PyHC Package Compatibility Effort Update

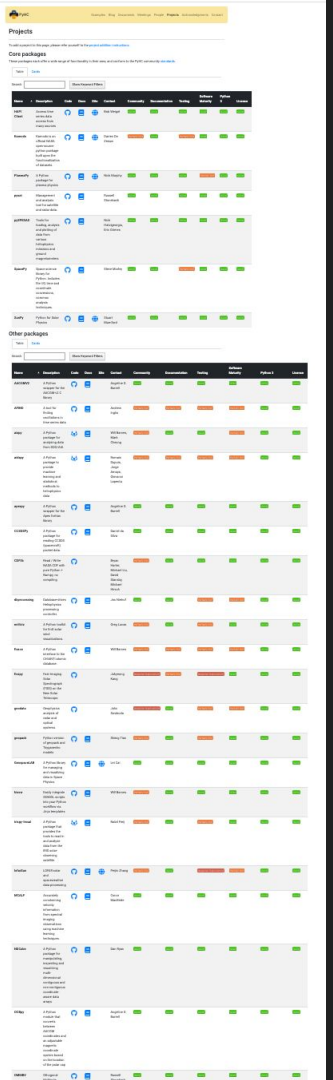
By Shawn Polson

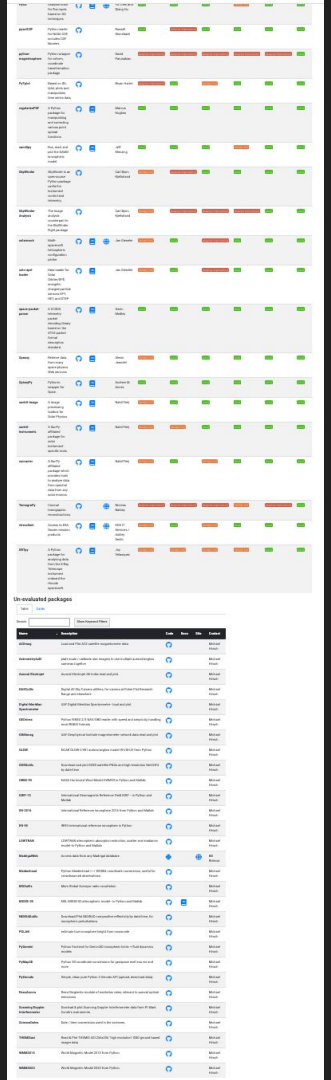
Introduction

Unified **Python environment**

Publishing images in **Docker Hub**

Putting packages in **Conda**





Lots of PyHC packages

generate-table.py

```python
def excel_spreadsheet_from_table_data(table_data):
    """
    :param table_data: The data structure returned from `generate_dependency_table_data()`
    :return: The Excel workbook that is the dependency conflict table
    """
    if not isinstance(table_data, dict) or not table_data:
        raise ValueError('Invalid table data.')
    if not isinstance(table_data['core_dependencies'], dict):
        raise ValueError('Invalid core_dependencies in table data.')
    if not isinstance(table_data['other_dependencies'], dict):
        raise ValueError('Invalid other_dependencies in table data.')
    if not isinstance(table_data['project_data'], dict):
        raise ValueError('Invalid project_data in table data.')

    # Extract data for Excel
    core_dependencies = table_data['core_dependencies']
    other_dependencies = table_data['other_dependencies']
    all_dependencies = {**other_dependencies, **core_dependencies}  # shouldn't be overlap, but core values would win
    project_data = table_data['project_data']

    # Create a new workbook
    workbook = openpyxl.Workbook()

    # Select the active worksheet
    worksheet = workbook.active

    # Write headers to the worksheet
    worksheet['A1'] = 'Package'
    worksheet['B1'] = 'Allowed Version Range'

    # Write data to the worksheet
    if core_dependencies:
        # Write core environment dependencies to the first two columns of the worksheet (shaded light gray)
        for package_name, (row, version_range) in core_dependencies.items():
            # Column 1 - Package
            cell = worksheet.cell(row=row, column=1)
            cell.value = package_name
            cell.fill = PatternFill(start_color="aaaaaa", end_color="aaaaaa", fill_type="solid")

            # Column 2 - Allowed Version Range
            cell = worksheet.cell(row=row, column=2)
            cell.value = version_range  # TODO: shouldn't ever be "N/A" but should I consider that case here anyway?
            cell.fill = PatternFill(start_color="aaaaaa", end_color="aaaaaa", fill_type="solid")

        # Add a dark gray separator before other dependencies
        cell = worksheet.cell(row=row+1, column=1)
        cell.fill = PatternFill(start_color="333333", end_color="333333", fill_type="solid")
        cell = worksheet.cell(row=row+1, column=2)
        cell.fill = PatternFill(start_color="333333", end_color="333333", fill_type="solid")

    # Write other environment dependencies to the first two columns of the worksheet
    # TODO: consider doing this the cell-oriented way like we do for core_dependencies?
    for package_name, (_, version_range) in other_dependencies.items():
        row_data = [package_name, version_range if version_range is not None else "N/A"]
        worksheet.append(row_data)

    # Write project data to the worksheet one column at a time
    for j, (project, dependency_data) in enumerate(project_data.items(), start=3):
        worksheet.cell(row=1, column=j, value=project)  # column header
        for package_name, (compatible, version_range) in dependency_data.items():
            row_num = all_dependencies[package_name][0]
            cell = worksheet.cell(row=row_num, column=j)
            if compatible is not None:
                cell.value = version_range
                if compatible:
                    cell.fill = PatternFill(start_color="00ff00", end_color="00ff00", fill_type="solid")
                else:
                    cell.fill = PatternFill(start_color="ff0000", end_color="ff0000", fill_type="solid")

    return workbook


if __name__ == '__main__':
    generate_requirements_file()
    core_packages = get_core_pyhc_packages()
    other_packages = get_other_pyhc_packages()
    all_packages = core_packages + other_packages
    table_data = generate_dependency_table_data(all_packages)

    # Write table_data
    import pickle
    with open('pyhc-dependency-table-may-11-2023.pkl', 'wb') as f:
        pickle.dump(table_data, f)

    table = excel_spreadsheet_from_table_data(table_data)
    table.save('pyhc-dependency-table-may-11-2023.xlsx')
    print("done")
```

Line 949, Column 1

Lots of PyHC packages

Needed a grip on **dependency conflicts**

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG	AH	AI	AJ	AK	AL	AM	AN	AO	AP	AQ	AR	AS	AT	AU	AV	AW	AX
1	Package	Allowed Version Range	hapiclient	kamodo	plasmapy	pysat	pyspedas	spacepy	sunpy	aacgmv2	aiapy	aidapy	apexpy	astrometry-ctfiib	dascutils	dbprocessir	dmsp	enlilviz	fiasco	geoinex	geospacela	goesutils	hissw	igrf	iri2016	iri90	inispy-imsal	lowtran	mcalf	msise00	ndcube	newradutils	octbpy	OMMBV	pydarn	pyfict	pytplot	pytplot-mpl	pyzenodo3	reesaurora	sciencedata	solarmach	solo-epd-lo	speasy	spicepyp	sunkit-imag	sunkit-instr	sunraster	themisasi
2	aacgmv2	>=2.6.2																				>=2.6.2													Any		Any													
3	aiohttp	Any							Any		Any	Any																Any															Any	Any			Any	Any		
4	aiesignal	>=1.1.2							>=1.1.2		>=1.1.2	>=1.1.2																>=1.1.2														>=1.1.2	>=1.1.2			>=1.1.2	>=1.1.2		
5	aniso8601	>=0.82		>=0.82																																															
6	antlr4-python3-runtime	==4.7		>=4.7																																															
7	anyio	>=3.1.0,<4			>=3.1.0,<4														>=3.1.0,<4																															
8	appdirs	Any																																											Any						
9	appnope	Any			Any														Any																																
10	argon2-cffi	Any			Any														Any																																
11	argon2-cffi-bindings	Any			Any														Any																																
12	asdf	>=2.8.1																										>=2.8.1				>=2.8.1																	>=2.8.1	
13	asdf-astropy	>=0.2.0																										>=0.2.0				>=0.2.0																	>=0.2.0	
14	asdf-coordinates-schemas	Any																										Any				Any																	Any	
15	asdf-standard	>=1.0.1																										>=1.0.1				>=1.0.1																	>=1.0.1	
16	asdf-transform-schemas	>=0.3.0																										>=0.3.0				>=0.3.0																	>=0.3.0	
17	asdf-unit-schemas	>=0.1.0																										>=0.1.0				>=0.1.0																	>=0.1.0	
18	asdf-wcs-schemas	Any																										Any				Any																	Any	
19	asteval	>=0.9.28			>=0.9.28														>=0.9.28																															
20	astropy	>=5.1			>=5.0.1		Any		>=4.2.1		>=4.2.1	>=4.2.1		Any		Any			>=5.0.1								>=5.1		>=4.2		>=5.1						Any				>=4.2.1	>=4.2.1	>=4.1		>=4.2.1	>=4.2.1	>=5.1	
21	astroquery	Any																																									Any		Any						
22	asttokens	>=2.1.0			>=2.1.0														>=2.1.0																															
23	async-timeout	>=4.0.0a3,<5.0							>=4.0.0a3,<5.0		>=4.0.0a3,-	>=4.0.0a3,<5.0																>=4.0.0a3,<5.0														>=4.0.0a3,-	>=4.0.0a3,<5.0			>=4.0.0a3,-	>=4.0.0a3,<5.0		
24	attrs	>=19.2.0		>=19.2.0	>=19.2.0	>=19.2.0			>=17.3.0		>=17.3.0	>=17.3.0							>=19.2.0									>=17.4.0				>=17.4.0			>=18.2.0						>=17.3.0	>=17.3.0			>=17.3.0	>=17.3.0	>=17.4.0	
25	babel	>=2.10			>=2.10														>=2.10																															
26	backcall	Any			Any														Any																															
27	beautifulsoup4	>=4.9.3			Any														Any			>=4.9.3																	Any			>=4.3.2	Any	>=4.3.2					
28	bleach	Any			Any														Any																															
29	blosc2	~=2.0.0					~=2.0.0																													~=2.0.0													
30	bokeh	>=1.1,<3.0					>=1.1,<3.0																															>=1.1	>=1.1,<3.0										
31	bottleneck	Any										Any																																						
32	bs4	Any																																									Any							
33	cdasws	>=1.7.24					>=1.7.24																																											
34	cdflib	>=0.4.3					>=0.4.3					Any										>=0.3.20																Any	Any				Any						>=0.3.13
35	certifi	>=2017.4.17		>=2017.4.1	>=2017.4.17		>=2017.4.17					>=2017.4.17							>=2017.4.17			>=2017.4.1	>=2017.4.17						>=2017.4.17		>=2017.4.17								>=2017.4.1	>=2017.4.17		>=2017.4.1	>=2017.4.1	>=2017.4.17					>=2017.4.1
36	cffi	>=1.12		>=1.12	>=1.0.1														>=1.0.1																															
37	cftime	Any				Any	Any										Any	Any				Any													Any															
38	charset-normalizer	>=2,<4		>=2,<4	>=2,<4		>=2,<4		>=2.0,<4.0		>=2.0,<4.0	>=2,<4							>=2,<4			>=2,<4	>=2,<4					>=2.0,<4.0			>=2,<4		>=2,<4						>=2,<4	>=2,<4		>=2,<4	>=2,<4	>=2,<4		>=2.0,<4.0	>=2.0,<4.0		>=2,<4	
39	click	>=8.0		>=5.1		>=7.0						>=8.0																														>=7.0									
40	cloudpickle	>=1.1.1				>=1.1.1																																				>=1.1.1									
41	comm	>=0.1.1			>=0.1.1														>=0.1.1																															
42	contourpy	>=1.0.1			>=1.0.1		>=1.0.1					>=1.0.1						>=1.0.1	>=1.0.1			>=1.0.1						>=1.0.1		>=1.0.1						>=1.0.1		>=1.0.1	>=1.0.1		>=1.0.1	>=1.0.1	>=1.0.1					
43	cryptography	>=38.0.0,<40		>=38.0.0,<40																																														
44	cycler	>=0.10			>=0.10		>=0.10					>=0.10						>=0.10	>=0.10			>=0.10						>=0.10		>=0.10						>=0.10		>=0.10	>=0.10		>=0.10	>=0.10	>=0.10					
45	cython	>=0.29.21					>=0.29.21															Any														>=0.29.21													
46	dask	Any				Any																													Any															
47	datetime	Any																																									Any							
48	debugpy	>=1.6.5			>=1.6.5														>=1.6.5																															
49	decorator	>=4.4.2		>=4.4.2	Any														Any																															
50	deepdish	Any																																		Any														
51	defusedxml	Any			Any														Any																															
52	dill	>=0.3.6																												>=0.3.6																				
53	diskcache	Any																																										Any						
54	drms	Any																																									Any							
55	entrypoints	Any			Any														Any																															
56	exceptiongroup	>=1.0.0rc8		>=1.0.0rc8	>=1.0.0rc8	>=1.0.0rc8													>=1.0.0rc8																>=1.0.0rc8													
57	executing	>=1.2.0			>=1.2.0														>=1.2.0																															
58	extension	Any										Any																																						
59	fastjsonschema	Any			Any														Any																															
60	flask	==1.1.2		>=1.1.2								>=1.0.2																																						
61	flask-cors	Any		Any																																															
62	flask-restful	==0.3.8		>=0.3.8																																															
63	fonttools	>=4.22.0			>=4.22.0		>=4.22.0					>=4.22.0						>=4.22.0	>=4.22.0			>=4.22.0						>=4.22.0		>=4.22.0						>=4.22.0		>=4.22.0	>=4.22.0		>=4.22.0	>=4.22.0	>=4.22.0					
64	fortranformat	Any																	Any																															
65	frozenlist	>=1.1.1							>=1.1.1		>=1.1.1	>=1.1.1																>=1.1.1														>=1.1.1	>=1.1.1			>=1.1.1	>=1.1.1		
66	fsspec	>=0.6.0				>=0.6.0																													>=0.6.0															
67	future	Any			Any														Any																															
68	geomagindices	>=1.4.0																													>=1.4.0										>=1.4.0								
69	geopack	>=1.0.9					>=1.0.9															>=1.0.8																											
70	greenlet	!=0.4.17															!=0.4.17																																	
71	gridaurora	Any																																							Any									
72	gwcs	>=0.15																										>=0.15				>=0.15																	>=0.15	
73	h5netcdf	Any																																									Any							
74	h5py	>=3.2.1			>=3											Any			>=3			>=3.2.1														Any						Any							
75	hapiclient	>=0.2.2					>=0.2.2																																											
76	hatanaka	Any																			Any																														
77	heliopy	>=0.12.0										>=0.12.0																																						
78	heliopy-multid	Any										Any																																						
79	html5lib	>=0.999																																								>=0.999		>=0.999						
80	hydra-core	==0.11.3		>=0.11.3																																															
81	idna	>=2.8,<4		>=2.5,<4	>=2.8,<4		>=2.5,<4		>=2.0		>=2.0	>=2.5,<4							>=2.8,<4			>=2.5,<4	>=2.5,<4					>=2.0			>=2.5,<4		>=2.5,<4						>=2.5,<4	>=2.5,<4	>=2.5,<4		>=2.0	>=2.0		>=2.5,<4	
82	imagesio	>=2.4.1																					>=2.1										>=2.3													>=2.4.1				
83	importlib-metadata	>=4.11.4			>=4.8.3							>=4.4							>=4.8.3									>=4.11.4				>=4.11.4										>=4.11.4		>=4.11.4				>=4.11.4	
84	importlib-resources	>=3.2.0			>=3.2.0		>=3.2.0					>=3.2.0						>=3.2.0	>=3.2.0	Any		>=3.2.0						>=3.0		>=3.2.0						>=3.2.0		>=3.2.0	>=3.2.0		>=3.2.0	>=3.2.0	>=3.2.0					
85	incremental	Any		Any																																															
86	inisnofix	Any		Any	Any	Any													Any																Any															

Sheet

Package	Allowed Version Range	hapiclient	kamodo	plasmapy	pysat	pyspedas	spacepy	sunpy	aacgmv2	aiapy	aidapy	apexpy	astrometry.net	astropy-ccffib	dascutils	dbprocessing	dmsp	enlilviz	fiasco	geopacela	geosutils	hissw	igrf	iri2016	iri90	inspy-imsat	lowtran	mcalf	msise00	ndcube	newradutils	octopy	OMMBV	pydarn	pyfiet	pytplot	pytplot-mpl	pyzenodo3	reesaurora	sciencedata	solarmach	solo-epd-lo	speasy	spicepy	sunkit-imag	sunkit-instr	sunraster	themisasi
aacgmv2	>=2.6.2																			>=2.6.2														Any														
aiohttp	Any							Any		Any	Any															Any														Any	Any			Any	Any		
aiosignal	>=1.1.2							>=1.1.2		>=1.1.2	>=1.1.2															>=1.1.2														>=1.1.2	>=1.1.2			>=1.1.2	>=1.1.2		
aniso8601	>=0.82		>=0.82																																													
antlr4-python3-runtime	==4.7		>=4.7																																													
anyio	>=3.1.0,<4			>=3.1.0,<4															>=3.1.0,<4																													
appdirs	Any																																										Any					
appnope	Any			Any															Any																													
argon2-cffi	Any			Any															Any																													
argon2-cffi-bindings	Any			Any															Any																													
asdf	>=2.8.1																									>=2.8.1				>=2.8.1																	>=2.8.1	
asdf-astropy	>=0.2.0																									>=0.2.0				>=0.2.0																	>=0.2.0	
asdf-coordinates-schemas	Any																									Any				Any																	Any	
asdf-standard	>=1.0.1																									>=1.0.1				>=1.0.1																	>=1.0.1	
asdf-transform-schemas	>=0.3.0																									>=0.3.0				>=0.3.0																	>=0.3.0	
asdf-unit-schemas	>=0.1.0																									>=0.1.0				>=0.1.0																	>=0.1.0	
asdf-wcs-schemas	Any																									Any				Any																	Any	
asteval	>=0.9.28			>=0.9.28															>=0.9.28																													
astropy	>=5.1			>=5.0.1		Any		>=4.2.1		>=4.2.1	>=4.2.1		Any		Any				>=5.0.1							>=5.1		>=4.2		>=5.1					Any				>=4.2.1	>=4.2.1	>=4.1		>=4.2.1	>=4.2.1	>=5.1	
astroquery	Any																																							Any		Any						
asttokens	>=2.1.0			>=2.1.0															>=2.1.0																													
async-timeout	>=4.0.0a3,<5.0							>=4.0.0a3,<5.0		>=4.0.0a3,<5.0	>=4.0.0a3,<5.0															>=4.0.0a3,<5.0												>=4.0.0a3,<5.0	>=4.0.0a3,<5.0			>=4.0.0a3,<5.0	>=4.0.0a3,<5.0		
attrs	>=19.2.0	>=19.2.0	>=19.2.0	>=19.2.0	>=19.2.0			>=17.3.0		>=17.3.0	>=17.3.0								>=19.2.0							>=17.4.0				>=17.4.0		>=19.2.0						>=17.3.0	>=17.3.0			>=17.3.0	>=17.3.0	>=17.4.0	
babel	>=2.10			>=2.10															>=2.10																													
backcall	Any			Any															Any																													
beautifulsoup4	>=4.9.3			Any															Any		>=4.9.3																Any		>=4.3.2	Any		>=4.3.2					
bleach	Any			Any															Any																													
blosc2	~=2.0.0					~=2.0.0																											~=2.0.0														
bokeh	>=1.1,<3.0					>=1.1,<3.0																														>=1.1	>=1.1,<3.0										
bottleneck	Any										Any																																					
bs4	Any																																															
cdasws	>=1.7.24					>=1.7.24																																										
cdflib	>=0.4.3					>=0.4.3					Any										>=0.3.20																									>=0.3.13	
certifi	>=2017.4.17		>=2017.4.17	>=2017.4.17		>=2017.4.17					>=2017.4.17								>=2017.4.17		>=2017.4.17	>=2017.4.17							>=2017.4.17		>=2017			>=2017.4.17	>=2017.4.17			>=2017.4.1	>=2017.4.17	>=2017.4.17						>=2017.4.1
cffi	>=1.12		>=1.12	>=1.0.1															>=1.0.1																													
cftime	Any				Any	Any											Any	Any			Any													Any														
charset-normalizer	>=2,<4	>=2,<4		>=2,<4		>=2,<4		>=2.0,<4.0		>=2.0,<4.0	>=2,<4								>=2,<4		>=2,<4					>=2.0,<4.0			>=2,<4						>=2,<4		>=2,<4	>=2,<4	>=2,<4			>=2.0,<4.0	>=2.0,<4.0		>=2,<4	
click	>=8.0		>=5.1		>=7.0						>=8.0																							>=7.0														
cloudpickle	>=1.1.1				>=1.1.1																													>=1.1.1														
comm	>=0.1.1			>=0.1.1																																												
contourpy	>=1.0.1			>=1.0.1		>=1.0.1					>=1.0.1					>=1.0.1											>=1.0.1						>=1.0.1		>=1.0.1				>=1.0.1	>=1.0.1	>=1.0.1						
cryptography	>=38.0.0,<40		>=38.0.0,<40																																													
cycler	>=0.10			>=0.10		>=0.10										>=0.10			>=0.10							>=0.10		>=0.10					>=0.10		>=0.10	>=0.10			>=0.10	>=0.10	>=0.10						
cython	>=0.29.21					>=0.28.21																											>=0.29.21															
dask	Any																																	Any														
datetime	Any																																									Any						
debugpy	>=1.6.5			>=1.6.5																																												
decorator	>=4.4.2		>=4.4.2	Any																																												
deepdish	Any																																															
defusedxml	Any			Any															Any																													
dill	>=0.3.6																											>=0.3.6																				
diskcache	Any																																										Any					
drms	Any																																									Any					
entrypoints	Any			Any															Any																													
exceptiongroup	>=1.0.0rc8	>=1.0.0rc8	>=1.0.0rc8	>=1.0.0rc8	>=1.0.0rc8														>=1.0.0rc8															>=1.0.0rc8													
executing	>=1.2.0			>=1.2.0															>=1.2.0																													
extension	Any										Any																																					
fastjsonschema	Any			Any															Any																													
flask	>=1.1.2		>=1.1.2								>=1.0.2																																					
flask-cors	Any		Any																																													
flask-restful	>=0.3.8		>=0.3.8																																													
fonttools	>=4.22.0			>=4.22.0		>=4.22.0					>=4.22.0							>=4.22.0	>=4.22.0		>=4.22.0					>=4.22.0		>=4.22.0					>=4.22.0		>=4.22.0	>=4.22.0			>=4.22.0	>=4.22.0	>=4.22.0						
fortranformat	Any																		Any																													
frozenlist	>=1.1.1							>=1.1.1		>=1.1.1	>=1.1.1															>=1.1.1												>=1.1.1	>=1.1.1			>=1.1.1	>=1.1.1		
fsspec	>=0.6.0				>=0.6.0																													>=0.6.0														
future	Any			Any															Any																													
geomagindices	>=1.4.0																												>=1.4.0								>=1.4.0										
geopack	>=1.0.9					>=1.0.9															>=1.0.8																										
greenlet	!=0.4.17																!=0.4.17																															
gridaurora	Any																																				Any											
gwcs	>=0.15																									>=0.15				>=0.15																	>=0.15	
h5netcdf	Any																																								Any							
h5py	>=3.2.1			>=3											Any				>=3		>=3.2.1													Any						Any							
hapiclient	>=0.2.2					>=0.2.2																																										
hatanaka	Any																			Any																												
hellopy	>=0.12.0										>=0.12.0																																					
hellopy-multid	Any										Any																																					
html5lib	>=0.999																																							>=0.999		>=0.999						
hydra-core	>=0.11.3		>=0.11.3																																													
idna	>=2.8,<4	>=2.8,<4		>=2.8,<4		>=2.5,<4		>=2.0		>=2.0	>=2.5,<4								>=2.8,<4		>=2.5,<4	>=2.5,<4				>=2.0			>=2.5,<4		>=2.5,<4					>=2.5,<4	>=2.5,<4	>=2.5,<4		>=2.5,<4	>=2.5,<4	>=2.5,<4			>=2.0	>=2.0		>=2.5,<4
imagesio	>=2.4.1																					>=2.1									>=2.3										>=2.4.1							
importlib-metadata	>=1.11.4			>=4.8.3							>=4.4										>=4.8.3					>=4.11.4				>=4.11.4								>=4.11.4		>=4.11.4					>=4.11.4	
importlib-resources	>=3.2.0			>=3.2.0		>=3.2.0					>=3.2.0							>=3.2.0	>=3.2.0	Any	>=3.2.0					>=3.0.0		>=3.2.0					>=3.2.0		>=3.2.0	>=3.2.0			>=3.2.0	>=3.2.0	>=3.2.0						
incremental	Any		Any																																													
isinonfis	Any		Any	Any	Any														Any															Any														

Sheet

Hackathon at the Spring Meeting

Hackathon at the Spring Meeting

```
[10]: import aacgmv2
      import aiapy
      import aidapy
      import apexpy
      import astrometry_azel
      import ccsdspy
      import cdflib
      import dascutils
      import dbprocessing
      import dmsp
      import enlilviz
      import fiasco
      import georinex
      import geospacelab
      import goesutils
      import hissw
      import igrf
      import iri2016
      import irispy
      import lowtran
      import mcalf
      import msise00
      import ndcube
      import nexradutils
      import ocbpy
      import OMMBV
      import pydarn
      import pyflct
      import pytplot  # should pull in pytplot_mpl_temp
      import pyzenodo3
      import reesaurora
      import regularizepsf
      import sciencedates
      import solarmach
      import solo_epd_loader
      import space_packet_parser
      import speasy
      import spiceypy
      import sunkit_image
      import sunkit_instruments
      import sunraster
      import themisasi
      import viresclient
      import wmm2015
      import wmm2020
      import hapiclient
      import kamodo
      import plasmapy
      import pysat
      import pyspedas
      import spacepy
      import sunpy

      print("\nAll the PyHC imports worked!\n")

      All the PyHC imports worked!

[ ]:
```

pyhc-environment-files Public

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main | 3 branches | 0 tags | Go to file | Add file | Code

sapols Add files related to pip/conda publishing 6ef49b8 on Aug 9 30 commits

pip-freeze-outputs	Add successful pip freeze folder	5 months ago
stats	Add files related to pip/conda publishing	2 months ago
README.md	Add note about PyGS	3 months ago
import-test.py	Uncomment pyspedas	5 months ago
pyhc-packages-requirements.txt	Rename pyhc-packages.txt to pyhc-packages-requirements.txt	5 months ago
pyhc-requirements.txt	Specify Heliopy <1	3 months ago

README.md

pyhc-environment-files

Repo with files trying to generate one virtual Python environment that can import every PyHC package.

Files:

1. `pyhc-requirements.txt` : All the package versions that the PyHC packages require
2. `pyhc-packages-requirements.txt` : The PyHC packages
3. `import-test.py` : A script that runs import statements for the PyHC packages before printing a success message

Steps:

1. `pip install -r pyhc-requirements.txt`
2. `pip install -r pyhc-packages-requirements.txt`
3. `python3 import-test.py`

Fixing ocbpy import (currently commented-out):

Problem:

It's failing on trying to get SpacePy to load the CDF C library

Solution:

Install CDF C library (see: https://spacepy.github.io/pycdf.html / https://spacepy.github.io/install_mac.html#install-mac-cdf)

Shawn's steps:

- Download Mac binaries "CDF3_9_0-binary-signed.pkg" (from:

About

Files for a unified Python virtual environment containing all published PyHC packages

Readme
Activity
0 stars
2 watching
0 forks

Releases

No releases published
Create a new release

Packages

No packages published
Publish your first package

Languages

Jupyter Notebook 83.2%
Python 16.8%

Suggested Workflows

Based on your tech stack

Python Package using Anaconda Configure
Create and test a Python package on multiple Python versions using Anaconda for package management.

Python package Configure
Create and test a Python package on multiple Python versions.

Publish Python Package Configure
Publish a Python Package to PyPI on release.

More workflows Dismiss suggestions

docker hub

Search Docker Hub

Explore Repositories Organizations Help

spolson

Search by repository name

All Content

Create repository

spolson / **pyhc-environment**
Contains: Image | Last pushed: 2 months ago

Inactive 0 4 Public

spolson / **pyhc-gallery-w-executable-paper**
Contains: Image | Last pushed: 2 months ago

Inactive 0 2 Public

spolson / **pyhc-gallery**
Contains: Image | Last pushed: 2 months ago

Inactive 0 7 Public

spolson / pyhc-environment

Description

A JupyterLab session using an environment containing every published PyHC package.

Last pushed: 2 months ago

Docker commands

Public View

To push a new tag to this repository:

```
docker push spolson/pyhc-environment:tagname
```

Tags

This repository contains 1 tag(s).

Tag	OS	Type	Pulled	Pushed
v2023.8.4		Image	2 months ago	2 months ago

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Upgrade

Repository overview

This `pyhc-environment` image runs a JupyterLab session with an environment containing every published PyHC package.

Inspiration

The environment used by this JupyterLab session is inspired by the work done in the `pyhc-environment-files` GitHub repo. That repo attempts to maintain up-to-date package version requirements for a unified Python virtual environment holding the latest versions of each PyHC package, although that is difficult to do in practice given how many packages there are and how frequently they make releases. Until we can automate this process, it is safe to assume the environment used here reflects the most recent successful `pip freeze` output from that repo.

Caveats

It is difficult with so many dependency requirements to create a valid Python virtual environment capable of even importing all these PyHC packages. There is one `import-test.ipynb` notebook added to demonstrate that all the imports do work, but no further compatibility testing has been done.

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spolson / pyhc-environment

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Edit

spolson / pyhc-gallery-w-executable-paper

Description

PyHC Gallery and EP running in JupyterLab using an environment with every published PyHC package.

Last pushed: 2 months ago

Docker commands

Public View

To push a new tag to this repository:

```
docker push spolson/pyhc-gallery-w-executable-paper:tagname
```

Tags

This repository contains 1 tag(s).

Tag	OS	Type	Pulled	Pushed
latest		Image	2 months ago	2 months ago

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Repository overview

This `pyhc-gallery-w-executable-paper` image has all the notebook examples from the Python in Heliophysics Community (PyHC) Gallery, along with the executable paper "Making an executable paper with the Python in Heliophysics Community to foster open science and improve reproducibility" by Polson et al., running in JupyterLab with an environment containing every published PyHC package.

Inspiration

The environment used by this JupyterLab session is inspired by the work done in the `pyhc-environment-files` GitHub repo. That repo attempts to maintain up-to-date package version requirements for a unified Python virtual environment holding the latest versions of each PyHC package, although that is difficult to do in practice given how many packages there are and how frequently they make releases. Until we can automate this process, it is safe to assume the environment used here reflects the most recent successful `pip freeze` output from that repo, with some additional system configurations to support the executable paper.

Caveats

It is difficult with so many dependency requirements to create a valid Python virtual environment capable of even importing all these PyHC packages. The Gallery notebooks and executable paper successfully execute, and there is an additional `import-test.ipynb` notebook added to demonstrate that all the imports do work, but no further compatibility testing has been done.

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Edit

File Edit View Run Kernel Git Tabs Settings Help

Launcher | import-test.ipynb

Code | git | Python 3 (ipykernel)

Filter files by name

/

Name

- executable-paper
- coordinate_systems.ipynb
- coordinates_demo.ipynb
- import-test.ipynb
- planet_locations.ipynb
- pyspedas_demo.ipynb
- pytplot_demo.ipynb
- retrieve_compress.ipynb
- units_demo.ipynb

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import wmm2015
import wmm2020
import hapiclient
import kamodo
import plasmapy
import pysat
import pyspedas
import spacepy
import sunpy


print("\nAll the PyHC imports worked!\n")
```

```
All the PyHC imports worked!
```

[ ]:

Simple | 0 | 1 | Python 3 (ipykernel) | Idle | Mode: Command | Ln 1, Col 1 | import-test.ipynb

File Edit View Run Kernel Git Tabs Settings Help

Launcher | import-test.ipynb

Code | Python 3 (ipykernel)

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import spacepy
import sunpy


print("\nAll the PyHC imports worked!\n")
```

```
All the PyHC imports worked!
```

[ ]:

Dockerfile

```dockerfile
# Use an official Anaconda runtime as a parent image
FROM continuumio/miniconda3

# Set the working directory in the container to /app
WORKDIR /app

# Update the packages in the base image and install the necessary compilers
RUN apt-get update && apt-get install -y gcc g++ gfortran ncurses-dev build-essential cmake

# Add the "contents" directory contents into the container at /app
ADD contents/ /app

# Configure CDF library
RUN mv /app/executable-paper/dependencies/cdf38_0-dist /usr/lib/
ENV CDF_BASE=/usr/lib/cdf38_0-dist
ENV CDF_LIB=$CDF_BASE/lib

# Configure package data directories
RUN mkdir -p /root/.sunpy
RUN mkdir -p /root/heliopy/data
RUN mkdir -p /root/Geospacelab/Data
RUN mkdir -p /root/.spacepy/data
RUN mv /app/executable-paper/pydata/spacepy/data/* /root/.spacepy/data/

# Create the conda environment using environment.yml
RUN conda env create -f /app/environment.yml

# Activate the created environment
RUN echo "source activate pyhc-all" > ~/.bashrc
ENV PATH /opt/conda/envs/pyhc-all/bin:$PATH

# Install additional packages with pip
RUN pip install --retries 5 --no-cache-dir -r requirements.txt

# Delete cruft
RUN rm /app/environment.yml
RUN rm /app/requirements.txt

# Make port 8888 available to the world outside this container
EXPOSE 8888

# Run Jupyter notebook when the container launches
CMD ["jupyter", "lab", "--ip='*'", "--port=8888", "--no-browser", "--allow-root"]
```

Simple | 0 | 1 | Python 3 (ipykernel) | Idle | Mode: Command | Ln 1, Col 1 | import-test.ipynb

Putting packages in Conda

pip-conda-spreadsheet.py

```python
import requests
import pandas as pd
import time
from openpyxl import load_workbook
from openpyxl.styles import PatternFill


def get_core_pyhc_packages():
    """
    TODO: consider scraping this from projects_core.yml online?
    :return: A list of the core PyHC package names.
    """
    return ["hapiclient", "kamodo", "plasmapy", "pysat", "pyspedas", "spacepy", "sunpy"]


def get_other_pyhc_packages():
    """
    TODO: consider scraping this from projects.yml online?
    :return: A list of the other non-core PyHC package names.
    """
    return ["acemag", "afino", "aeindex", "geodata", "gimamag", "polan", "pygemini", "pyglow", "python-mag


def is_package_in_pypi(package_name):
    response = requests.get(f'https://pypi.org/pypi/{package_name}/json')
    return response.status_code == 200


def is_package_in_conda(package_name):
    response = requests.get(f'https://api.anaconda.org/package/conda-forge/{package_name}')
    return response.status_code == 200


# ----------------------------------------------------------------------------------------------------------


core_packages = get_core_pyhc_packages()
other_packages = get_other_pyhc_packages()
packages = core_packages + other_packages

results = []

for package in packages:
    in_pypi = is_package_in_pypi(package)
    time.sleep(2)  # wait to avoid API rate limit
    in_conda = is_package_in_conda(package)
    time.sleep(2)  # wait to avoid API rate limit

    results.append({
        'Package': package,
        'PyPI': in_pypi,
        'Conda': in_conda,
    })
    print(f"Appended: {package}")

df = pd.DataFrame(results).set_index('Package')  # The pip/conda True/False results

# Use pd options to avoid truncating printout
pd.set_option('display.max_rows', None)
print("\n\nRESULTS:\n")
print(df)
pd.reset_option('display.max_rows')

# first, export the DataFrame to an Excel file
excel_file = "output.xlsx"
df.to_excel(excel_file)

# load the workbook and select the sheet
book = load_workbook(excel_file)

# define the fill colors
green_fill = PatternFill(start_color="00FF00", end_color="00FF00", fill_type="solid")
red_fill = PatternFill(start_color="FF0000", end_color="FF0000", fill_type="solid")

# get the active worksheet
sheet = book.active

# iterate over the cells in the sheet
for row in sheet.iter_rows(min_row=2):  # start from 2 to skip the header
    for cell in row:
        if cell.value is True:
            cell.fill = green_fill
        elif cell.value is False:
            cell.fill = red_fill

# save the changes
book.save(excel_file)

print("done")
```

	A	B	C
1	Package	PyPI	Conda
2	aacgmv2	TRUE	FALSE
3	acemag	FALSE	FALSE
4	aeindex	FALSE	FALSE
5	afino	FALSE	FALSE
6	aiapy	TRUE	TRUE
7	aidapy	TRUE	FALSE
8	apexpy	TRUE	FALSE
9	astrometry-azel	TRUE	FALSE
10	cdflib	TRUE	TRUE
11	dascutils	TRUE	FALSE
12	dbprocessing	TRUE	FALSE
13	dmsp	TRUE	FALSE
14	enlilviz	TRUE	FALSE
15	fiasco	TRUE	FALSE
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19	georinex	TRUE	FALSE
20	geospacelab	TRUE	FALSE
21	gimamag	FALSE	FALSE
22	goesutils	TRUE	FALSE
23	hapiclient	TRUE	TRUE
24	hissw	TRUE	FALSE
25	hwm93	TRUE	FALSE
26	igrf	TRUE	FALSE
27	iri2016	TRUE	FALSE
28	iri90	TRUE	FALSE
29	irispy-lmsal	TRUE	TRUE
30	kamodo	TRUE	FALSE
31	lowtran	TRUE	FALSE
32	madrigalWeb	TRUE	FALSE
33	maidenhead	TRUE	FALSE
34	mcalf	TRUE	TRUE
35	mgsutils	TRUE	FALSE
36	msise00	TRUE	FALSE
37	ncarglow	TRUE	FALSE
38	ndcube	TRUE	TRUE
39	nexradutils	TRUE	FALSE
40	ocbpy	TRUE	FALSE
41	OMMBV	TRUE	FALSE
42	plasmapy	TRUE	TRUE
43	polan	FALSE	FALSE
44	pydarn	TRUE	FALSE
45	pyfict	TRUE	TRUE
46	pygemini	TRUE	FALSE
47	pyglow	TRUE	FALSE
48	pymap3d	TRUE	TRUE
49	pysat	TRUE	FALSE
50	pysatCDF	TRUE	FALSE
51	pyspedas	TRUE	FALSE
52	python-magnetosphere	FALSE	FALSE
53	pytplot	TRUE	FALSE
54	pytplot-mpl-temp	TRUE	FALSE
55	pyzenodo3	TRUE	TRUE
56	reesaurora	TRUE	FALSE
57	sami2py	FALSE	FALSE
58	scanning-doppler-interferometer	FALSE	FALSE
59	sciencedates	TRUE	FALSE
60	SkyWinder	TRUE	FALSE
61	SkyWinder-Analysis	TRUE	FALSE
62	solarmach	TRUE	TRUE
63	solo-epd-loader	TRUE	TRUE
64	spacepy	TRUE	FALSE
65	speasy	TRUE	FALSE
66	spiceypy	TRUE	TRUE
67	sunkit-image	TRUE	TRUE
68	sunkit-instruments	TRUE	TRUE
69	sunpy	TRUE	TRUE
70	sunraster	TRUE	TRUE
71	themisasi	TRUE	FALSE
72	TomoGraPy	TRUE	FALSE
73	viresclient	TRUE	TRUE
74	wmm2015	TRUE	FALSE
75	wmm2020	TRUE	FALSE
76			

Where packages publish

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    response = requests.get(f'https://api.anaconda.org/package/conda-forge/{package_name}')
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        'Package': package,
        'PyPI': in_pypi,
        'Conda': in_conda,
    })
    print(f"Appended: {package}")

df = pd.DataFrame(results).set_index('Package')  # The pip/conda True/False results

# Use pd options to avoid truncating printout
pd.set_option('display.max_rows', None)
print("\n\nRESULTS:\n")
print(df)
pd.reset_option('display.max_rows')

# first, export the DataFrame to an Excel file
excel_file = "output.xlsx"
df.to_excel(excel_file)

# load the workbook and select the sheet
book = load_workbook(excel_file)

# define the fill colors
green_fill = PatternFill(start_color="00FF00", end_color="00FF00", fill_type="solid")
red_fill = PatternFill(start_color="FF0000", end_color="FF0000", fill_type="solid")

# get the active worksheet
sheet = book.active

# iterate over the cells in the sheet
for row in sheet.iter_rows(min_row=2):  # start from 2 to skip the header
    for cell in row:
        if cell.value is True:
            cell.fill = green_fill
        elif cell.value is False:
            cell.fill = red_fill

# save the changes
book.save(excel_file)

print("done")
```

	A	B	C
1	Package	PyPI	Conda
2	aacgmv2	TRUE	FALSE
3	acemag	FALSE	FALSE
4	aeindex	FALSE	FALSE
5	afino	FALSE	FALSE
6	aiapy	TRUE	TRUE
7	aidapy	TRUE	FALSE
8	apexpy	TRUE	FALSE
9	astrometry-azel	TRUE	FALSE
10	cdflib	TRUE	TRUE
11	dascutils	TRUE	FALSE
12	dbprocessing	TRUE	FALSE
13	dmsp	TRUE	FALSE
14	enlilviz	TRUE	FALSE
15	fiasco	TRUE	FALSE
16	fisspy	TRUE	TRUE
17	geodata	TRUE	FALSE
18	geopack	TRUE	FALSE
19	georinex	TRUE	FALSE
20	geospacelab	TRUE	FALSE
21	gimamag	FALSE	FALSE
22	goesutils	TRUE	FALSE
23	hapiclient	TRUE	TRUE
24	hissw	TRUE	FALSE
25	hwm93	TRUE	FALSE
26	igrf	TRUE	FALSE
27	iri2016	TRUE	FALSE
28	iri90	TRUE	FALSE
29	irispy-lmsal	TRUE	TRUE
30	kamodo	TRUE	FALSE
31	lowtran	TRUE	FALSE
32	madrigalWeb	TRUE	FALSE
33	maidenhead	TRUE	FALSE
34	mcalf	TRUE	TRUE
35	mgsutils	TRUE	FALSE
36	msise00	TRUE	FALSE
37	ncarglow	TRUE	FALSE
38	ndcube	TRUE	TRUE
39	nexradutils	TRUE	FALSE
40	ocbpy	TRUE	FALSE
41	OMMBV	TRUE	FALSE
42	plasmapy	TRUE	TRUE
43	polan	FALSE	FALSE
44	pydarn	TRUE	FALSE
45	pyfict	TRUE	TRUE
46	pygemini	TRUE	FALSE
47	pyglow	TRUE	FALSE
48	pymap3d	TRUE	TRUE
49	pysat	TRUE	FALSE
50	pysatCDF	TRUE	FALSE
51	pyspedas	TRUE	FALSE
52	python-magnetosphere	FALSE	FALSE
53	pytplot	TRUE	FALSE
54	pytplot-mpl-temp	TRUE	FALSE
55	pyzenodo3	TRUE	TRUE
56	reesaurora	TRUE	FALSE
57	sami2py	FALSE	FALSE
58	scanning-doppler-interferometer	FALSE	FALSE
59	sciencedates	TRUE	FALSE
60	SkyWinder	TRUE	FALSE
61	SkyWinder-Analysis	TRUE	FALSE
62	solarmach	TRUE	TRUE
63	solo-epd-loader	TRUE	TRUE
64	spacepy	TRUE	FALSE
65	speasy	TRUE	FALSE
66	spiceypy	TRUE	TRUE
67	sunkit-image	TRUE	TRUE
68	sunkit-instruments	TRUE	TRUE
69	sunpy	TRUE	TRUE
70	sunraster	TRUE	TRUE
71	themisasi	TRUE	FALSE
72	TomograPy	TRUE	FALSE
73	viresclient	TRUE	TRUE
74	wmm2015	TRUE	FALSE
75	wmm2020	TRUE	FALSE
76			

Where packages publish

Eventually want **all packages** published in both **pip** and **conda**

Planning to hire an **intern**

Future Work

Further **testing** of PyHC environment
Incorporate package **unit tests**?

All packages in **pip** and **conda**

CI/CD to monitor when package updates **“break the build”**
Community discussions when it happens

Require compatibility with environment (at some level)

Links

https://hub.docker.com/u/spolson

https://github.com/sapols/pyhc-environment-files