



Science Platforms Coordination

IHDEA Working Group Update



GOAL

To develop international standard software computing environments for Heliophysics





MEMBERS

Jan Reerink
Shawn Polson

Anne Spalding
Arnaud Masson
Brian Thomas
James Parr
Jeffrey Bradford
Jim Colliander
Julie Barnum
Rebecca Ringuette
Sandy Antunes
Sarah Rourke



INTRODUCTION

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INSPIRATION

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WHAT WE'DONE

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04

FUTUREWORK




01

INSPIRATION



IHDEA Cloud Workshop July:

“We want a shared Heliophysics software environment for cloud computing”



DASH/IHDEA Meeting October:



PyHC Package Compatibility Effort Update

By Shawn Polson



pyhc-docker-environment Public[Edit Pins](#) [Unwatch 4](#) [Fork 0](#) [Star 1](#)main 2 Branches 0 Tags

Go to file

Add file

Code

About

Pipeline to generate and dockerize Python environments containing all published PyHC packages

[Readme](#)
[Activity](#)
[Custom properties](#)
★ 1 star
👁 4 watching
🍴 0 forks

[Report repository](#)

Releases

No releases published
[Create a new release](#)

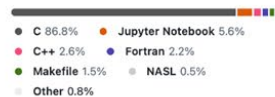
Packages












No packages published
[Publish your first package](#)

Contributors 2

 **sapols** Shawn Polson **github-actions[bot]**

Languages



File	Commit Message	Commit Date
 github-actions[bot]	Update Docker image requirements, spreadsheet, README	50f5e55 · 2 weeks ago
 .github/workflows	Update to Python 3.10	4 months ago
 docker	Update Docker image requirements, spreadsheet, README	2 weeks ago
 spreadsheets	Update Docker image requirements, spreadsheet, README	2 weeks ago
 utils	Temporarily remove OMMBV	3 weeks ago
 .gitattributes	Manage executable paper with Git LFS	8 months ago
 .gitignore	Initial commit	8 months ago
 README.md	Update Docker image requirements, spreadsheet, README	2 weeks ago
 __init__.py	Initial commit	8 months ago
 pipeline.py	Temporarily specify numpy==1.26.4	3 months ago
 pipeline_requirements.txt	Setuptools<60.0 didn't fix anything	3 weeks ago

README

PyHC Environment Pipeline

Overview

The PyHC Environment Pipeline automates the creation of Docker images with Python environments that come pre-loaded with the latest versions of all published PyHC ([Python in Heliophysics Community](#)) packages. The GitHub Actions workflow rebuilds and pushes the Docker images to [Docker Hub](#) each time a PyHC package releases a new update. It also keeps the source files in this repo in-sync with what's in Docker Hub.

Features



spolson/pyhc-environment ☆0

By [spolson](#) · Updated 13 days ago

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

[IMAGE](#)

Manage Repository

↓ Pulls 191

Overview Tags

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 backed by the [pyhc-docker-environment](#) GitHub repo. That repo maintains up-to-date package version requirements for a unified Python virtual environment holding the latest versions of each PyHC package, automated by GitHub Actions.

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 little further compatibility testing has been done.

Docker Pull Command

```
docker pull spolson/pyhc-environment
```

Copy



“Sounds like a new working group”

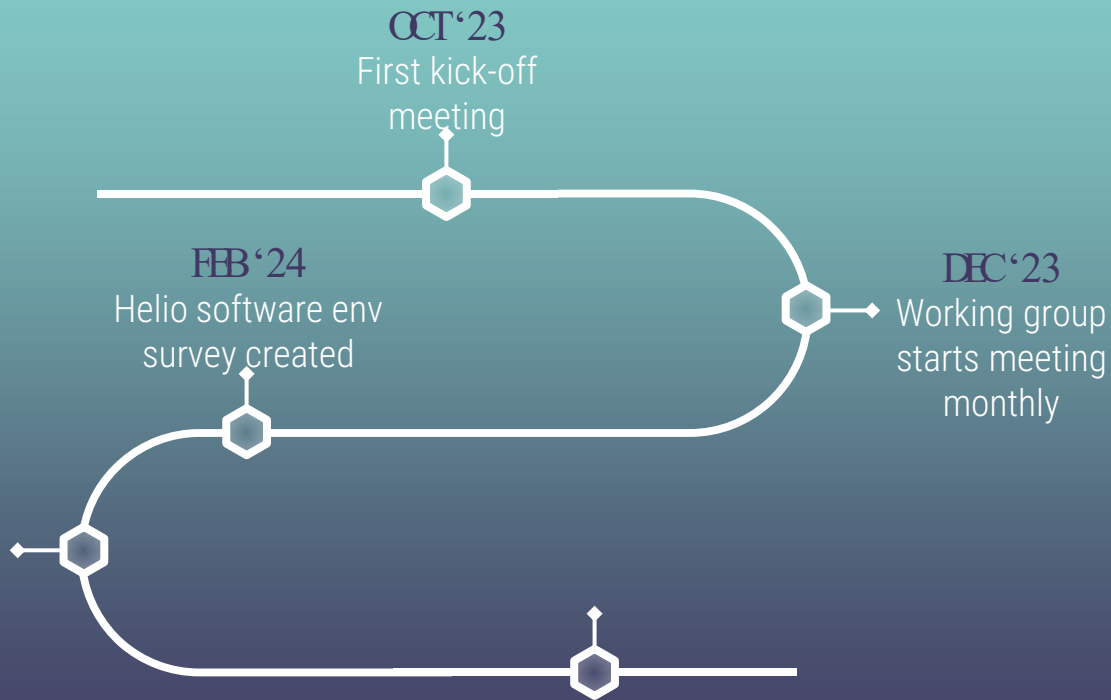




02

WHAT WE'DONE

WHAT WE'VE DONE



SURVEY: Software Environments for Heliophysics



“We are developing multiple Python-based software environments tailored to current research in our fields, so we are interested in which Python packages you currently use in your research. By developing these software environments based on community input, we intend to increase the reproducibility of your research for others, which research shows is expected to increase citations to your work and increase collaboration across our communities. So please open up your favorite software environment and answer the brief questions below”



Software Environments for Heliophysics

Hi there!

We are an international working group that is working to create sharable science platforms for the Heliophysics, Space Physics, and related communities. We are developing multiple Python-based software environments tailored to current research in our fields, so we are interested in which Python packages you currently use in your research. By developing these software environments based on community input, we intend to increase the reproducibility of your research for others, which research shows is expected to increase citations to your work and increase collaboration across our communities. So please open up your favorite software environment and answer the brief questions below. If you have more than one environment, please enter your answers for those environments on separate forms. We intend to give reports on our progress at the DASH workshop and at AGU. Thanks for your input!

IHDEA Science Platforms Coordination Working Group

Co-chairs: Shawn Polson and Jan Reerink

<https://ihdea.net/>

shp09723@colorado.edu [Switch account](#)



The name and photo associated with your Google account will be recorded when you upload files and submit this form. Your email is not part of your response.

Any files that are uploaded will be shared outside of the organization they belong to.

* Indicates required question

If you would like us to contact you about this information, please enter your email address.

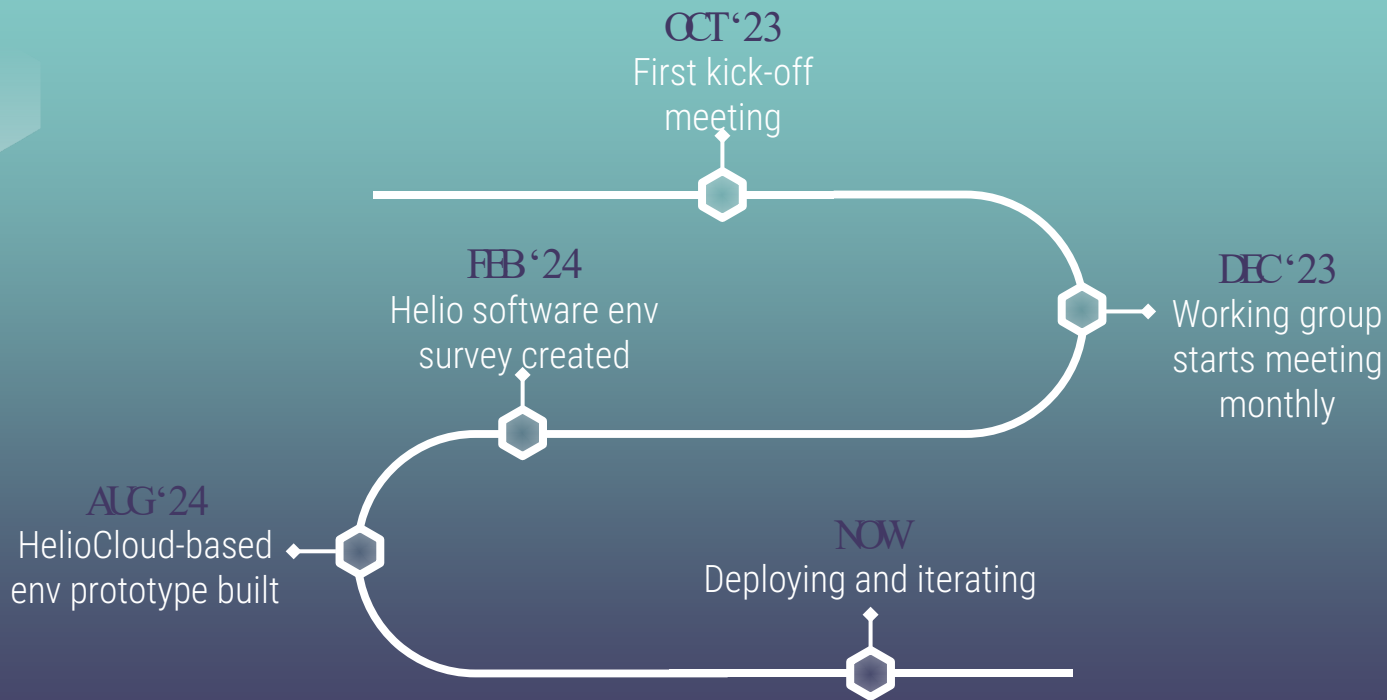
Your answer _____

What broad science category(ies) does the work you perform in this software environment fall into? *

- Solar
- Heliophysics
- Geospace
- Space Physics
- Magnetosphere
- Ionosphere/Thermosphere



WHAT WE'VE DONE



DEPLOYMENT PARTNERS



2i2c

The International Interactive Computing Collaboration—offer scalable and access-controlled Binder/Jupyter resources



ESADatalabs

A “public moderated beta” of browser-based tools for scientists with a focus on bringing questions and code to data



A global network of community hubs for interactive learning and discovery

Our interactive computing platform gives research and education communities a digital home to create and share knowledge with a global network of communities to learn from.

[Learn about our interactive computing platform](#)

[Join our network >](#)

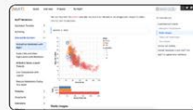
We help communities build their own interactive computing hub in the cloud with open infrastructure



Resource and user management



Interactive interfaces



Computational knowledge bases

2i2c's [community hub platform and consultancy services](#) ensure your community makes the best use of open infrastructure for interactive computing in the cloud.

We serve **over 90 communities across the globe** with **over 7000 active users** dedicated to creating and sharing knowledge. See [our community impact stories](#) for inspiration.



hhmi Howard Hughes Medical Institute

National Center for **Atmospheric Sciences**

PANGEO

UNIVERSITY OF **TORONTO**



[Join our network of community hubs](#)

THE EUROPEAN SPACE AGENCY

esa

ESA Datalabs [0.13.0/BETA]

ESA Datalabs is available as "Public Moderated Beta"
If you wish to apply for access, please [submit your request here](#).

«YOU CAN EITHER MOVE YOUR QUESTIONS OR THE DATA. [...] OFTEN IT TURNS OUT TO BE MORE EFFICIENT TO MOVE THE QUESTIONS THAN TO MOVE THE DATA.»

Jim Gray, eScience: A Transformed Scientific Method

BRING YOUR QUESTIONS TO THE DATA

There is a new paradigm, opening completely new opportunities for discovery – a data-intensive approach to science. In many domains, we have entered what could be called the golden age of surveys, with several large-scale projects, spanning decades, between finished, ongoing, and planned activities. ESA is responsible, or is a major partner, in several of these initiatives.

There is, however, a new profound change: data has become a major technological challenge. Increases by multiple orders of magnitude in dataset size means that transferring data to a scientist is often unfeasible.

ESA datalabs gives you a privileged position; bring your code directly to ESA's infrastructure – there is a great set of tools and programming languages are flexible – and execute it with direct access to ESA's archives.

DEPLOYMENTS



2i2c Binder

BinderHub where
NASA foots the bill
(small & big)



2i2c JupyterHub

Authenticated hub
with many images,
resource options



ESADATALABS

JupyterLab platform
connected to ESA
infrastructure



Turn a Git repo into a collection of interactive notebooks

Have a repository full of Jupyter notebooks? With Binder, open those notebooks in an executable environment, making your code immediately reproducible by anyone, anywhere.

New to Binder? Get started with a [Zero-to-Binder tutorial](#) in Julia, Python, or R.

Build and launch a repository

GitHub repository name or URL

GitHub

Git ref (branch, tag, or commit)

Path to a notebook file (optional)

File

Copy the URL below and share your Binder with others:

Expand to see the text below, paste it into your README to show a binder badge:

How it works

1

Enter your repository information

Provide in the above form a URL or a GitHub repository that contains

science-platforms-coordination Public[Edit Pins](#) [Unwatch](#) 2 [Fork](#) 0 [Star](#) 0

heliocloud-base 4 Branches 0 Tags

Go to file

Add file

<> Code

About

This branch is 13 commits ahead of main.

Contribute

sapols Update README.md

1e558b7 · 1 hour ago

18 Commits

Dockerfile	Fix typo	last month
LICENSE	Initial commit	2 months ago
README.md	Update README.md	1 hour ago
apt.txt	First implementation with HelioCloud/Pangeo base	last month
conda-lock.yml	Upload conda-lock.yml	2 weeks ago
environment.yml	First implementation with HelioCloud/Pangeo base	last month
install_cdfilib.sh	First implementation with HelioCloud/Pangeo base	last month
jupyter_notebook_config.py	Add jupyter_notebook_config.py	last month
start	First implementation with HelioCloud/Pangeo base	last month

README License

Science Platforms Coordination Base Image

(For Binder/JupyterHub)

A Docker image inspired by HelioCloud's base image to be used by the Science Platforms Coordination IHDEA working group.

No description, website, or topics provided.

Readme
MIT license
Activity
Custom properties
0 stars
2 watching
0 forks

[Report repository](#)

Releases

No releases published
[Create a new release](#)

Packages

No packages published
[Publish your first package](#)

Languages

Dockerfile 100.0%

Suggested workflows

Based on your tech stack

**Docker image**[Configure](#)

Build a Docker image to deploy, run, or push to a registry.



Turn a Git repo into a collection of interactive notebooks

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How it works

1

Enter your repository information

Provide in the above form a URL or a GitHub repository that contains

hub.binder.opensci.212c.cloud

JupyterLab

File Edit View Run Kernel Git Tabs Settings Help

Filter files by name

Name	Last Modified
joovyan	12 minutes ago
README.md	17 minutes ago

Launcher

Notebook

- Python 3 (ipykernel)
- panel [x]

Console

- Python 3 (ipykernel)

Other

- Terminal
- Text File
- Markdown File
- Python File
- Show Contextual Help

Simple 0 0 Mem: 217.98 / 4096.00 MB Launcher

hub.binder.opensci.212c.cloud

Untitled.ipynb - JupyterLab

File Edit View Run Kernel Git Tabs Settings Help

Filter files by name

Name	Last Modified
joyvan	13 minutes ago
README.md	18 minutes ago
Untitled.ipynb	seconds ago

```
[2]: !pip list
```

Package	Version
accessible-pygments	0.0.5
adal	1.2.7
adlfs	2024.7.0
aiapy	0.7.4
aiobotocore	2.13.2
aiofiles	24.1.0
aioftp	0.22.3
aiohappyeyeballs	2.3.5
aiohttp	3.10.3
aiointertools	0.11.0
aiosignal	1.3.1
alabaster	0.7.16
alembic	1.13.2
annotated-types	0.7.0
anyio	3.7.1
appdirs	1.4.4
argon2-cffi	23.1.0
argon2-cffi-bindings	21.2.0
asciitree	0.3.3
asdf	3.4.0
asdf-astropy	0.6.1
asdf_coordinates_schemas	0.3.0
asdf_standard	1.1.1
asdf_transform_schemas	0.5.0
asteval	1.0.2
astropy	6.1.2
astropy_healpix	1.0.3
astropy-iers-data	0.2024.8.5.0.32.23
asttokens	2.4.1
async_generator	1.10
async-timeout	4.0.3
attrs	24.2.0
awscli	2.17.30
awscli	0.21.2
azure-core	1.30.2
azure-datalake-store	0.0.51
azure-identity	1.17.1
azure-storage-blob	12.22.0
Babel	2.14.0
backcall	0.2.0
backports.tarfile	1.0.0
beautifulsoup4	4.12.3
black	24.8.0
bleach	6.1.0
blinker	1.8.2
blosc	1.11.2
bokeh	2.4.3

Simple 0 1 Python 3 (ipykernel) | Idle Mem: 280.70 / 4096.00 MB Mode: Command Ln 1, Col 1 Untitled.ipynb

Filter files by name 🔍

Name	Last Modified
/	
data	an hour ago
my_workspace	an hour ago
team_workspaces	an hour ago
notebooks	an hour ago

📄 Launcher

Notebook

- Python 3 (ipykernel)
- panel [?]

Console

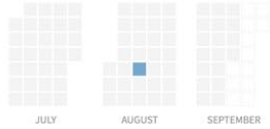
- Python 3 (ipykernel)

Other

- Terminal
- Text File
- Markdown File
- Python File
- Show Contextual Help



Repository Activity



Recent Repo Builds

No builds have been run for this repository.

Click on the Builds tab to start a new build.



Description

[Click to set repository description](#)

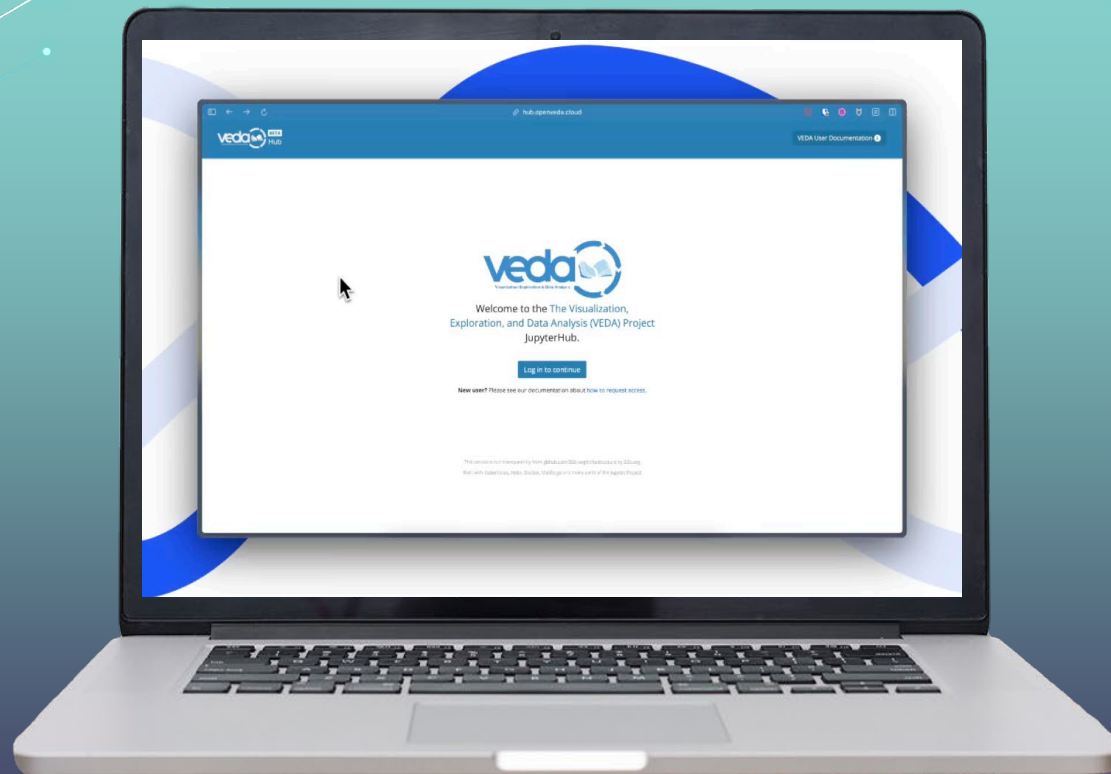
Pull this container with the following Podman command:

```
podman pull quay.io/sapols/helio-science-platform
```

Pull this container with the following Docker command:

```
docker pull quay.io/sapols/helio-science-platform
```

2i2c



Imagining multiple flavors:
HelioCloud, PyHC, Survey results



03

SURVEY RESULTS

META ANALYSIS

(#) = number of respondents

DATA PROCESSING & ANALYSIS TOOLS



MODELING SIMULATIONS

- (6) Specific science questions
- (5) Comparing models/theory
- (2) Performing model/sim runs
- (2) Event detection & forecasts

SOFTWARE DEVELOPMENT & DATA PRODUCTION

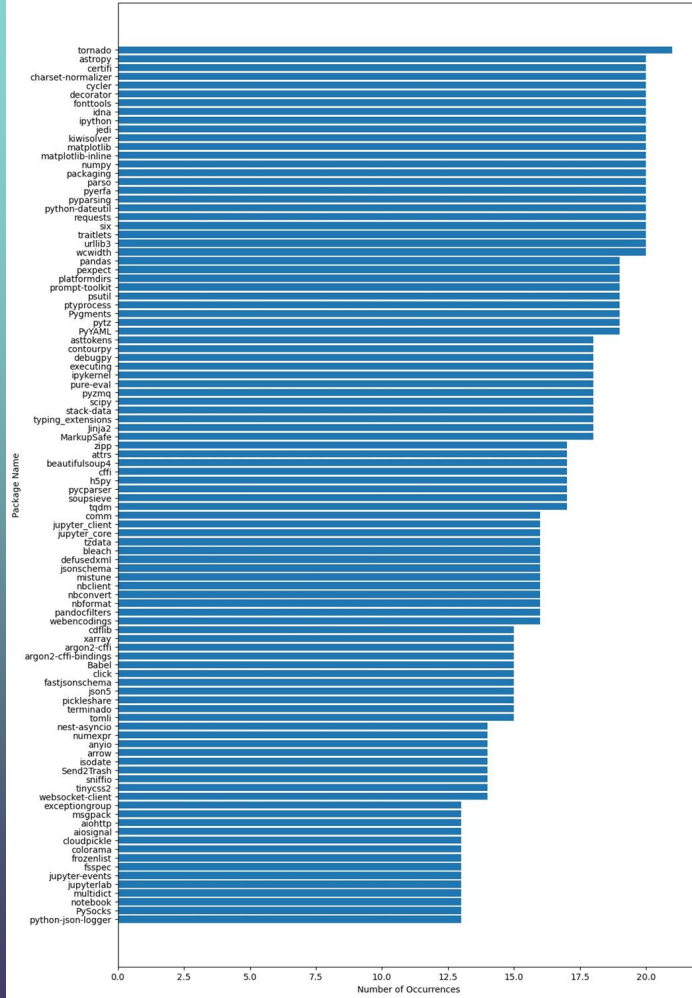
- (2) Improve specific packages
- (2) Create data from telemetry
- (1) Operationalize research s/w
- (1) Quality check data

- Specific science questions (10)
- In Situ data analysis (7)
- Data & image processing (5)
- Event labeling & ML (3)

DATA FUSION & VISUALIZATION

- Data, images, & datacubes (5)
- Data wrangling (3)
- Making spacecraft data interoperable (3)
- Time-series data (2)
- Publication-quality data (2)
- Plotting telemetry (1)
- FAIR data (1)

Top 100 Packages by Occurrence





04

FUTURE WORK

FUTURE WORK

- Put it in peoples' hands, collect feedback, iterate
- Make environments citable, e.g. DOIs (reproducibility!)
- Build environment based on survey results
- Finish gathering survey results



THANKS

Any questions?

shawn.polson@lasp.colorado.edu

Heliophysics
env survey:



HelioCloud base
image in Binder:



2i2c
website:



ESA Datalabs
website:

