PYSAT: Python Satellite Data Analysis Toolkit

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Abstract. A common problem in space science data analysis is combin-1 ing complementary data sources that are provided and analyzed in differ-2 ent formats and programming languages. The Python Satellite Data Anal-3 ysis Toolkit (pysat) addresses this issue by providing an open source toolkit that implements the general process of space science data analysis, from be-5 ginning to end, in an instrument independent manner. This toolkit uses an 6 Instrument object that enables systematic analysis of science data from a 7 variety of platforms within a single interface. Basic functions such as down-8 loading, loading, and cleaning are included for all supported instruments. Com-9 mon analysis routines are also included, which are instrument and data source 10 independent. A nano-kernel is used to provide instrument independence, it 11 is attached to the Instrument object and mediates the systematic and ar-12 bitrary modification of loaded data. Pysat uses the nano-kernel to improve 13 the rigor of time series analysis, support on-the-fly orbit determination, and 14 cleanly span file breaks. Pysat's functions and higher level scientific analy-15 sis features are validated through the use of unit testing. Further adoption 16 by the community provides a set of scientific results produced by a common 17 core, constituting a distributed heritage that supports the validity of the un-18 derlying processing and scientific output. These features are used to demon-19 strate consistency between derived electron density profiles and measured 20 ion drifts, particularly downward ion drifts in the afternoon hours during ex-21 treme solar minimum. Pysat builds upon open source Python software that 22 is freely available and encourages community driven development. 23

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1. Introduction

The study of the geospace environment requires a wide variety of measurement tech-24 niques and a large number of measurement platforms. The quantity of data itself can be a 25 problem due to the variety of file formats and the unique characteristics of the underlying 26 data. These practical difficulties hinder scientific advancement and result in duplicated 27 efforts, as individual scientists or research groups create their own tools to solve old prob-28 lems. The scale and impact of these duplicated efforts has become intolerable now that 29 the geospace community has begun to take a system science approach, which requires inte-30 grating measurements from multiple platforms to understand the environment as a whole 31 CEDAR, 2010; Gil et al, 2016]. Thus, there is a need for a framework to accommodate 32 these varied data sets in an open and reproducible manner, while enabling versatility to 33 pursue various avenues of scientific investigation. 34

To support these goals, a variety of open source python packages have been released. Py-35 Glow collects a variety of space science models in one place, simplifies installation, and pro-36 vides a python interface [Duly et. al., 2013]. Apexpy [Mereen et al, 2018] and AACGMv2 37 Burrell and Meeren, 2018 provide interfaces to magnetic field models. OCBPy is a 38 Python module that converts between AACGM coordinates and a magnetic coordinate 39 system that adjusts latitude and local time relative to the Open Closed field line Boundary 40 (OCB) [Burrell and Chisham, 2018]. DaViTPy [DaViTPy, 2012] provides a suite of tools 41 designed to support the Super Dual Auroral Radar Network (SuperDARN) [Greenwald 42 et al., 1995; Chisham et al., 2007]. GeoData [Swoboda et al, 2016] is an API for obtain-43 ing and visualizing space science data, with current support for ground based systems. 44

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The Madrigal database, a repository of many space science measurements, has a python 45 interface [Rideout, 2004]. SpacePy [Morely et al, 2010] includes a variety of tools to support space science, a partial list includes field line tracing, file format support, coordinate 47 conversions, superposed epoch analysis support, and time support functions. pysatCDF Stoneback and Depew, 2018] provides a python interface to NASA CDF libraries and ad-49 ditional functionality to format this data for coupling with pysat. To simplify installation 50 the NASA CDF source code is included within pysatCDF and compiled automatically 51 using standard community tools. A pure python implementation for CDF reading and 52 writing without the use of the NASA C library is under development [Harter and Liu, 53 2018]. 54

The Python Satellite Data Analysis Toolkit (pysat) presented here is an open source 55 software package that handles the tedious details of file and data handling with a consistent 56 front end, allowing researchers to focus on the unique aspects of their scientific research. 57 Pysat's design evolved through years of data analysis using a variety of space and ground 58 based platforms and data types to enable the versatility required to address scientific 59 questions within a single interface. The generalized treatment of data sets and processing 60 by pysat provides the common ground needed to integrate many python package and 61 sources of data and into a cohesive whole that enables system science. 62

Pysat support begins with assisting users in obtaining data. Each instrument supported
 by pysat includes routines to download data from appropriate public locations, organize
 the files on the local computer, and clean the data.

⁶⁶ Pysat handles both data and metadata, data about the loaded data, with support for ⁶⁷ handling files of differing metadata standards in a consistent and robust manner. Even within the same file standard, differing capitalization (case) may be found across files from different teams. Pysat handles metadata in a case preserving manner that is also case-insensitive, enabling ease of use.

To enable the custom processing required by novel scientific investigations pysat includes funcitonality that mediates the application of custom functions upon data as it loaded. This design pattern ensures the availability of the newly processed parameters across all levels of pysat, with no additional effort required by the user.

To ease data distribution, routines have been created that transparently write a pysat 75 Instrument object to disk in a netCDF4 file, as well as load that file and produce the same 76 pysat Instrument object. These routines are written to be consistent with a combined 77 netCDF4 and NASA CDAWeb standard employed by the upcoming NASA ICON mission. 78 The validity of pysat functions and instrument independent analysis is verified through 79 the use of unit testing. Automated tests have been developed that test instrument support 80 routines, assisting new users in developing new instrument routines, while also ensuring 81 that these routines continue to work. In addition to isolated unit tests that verify specific 82 outputs from isolated functions, simulated instruments have been developed to support 83 the testing of pysat and associated functions as users would interact with the system. As 84 changes are committed to pysat, the test suite is automatically run, ensuring validity and 85 compatibility throughout the development process. 86

These features support the development and use of instrument independent analysis routines allowing users to focus on the unique aspects of their research project. Pysat's openness to community development also provides a place for researchers to disseminate their analysis routines used in their work. The application of an instrument independent

seasonal bin averaging routine is demonstrated here as an example of one such routine, 91 using remote measurements from COSMIC [Yue et al., 2010] and in situ measurements 92 from C/NOFS [de La Beaujardire et. al., 2004]. Despite the large difference in measure-93 ment type and data format, the same seasonal routine is used on both platforms. This 94 demonstrates geophysical consistency between the platforms. The use of seasonal bin 95 averaging is widespread in space science data analysis, thus pysat's validated instrument 96 independent implementation of this technique could assist many scientific studies using 97 the same underlying code. 98

2. Instrument Object

⁹⁹ The core functionality of pysat lies in the Instrument object. The intent of the In-¹⁰⁰ strument object is to offer a single interface for interacting with science data that is ¹⁰¹ independent of measurement platform. The layer of abstraction presented by the Instru-¹⁰² ment object is required for instrument independent analysis procedures, but it can also ¹⁰³ make science data analysis simpler and more rigorous.

As a simple metaphor, a software object is like a box with buttons. Inside the box the 104 object stores required data and the buttons on the box call methods that understand how 105 to interact with the data and produce the desired products. The pysat Instrument object 106 follows this guideline by storing science data within an object that also includes a number 107 of basic functions designed to load, modify, and analyze the data over arbitrary periods. 108 Data is stored internally in a Python Data Analysis Library (pandas) DataFrame, a format 109 chosen due to its time based array indexing and its ability to align multiple data products. 110 The pandas DataFrame is capable of storing higher dimensional objects, enabling mixed 111 dimensionality data sets [McKinney, 2010]. 112

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Pysat supports one data set per Instrument object, where a data set is defined as having 113 a single platform, instrument, measurement type, and satellite identifier, as appropriate. 114 Though the particulars of the files and data differ greatly between missions, the interface to 115 the data through the Instrument object remains constant. As an example, consider how to 116 initialize Instrument objects for magnetometer data from the Vector Electric Field Instru-117 ment (VEFI) or electron data from the Planar Langmuir Probe (PLP) that flew onboard 118 the Communications/Navigation Outage Forecasting System (C/NOFS), thermal plasma 119 measurement from the Ion Velocity Meter (IVM) also on C/NOFS; Global Positioning 120 Signals (GPS) from the Constellation Observing System for Meteorology, Ionosphere, and 121 Climate (COSMIC) satellites, or high-level, ground-based radar measurements from the 122 northern hemispheric portion of Super Dual Auroral Radar Network (SuperDARN): 123 vefi = pysat.Instrument(platform='cnofs', name='vefi', tag='dc_b') 124 ivm = pysat.Instrument(platform='cnofs', name='ivm') 125 cosmic = pysat.Instrument(platform='cosmic2013', name='gps', tag='ionprf') 126 darn = pysat.Instrument(platform='superdarn', name='grdex', tag='north') 127 Note how each instrument requires a different level of specificity based on the division 128 of data products within each mission. The full list of supported instruments is available 129 directly in python by inspecting the submodules, as well as within the pysat documenta-130 tion. Details about the options available for each instrument are stored directly within 131 the code through a python commenting standard called a docstring. These docstrings are 132 automatically collected and presented in the pysat documentation, reflecting the current 133 state of the instrument suite. The pysat documentation is integrated with a continuous 134 documentation service and is automatically generated as versions are released. 135

For each instrument, pysat looks for supporting routines that understand the unique qualities of the data set and handles the translation into a pysat compatible format. When no existing routines are available, they may be added to pysat. However, if no pysat specific support exists but there are already existing packages to support the loading of a data set, this functionality does not need to be recreated. For example, support for SuperDARN is fundamentally enabled by DaViT Python Project routines, which obtain and load the SuperDARN files.

Pysat support for some public data sources may be generalized. In these cases adding a new instrument to pysat may only involve little effort. Routines have been created for NASA's CDAWeb Common Data Format (CDF) and included with pysat. Pysat's support of C/NOFS' IVM, VEFI, PLP, and NASA's OMNI data sets are all driven by these routines. The only differences in pysat's support for each instrument are the cleaning routines, public data locations, and filename details.

Though the particulars of VEFI magnetometer data, IVM plasma parameters, COS-149 MIC atmospheric measurements, and SuperDARN backscatter measurements are very 150 different, the processes for high level operations on these data are the same. Data for any 151 Instrument may be obtained from data servers intended for public distribution and stored 152 locally by using the 'download' function, and data may be loaded for each instrument 153 using the 'load' function. There are multiple options available when instantiating objects 154 and when loading data that are fully explained in the pysat documentation, but outside 155 the scope of this document. 156

As mentioned previously, pysat uses the pandas DataFrame to store information internally. The DataFrame is similar to a spreadsheet, possessing labeled columns and rows. ¹⁵⁹ Pysat labels labels columns by the data name and rows by date and time. When opera-¹⁶⁰ tions are performed on the underlying data, row indices are aligned before performing the ¹⁶¹ operation. The loaded data may be accessed at the object level using strings. Support ¹⁶² for slicing and other operations is included.

For the one dimensional measurements in time, each column in the pandas DataFrame is a simple indexed array of numbers. However, the pandas DataFrames also support general collections of objects, used here to support higher dimensional data structures, such as the two dimensional electron density profiles from COSMIC. This is shown below for the first four elements of a COSMIC electron density profile. Note that the profile for this single time is also indexed by altitude.

169 In[]: cosmic[0, 'profiles']

170 Out[]:

171		ELEC_dens	GEO_lat
172	MSL_alt		
173	59.592628	34801.515625	49.295200
174	62.223614	31884.595703	49.303425
175	64.850388	32775.335938	49.311638
176	67.472939	29608.988281	49.319843

2.1. MetaData

Maintaining information about the data set is important. Pysat has built-in support to keep track of metadata, stored in a Meta object attached to the Instrument object. Metadata may be accessed by name at the object level, similar to standard data. Metadata may be assigned when data is assigned, or as needed. By default, units, name, notes, description, plot label, axis label, fill value, and plot scaling (linear vs log) are always tracked by the Instrument object, though arbitrary additional parameters may be added. When writing to a file, these metadata parameters are translated into a mixed standard spanning file requirements for the netCDF4 files as well as the International Solar Terrestrial Physics (ISTP) standard employed by NASA's CDAWeb. Parameters that may be determined through simple inspection of the data are not tracked.

¹⁸⁷ To help maintain compatibility with multiple standards, the pysat Meta object allows ¹⁸⁸ for user specified string labels to identify particular metdata types (fill, units, notes). ¹⁸⁹ As an example for fill values, netCDF4 files should use '_FillValue' while ISTP specifies ¹⁹⁰ 'FillVal'. Case is preserved for these labels however data access is case-insensitive, thus ¹⁹¹ 'units' works in code even if the label is strictly 'Units'. Label independent access is also ¹⁹² provided, thus users can use attributes attached to the pysat Meta object to access the ¹⁹³ desired metadata type without specifying the string used to label those values.

2.2. Modifying Data

Frequently, data sets need to be modified before a larger analysis may be completed. 194 Instrument specific modifications are handled in pysat by a nano-kernel with a custom 195 processing queue. Functions may be added to the queue as needed, and whenever new 196 data is loaded the nano-kernel will apply the ordered functions before making the data 197 available to the user. This configuration ensures that the newly calculated data has 198 the same properties and availability as parameters that are native to the file. A data 199 cleaning example is shown below. This code segment selects only VEFI magnetometer 200 measurements made at times when the magnetic torque rods on the spacecraft, used for 201 momentum control, were not contaminating the magnetic field environment. 202

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```
# define function to remove flagged values
def filter_vefi(vefi):
    idx, = np.where(vefi['B_flag']==0)
    vefi.data = vefi[idx, :]
    return
# add custom function to instrument
vefi.custom.add(filter_vefi, 'modify')
```

Once added, this function will filter the available VEFI data, modifying it in place, every time vefi.load is called.

2.3. Data Flow

The full data flow through the Instrument object when a load call is invoked is shown in Figure 1. Instrument specific functions (purple) translate the specifics of the given data set into a format suitable for pysat. Options and other parameters provided by the user are supplied as needed, shown in green. Pysat invokes the instrument specific functions as needed to provide the user with data in the desired form. Functions handled by pysat are shown in blue.

3. Generalized Space Science Solutions

Pysat builds upon the consistent object interface across data sets to enable generalized solutions for space science data analysis and visualization. At a basic level, all analysis routines that use the pysat Instrument object gain some independence from the particulars of the analyzed data. For example, string based data access makes it easy to support programmatic use of data. This and other pysat features allow many analytical processes to be generalized. Several examples of pysat generalized solutions to common space science
data problems are discussed in this section.

3.1. Recreating Continuous Data from Files

Measurements of continuous processes by scientific instruments are eventually divided into chunks and stored separately on a file system. These file boundaries can interfere with calculations, particularly for those times near the file edges. For example, consider a simple centered smoothing filter that averages a set number of measurements in time. The start and end of the time series will not have enough samples to obtain the result. To handle this problem, as well as the possibility of data gaps, a user must choose how to balance the quality and coverage of the output.

Pysat offers a solution to the problem of file breaks in a data set that requires no specific 232 support by any user supplied routine. When activated, pysat maintains an internal data 233 buffer that spans three files/days, depending upon user selected parameters. Each time 234 a user loads data, pysat centers the data buffer on the requested time, downselects from 235 this full buffer the requested data plus a user specified amount of data padding, applies 236 any user directed custom functions, and then removes the padded data before making the 237 full results available to the user (see Figure 1). This solution does not fix the calculation 238 everywhere, but rather pushes the boundaries where the calculation degrades outside the 239 desired time range and then removes the degraded calculations. 240

The resulting output is equivalent to a continuous data set, barring measurement gaps. The time period for this padding is arbitrary up to a maximum additional file or day. While this limits the maximum continuous data period available for a time based calculation, shorter period calculations may be applied without error over an effectively infinite time series while only using a small amount of computer memory. Applying this feature over N days only requires N+2 loads from the filesystem. Custom functions applied by the nano-kernel when data padding is enabled do not need to explicitly support the feature, as the data padding is removed after the custom functions are applied.

3.2. Iterating over Time Periods and Orbits

Seasons are one of the natural temporal divisions of geophysical data. To assist the 249 production of seasonally averaged pictures of the upper atmosphere, the temporal analysis 250 loop can be used to load data for a specified range of dates, one file at a time, and operated 251 on as needed for the desired analysis. The temporal analysis loop is a special case of the 252 iteration that is built into the pysat Instrument object. A simple pair of dates may be set 253 for a single season, or a range of dates may be provided for a more distributed temporal 254 analysis. The iteration is activated through standard Python functionality, using the same 255 mechanism employed when iterating over Python list elements. Each loop triggers a load 256 data call on the pysat Instrument object for the next day of data within the desired date 257 range. 258

This basic data iteration support is sufficient for daily or orbit-based analysis of science data sets. Since not all data sets are stored by day, pysat includes functionality to parse from multiple files the data that corresponds to the requested day. Similarly, pysat is designed to support real-time determination of orbit breaks from the data set, and then iterate over these orbits as desired. Orbits that cross file boundaries are handled using the pysat Instrument's iterative functions, moving forward or backward within the data to determine if the desired orbit begins or ends across one of these filebreaks and then includes the appropriate data. This combination of features makes it straightforward to make an orbit by orbit plot for any of the satellite missions supported by pysat. A simple code example for plotting the entirety of the VEFI data set by orbit is shown below, while the results are shown in Figure 2. For this particular example the orbits are set to begin and end at 0° geographic longitude.

instantiate instrument with desired orbit breakdown 272 orbit_info = {'index':'longitude', 'kind':'longitude'} 273 vefi = pysat.Instrument(platform='cnofs', name='vefi', tag='dc_b', 274 clean_level=None, orbit_info=orbit_info) 275 # iterate over dataset, orbit by orbit 276 for count, vefi in enumerate(vefi.orbits): 277 # One orbit of data is now accessible via vefi.data 278 # To ensure data gaps do not have a line drawn across the gap, 279 # resample data onto constant 1 second cadence, filling in gaps with NaN 280 vefi.data = vefi.data.resample('1S', fill_method='ffill', 281 limit=1, label='left') 282

283 # data is ready to be plotted

3.3. Instrument Independent Seasonal Analysis

²⁸⁴ Pysat functionality has been used to develop several seasonal analysis routines that are ²⁸⁵ instrument and iteration independent. An example using a pysat occurrence probability ²⁸⁶ routine is shown, reproducing the fundamental processing used to obtain published results ²⁸⁷ by *Stoneback and Heelis* [2014]. Note that the pysat analysis covers all of the data loading, ²⁸⁸ iteration, and analysis. No specific support for VEFI was included in the routine. The ²⁸⁹ routine calculates the number of times a given value exceeds a supplied threshold at ²⁹⁰ least once per temporal period (day, file, or orbit), divided by the number of times a ²⁹¹ given spatial bin is visited per temporal period. As a demonstration, the probability of ²⁹² a positive perturbation in the meridional component of the geomagnetic field by orbit is ²⁹³ shown over a week for VEFI in Figure 3.

To help ensure the plotted data is geophysical, the VEFI torque rod exclusion function introduced earlier is attached to a VEFI pysat object. This function selects data when magnetic torquers on C/NOFS were idle. The torque rod firings interfered with the electromagnetic measurements and are generally located near the magnetic equator. The reduction in counts in Figure 3(b) along the magnetic equator demonstrates that the custom function is properly selecting data. The code to produce Figure 3 follows:

300 # instantiate instrument with desired orbit breakdown

301 orbit_info = {'index':'longitude', 'kind':'longitude'}

- vefi = pysat.Instrument(platform='cnofs', name='vefi', tag='dc_b',
- 303

clean_level=None, orbit_info=orbit_info)

³⁰⁴ # add custom torque rod filter function to instrument

vefi.custom.add(filter_vefi, 'modify')

306 # set time limits on data analysis

307 start = pysat.datetime(2010,5,9)

stop = pysat.datetime(2010,5,15)

309 # download data for specified time period

310 vefi.download(start, stop)

311 # perform probability calculation. Any data added by custom functions is

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312 # available within routine below

ans = ssnl.occur_prob.by_orbit2D(vefi, [0,360,144], 'longitude',

³¹⁴ [-13,13,104], 'latitude', ['dB_mer'], [0.], returnBins=True)

³¹⁵ # a dictionary object with keys corresponding

316 # to data labels is returned

317 # results are ready for plotting

Pysat also includes generalized seasonal analysis routines that support averaging mul-318 tiple instrument parameters of various dimensionality over a season. Here we use this 319 functionality to average both IVM and COSMIC data, enabling comparisons between the 320 average distributions of ion density and ion drift. The same general process used to ob-321 tain the VEFI occurrence probability is used; both IVM and COSMIC pysat objects are 322 instantiated and passed along to the seasonal pysat routines for analysis. The COSMIC 323 data set does not come with location information in geomagnetic coordinates, or with 324 information on the topside scale height, so these parameters are calculated using custom 325 functions and applied to the data set automatically using the nano-kernel functionality. 326 The nano-kernel functionality ensures that the custom COSMIC parameters are available 327 for averaging within the seasonal bin averaging routine. 328

Figure 4 includes ion drift measurements from IVM and electron density profile parameters from COSMIC, seasonally averaged over apex longitude and local time. The use of apex longitude organizes the data based upon the apex location of the geomagnetic field line at the measurement location. IVM derived vertical ion drifts are at the top followed by the COSMIC derived ion density maximum, height of the density maximum, and the thickness of the density distribution. This ion drift average displays downward ³³⁵ afternoon ion drifts, a characteristic of the ionosphere during very low solar activity levels ³³⁶ Stoneback et al [2011]. These ion drifts employ a geophysically motivated calibration to ³³⁷ appropriately set the zero ion drift level used when translating raw IVM measurements ³³⁸ to geophysical ion drifts [Stoneback et al, 2011].

In the late afternoon and evening sector, longitudinal and local time variations in the 339 meridional ion drift recorded by IVM have equivalent variations in the altitude of the 340 density maximum recorded by COSMIC. A strong correlation between drifts and density 341 is not expected during the morning through afternoon as plasma production from sunlight 342 is a dominant driver of density. In the late afternoon and evening hours, when plasma 343 production and loss processes are small or nearly equal, redistribution of the plasma to 344 different altitudes through transport by ion drifts are expected to have a measurable 345 impact upon the ionosphere. The results in Figure 4 between 15 - 24 local time have 346 a strong apparent correlation between areas with upward (downward) ion drifts and an 347 increase (decrease) in the height of the density maximum across all longitudes. 348

The full electron density profiles from COSMIC are shown in Figure 5 and correspond 349 to the first four longitude sectors $(0^{\circ} - 60^{\circ})$ in Figure 4. The first two longitude sectors 350 top panel) have upward slants in the bottomside density distribution at night, consistent 351 with the upward drifts after sunset in Figure 4. In contrast, the bottom two panels, show 352 longitudes associated with downward drifts in the evening and have flat bottomside ion 353 distributions at night. These changes in the bottomside density profiles are consistent 354 with the meridional plasma drift, because a negative drift moves plasma to lower altitude 355 field lines with higher neutral densities, where loss processes rise exponentially. This effec-356 tively produces a minimum viable altitude for the night ime ionosphere. The consistency 357

demonstrated between IVM and COSMIC measurements provides supporting evidence 358 that both platforms are reporting measurements with geophysical significance that have 359 been analyzed in a consistent and appropriate manner. The same generalized seasonal 360 analysis code was used for both IVM and COSMIC. The complete code to produce these 361 figures is included in the pysat repository under demos. 362

3.4. Validating Results

To validate space science results, both the code and the underlying data must be tested. 363 A suite of unit tests have been developed to help ensure robust performance of pysat and 364 its features. These tests initialize the system in a known state, perform a limited set of 365 operations, and then compare the result of those operations against a known output. The 366 pysat development repository is connected to a continuous integration service, which runs 367 the test suite after every change to the codebase. Currently, 460 unit tests cover 82% of 368 pysat's code, as determined using standard community tools. Basic tests cover options for 369 instantiating the pysat Instrument object and its handling of data, metadata, and files. 370 To facilitate the testing of pysat features that require science data, such as the nano-371 kernel support, orbit-by-orbit iteration, and instrument independent analysis functions, 372 testing instrument platforms are also included. These pysat test instruments operate like 373 a normal pysat Instrument object. However, the typical load routines that read science 374 data from the filesystem are replaced with a basic simulation of satellite motion. Signals 375 representing the large scale periodic features of local time, longitude, latitude, altitude, 376 etc. are generated. These routines produce infinite continuous streams of reproducible 377 data that may be used as known inputs in a unit testing framework.

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The general process of determining orbits from a random science data set faces a number 379 of data and file issues. Accounting for these variables, along with the various input options 380 that can be selected, required a significant testing suite. Iterating by orbit requires, in part, 381 determining where orbit breaks occur, completing orbits across file breaks, accounting for 382 data gaps, and ensuring consistent orbit numbering. To cover all of these options a 383 general class of orbit tests were created that produced a wide range of data and file gaps. 384 Each problem type is expanded upon to ensure coverage for edge and pathological cases. 385 This whole suite of tests is then run using each type of orbit pysat supports (local time, 386 longitude, latitude, orbit number), ensuring that loading or processing data by orbit will 387 not affect the scientific analysis. 388

³⁸⁹ Unit tests have also been developed to monitor the instrument specific routines that ³⁹⁰ download, load, and clean science data as part of the pysat process. Each run of the unit ³⁹¹ testing suite downloads, loads, and cleans test days for pysat supported instruments using ³⁹² data obtained from the appropriate public data source. General pysat compliance is also ³⁹³ checked, assisting users developing code to support new instruments. Some instruments ³⁹⁴ have to be excluded from parts of the testing process, as access to the data sources requires ³⁹⁵ authentication.

3.5. Creating Data for Distribution

³⁹⁶ Creating data sets suitable for distribution has remained a challenge. Files that are easy ³⁹⁷ to put together lack the metadata for a self-supporting specification of the data. Formats ³⁹⁸ that are capable of storing a wide variety of data, formats, and metadata generally require ³⁹⁹ significant effort to provide this information. Pysat approaches this issue on two fronts. ⁴⁰⁰ Pysat includes metadata by default. Thus, as a routine to create a dataset is written,

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⁴⁰¹ both the data and metadata may be specified naturally. Following best coding practices,
⁴⁰² the data specification work is distributed across the whole development effort.

When a pysat Instrument object loads data both the instrument data and metadata 403 are pulled from the file and attached to the pysat Instrument object. File routines have 404 been created to reverse this process and transparently store a pysat object to disk as a 405 netCDF. As many different data schemes may be stored within pysat, a translation layer 406 has been developed that stores the data in the netCDF in a format intuitive to humans. 407 A complementary netCDF load routine is also included with pysat, making it possible 408 to recover the original pysat Instrument object state without any additional processing. 409 Recovery back to the original pysat object relies upon a variable naming pattern, and 410 thus is not guaranteed for non-pysat netCDFs. 411

4. Future Possibilities

Pysat provides a systematic and versatile framework for the arbitrary modification and 412 analysis of data. A selection of instruments and analyses are included that currently 413 reflect the research interests of the authors. The list is not exhaustive. Since instrument 414 data types ranging from in situ satellite data, satellite based remote sensing data, and 415 ground based data have already been successfully integrated into pysat, a wide range of 416 instruments are expected to be supported without significant changes to pysat's structure. 417 With community support, the full range of space science data sets could be available from a 418 single, consistent interface. Additional analysis types, such as superposed epoch analysis, 419 can also be added to pysat. 420

⁴²¹ Pysat's support for test instruments and inclusion of unit testing provides a mechanism
 ⁴²² to validate analysis code. Details of exhaustive test procedures are not typically included

⁴²³ in scientific publications, limiting the ability of the audience to audit the analysis. Adop-⁴²⁴ tion of open source analyses such as pysat by the community provides a verifiable code ⁴²⁵ standard that minimizes both the effort required by the author, as well as the innate ⁴²⁶ level of trust required by the reader. The sum total of publications based upon pysat ⁴²⁷ code provides a heritage base that supports future publications. This can be of particular ⁴²⁸ importance for analyses that produce controversial results.

Pysat's structure enables a common ground and a single interface for all space science 429 data sets. This does not preclude the development and use of instrument specific packages, 430 as desired by the community. In these situations pysat can and will make use of the 431 instrument specific tools when adding support for that instrument. In most cases, a thin 432 translation layer from the native data format to the pandas DataFrame will provide the 433 majority of the required functionality. A pair of functions that translate the data back 434 and forth between standards would even enable the use of instrument specific processing 435 functions from within pysat. While the instrument specific package may be optimal for 436 primary instrument users, outside users could utilize the standard interface provided by 437 pysat and still benefit from the creation of the instrument specific tools. 438

The range of file management features required to support pysat also provide an underlying basis for a CubeSat data processing system. While Explorer-level missions supported by NASA typically have enough funds to produce a dedicated software ecosystem to support the processing of data, funding levels typically employed for CubeSats are insufficient for this level of software development. Pysat provides a foundation for file and data processing management that reduces the workload required to create a system capable of delivering upon the science goals of the mission. If leading CubeSat missions are willing to use pysat for this purpose as well as contribute code back to the repository, this community resource could increase both the dollar and science efficiency of future CubeSat missions.

The functions provided by pysat constitute the underlying functionality needed to drive a Graphical User Interface (GUI) for easy visualization of data. In this scenario if a user finds something interesting visually and wanted to complete a more rigorous analysis the exact same tools would be available at the command line, providing continuity for scientific analysis. Given that user interface requirements can differ significantly based upon the analysis or instrument type, a range of specialized GUIs all powered by the same underlying pysat code would be ideal.

Functionality provided by pysat also supports the creation of a Constellation object, a heterogenous collection of pysat Instrument objects. This abstraction will allow custom collections of instruments to be operated upon as a whole. As the processing required for each instrument within the constellation could be unique, custom functions may be attached to the Constellation object and applied to individual instruments automatically. Analysis functions and orbit determination on the constellation level are also planned.

5. Conclusion

Pysat provides a systematic process for custom analysis of science data sets. The pysat Instrument object enables a complex flow for each user request of data, providing for an arbitrary relationships between the requested and archived data. This processing flow is used to solve problems associated with multiple data sets, data distribution in files, accurate time-series calculations, orbit determination, data modification, and the calculation of new scientific products. The combination of the pysat Instrument object,

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⁴⁶⁸ pandas DataFrame, and this computational versatility enables instrument independent
⁴⁶⁹ analysis and simplifies the comparison of results across data sets. These features are
⁴⁷⁰ expected to be sufficient to enable integration of data sets across space science into a
⁴⁷¹ single common platform.

The adoption of unit testing across the package provides a verification chain to ensure 472 results are robust. Tests are applied to the Instrument object as well as the higher order 473 analysis routines (seasonal bin averaging, etc.) The public availability of both the code 474 and the tests provides a mechanism for verifiable and reproducible science. Should pysat 475 be adopted by the wider community, additional validation is gained as scientists use and 476 individually verify the tools as part of their own research. Thus, scientific papers that 477 incorporate pysat not only benefit from the heritage established by previous use, each new 478 use of pysat also provides validation that the outputs provided by pysat are scientifically 479 valid. 480

⁴⁸¹ Pysat is being used as a foundational framework for ground station processing of IVM ⁴⁸² measurements for the upcoming ICON and COSMIC-2 missions. While work is still ⁴⁸³ underway, pysat has been integrated by both CDAAC and the Berkeley ground software ⁴⁸⁴ system in anticipation of these missions. The data flow generated by these missions will ⁴⁸⁵ provide a strong heritage that future missions and science data analyses can build upon.

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 The data used in this article may be obtained at:

488 CDAWeb: http://cdaweb.gsfc.nasa.gov

489 CDF Library: http://cdf.gsfc.nasa.gov.

490 CDAAC: http://cosmic-io.cosmic.ucar.edu/cdaac/index.html

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- ⁴⁹¹ pysat : https://github.com/rstoneback/pysat
- ⁴⁹² pysatCDF : https://github.com/rstoneback/pysatCDF
- ⁴⁹³ DaViTpy : https://github.com/vtsuperdarn/davitpy
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Figure 1. Pysat program flow when an pysat.Instrument.load() routine is called.

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Figure 2. Sample orbit figure using VEFI data, where the interp flag reflects times when spacecraft operations could interfere with measurements.





Figure 3. Seasonal occurrence probability demo using VEFI data. The location of the magnetic equator may be seen in the lower data counts for the data distribution.



Figure 4. Comparison of seasonal averages of IVM meridional ion drifts (top) and averages of COSMIC profiles covering NmF2, hmF2, and topside scale height.



Figure 5. Seasonal average of COSMIC electron density profiles.