcreate("test_file.h5", H5F_ACC_TRUNC, H5P_DEFAULT, H5P_DEFAULT);
/* define array dimensions */
int Nblts = 10;
int Nfreqs = 16;
int Npols = 4;
hsize_t dims[3] = {Nblts, Nfreqs, Npols};
/* initialize data array with FALSE values */
bool_t data[Nblts][Nfreqs][Npols];
for (int i=0; i<Nblts; i++) {</pre>
  for (int j=0; k<Nfreqs; j++) {</pre>
    for (int k=0; l<Npols; k++) {</pre>
      data[i][j][k] = FALSE;
    }
 }
}
/* make dataspace and write out data */
dspace_id = H5Screate_simple(3, dims, dims);
flags_id = H5Dcreate(file_id, "flags", boolenumtype, dspace_id,
                     H5P_DEFAULT, H5P_DEFAULT, H5P_DEFAULT);
status = H5Dwrite(flags_id, boolenumtype, H5S_ALL, H5S_ALL,
                  H5P_DEFAULT, data);
/* close down */
H5Dclose(flags_id);
H5Sclose(dspace_id);
H5Fclose(file_id);
return 0;
```

}