The Advanced Scientific Data Format (ASDF): An Update

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Abstract—We report on progress in developing and extending the new (ASDF) format we have developed for the data from the James Webb and Nancy Grace Roman Space Telescopes since we reported on it at a previous Scipy. While the format was developed as a replacement for the long-standard FITS format used in astronomy, it is quite generic and not restricted to use with astronomical data. We will briefly review the format, and extensions and changes made to the standard itself, as well as to the reference Python implementation we have developed to support it. The standard itself has been clarified in a number of respects. Recent improvements to the Python implementation include an improved framework for conversion between complex Python objects and ASDF, better control of the configuration of extensions supported and versioning of extensions, tools for display and searching of the structured metadata, better developer documentation, tutorials, and a more maintainable and flexible schema system. This has included a reorganization of the components to make the standard free from astronomical assumptions. A important motivator for the format was the ability to support serializing functional transforms in multiple dimensions as well as expressions built out of such transforms, which has now been implemented. More generalized compression schemes are now enabled. We are currently working on adding chunking support and will discuss our plan for further enhancements.

Index Terms—data formats, standards, world coordinate systems, yaml

Introduction

The Advanced Scientific Data Format (ASDF) was originally developed in 2015. That original version was described in a paper [Gre15]. That paper described the shortcomings of the widely used astronomical standard format FITS [FIT16] as well as those of existing potential alternatives. It is not the goal of this paper to rehash those points in detail, though it is useful to summarize the basic points here. The remainder of this paper will describe where we are using ASDF, what lessons we have learned from using ASDF for the James Webb Space Telescope, and summarize the most important changes we have made to the standard, the Python library that we use to read and write ASDF files, and best practices for using the format.

We will give an example of a more advanced use case that illustrates some of the powerful advantages of ASDF, and that its application is not limited to astronomy, but suitable for much of scientific and engineering data, as well as models. We finish by outlining our near term plans for further improvements and extensions.

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Summary of Motivations

- Suitable as an archival format:
  - Old versions continue to be supported by libraries.
  - Format is sufficiently transparent (e.g., not requiring extensive documentation to decode) for the fundamental set of capabilities.
  - Metadata is easily viewed with any text editor.
- Intrinsically hierarchical
- Avoids duplication of shared items
- Based on existing standard(s) for metadata and structure
- No tight constraints on attribute lengths or their values.
- Clearly versioned
- Supports schemas for validating files for basic structure and value requirements
- Easily extensible, both for the standard, and for local or domain-specific conventions.

Basics of ASDF Format

- Format consists of a YAML header optionally followed by one or more binary blocks for containing binary data.
- The YAML [http://yaml.org] header contains all the metadata and defines the structural relationship of all the data elements.
- YAML tags are used to indicate to libraries the semantics of subsections of the YAML header that libraries can use to construct special software objects. For example, a tag for a data array would indicate to a Python library to convert it into a numpy array.
- YAML anchors and alias are used to share common elements to avoid duplication.
- JSON Schema [http://json-schema.org/specification.html], [http://json-schema.org/understanding-json-schema/] is used for schemas to define expectations for tag content and whole headers combined with tools to validate actual ASDF files against these schemas.
- Binary blocks are referenced in the YAML to link binary data to YAML attributes.
- Support for arrays embedded in YAML or in a binary block.

- Streaming support for a single binary block.
- Permit local definitions of tags and schemas outside of the standard.
- While developed for astronomy, useful for general scientific or engineering use.
- Aims to be language neutral.

Current and planned uses

James Webb Space Telescope (JWST)

NASA requires JWST data products be made available in the FITS format. Nevertheless, all the calibration pipelines operate on the data using an internal objects very close to the the ASDF representation. The JWST calibration pipeline uses ASDF to serialize data that cannot be easily represented in FITS, such as World Coordinate System information. The calibration software is also capable of reading and producing data products as pure ASDF files.

Nancy Grace Roman Space Telescope

This telescope, with the same mirror size as the Hubble Space Telescope (HST), but a much larger field of view than HST, will be launched in 2026 or thereabouts. It is to be used mostly in survey mode and is capable of producing very large mosaicked images. It will use ASDF as its primary data format.

Daniel K Inoue Solar Telescope

This telescope is using ASDF for much of the early data products to hold the metadata for a combined set of data which can involve many thousands of files. Furthermore, the World Coordinate System information is stored using ASDF for all the referenced data.

Vera Rubin Telescope (for World Coordinate System interchange)

There have been users outside of astronomy using ASDF, as well as contributors to the source code.

Changes to the standard (completed and proposed)

These are based on lessons learned from usage.

The current version of the standard is 1.5.0 (1.6.0 being developed).

The following items reflect areas where we felt improvements were needed.

Changes for 1.5

Moving the URI authority from `stsci.edu` to `asdf-format.org`

This is to remove the standard from close association with STScI and make it clear that the format is not intended to be controlled by one institution.

Moving astronomy-specific schemas out of standard

These primarily affect the previous inclusion of World Coordinate Tags, which are strongly associated with astronomy. Remaining are those related to time and unit standards, both of obvious generality, but the implementation must be based on some standards, and currently the astropy-based ones are as good or better than any.

Changes for 1.6

Addition of the manifest mechanism

The manifest is a YAML document that explicitly lists the tags and other features introduced by an extension to the ASDF standard. It provides a more straightforward way of associating tags with schemas, allowing multiple tags to share the same schema, and generally making it simpler to visualize how tags and schemas are associated (previously these associations were implied by the Python implementation but were not documented elsewhere).

Handling of null values and their interpretation

The standard didn't previously specify the behavior regarding null values. The Python library previously removed attributes from the YAML tree when the corresponding Python attribute has a `None` value upon writing to an ADSF file. On reading files where the attribute was missing but the schema indicated a default value, the library would create the Python attribute with the default. As mentioned in the next item, we no longer use this mechanism, and now when written, the attribute appears in the YAML tree with a null value if the Python value is `None` and the schema permits null values.

Interpretation of default values in schema

The use of default values in schemas is discouraged since the interpretation by libraries is prone to confusion if the assemblage of schemas conflict with regard to the default. We have stopped using defaults in the Python library and recommend that the ASDF file always be explicit about the value rather than imply it through the schema. If there are practical cases that preclude always writing out all values (e.g., they are only relevant to one mode and usually are irrelevant), it should be the library that manages whether such attributes are written conditionally rather using the schema default mechanism.

Add alternative tag URI scheme

We now recommend that tag URIs begin with `asdf://`

Be explicit about what kind of complex YAML keys are supported

For example, not all legal YAML keys are supported. Namely YAML arrays, which are not hashable in Python. Likewise, general YAML objects are not either. The Standard now limits keys to string, integer, or boolean types. If more complex keys are required, they should be encoded in strings.

Still to be done

Upgrade to JSON Schema draft-07

There is interest in some of the new features of this version, however, this is problematic since there are aspects of this version that are incompatible with *draft-04*, thus requiring all previous schemas to be updated.

Replace extensions section of file history

This section is considered too specific to the concept of Python extensions, and is probably best replaced with a more flexible system for listing extensions used.

Changes to Python ASDF package

Easier and more flexible mechanism to create new extensions (2.8.0)

The previous system for defining extensions to ASDF, now deprecated, has been replaced by a new system that makes the association between tags, schemas, and conversion code more straightforward, as well as providing more intuitive names for the methods and attributes, and makes it easier to handle reference cycles if they are present in the code (also added to the original Tag handling classes).

Introduced global configuration mechanism (2.8.0)

This reworks how ASDF resources are located, and makes it easier to update the current configuration, as well as track down the location of the needed resources (e.g., schemas and converters), as well as removing performance issues that previously required extracting information from all the resource files thus slowing the first `asdf.open` call.

Added `info/search` methods and command line tools (2.6.0)

These allow displaying the hierarchical structure of the header and the values and types of the attributes. Initially, such introspection stopped at any tagged item. A subsequent change provides mechanisms to see into tagged items (next item). An example of these tools is shown in a later section.

Added mechanism for info to display tagged item contents (2.9.0)

This allows the library that converts the YAML to Python objects to expose a summary of the contents of the object by supplying an optional "dunder" method that the info mechanism can take advantage of.

Added documentation on how ASDF library internals work

These appear in the readthedocs under the heading "Developer Overview".

Plugin API for block compressors (2.8.0)

This enables a localized extension to support further compression options.

Support for `asdf://` URI scheme (2.8.0)

Support for ASDF Standard 1.6.0 (2.8.0)

This is still subject to modifications to the 1.6.0 standard.

Modified handling of defaults in schemas and `None` values (2.8.0)

As described previously.

Using ASDF to store models

This section highlights one aspect of ASDF that few other formats support in an archival way, e.g., not using a language-specific mechanism, such as Python's pickle. The astropy package contains a modeling subpackage that defines a number of analytical, as well as a few table-based, models that can be combined in many ways, such as arithmetically, in composition, or multi-dimensional. Thus it is possible to define fairly complex multi-dimensional models, many of which can use the built in fitting machinery.

These models, and their compound constructs can be saved in ASDF files and later read in to recreate the corresponding astropy objects that were used to create the entries in the ASDF file. This is made possible by the fact that expressions of models are straightforward to represent in YAML structure.

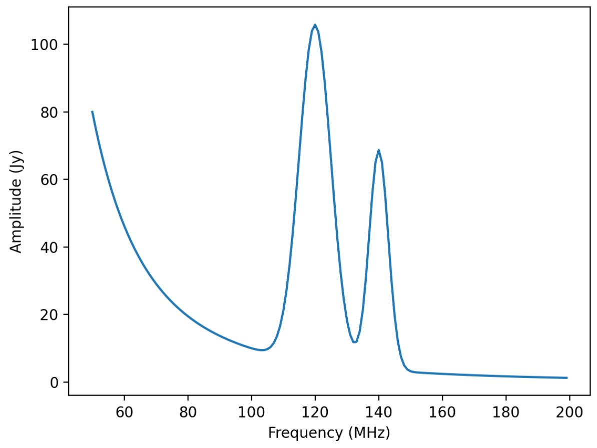


Fig. 1: *A plot of the compound model defined in the first segment of code.*

Despite the fact that the models are in some sense executable, they are perfectly safe so long as the library they are implemented in is safe (e.g., it doesn't implement an "execute any OS command" model). Furthermore, the representation in ASDF does not explicitly use Python code. In principle it could be written or read in any computer language.

The following illustrates a relatively simple but not trivial example.

First we define a 1D model and plot it.

```python
import numpy as np
import astropy.modeling.models as amm
import astropy.units as u
import asdf
from matplotlib import pyplot as plt

# Define 3 model components with units
g1 = amm.Gaussian1D(amplitude=100*u.Jy,
                    mean=120*u.MHz,
                    stddev=5.*u.MHz)
g2 = amm.Gaussian1D(65*u.Jy, 140*u.MHz, 3*u.MHz)
powerlaw = amm.PowerLaw1D(amplitude=10*u.Jy,
                          x_0=100*u.MHz,
                          alpha=3)
# Define a compound model
model = g1 + g2 + powerlaw
x = np.arange(50, 200) * u.MHz
plt.plot(x, model(x))
```

The following code will save the model to an ASDF file, and read it back in

```python
af = asdf.AsdfFile()
af.tree = {'model': model}
af.write_to('model.asdf')
af2 = asdf.open('model.asdf')
model2 = af2['model']
model2 is model
    False
model2(103.5) == model(103.5)
    True
```

Listing the relevant part of the ASDF file illustrates how the model has been saved in the YAML header (reformatted to fit in this paper column).

```
model: !transform/add-1.2.0
  forward:
```

```
  - !transform/add-1.2.0
    forward:
    - !transform/gaussian1d-1.0.0
      amplitude: !unit/quantity-1.1.0
        {unit: !unit/unit-1.0.0 Jy, value: 100.0}
      bounding_box:
      - !unit/quantity-1.1.0
        {unit: !unit/unit-1.0.0 MHz, value: 92.5}
      - !unit/quantity-1.1.0
        {unit: !unit/unit-1.0.0 MHz, value: 147.5}
      bounds:
        stddev: [1.1754943508222875e-38, null]
      inputs: [x]
      mean: !unit/quantity-1.1.0
        {unit: !unit/unit-1.0.0 MHz, value: 120.0}
      outputs: [y]
      stddev: !unit/quantity-1.1.0
        {unit: !unit/unit-1.0.0 MHz, value: 5.0}
    - !transform/gaussian1d-1.0.0
      amplitude: !unit/quantity-1.1.0
        {unit: !unit/unit-1.0.0 Jy, value: 65.0}
      bounding_box:
      - !unit/quantity-1.1.0
        {unit: !unit/unit-1.0.0 MHz, value: 123.5}
      - !unit/quantity-1.1.0
        {unit: !unit/unit-1.0.0 MHz, value: 156.5}
      bounds:
        stddev: [1.1754943508222875e-38, null]
      inputs: [x]
      mean: !unit/quantity-1.1.0
        {unit: !unit/unit-1.0.0 MHz, value: 140.0}
      outputs: [y]
      stddev: !unit/quantity-1.1.0
        {unit: !unit/unit-1.0.0 MHz, value: 3.0}
    inputs: [x]
    outputs: [y]
  - !transform/power_law1d-1.0.0
    alpha: 3.0
    amplitude: !unit/quantity-1.1.0
      {unit: !unit/unit-1.0.0 Jy, value: 10.0}
    inputs: [x]
    outputs: [y]
    x_0: !unit/quantity-1.1.0
      {unit: !unit/unit-1.0.0 MHz, value: 100.0}
  inputs: [x]
  outputs: [y]
...
```

Note that there are extra pieces of information that define the model more precisely. These include:

- many tags indicating special items. These include different kinds of transforms (i.e., functions), quantities (i.e., numbers with units), units, etc.
- definitions of the units used.
- indications of the valid range of the inputs or parameters (bounds)
- each function shows the mapping of the inputs and the naming of the outputs of each function.
- the addition operator is itself a transform.

Without the use of units, the YAML would be simpler. But the point is that the YAML easily accommodates expression trees. The tags are used by the library to construct the astropy models, units and quantities as Python objects. However, nothing in the above requires the library to be written in Python.

This machinery can handle multidimensional models and supports both the combining of models with arithmetic operators as well as pipelining the output of one model into another. This system has been used to define complex coordinate transforms from telescope detectors to sky coordinates for imaging, and wavelengths for spectrographs, using over 100 model components, something that the FITS format had no hope of managing, nor any other scientific format that we are aware of.

Displaying the contents of ASDF files

Functionality has been added to display the structure and content of the header (including data item properties), with a number of options of what depth to display, how many lines to display, etc. An example of the info use is shown in Figure 2.

There is also functionality to search for items in the file by attribute name and/or values, also using pattern matching for either. The search results are shown as attribute paths to the items that were found.

ASDF Extension/Converter System

There are a number of components that are involved. Converters encapsulate the code that handles converting Python objects to and from their ASDF representation. These are classes that inherit from the basic `Converter` class and define two Class attributes: tags, types each of which is a list of associated tag(s) and class(es) that the specific converter class will handle (each converter can handle more than one tag type and more than one class). The ASDF machinery uses this information to map tags to converters when reading ASDF content, and to map types to converters when saving these objects to an ASDF file.

Each converter class is expected to supply two methods: `to_yaml_tree` and `from_yaml_tree` that construct the YAML content and convert the YAML content to Python class instances respectively.

A manifest file is used to associate tags and schema ID's so that if a schema has been defined, that the ASDF content can be validated against the schema (as well as providing extra information for the ASDF content in the info command). Normally the converters and manifest are registered with the ASDF library using standard functions, and this registration is normally (but is not required to be) triggered by use of Python entry points defined in the `setup.cfg` file so that this extension is automatically recognized when the extension package is installed.

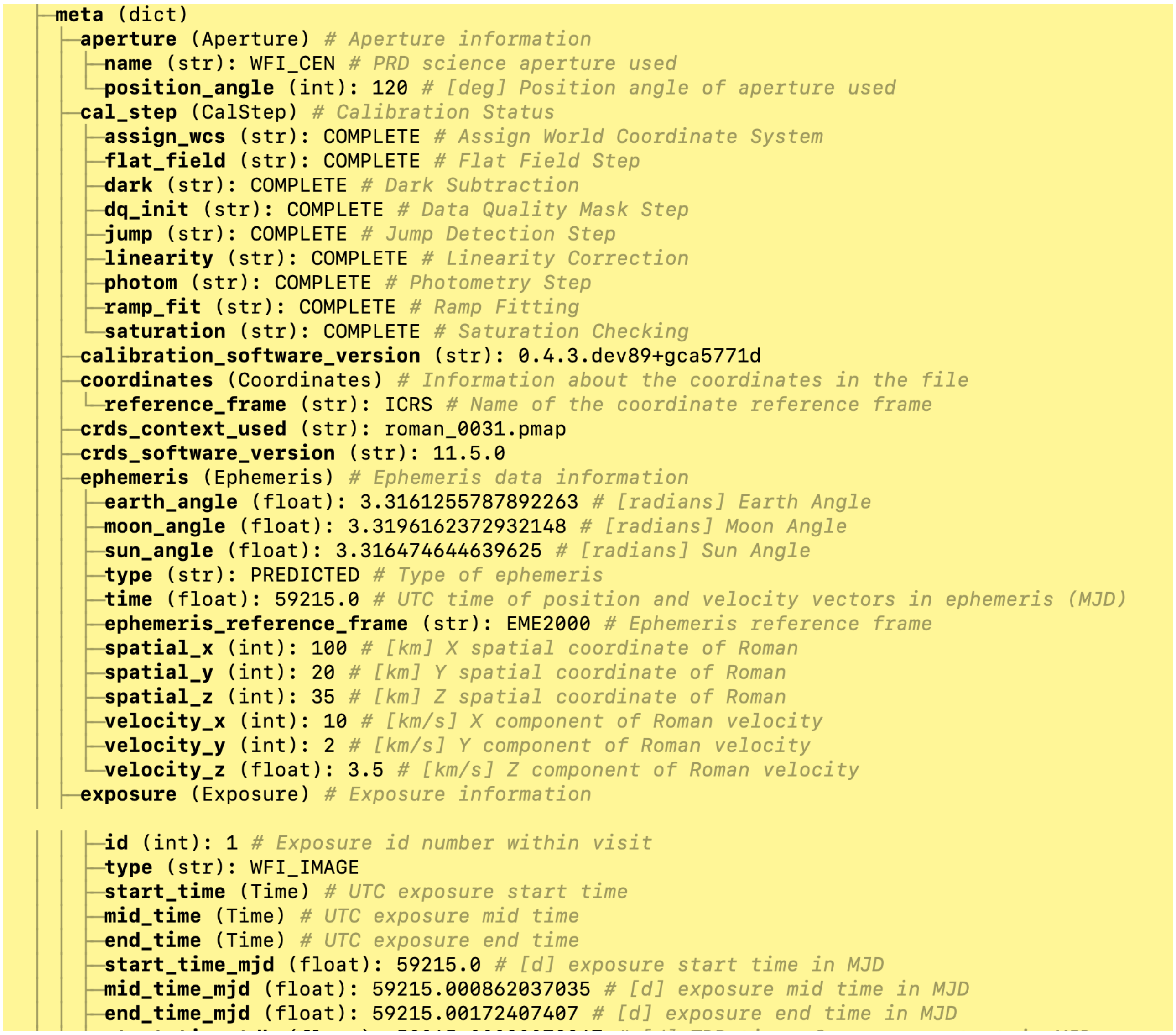
One can of course write their own custom code to convert the contents of ASDF files however they want. The advantage of the tag/converter system is that the objects can be anywhere in the tree structure and be properly saved and recovered without having any implied knowledge of what attribute or location the object is at. Furthermore, it brings with it the ability to validate the contents by use of schema files.

Jupyter tutorials that show how to use converters can be found at:

- https://github.com/asdf-format/tutorials/blob/master/Your_first_ASDF_converter.ipynb
- https://github.com/asdf-format/tutorials/blob/master/Your_second_ASDF_converter.ipynb

ASDF Roadmap for STScI Work

The planned enhancements to ASDF are understandably focussed on the needs of STScI missions. Nevertheless, we are particularly interested in areas that have wider benefit to the general scientific and engineering community, and such considerations increase the priority of items necessary to STScI. Furthermore, we are eager to aid others working on ASDF by providing advice, reviews, and



```
├─meta (dict)
│ ├─aperture (Aperture) # Aperture information
│ │ ├─name (str): WFI_CEN # PRD science aperture used
│ │ └─position_angle (int): 120 # [deg] Position angle of aperture used
│ ├─cal_step (CalStep) # Calibration Status
│ │ ├─assign_wcs (str): COMPLETE # Assign World Coordinate System
│ │ ├─flat_field (str): COMPLETE # Flat Field Step
│ │ ├─dark (str): COMPLETE # Dark Subtraction
│ │ ├─dq_init (str): COMPLETE # Data Quality Mask Step
│ │ ├─jump (str): COMPLETE # Jump Detection Step
│ │ ├─linearity (str): COMPLETE # Linearity Correction
│ │ ├─photom (str): COMPLETE # Photometry Step
│ │ ├─ramp_fit (str): COMPLETE # Ramp Fitting
│ │ └─saturation (str): COMPLETE # Saturation Checking
│ ├─calibration_software_version (str): 0.4.3.dev89+gca5771d
│ ├─coordinates (Coordinates) # Information about the coordinates in the file
│ │ └─reference_frame (str): ICRS # Name of the coordinate reference frame
│ ├─crds_context_used (str): roman_0031.pmap
│ ├─crds_software_version (str): 11.5.0
│ ├─ephemeris (Ephemeris) # Ephemeris data information
│ │ ├─earth_angle (float): 3.3161255787892263 # [radians] Earth Angle
│ │ ├─moon_angle (float): 3.3196162372932148 # [radians] Moon Angle
│ │ ├─sun_angle (float): 3.316474644639625 # [radians] Sun Angle
│ │ ├─type (str): PREDICTED # Type of ephemeris
│ │ ├─time (float): 59215.0 # UTC time of position and velocity vectors in ephemeris (MJD)
│ │ ├─ephemeris_reference_frame (str): EME2000 # Ephemeris reference frame
│ │ ├─spatial_x (int): 100 # [km] X spatial coordinate of Roman
│ │ ├─spatial_y (int): 20 # [km] Y spatial coordinate of Roman
│ │ ├─spatial_z (int): 35 # [km] Z spatial coordinate of Roman
│ │ ├─velocity_x (int): 10 # [km/s] X component of Roman velocity
│ │ ├─velocity_y (int): 2 # [km/s] Y component of Roman velocity
│ │ └─velocity_z (float): 3.5 # [km/s] Z component of Roman velocity
│ ├─exposure (Exposure) # Exposure information

│ │ ├─id (int): 1 # Exposure id number within visit
│ │ ├─type (str): WFI_IMAGE
│ │ ├─start_time (Time) # UTC exposure start time
│ │ ├─mid_time (Time) # UTC exposure mid time
│ │ ├─end_time (Time) # UTC exposure end time
│ │ ├─start_time_mjd (float): 59215.0 # [d] exposure start time in MJD
│ │ ├─mid_time_mjd (float): 59215.000862037035 # [d] exposure mid time in MJD
│ │ ├─end_time_mjd (float): 59215.00172407407 # [d] exposure end time in MJD
```

Fig. 2: *This shows part of the output of the info command that shows the structure of a Roman Space Telescope test file (provided by the Roman Telescopes Branch at STScI). Displayed is the relative depth of the item, its type, value, and a title extracted from the associated schema to be used as explanatory information.*

possibly collaborative coding effort. STScI is committed to the long-term support of ADSF.

The following is a list of planned work, in order of decreasing priority.

Chunking Support

Since the Roman mission is expected to deal with large data sets and mosaicked images, support for chunking is considered essential. We expect to layer the support in our Python library on `zarr` [https://zarr.dev/], with two different representations, one where all data is contained within the ADSF file in separate blocks, and one where the blocks are saved in individual files. Both representations have important advantages and use cases.

Improvements to binary block management

These enhancements are needed to enable better chunking support and other capabilities.

Redefining versioning semantics

Previously the meaning of different levels of versioning were unclear. The normal inclination is to treat schema version using the typical semantic versioning system defined for software. But schemas are not software and we are inclined to use the proposed system for schemas [url: https://snowplowanalytics.com/blog/2014/05/13/introducing-schemaver-for-semantic-versioning-of-schemas/] To summarize: in this case the three levels of versioning correspond to:

Model.Revision.Addition where a schema change:

- [Model] prevents working with historical data
- [Revision] may prevent working with historical data
- [Addition] is compatible with all historical data

Integration into astronomy display tools

It is essential that astronomers be able to visualize the data contained within ASDF files conveniently using the commonly available tool, such as SAOImage DS9 [Joy03] and Ginga [Jes13].

Cloud optimized storage

Much of the future data processing operations for STScI are expected to be performed on the cloud, so having ASDF efficiently support such uses is important. An important element of this is making the format work efficiently with object storage services such as AWS S3 and Google Cloud Storage.

IDL support

While Python is rapidly surpassing the use of IDL in astronomy, there is still much IDL code being used, and many of those still using IDL are in more senior and thus influential positions (they aren't quite dead yet). So making ASDF data at least readable to IDL is a useful goal.

Support Rice compression

Rice compression [Pen09], [Pen10] has proven a useful lossy compression algorithm for astronomical imaging data. Supporting it will be useful to astronomers, particularly for downloading large imaging data sets.

Pandas Dataframe support

Pandas [McK10] has proven to be a useful tool to many astronomers, as well as many in the sciences and engineering, so support will enhance the uptake of ASDF.

Compact, easy-to-read schema summaries

Most scientists and even scientific software developers tend to find JSON Schema files tedious to interpret. A more compact, and intuitive rendering of the contents would be very useful.

Independent implementation

Having ASDF accepted as a standard data format requires a library that is divorced from a Python API. Initially this can be done most easily by layering it on the Python library, but ultimately there should be an independent implementation which includes support for C/C++ wrappers. This is by far the item that will require the most effort, and would benefit from outside involvement.

Provide interfaces to other popular packages

This is a catch all for identifying where there would be significant advantages to providing the ability to save and recover information in the ASDF format as an interchange option.

Sources of Information

- ASDF Standard: https://asdf-standard.readthedocs.io/en/latest/
- Python ASDF package documentation: https://asdf.readthedocs.io/en/stable/
- Repository: https://github.com//asdf-format/asdf
- Tutorials: https://github.com/asdf-format/tutorials

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