

The Hubble Space Telescope (HST) Advanced Camera for Surveys (ACS) Quicklook Project

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Abstract—The Hubble Space Telescope (HST) Advanced Camera for Surveys (ACS) instrument has been acquiring thousands of astronomical images each year since its installation in 2002 and subsequent restoration in 2009. The ACS Quicklook Project (`acsq1`) provides a means for users to discover and interact with these data via a database-driven web application. This is accomplished via several `acsq1` components: (1) A ~ 40 TB network file system, which stores all on-orbit ACS data files on disk, (2) a `MySQL` database, which stores observational metadata in a normalized relational form, allowing users to build custom datasets based on observational parameters, (3) A `Python/Flask`-based web application, which allows users to view “Quicklook” JPEG images of any publicly-available ACS data along with its metadata, and (4) a `Python` code library, which provides a platform on which users can build automated instrument calibration and monitoring routines. The `acsq1` project may be extended to support the forthcoming James Webb Space Telescope (JWST) mission, which is scheduled to launch in 2018.

1 INTRODUCTION

The Advanced Camera for Surveys (ACS) is a third-generation imaging instrument on board the Hubble Space Telescope (HST), installed in 2002 during Servicing Mission 3B. It is comprised of three detectors: (1) the Wide Field Camera (WFC), which is designed for wide-field imaging and spectroscopy in visible to near-infrared wavelengths, (2) the High Resolution Channel, which is designed for high resolution near-ultraviolet to near-infrared wavelength images and coronagraphy, and (3) the Solar Blind Channel (SBC), designed for far-ultraviolet imaging and spectroscopy. ACS experienced an electronics failure in 2007 that affected the WFC and HRC detectors, until 2009 when astronauts successfully restored the WFC detector during Servicing Mission 4; the HRC still remains unoperational.

Besides these few hiccups, the ACS instrument has been steadily acquiring astronomical images over its 15 on-orbit lifetime. Figure 1 shows an estimates of the number of observations over time for each of the three detectors. To date, there have been nearly 200,000 of observations total. Further information about the ACS instrument including its history, configuration, performance, and scientific capability can be found in the ACS Instrument Handbook (Avila et al., 2017).

ACS data, along with all other data from the other HST instruments past and present (e.g. The Wide Field Camera 3 (WFC3), The Cosmic Origins Spectroscopy (COS), etc.), are primarily stored and publicly-available in the Barbara A. Mikulski Archive for Space Telescopes (MAST)¹ (Barbara, 2017). Through MAST, users can request and retrieve data

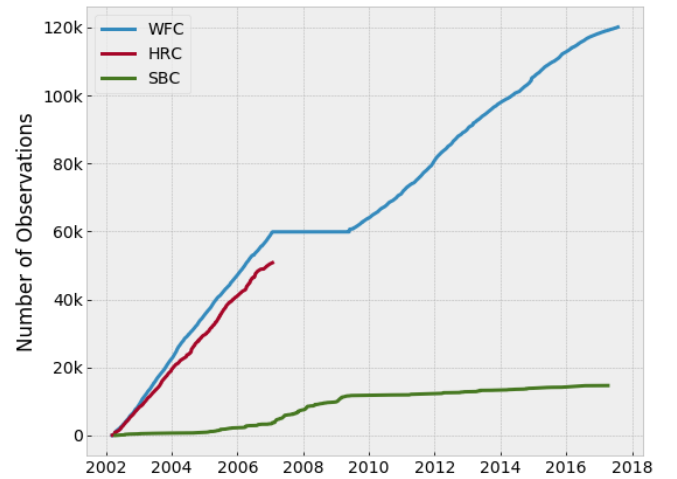


Fig. 1: The number of observations over time for each of the three detectors on ACS.

for any publicly-available dataset via `ftp`, `sftp`, or DVD by mail². The ACS data, like most all other astronomical data, are stored in the Flexible Image Transport System (FITS) filetype (FITS, 2008). This filetype has several unique characteristics, as will be discussed in section 1.1.

The ACS Quicklook Project is a `python`-based application for discovering, viewing, and querying all publicly-available ACS data. It consists of several subsystems: (1) A filesystem that stores ACS instrument data files and “Quick-

Manuscript received Month DD, YYYY

1. named after the U.S. Senator from Maryland who has been a pivotal political driving force behind the manned servicing missions, the Hubble Space Telescope, and the forthcoming James Webb Space Telescope

2. Not all HST data are publicly available; most HST data of scientific targets are considered proprietary for up to one calendar year, after which they are publicly released.

look” JPEGs in an organized Network File System (NFS), (2) A MySQL database that stores image metadata of each observation, (3) A python/Flask-based web application for interacting with the filesystem and database, and (4) A python code library (named `acsq`) that contains code for connecting to the database, ingesting new data, logging production code execution, and building/maintaining the database and web application. Each of these subsystems are explained in further detail in the Methodology section of this paper.

This paper aims to outline and detail the ACS Quicklook project as part of the Towson University Computer Science Masters Program Graduate Project. The remaining subsections in this chapter discuss the motivation and use cases for this application, as well as details on the underlying data structure on top of which this project was built. Chapter 2 discusses related work to this project and how the ACS Quicklook project differs from existing similar applications. Chapter 3 details the implementations of each of the ACS Quicklook subsystems. Chapter 4 outlines the results of the project, namely the project deliverables. Lastly, chapters 5 and 6 conclude the paper with a discussion of possible extensions and modifications to the application.

It should be noted that the work that went into this project by the authors was accomplished on behalf of the Space Telescope Science Institute (STScI) located in Baltimore, Maryland. STScI is the home institution for instrument, data, and user support of HST, the forthcoming James Webb Space Telescope (JWST), and MAST. STScI is part of the Association of Universities for Research in Astronomy (AURA).

1.1 Data Structure

The design of the ACS Quicklook application, especially the database, is heavily dependant on the underlying data structure of ACS FITS files. As such, it is important for the reader to understand this data structure and thus the next four sections are dedicated to giving an overview on the subject.

1.1.1 Filenames

Each ACS data file is named in a consistent fashion:

```
<rootname>_<filetype>.fits
```

where each `<rootname>` consists of nine unique alphanumeric characters, and `<filetype>` is one of several three-character filetype options (discussed in proceeding section 1.1.4). For example, one ACS observation has the rootname `j6mf16lhq_raw.fits` (Principle Investigator Gary Bernstein, observation date 2016-09-22). Each character in the 9-character rootname has meaning, and is discussed in section 5.2 of the Introduction to the HST Data Handbooks (Smith et al., 2011). The `.fits` extension at the end of the filename signifies that the file is of FITS format.

Note about rootname caveat.

1.1.2 FITS file structure

Each ACS FITS file consists of several “Extensions”, with each extension serving a purpose to describe a particular

TABLE 1: ACS/WFC FITS file extensions

Extension	Purpose	Image Dimensions (pixels)	Data Type
0	Primary header	–	String
1	SCI, Chip 2	(4096, 2048)	Float
2	ERR, Chip 2	(4096, 2048)	Float
3	DQ, Chip 2	(4096, 2048)	Integer
4	SCI, Chip 1	(4096, 2048)	Float
5	ERR, Chip 1	(4096, 2048)	Float
6	DQ, Chip 1	(4096, 2048)	Integer

TABLE 2: ACS/HRC and ACS/SBC FITS file extensions

Extension	Purpose	Image Dimensions (pixels)	Data Type
0	Primary header	–	String
1	SCI	(1024, 1024)	Float
2	ERR	(1024, 1024)	Float
3	DQ	(1024, 1024)	Integer

aspect of the observation. Each extension consists of two parts: (1) an extension “header”, which contain key/value pairs describing image metadata (for example, `DATE-OBS = '2016-09-22'` indicates that the observation date was 2016-09-22) (discussed in the next section), and (2) the extension data, which may be a binary table or, more commonly, a multi-dimensional array of detector pixel values.

The type of extension data can also vary. The most common extension data types are (1) ‘science’ (SCI), in which the extension data describe a scientific observation, (2) ‘error’ (ERR), in which the extension data describe the uncertainty in the pixel values of the SCI data, and (3) ‘data quality’ (DQ), in which the extension data describe the quality of the pixel values for the detector (for example, they may indicate that certain pixels were affected by cosmic rays during the observation). Typically, for a given file, the 1st extension is the SCI extension, the 2nd extension is the ERR extension, and the 3rd extension is the DQ extension. Furthermore, the 0th extension typically has no extension data and only an extension header that contains metadata that is common to all extensions. This is referred to as the ‘Primary Header’.

Tables 1-3 describe the different extensions of ACS FITS files for each of the three ACS detectors. Note that there are two sets of SCI/ERR/DQ extensions for WFC since WFC is comprised of two separate CCD chips.

Over the years, there have been several tools written in various programming languages to read in FITS files and automatically convert their extension data to multi-dimensional array data types and their extension headers to dictionary data types. For this project, the `astropy.fits` python library is used extensively to read and interact with ACS FITS files (Robitaille et al., 2013).

```

SIMPLE =      T / data conform to FITS standard
BITPIX =     16 / bits per data value
NAXIS =       0 / number of data axes
EXTEND =      T / File may contain standard extensions
NEXTEND =     6 / Number of standard extensions
GROUPS =      F / image is in group format
DATE = '2016-09-22' / date this file was written (yyyy-mm-dd)
FILENAME = 'j6mf16lhq_raw.fits' / name of file
FILETYPE = 'SCI' / type of data found in data file

TELESCOP = 'HST' / telescope used to acquire data
INSTRUME = 'ACS' / identifier for instrument used to acquire data
EQUINOX = 2000.0 / equinox of celestial coord. system

/ DATA DESCRIPTION KEYWORDS

ROOTNAME = 'j6mf16lhq' / rootname of the observation set
IMAGETYP = 'DARK' / type of exposure identifier
PRIME1 = 'ACS' / instrument designated as prime

/ TARGET INFORMATION

TARGNAME = 'DARK' / proposer's target name
RA_TARG = 0.000000000000E+00 / right ascension of the target (deg) (J2000)
DEC_TARG = 0.000000000000E+00 / declination of the target (deg) (J2000)

/ PROPOSAL INFORMATION

PROPOSID = 9433 / PEP proposal identifier
LINENUM = '16.055' / proposal logsheet line number
PR_INV_L = 'Bernstein' / last name of principal investigator
PR_INV_F = 'Gary' / first name of principal investigator
PR_INV_M = ' / middle name / initial of principal investigator

/ EXPOSURE INFORMATION

SUNANGLE = 93.563698 / angle between sun and V1 axis
MOONANGLE = 33.222004 / angle between moon and V1 axis
SUN_ALT = 68.062172 / altitude of the sun above Earth's limb
FGSLOCK = 'FINE' / commanded FGS lock (FINE, COARSE, GYROS, UNKNOWN)
GYROMODE = '3' / number of gyros scheduled, T=3+0BAD
REFFRAME = 'GSC1' / guide star catalog version
MTFLAG = ' ' / moving target flag; T if it is a moving target

DATE-OBS = '2003-01-27' / UT date of start of observation (yyyy-mm-dd)
TIME-OBS = '15:20:01' / UT time of start of observation (hh:mm:ss)
EXPSTART = 5.266663890058E+04 / exposure start time (Modified Julian Date)
EXPEND = 5.266665048715E+04 / exposure end time (Modified Julian Date)
EXPTIME = 1000.000000 / exposure duration (seconds)—calculated

```

Fig. 2: An example header.

1.1.3 FITS file extension headers

As mentioned in the previous section, each FITS extension contains a “header”, which contains key/value pairs of metadata associated with the extension data. Such metadata includes various data that describes the astronomical observation (e.g. target name, exposure time, principle investigator name, etc.), telemetry of ACS or HST in general at the time of observation (e.g. temperature of the ACS instrument, orientation of the telescope pointing, position of the telescope relative to Earth, etc.) or the FITS file itself (e.g. the number of extensions, file creation date, etc.). A subsection of an example header is shown in Figure 2.

Extension headers may contain a large number of key-word/value pairs. Some extension headers contain upwards of 300 keywords, while others may contain only ~40 keywords.

1.1.4 FITS filetypes for ACS

As discussed in section 1.1.1, each ACS observation may result in several FITS filetypes. Each filetype describes the observation in a different way. The set of available filetypes for a given observation is dependent on the characteristics of the observation, the details of which are beyond the scope of this paper. Also beyond the scope of this paper are the vast details that surround each filetype; each one has a different scientific application that is not important to understanding the ACS Quicklook project. However, to provide at least some context, below we give a brief description of each possible filetype that a given observation may contain:

- **raw** - The raw, uncalibrated data that comes directly from HST
- **flt** - nominally calibrated data
- **flc** - nominally calibrated data plus corrected for Charge Transfer Efficiency (CTE) deficits.
- **drz** - Geometric distortion-corrected data
- **drc** - Geometric distortion-corrected plus CTE corrected data
- **spt** - Telescope telemetry data
- **jlt** - Telescope pointing data
- **jif** - Telescope drifting data
- **crj** - Cosmic ray rejected data
- **crc** - Cosmic ray rejected plus CTE corrected data
- **asn** - Observation association table.

As noted earlier, a given observation may not result in the set of all possible filetypes. For example, the observation j6mf16lhq only has the filetypes raw, flt, jlt, jif, and spt.

1.2 Key Metadata

There are several metadata key/value pairs that are particularly important for the ACS Quicklook application, specifically the web application. For some reference, and context, these metadata are briefly described below. Note that the `rootname` and `proposal_type` are not metadata from extension headers, but rather are metadata that were explicitly added to the database schema.

APERTURE - The portion of the WFC, HRC, or SBC detector that was used during an observation. Can either be the entire detector (called a “full-frame image”) (e.g. WFC), or a subsection of the detector (called a “subarray”) (e.g. WFC1-1K).

DATE-OBS - The date of the observation in the format YYYY-MM-DD, measured in Universal Time (e.g. '2017-08-05').

DEC_TARG - The declination of the target (i.e. the angular distance the target north or south of the celestial equator) (e.g. 41.2842).

DETECTOR - The detector used for the observation. Can either be WFC, HRC, or SBC.

EXPFLAG - Indicates if an observation was interrupted (e.g. INTERRUPTED) or not (e.g. NORMAL).

EXPSTART - The exposure start time of the observation, in units of Modified Julian Date (e.g. 52473.8).

EXPTIME - The exposure duration of the observation, in units of seconds (e.g. 1000.0).

FILTER1 - The selected element from the ACS filter wheel # 1 (e.g. F606W).

FILTER2 - The selected element from the ACS filter wheel # 1 (e.g. F814W).

IMAGETYP - The type of exposure for the observation (e.g. BIAS, EXT, etc.).

OBSTYPE - The type of observation, either IMAGING, SPECTROSCOPIC, CORONOGRAPHIC, or INTERNAL.

proposal_type - The type of proposal that the observation belongs to, such as Calibration (i.e. CAL) or General Observer (i.e. GO).

PROPOSID - The proposal number that the observation belongs to (e.g. 10695).

RA_TARG - The right ascension of the target (i.e. the angular distance of the target east and west on the celestial sphere) (e.g. 49.5375).

rootname - The 8-character unique rootname of the observation (e.g. j5915401).

SUBARRAY - A boolean flag that indicates if the observation is a full-frame APERTURE (i.e. 0) or a subarray APERTURE (i.e. 1).

TARGNAME - The name of the target (e.g. M87, NGC-4536, ANDROMEDA-I, etc.).

TIME-OBS - The time of the start of the observation in the format HH:MM:SS, measured in Universal Time (e.g. 14:21:56).

1.3 Motivation

The motivation for the ACS Quicklook system is driven by several shortcomings of the FITS file structure as well as the current capabilities of MAST from a specific user perspective (intended users and their use cases are discussed in section 1.2). Some of these shortcomings are described below along with the intended way the ACS Quicklook application will address them.

Data retrieval latency: Currently, users who wish to retrieve data from the MAST archive must submit a retrieval request via the MAST online interface. Once the retrieval request is processed (usually automatically unless it is a request of a large number of datasets), the data are either transferred to the user directly via *sftp*, transferred to a "staging area" in which the user can log into and copy the data via *ftp* at their leisure, or sent by mail via DVD, depending on which option the user selects. In the case of any one of these options, the time between a download request and the time in which the user has fully retrieved the data is a non-significant amount of time. In the fastest scenario of the *sftp* option, a typical request can take minutes to hours to be completed. The ACS Quicklook system attempts to circumnavigate this retrieval process by making the full data products instantly available via read-only access of the filesystem subsystem, as well as a subset of the data products (and corresponding metadata) instantly available to view through the web application.

File I/O: Users who

Data redundancy: Something.

Data discovery: Something

1.4 Use Cases

The intended user of ACS Quicklook are ACS instrument scientists, analysts, or scientific users who wish to perform one or more of the following use cases:

1. View

2 RELATED WORK

Topics to discuss:

1. The MAST archive
2. The MAST portal
3. The WFC3/Quicklook project
4. Other Astronomy Institutions
5. How ACS/Quicklook is different

3 METHODOLOGY

In this chapter, we discuss the methods by which we implemented the various subsystems of the ACS Quicklook system. Additionally, we discuss the programming standards and standard workflows that were employed to promote code quality such as readability, maintainability, extensibility, etc; we believe that this aspect of the project is at least equally important to the system as its individual components.

3.1 Version control

All code associated with this project (including this paper itself) is version controlled using the *git* Version Control System (VCS) (*git*, 2017). The *git* repository for the project is named *acsq*. The *git* repository is also hosted on GitHub, a repository hosting service (GitHub, 2017), and is publicly available at <http://github.com/spacetelescope/acsq/>.

Several feature branches of the code were created throughout the building of this project such that the *master* branch (which is considered the "production" branch) always contained operational code (while the code in the branches may contain unfinished implementations). Such branches include *create-database* (for implementation of the database schema), *add-logging* (for implementation of system logging), *build-ingest* (for implementation of data ingestion software), and *web-application* (for implementation of the web application). For each merge of a feature branch, a *tag* and *release* was created for the *master* branch, which allows a specific version of the *master* branch to be saved in the repository. These releases are available at <https://github.com/spacetelescope/acsq/releases>.

Additionally, using GitHub allowed for issue tracking of bugs, features, and potential enhancements to the code repository. Current open issues of the repository can be found at <https://github.com/spacetelescope/acsq/issues>.

```
def get_proposal_type(proposid):
    """Return the ``proposal_type`` for the given ``proposid``.

    The ``proposal_type`` is the type of proposal (e.g. ``CAL``,
    ``GO``, etc.). The ``proposal_type`` is scraped from the MAST
    proposal status webpage for the given ``proposid``. If the
    ``proposal_type`` cannot be determined, a ``None`` value is returned.

    Parameters
    -----
    proposid : str
        The proposal ID (e.g. ``12345``).

    Returns
    -----
    proposal_type : int or None
        The proposal type (e.g. ``CAL``).
    """
```

Fig. 3: An example of the PEP257 and numpydoc docstring conventions, using the `get_proposal_type` function from `acsq1.ingest.ingest`.

3.2 Programming and Documentation Standards

All code contained within this project was written to adhere to specific standards and conventions, namely (1) the PEP8 Style Guide for python code (van Rossum, 2001), (2) The PEP257 python guide for module and function docstring conventions (Goodger, 2001), and (3) the numpydocs documentation standard (NumPy Documentation, 2017). More details on each of these standards and conventions are given below.

The PEP8 Style Guide for python code (abbreviated for ‘Python Enhancement Proposal #8’) documents python coding conventions including variable naming, spacing, line length, module layout, function layout, comments, and design patterns. Only in specific cases were these conventions not followed, such as using a single line of code, even if it exceeded the recommended 80 characters, to allow for greater readability. By following these conventions, the style of the `acsq1` code is consistent amongst each module and attempts to reflect the style of industry-grade python code.

The PEP257 guide for docstring conventions describes standard conventions used for function and module docstrings (i.e. the API documentation found in block comments at the beginning of modules or immediately after function declarations). Like PEP8, following these conventions ensure consistency amongst the `acsq1` code documentation. Furthermore, the numpydocs documentation convention provides some additional details on top of the PEP257 conventions and is used in many python packages including the `numpy` (numerical python) and `scipy` (scientific python) packages (van der Walt et al., 2011). Figure N shows an example of these conventions, taken from the `acsq1.ingest.ingest.get_proposal_type` function.

Another benefit to using PEP257 and numpydoc docstring conventions is that API documentation creation tools such as `sphinx` (Brandt et al., 2007) or `epydoc` (Loper, 2004) can automatically convert the docs into other output formats such as HTML and PDF. For this project, we use `sphinx` to convert API documentation to HTML, and host the webpages online using the `readthedocs`, which is an open-

```
ingest.ingest.get_proposal_type(proposid)

Return the proposal_type for the given proposid.

The proposal_type is the type of proposal (e.g. CAL, GO, etc.). The proposal_type is scraped from the MAST proposal status webpage for the given proposid. If the proposal_type cannot be determined, a None value is returned.

Parameters: proposid : str
    The proposal ID (e.g. 12345).

Returns: proposal_type : int or None
    The proposal type (e.g. CAL).
```

Fig. 4: The `readthedocs` documentation for the `acsq1` example function seen in Figure N.

```
filesystem/
  jcp0/
    jcp001kwq/
      jcp001kwq_flg.fits
      jcp001kwqflt.fits
      jcp001kwq_raw.fits
      jcp001kwq_spt.fits
      jcp001kwj_jit.fits
      jcp001kwj_jif.fits
    jcp001010/
      jcp001010_asn.fits
      jcp001010_drc.fits
      jcp001010_drz.fits
      jcp001010_jif.fits
      jcp001010_jit.fits
    jcp014tyq/
      ...
    jcp001ktq/
      ...
  jcp3/
    ...
  jcp7/
    ...
  ...
```

Fig. 5: A representation of the directory structure within the `acsq1` filesystem, using a few observations as an example.

source, community supported tool for hosting and browsing documentation (Read the Docs, 2017). The documentation for `acsq1` is hosted at <http://acsq1.readthedocs.io/>. The output documentation as seen on `readthedocs` for the example function in figure N is provided in Figure N.

3.3 Filesystem: Archive of ACS data

The `acsq1` filesystem is a Network File System (NFS) that stores all on-orbit ACS data on disk in an organized set of directories and subdirectories hosted at STScI. Figure N shows an example of this directory structure: The parent directory is the first four characters of the 9-character `rootname`, which maps directly to an individual `PROPOSID`. The subdirectories of the parent directories are named after the full 9-character `rootname` such that each parent directory contains the `rootname` subdirectories that were observed for that particular `PROPOSID`. Each `rootname` subdirectory contains every available filetype (as described in Section 1.1.4) for the particular observation is stored.

Figure N shows how the total size of the filesystem has evolved over the lifetime of the mission; currently, the filesystem occupies ~40 TB of storage space. Note that the file sizes across the detectors and across the various filetypes

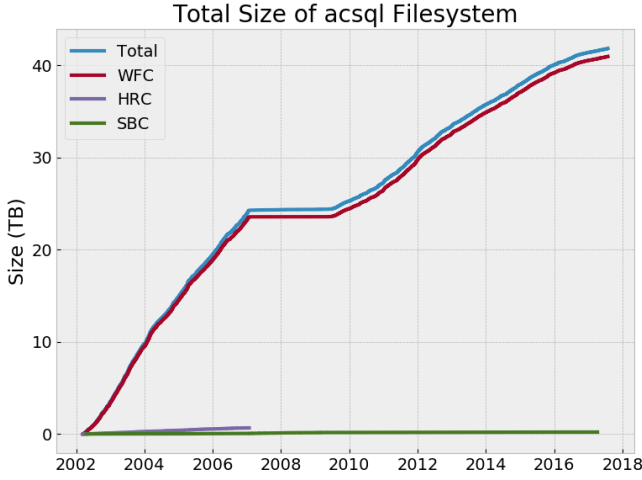


Fig. 6: The size of the `acsdl` filesystem as a function of observation date.

may vary depending on the nature of the particular observation (for example, full-frame observations result in larger file sizes than subarray observations, calibrated filetypes have larger file sizes than un-calibrated filetypes, etc.).

3.4 Filesystem: Archive of JPEGs and Thumbnails

In addition to the ACS data products described in the last section, the `acsdl` filesystem also stores “Quicklook” JPEG and thumbnail images of each RAW, FLT, and FLC filetype (when applicable) in an organized directory structure. These images are used by the `acsdl` web application to allow users to quickly and easily view the contents of the data without having to physically open the corresponding `.fits` files.

The JPEG images are generated by taking the two-dimensional data from the SCI extension(s), sigma-clipping the top and bottom 1% of the values (as to avoid large outlier values and enhance the scaling of the image), and saving the data to a JPEG format. The thumbnail images are created by simply resizing the corresponding JPEG into a 128x128 pixel image and saving to a `.thumb` extension; the purpose of these thumbnail images are to be able to view many of them on a single webpage in the `acsdl` web application. An example of a JPEG image and its corresponding thumbnail is shown in Figure N.

Unlike the ACS data products portion of the filesystem, the JPEG and thumbnail portions of the filesystem are organized based on the 5-digit PROPOSID of the corresponding observation instead of the first four characters of the rootname. This design was chosen as a means to simplify the design of the web application; users often view data based on the 5-digit PROPOSID and less often on the details of the rootname. An example of this structure is shown in Figure N. Note that the thumbnail filesystem only contains thumbnails created from FLT filetypes, since thumbnails are only intended for navigation and quick-viewing.

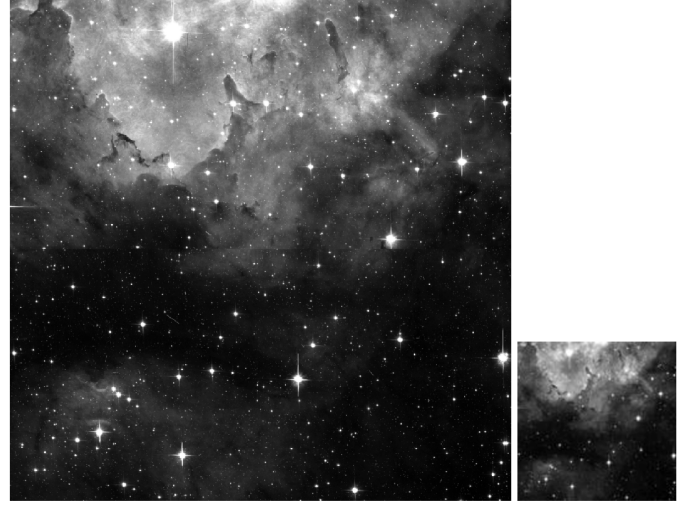


Fig. 7: An example of a JPEG image (left) and its corresponding thumbnail image using example dataset `jcs718koq`.

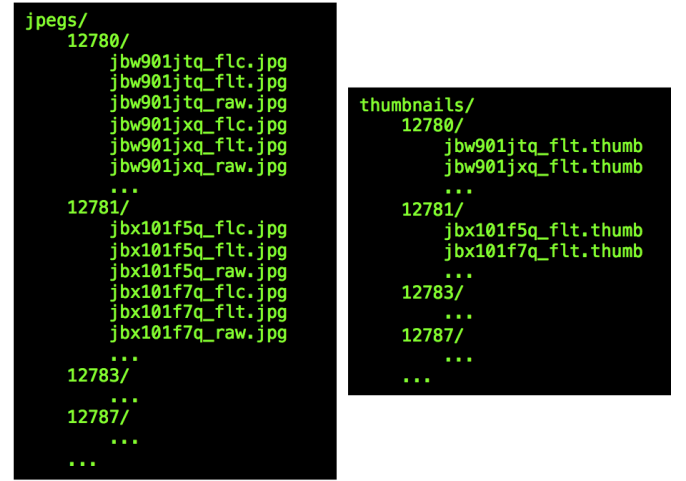


Fig. 8: A representation of the directory structure for the JPEG (left) and thumbnail (right) portion of the `acsdl` filesystem, using a few observations as an example.

3.5 Database: Relational Schema

Another major component of the `acsdl` project is a relational database that stores all FITS header key/value pairs for each ACS filetype and FITS file extension across all on-orbit ACS observations. Such a database allows users to perform relational queries for any observational metadata.

To accomplish this, we implemented the relational schema shown in Figure N. The `acsdl` database contains 111 tables in total: one master table which contains basic information about each rootname that is important for the `acsdl` database in general, one datasets table which indicate which filetypes are available for a particular rootname, and 109 ‘header’ tables which stores the header key/value pairs, one for each detector/filetype/extension combination (e.g. `wfc_raw_0`). Each of these tables are described in detail below.

The master table contains information that is particularly useful for maintaining and using the `acsdl` database.

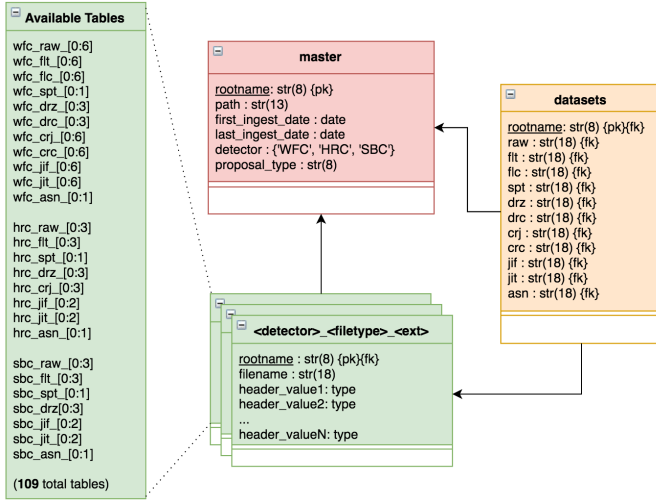


Fig. 9: The relational database schema for the acsql database.

Its primary key is the first 8 characters of the 9-character rootname for the particular observation (recall from section 1.1.1 that only the first 8 characters of a rootname are actually unique). The path column contains the location of the observation in the acsql filesystem. The first_ingest_date and last_ingest_date contains the date in which the observation was first inserted into the database and the date in which the observation was most recently updated in the database, respectively. The last_ingest_date allows the database maintainer to determine when data in the database may become outdated and require re-ingestion.

The datasets table lists which filetypes are available for each observation. If a particular filetype is available for the given rootname, the value for the appropriate column in the table is the full <rootname>_<filetype>.fits filename (for example, the raw column contains the value jcs718koq_raw.fits for rootname jcs718ko). If a particular filetype is not available, the value of the column is NULL. This table allows a user to determine which header tables are queryable for a given rootname. The rootname in the datasets table acts as both a primary key for the table as well as a foreign key that maps to the rootname of the master table.

The remaining 109 tables were designed to be in direct correspondance with the header metadata key/value pairs found in observations files; each column is named in the same manner as the header keys, with the value of that column reflecting the header value. There is one table for each detector, filetype, and extension combination; collectively, these are referred to as the 'header' tables. Like with the datasets table, the rootname column serves as a primary key for the header tables as well as a foreign key that maps to the rootname of the master table.

3.6 Database: MySQL + SQLAlchemy

The acsql database is stored on a MySQL server (Version 5.6) (Oracle, 2017) that is hosted at STScI. The database schema was implimented using SQLAlchemy, which is

an open-source SQL toolkit and Object Relational Mapper (ORM) for python (Bayer, 2006). As an ORM, SQLAlchemy enables python classes to be easily translated to SQL-based database tables, and vice versa. Additionall, SQLAlchemy provides python methods for connecting to a SQL-based database and performing typical SQL tasks such as inserts, updates, and queries.

There are several key functions and classes that were used to construct the acsql database (all of which can be found in the acsql.database.database_interface.py module). One such function is the load_connection, as shown in Figure N. This function creates three SQLAlchemy objects that are used to establish a connection with the acsql database: engine, base, and session, each described below.

The engine object contains the Python Database API Specification (also known as DBAPI), which provides a low-level API for python-specific, commonly-used database tasks (Lemburg, 2017). It is created from the sqlalchemy.create_engine method, which requires a user-supplied connection_string. The connection_string is a string that contains information about the type of database, the specific database dialect being used, and the user credentials (e.g. username, password, port number, and host server name). In the case of the acsql, this connection string takes the form of 'mysql+pymysql://username:password@host:port/acsql'. The connection_string is imported from a user supplied config file within the acsql library (as will be discussed in section 3.9).

The base object serves as a base class for declarative class definitions (i.e. the classes that are used to define the database tables). It is created from the sqlalchemy.ext.declarative.declarative_base method. Perhaps most importantly, the base object contains methods for creating and dropping tables from the class definitions (e.g. base.metadata.create_all() and base.metadata.drop_all(), respectively).

The session object provides a primary usage interface for database operations, and is created via the sqlalchemy.sessionmaker method, which takes as a parameter the engine object. The methods of the session object are primarily used to query the database (i.e. session.query()) as well as committing inserts or updates (i.e. session.commit()).

The master and datasets tables were implemented via explicit class definitions in database_interface, and are shown in Figures N and N, respectively. Each table column is defined using the sqlalchemy.Column object, which is a class that can be initialized with the datatype that will be stored in the column (e.g. String, Float, Integer, etc.) as well as parameters that set SQL-like constraints and parameters on the column values. These include, but are not limited to, primary keys (e.g. the primary_key=True parameter in the master.rootname column), foreign key constrains (e.g. the ForeignKey constraint in the datasets.rootname column), uniqueness constraints (e.g. the unique=True parameters in the master.path column), and NULL constraints (e.g. the nullable=False parameter in the master.first_ingest_date column).

```
def load_connection(connection_string):
    """Return ``session``, ``base``, and ``engine`` objects for
    connecting to the ``acsql`` database.

    Create an ``engine`` using an given ``connection_string``. Create a
    ``base`` class and ``session`` class from the ``engine``. Create an
    instance of the ``session`` class. Return the ``session``,
    ``base``, and ``engine`` instances.

    Parameters
    -----
    connection_string : str
        The connection string to connect to the ``acsql`` database. The
        connection string should take the form:
        ``dialect+driver://username:password@host:port/database``

    Returns
    -----
    session : session object
        Provides a holding zone for all objects loaded or associated
        with the database.
    base : base object
        Provides a base class for declarative class definitions.
    engine : engine object
        Provides a source of database connectivity and behavior.
    """

    engine = create_engine(connection_string, echo=False, pool_timeout=100000)
    base = declarative_base(engine)
    Session = sessionmaker(bind=engine)
    session = Session()

    return session, base, engine
```

Fig. 10: The `load_connection` function, which is used to build a connection to the `acsql` database

```
class Master(base):
    """ORM for the master table."""
    def __init__(self, data_dict):
        self.__dict__.update(data_dict)

    __tablename__ = 'master'
    rootname = Column(String(8), primary_key=True, index=True, nullable=False)
    path = Column(String(15), unique=True, nullable=False)
    first_ingest_date = Column(Date, nullable=False)
    last_ingest_date = Column(Date, nullable=False)
    detector = Column(Enum('WFC', 'HRC', 'SBC'), nullable=False)
    proposal_type = Column(Enum('CAL/ACS', 'CAL/OTA', 'CAL/STIS', 'CAL/WFC3',
                               'ENG/ACS', 'GO', 'GO/DD', 'GO/PAR', 'GTO/ACS',
                               'GTO/COS', 'NASA', 'SM3/ACS', 'SM3/ERO',
                               'SM4/ACS', 'SM4/COS', 'SM4/ERO', 'SNAP'),
                          nullable=True)
```

Fig. 11: The class definition for constructing the master table via SQLAlchemy.

SQLAlchemy determines the name of the table via the `__tablename__` attribute, and determines the name of the columns by the name of the variable used to initialize each Column object.

Since there are 109 header tables, some of which have hundreds of columns, it is not practical to construct a class definition for each table in a similar manner to that of the master and datasets table. Instead, these class definitions were implemented via the `database_interface.orm_factory` function, which is a factory function that creates and returns a class definition

```
class Datasets(base):
    """ORM for the datasets table."""
    def __init__(self, data_dict):
        self.__dict__.update(data_dict)

    __tablename__ = 'datasets'
    rootname = Column(String(8), ForeignKey('master.rootname'),
                      primary_key=True, index=True, nullable=False)
    raw = Column(String(18), nullable=True)
    flt = Column(String(18), nullable=True)
    flc = Column(String(18), nullable=True)
    spt = Column(String(18), nullable=True)
    drz = Column(String(18), nullable=True)
    drc = Column(String(18), nullable=True)
    crj = Column(String(18), nullable=True)
    crc = Column(String(18), nullable=True)
    jif = Column(String(18), nullable=True)
    jit = Column(String(18), nullable=True)
    asn = Column(String(18), nullable=True)
```

Fig. 12: The class definition for constructing the datasets table via SQLAlchemy.

```
def orm_factory(class_name):
    """Create a SQLAlchemy ORM Classes with the given ``class_name``.

    Parameters
    -----
    class_name : str
        The name of the class to be created

    Returns
    -----
    class : obj
        The SQLAlchemy ORM
    """

    data_dict = {}
    data_dict['__tablename__'] = class_name.lower()
    data_dict['rootname'] = Column(String(8), ForeignKey('master.rootname'),
                                  primary_key=True, index=True,
                                  nullable=False)
    data_dict['filename'] = Column(String(18), nullable=False, unique=True)
    data_dict = define_columns(data_dict, class_name)
    data_dict['__table_args__'] = {'mysql_row_format': 'DYNAMIC'}

    return type(class_name.upper(), (base,), data_dict)
```

Fig. 13: The `orm_factory` function, used to define class definitions for header tables.

for each header table, based on the given `class_name` that reflects the detector/filetype/extension combination (e.g. `wfc_raw_0`). The `orm_factory` function is shown in Figure N. Similar to the Master and Datasets classes, some of the columns in the `orm_factory` function are explicitly defined via the SQLAlchemy Column class. However, the columns that correspond to header key/value pairs are defined in a separate function named `define_columns`, shown in Figure N.

The purpose of the `define_columns` function is to define SQLAlchemy Column objects for each header keyword in the headers of the particular detector/filetype/extension combination


```

def define_columns(data_dict, class_name):
    """Dynamically define the class attributes for the ORM

    Parameters
    -----
    data_dict : dict
        A dictionary containing the ORM definitions
    class_name : str
        The name of the class/ORM.

    Returns
    -----
    data_dict : dict
        A dictionary containing the ORM definitions, now with header
        definitions added.
    """

    special_keywords = ['RULEFILE', 'FWERROR', 'FW2ERROR', 'PROPTTL1',
                        'TARDESCR', 'QUALCOM2']

    with open(os.path.join(os.path.split(__file__)[0], 'table_definitions',
                           class_name.lower() + '.txt'), 'r') as f:
        data = f.readlines()
    keywords = [item.strip().split(', ') for item in data]
    for keyword in keywords:
        if keyword[0] in special_keywords:
            data_dict[keyword[0].lower()] = get_special_column(keyword[0])
        elif keyword[1] == 'Integer':
            data_dict[keyword[0].lower()] = Column(Integer())
        elif keyword[1] == 'String':
            data_dict[keyword[0].lower()] = Column(String(50))
        elif keyword[1] == 'Float':
            data_dict[keyword[0].lower()] = Column(Float(precision=32))
        elif keyword[1] == 'Decimal':
            data_dict[keyword[0].lower()] = Column(Float(precision='13,8'))
        elif keyword[1] == 'Date':
            data_dict[keyword[0].lower()] = Column(Date())
        elif keyword[1] == 'Time':
            data_dict[keyword[0].lower()] = Column(Time())
        elif keyword[1] == 'DateTime':
            data_dict[keyword[0].lower()] = Column(DateTime)
        elif keyword[1] == 'Bool':
            data_dict[keyword[0].lower()] = Column(Bool)
        else:
            raise ValueError('unrecognized header keyword type: {}'.format(
                keyword[0], keyword[1]))

    if 'aperture' in data_dict:
        data_dict['aperture'] = Column(String(50), index=True)

    return data_dict

```

Fig. 14: The `define_columns` function, used to define columns used in the header tables.

(provided in the given `class_name` parameter). This is accomplished by reading in a text file (named `<class_name>.txt` that contains the header keywords and their datatype (one per line) for the given `class_name`. An portion of an example text file is shown in Figure N.

Furthermore, the 109 text files used to define the header table columns are also generated in an automated fashion via the `acsql.database.make_tabledefs.py` module. This module uses a set of example FITS files to scrape its header contents, determine all of the header keywords and their datatypes, and write the results to a text file. Similarly, the `acsql.database.update_tabledefs.py` is used to add new header keywords by comparing the header contents of a given FITS file and the existing column

```

DETECTOR, String
NEXTEND, Integer
EXTEND, Bool
SIMPLE, Bool
NAXIS, Integer
LINENUM, String
GROUPS, Bool
DATE, String
EQUINOX, Float
INSTRUME, String
PROPOSID, Integer
ASN_ID, String
ASN_PROD, Bool
ASN_STAT, String
DEC_TARG, Float
FILETYPE, String
ASN_TAB, String
PRIMESI, String
RA_TARG, Float
TARGNAME, String
TELESCOP, String
PR_INV_F, String
BITPIX, Integer
PR_INV_M, String
PR_INV_L, String

```

Fig. 15: The contents of an example text file used to define the columns of a header table in the `define_columns` function. The example table used here is the `wfc_asn_0` table.

```

WFC_raw_0 = orm_factory('WFC_raw_0')
WFC_raw_1 = orm_factory('WFC_raw_1')
WFC_raw_2 = orm_factory('WFC_raw_2')
WFC_raw_3 = orm_factory('WFC_raw_3')
WFC_raw_4 = orm_factory('WFC_raw_4')
WFC_raw_5 = orm_factory('WFC_raw_5')
WFC_raw_6 = orm_factory('WFC_raw_6')

WFCflt_0 = orm_factory('WFCflt_0')
WFCflt_1 = orm_factory('WFCflt_1')
WFCflt_2 = orm_factory('WFCflt_2')
WFCflt_3 = orm_factory('WFCflt_3')
WFCflt_4 = orm_factory('WFCflt_4')
WFCflt_5 = orm_factory('WFCflt_5')
WFCflt_6 = orm_factory('WFCflt_6')

WFCflc_0 = orm_factory('WFCflc_0')
WFCflc_1 = orm_factory('WFCflc_1')
WFCflc_2 = orm_factory('WFCflc_2')
WFCflc_3 = orm_factory('WFCflc_3')
WFCflc_4 = orm_factory('WFCflc_4')
WFCflc_5 = orm_factory('WFCflc_5')
WFCflc_6 = orm_factory('WFCflc_6')

```

Fig. 16: An example of how the `orm_factory` function is called to create class definitions for the header tables.

definition text files³.

With the implementation of the `orm_factory` and `define_columns` function, it is then trivial to create class definitions for each of the 109 header tables. An example of this is shown in Figure N, where the several of the WFC header tables are defined.

With the `master`, `datasets`, and each of the 109 header tables defined in the `database_interface` module, creating the database tables on the MySQL server is accom-

3. New header keywords are occasionally introduced to ACS data proceeding updates to its calibration software

plished by executing the `base.metadata.create_all()` method.

3.7 Data ingestion software: Algorithm

Another critical component of the ACS Quicklook system are the modules that are used to ingest data into the `acsqsl` database and to create the “Quicklook” JPEGs and thumbnails. By the term ‘ingest’, we refer to the following algorithm:

1. *Identify newly available public ACS data in the filesystem:* This is accomplished by comparing the list of `rootnames` in the filesystem with the list of `rootnames` in the master table of the `acsqsl` database. Any `rootnames` that exist in the filesystem but not in the database are considered new `rootnames` to be ingested.

2. *Loop over each **rootname** (in a parallelized manner):* The ingestion software (i.e. the `acsqsl.ingest.ingest` module), takes as input a single `rootname`, such that if there are multiple `rootnames` to be ingested, the calls to the ingestion module can be parallelized over many CPUs. The ingestion of one `rootname` does not depend on the ingestion of another, nor is the order of which files are ingested important. Please note that steps 3 through N are written from the perspective that a single `rootname` is being ingested (i.e. inside of the loop.)

3. *Update the **master** table with information about the **rootname**:* At this point, the master table can be updated with metadata pertaining to the `rootname`. A generic `insert_or_update` function was written (available in the `acsqsl.utils.utils` module) to determine if an entry should be inserted (in the case of first-time ingestion) or updated (in the case of re-ingestion). This function uses various `sqlalchemy` methods and the class definitions described in section 3.6 to perform the insert or update operation. The `insert_or_update` function is shown in Figure N.

4. *Loop over the available **filetypes** for the given **rootname**:* The available `filetypes` are determined by traversing down a level in the tree structure of the filesystem and identifying which files are present. Once determined, the ingestion algorithm processes each `<rootname>_<filetype>.fits` file individually. Please note that steps 5 through N are written from the perspective that a single file is being ingested (i.e. inside of the next nested loop).

5. *Create a **python** dictionary with metadata about the file:* To reduce the amount of variables being passed around to various functions, a data container in the form of a `python` dictionary data type is created to hold metadata needed by the remainder of the ingestion process. We refer to this data container as the `file_dict`. The `file_dict` contains metadata such as the absolute path of the file in the filesystem, the `filetype`, the available FITS file extensions of the file, and the absolute paths to which the “Quicklook” JPEGs and Thumbnails will be written.

6. *For each **FITS** file extension, extract the header information and update the appropriate header table in the **acsqsl** database:* The header information is read into a `python` dictionary via the `astropy.io.fits` module. Besides some minor fixes for a few corner cases (such as

```
def insert_or_update(table, data_dict):
    """Insert or update a record in the given ``table`` with the data
    in the ``data_dict``.

    A record is inserted if the primary key of the record does not
    already exist in the ``table``. A record is updated if it does
    already exist.

    Parameters
    -----
    table : str
        The name of the table to insert/update into.
    data_dict : dict
        A dictionary containing the data to insert/update.
    """

    table_obj = getattr(acsqsl.database.database_interface, table)
    session, base, engine = acsqsl.database.database_interface.\
        load_connection(SETTINGS['connection_string'])

    # Check to see if a record exists for the rootname
    query = session.query(table_obj)\
        .filter(getattr(table_obj, 'rootname') == data_dict['rootname'])
    query_count = query.count()

    # If there are no results, then perform an insert
    if not query_count:
        tab = Table(table.lower(), base.metadata, autoload=True)
        insert_obj = tab.insert()
        try:
            insert_obj.execute(data_dict)
        except (DataError, IntegrityError, InternalError) as e:
            logging.warning('\tUnable to insert {} into {}: {}'.format(
                data_dict['rootname'], table, e))

    else:
        query.update(data_dict)

    session.commit()
    session.close()
    engine.dispose()
```

Fig. 17: The `insert_or_update` function from the `acsqsl.utils.utils` module, used at various times during the data ingestion process to determine if an entry should be inserted or updated in the `acsqsl` database.

converting hypens in header keys to underscores as to avoid python errors), it is rather trivial to perform an insert or update operation via the `insert_or_update` function (see Figure N).

7. *Update the **datasets** table for the given **filetype**:* At this point, an entry in the `datasets` table is either inserted if it is the first `filetype` for the `rootname` being ingested, or updated if a `filetype` under the same `rootname` had already been ingested.

8. *If the **filetype** is either **raw**, **flt**, or **flc**, then create a “Quicklook” JPEG image:* JPEGs are produced only for `raw`, `flt`, and `flc` `filetypes`, since it are these `filetypes` that contain actual two-dimensional image data. The image data are read into multidimensional `numpy` array data types via the `astropy.io.fits` module. The data are then rescaled as to avoid an undesirable image stretch caused by extremely high or low-valued pixels, and

saved to a .jpg format. The JPEGs are saved to the JPEG portion of the `acsq1` filesystem (described in section 3.4).

9. *If the filetype is flt, then create a "Quicklook" Thumbnail image:* Thumbnail images are only produced for `flt` filetypes since they are only meant to be viewed as a means to discover the larger JPEG images via the `acsq1` web application. Thumbnails are generated by simply opening up the corresponding `flt` JPEG and resizing it to 128x128 pixels. The Thumbnailss are saved to the Thumbnail portion of the `acsq1` filesystem (described in section 3.4).

This workflow is encapsulated within several modules across the `acsq1.scripts` and `acsq1.ingest` subpackages, as will be described in section 3.9. These modules are intended to be executed daily (as an automatically-spawned process) as to keep the ACS Quicklook system up-to-date on any public data as it becomes available.

3.8 Data ingestion software: logging

Since the data ingestion software is intended to be executed by an automatic process and not by a human, we implemented a system by which the status of the ingestion process can be logged to an output text file and analyzed at a later time. Such log files can be used to assess if there were any issues with the ingestion process, such as if a new header keyword has appeared (requiring an update to the appropriate header table in the database). An example log file showing the ingestion of a single rootname (`j8zh21xv`) is provided in Figure N.

When the ingestion module gets executed, an empty log file is created with the filename `<module_name>_<timestamp>.log`, where `<module_name>` is the name of the ingestion module (in production, this is `ingest_production.py`, as will be discussed in section 3.9), and `<timestamp>` is the current time in the format `YYYY-MM-DD-HH-MM`. The naming convention of the log file allows system maintainers to determine which log file corresponds to which ingestion run.

Next, the `python` logging module is used to configure the format of the log statements. It does this by (1) setting the default logging level to `INFO` (meaning that, unless otherwise specified, each call to logging by the ingestion module will result in an `INFO` statement.), (2) setting the timestamp format to `YYYY-MM-DD HH:MM:SS`, and (3) setting the logging message format to `<timestamp> <level>: <message>`.

With the logging settings configured, any call to the logging module within the ingestion software results in a log statement. For example, the code `logging.info('Gathering files to ingest')` results in a timestamped log message, e.g. `08/15/2017 11:05:26 INFO: Gathering files to ingest` (as shown in Figure N.)

Calls to the logging module are strategically placed within the ingestion software to provide enough context to the status of the ingestion without cluttering the log file with too much detail. In most cases, logging statements only occur after a change of state to the system (i.e. an updated database table, the creation of a JPEG or Thumbnail.)

3.9 Web Application

3.10 acsq1 Library

4 RESULTS

Topics to discuss: 1. GitHub repository 2. ReadTheDocs documentation repository 3. Quantification of Database records 4. Quantification of Code repository 5. Website location

5 CONCLUSION

The conclusion goes here.

6 DISCUSSION

Topics to discuss:

1. Possible simplification based on MAST archive 2. Possible extensions to other instruments

APPENDIX A

acsq1 CODE

Appendix one text goes here.

ACKNOWLEDGMENTS

The authors would like to thank...

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```

08/15/2017 11:05:26 INFO: User: bourque
08/15/2017 11:05:26 INFO: Python Version: 3.5.2 [Continuum Analytics, Inc.] (default, Jul 2 2016, 17:53:06) [GCC 4.4.7 20120313 (Red Hat 4.4.7-1)]
08/15/2017 11:05:26 INFO: Python Path: /bourque/envs/anaconda3/envs/astroconda3/bin/python
08/15/2017 11:05:26 INFO: Numpy Version: 1.11.2
08/15/2017 11:05:26 INFO: Numpy Path: /bourque/envs/anaconda3/envs/astroconda3/lib/python3.5/site-packages/numpy
08/15/2017 11:05:26 INFO: Astropy Version: 1.2.1
08/15/2017 11:05:26 INFO: Astropy Path: /bourque/envs/anaconda3/envs/astroconda3/lib/python3.5/site-packages/astropy
08/15/2017 11:05:26 INFO: SQLAlchemy Version: 1.1.4
08/15/2017 11:05:26 INFO: SQLAlchemy Path: /bourque/envs/anaconda3/envs/astroconda3/lib/python3.5/site-packages/SQLAlchemy-1.1.4-py3.5-linux-x86_64.egg/sqlalchemy
08/15/2017 11:05:26 INFO: Gathering files to ingest
08/15/2017 11:05:52 INFO: j8zh21xv: Begin ingestion
08/15/2017 11:06:00 INFO: j8zh21xv: Updated master table.
08/15/2017 11:06:01 INFO: j8zh21xv: Updated HRC_flt_0 table.
08/15/2017 11:06:01 INFO: j8zh21xv: Updated HRC_flt_1 table.
08/15/2017 11:06:01 INFO: j8zh21xv: Updated HRC_flt_2 table.
08/15/2017 11:06:01 INFO: j8zh21xv: Updated HRC_flt_3 table.
08/15/2017 11:06:01 INFO: j8zh21xv: Updated datasets table for flt.
08/15/2017 11:06:01 INFO: j8zh21xv: Creating JPEG
08/15/2017 11:06:02 INFO: j8zh21xv: Creating Thumbnail
08/15/2017 11:06:02 INFO: j8zh21xv: Updated HRC_raw_0 table.
08/15/2017 11:06:02 INFO: j8zh21xv: Updated HRC_raw_1 table.
08/15/2017 11:06:03 INFO: j8zh21xv: Updated HRC_raw_2 table.
08/15/2017 11:06:03 INFO: j8zh21xv: Updated HRC_raw_3 table.
08/15/2017 11:06:03 INFO: j8zh21xv: Updated datasets table for raw.
08/15/2017 11:06:03 INFO: j8zh21xv: Creating JPEG
08/15/2017 11:06:04 INFO: j8zh21xv: Updated HRC_spt_0 table.
08/15/2017 11:06:05 INFO: j8zh21xv: Updated HRC_spt_1 table.
08/15/2017 11:06:05 INFO: j8zh21xv: Updated datasets table for spt.
08/15/2017 11:06:05 INFO: j8zh21xv: End ingestion

```

Fig. 18: An example log file for the ingestion of a single file (j8zh21xv).