plasmapy

Open source software and data for fusion energy sciences

Nick Murphy

Center for Astrophysics | Harvard & Smithsonian

This work has been supported by:

NSF, Department of Energy, NASA

With thanks to: S. Harihareswara, D. Stańczak, E. Everson, D. Coster, S. de Witt, P. Strand, J. Barnum, A. Roberts, A. Ware, D. Bouquin, R. W. James, S. Mumford, A. Leonard, S. Smith, A. Huebl, R. Lehe, G. Wilson, the PlasmaPy, SunPy, and Astropy communities, Fair4Fusion, APS DPP DEI OCC, US-RSE, Software Carpentry, the Python in Heliophysics Community, and the organizers/participants of Plasma Hack Week 2021.

My background

- Graduate school in astronomy (U. Wisconsin)
  - Studied connections between laboratory & astrophysical plasma physics
- Postdoc and researcher (Center for Astrophysics)
  - Studied solar physics and fundamental plasma science
- Last 3.1 ± 0.7 (3σ) years
  - Research software engineering for PlasmaPy
  - Advocating for open & reproducible plasma science
- Most recent pandemic hobby
  - Reading tokamak data management plans 🥳 😫 😱 😐

Main point for the next ~71 minutes

The fusion energy sciences community does not yet have a culture that supports open sharing of software and data.

But we will!

Topics for the next ~70 minutes

- Data and software environment comparison
  - Solar physics
  - Fusion energy sciences
- Open science
  - Motivation
  - Barriers
- FAIR principles for data stewardship
  - Example: Fair4Fusion
- Open source software
  - Example: PlasmaPy

Case study: solar physics

- Similarities with fusion energy sciences
  - Plasma physics is foundational
  - Diagnostics (e.g., spectroscopy)
  - Comparisons between simulations and reality
- Differences with fusion energy sciences
  - Solar observations are more homogeneous
    - Images, spectra, and time series
  - No experimental control
  - “There’s only one Sun.” — D. Coster

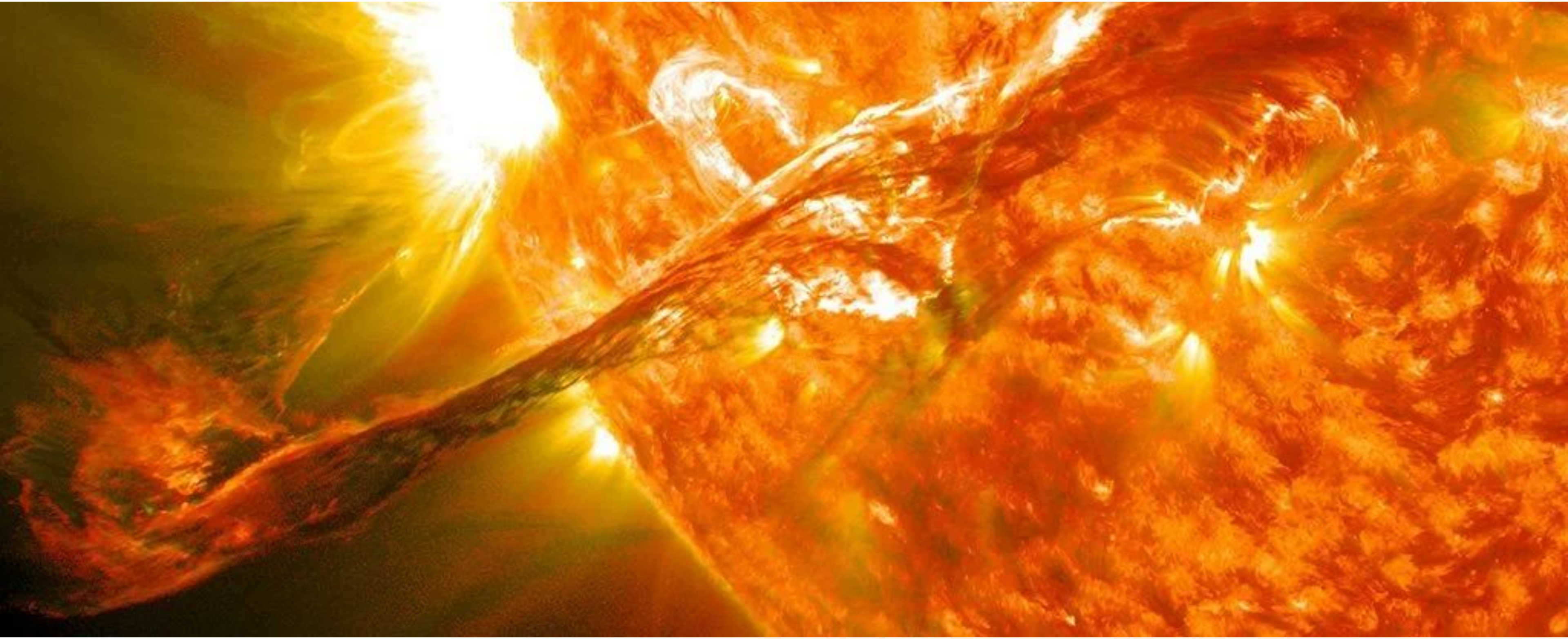
The solar physics software environment

- **SolarSoft**
  - Community-developed (unclear licensing)
  - Developed since the 1990s
  - Written in IDL (proprietary language)
  - Monolithic architecture
- **SunPy**
  - Community-developed (open source license)
  - Developed since 2011
  - Written in Python (open source language)
  - Modular architecture
  - Written using modern software engineering best practices

The solar physics data environment

- Most observational data sets are openly available
- The **Virtual Solar Observatory** (VSO) allows us to:
  - Simultaneously search multiple databases
  - Download data from multiple observatories
- Multiple ways to use VSO
  - Web interface
  - SolarSoft
  - SunPy
- Data sets are mostly standardized

Can start downloading solar data in minutes



Consequences for solar physics

- Data sets are widely used and re-used
- Multiple groups can study the same event
- Customary to use data from multiple sources
- Data sets well-suited for machine learning studies
- Well-documented and well-tested community software
- Less software duplication
- Data access not restricted by major institutions

Fusion energy sciences data environment

- Access to most experimental data is restricted
  - Can often request permission
- User agreements often contain restrictions such as:
  - No commercial use (without prior approval)
  - No redistribution of data (without prior approval)
  - Internal approval required for presentations & papers
- Data sets usually not standardized
- Difficult to search archives

Fusion energy sciences software environment

- Dependence on legacy codes
  - Often not open source
  - Different degrees of documentation, testing, and usability
- Software and many data sets bridged together by OMFIT
  - Likely to become open source soon!
- Common license customizations
  - Restrictions on commercial use
  - Limits on redistribution rights
- Difficult to find out which codes do what

Consequences for fusion energy sciences

- Hard to find data
  - Cannot simultaneously search across tokamak data archives
- Hard to access data
  - Need to request permissions
  - Difficult to perform cross-device studies
- Hard to write analysis software for multiple devices
  - Need partially met by OMFIT
- Reduced scientific reproducibility

Increasing number of open source software projects

- PlasmaPy
- OMFIT (soon!)
- OMAS
- tofu
- PyMethes
- FIDASIM
- Aurora
- simsopt
- BOUT++
- Gkeyll
- VPIC
- bapsflib
- gptools
- profiletools
- divHretention
- MOOSE

Open science principles

- Open access data
- Open source software
- Open methodology
- Open peer review
- Open access publications
- Open educational resources

Open science principles

- **Open access data**
- **Open source software**
- Open methodology
- Open peer review
- Open access publications
- Open educational resources

Why open science?

- Reduce barriers to access
- Broaden research impact
- Improve scientific reproducibility
- Make research more transparent
- Make publicly funded research available to the public
- Maximize use of data
- Allow community review of results
- Invest in our future

Barriers to open science

- Pressure to publish
  - Fear of being scooped
- Time pressure
- Financial pressure
  - Open access publication often costs extra
- Bureaucracy and institutional inertia
  - Decisions might need approval of ITER Council
- Power imbalances
  - Early career scientists more likely to support open science

Barriers to open science

- Toxic culture
  - Blatant or subtle acts of racism, sexism, etc.
  - Bullying, harassment, and discrimination
  - Retaliation
- Equity gaps
- Language barriers
  - Scientific information sometimes only available in English
- National security and intellectual property rights

Academic reward system

- What's good for *science* ≠ what's good for *scientists*
- Good for career
  - New and exciting results
  - Not "wasting time" making data & software available
- Good for science
  - Writing software documentation
  - Investing time to make data & software available
- How can we make what's good for science also what's good for scientists?

Open science is an investment

- It takes time and resources to:
  - Make data FAIR
  - Write documentation
  - Write tests
  - Maintain software
  - Learn necessary skills
- Open science will not happen right away…
- ...but it is worth the effort!

How do we get closer open science?

- Change our culture
  - Ensure psychological safety
  - Eliminate equity gaps
- Change our institutions
- Collaborate on technical infrastructure
  - Open access data
  - Open source software

How do we get closer to open science?

- Change our culture
  - Ensure psychological safety
  - Eliminate equity gaps
- Change our institutions
- Collaborate on technical infrastructure
  - **Open access data**
  - **Open source software**

The FAIR principles for data stewardship

- Findability
- Accessibility
- Interoperability
- Reusability

Findability

- Before being able to reuse a data set…we have to find it!
- Assign digital resources a **persistent identifier**
    - Digital Object Identifiers (DOIs)
- Describe data sets with **rich metadata**
- Index data sets **in a searchable resource**
    - Zenodo ← online repository operated by CERN
    - Virtual Solar Observatory

Accessibility

- Can access a data set using its persistent identifier
- Can access metadata even if original data set is gone
- *Accessible* is not the same as *open*
    - Authentication and authorization sometimes required

Data should be openly available when possible

- Data sets from most fusion devices are *not* openly available
- Should each device create its own online open archive?
  - Possible duplication of effort
  - Potential limitations on cross-device searchability
- Could we create a community-wide portal to access open fusion/plasma data sets?
  - Improve findability, accessibility, & reproducibility
  - Enable cross-device studies
  - Allow wide re-use of data

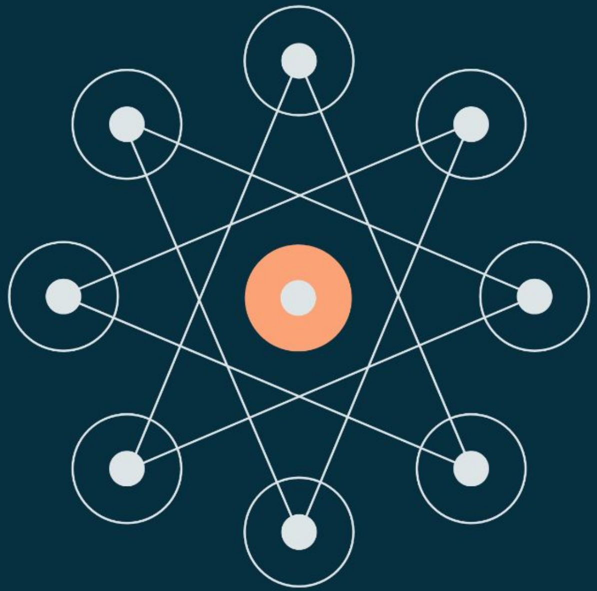
Some data from MAST is now open

UKAEA Open Data

Published Data | MAST Data | License

MAST Data

These pages provide an access point to publicly funded MAST research data. By selecting a Program or Objective, and then a specific experiment number, you can request the related underlying shot data if it is available for release.



MAST ≡ Mega Ampere Spherical Tokamak

Some data from MAST is now open

UKAEA Open Data

Published Data | MAST Data | License

amh	Analysed	Halo current Measurements (HAL), P2/P3 Halo Current Measurements (HALO)	amh27027.nc	netcdf4/hdf5	1	0	3	Download
amm	Analysed	Output from EFIT's wall model: calculated induced currents in toroidal vessel elements for input to EFIT	amm27027.nc	netcdf4/hdf5	18	0	83	Download
ane	Analysed	CO2 Interferometry	ane27027.nc	netcdf4/hdf5	1	0	7	Download
anu	Analysed	Neutron measurement	anu27027.nc	netcdf4/hdf5	2	0	3	Download
asb	Analysed	Spectroscopy CII, OII	asb0270.27	IDA3	1	0	5	Request Data

Interoperability

- Fusion facilities often have their own way of storing and organizing data
  - Hard to perform cross-device studies
  - Hard to develop shared software
- Approach #1: develop software to serve as an interface
  - OMFIT bridges different data types and software packages
- Approach #2: adopt shared standards for data

Why do we need data interoperability?

- Suppose we are doing experiments at two facilities
  - Basic Plasma Science Facility (BaPSF)
  - Wisconsin Plasma Physics Laboratory (WiPPL)
- We're studying the same physical process…
- …but data from BaPSF & WiPPL are structured differently!
- We need to write separate software to perform the same analysis
- A *common data model* would enable shared software and promote cross-device collaborations
  - Examples: IMAS, Plasma-MDS, OpenPMD, SPASE, MetaSat

Plasma science needs *open metadata standards*

- A **metadata standard** describes an agreed-upon way to structure and understand data
- A meaning is assigned to each variable name
  - Reduces ambiguity
- Greatly improves interoperability
  - Allows different groups to use and interpret data
- **Metadata crosswalks** convert between different standards

Why should metadata standards be *open*?

- Some standards like IMAS (for ITER) are not open
- Open standards allow for wider adoption
  - PDF, Blu-Ray, etc.
- Restricting access to metadata standards limits adoption
  - May lead to creation of competing standards

Reusability

- Describe data with sufficient **metadata**
- Metadata meet **community standards**
- Data sets have a clear **license**
- Data sets include detailed **provenance**
  - Where did the data come from?

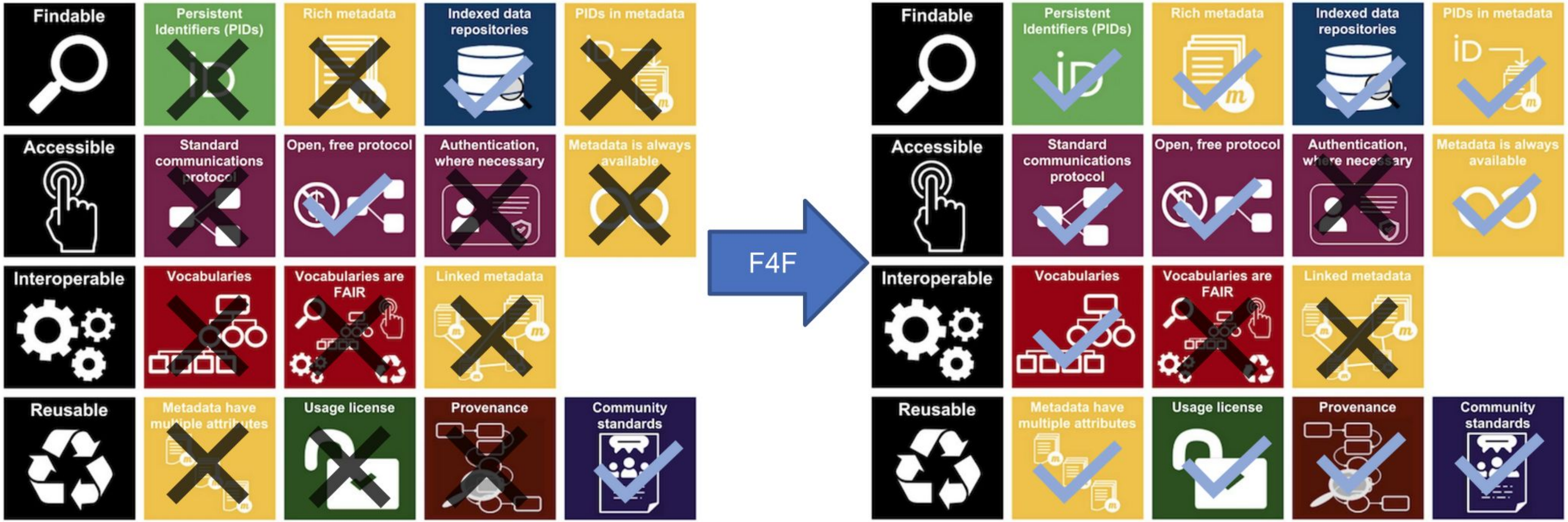
Benefits of reusable data

- Broaden access to research data
- Maximize knowledge gained from data sets
- Improve scientific reproducibility
- Enable machine learning studies

Fair4Fusion

- Objective: Make European-funded fusion data more widely available & FAIR
    - Raise awareness of open data within the fusion program
    - Develop tools needed for an open data approach
    - Lay foundations for an open data policy
- Subset of tasks
    - Outreach to community
    - Define use cases
    - Create blueprint architecture for open fusion data
    - Build data foundation for open access
    - Develop open data demonstrators

Fair4Fusion



Fair4Fusion is laying the groundwork to improve the data environment for fusion

Use cases from F4F show need for open access

- As a member of the general public, I would like to know how many shots per day and per year are performed by each of the experiments.
- As a researcher, I want to locate all H-mode shots that had a flat-top phase of longer than 0.5 seconds, across a selection of devices.
- As a data provider, I want to ensure the appropriate availability of my data without breaking the law (e.g. GDPR).

Efforts to make fusion data FAIR need to continue

- The Fair4Fusion project ends later this year
  - All deliverables to be completed on schedule
- Lesson: *It's very difficult to change an established community with "working" practices...but the astronomical and meteorological communities show it can be done.*
- Significant potential for international collaboration
  - As with International Heliophysics Data Environment Alliance

Open Source Definition

- Software is **open source** if anyone is free to use, modify, and/or redistribute it
  - Including source code
- An open source license does not discriminate against persons, groups, or fields of endeavor
  - No restrictions on commercial use
- The Open Source Initiative maintains a list of approved licenses
  - Customizing licenses causes problems

Two categories of licenses

- **Permissive** licenses have few restrictions
  - Examples: MIT and BSD 2-clause license
- **Copyleft** licenses require derived works to be released under the same license
  - Example: GNU General Public License version 3 (GPLv3)
- Two licenses are compatible if they allow both programs to be combined into a single program
  - Permissive licenses maximize license compatibility

Pain points with scientific software

- Lack of user-friendliness
- Difficult to compile & install
- Inadequate documentation
- Unreadable code
- Cryptic error messages
- Licensing issues
- Packages not written to work with each other
- Unvalidated code

Consequences of pain points

- Beginning research is hard
- Collaboration is difficult
- Duplication of functionality
- Research is less reproducible
- Research can be frustrating

How can we address these pain points?

- Make our software open source
- Write readable, usable, & maintainable code
- Use a high-level language, where appropriate
- Prioritize documentation
- Create an automated test suite
- Develop code as a community
- Build a shared software framework...

A software ecosystem!

What is PlasmaPy?

plasmapy

Mission

*To grow an open source **software ecosystem** for plasma research & education*

Many ways to be part of the community

- Come to PlasmaPy's...
  - Community meeting (Tuesdays at 18 UTC)
  - Office hours (Thursdays at 18 UTC)
- Join our Element chat
- Request new features on GitHub
- Organize community events
- Contribute!

Current & planned PlasmaPy subpackages

`plasmapy.particles`

- Object-oriented representations of ions, electrons, and fundamental particles

`plasmapy.formulary`

- Commonly needed formulae for plasma parameters and transport coefficients

`plasmapy.simulation`

- To include building blocks of plasma simulations and an improved particle tracker

Current & planned PlasmaPy subpackages

`plasmapy.analysis`

- Analysis techniques for data from simulations, experiments, and observations

`plasmapy.diagnostics`

- For representations of plasma diagnostics such as Langmuir and magnetic flux probes, as well as synthetic diagnostics

`plasmapy.dispersion`

- To contain dispersion relation solvers for plasma waves

Current & planned PlasmaPy subpackages

`plasmapy.plasma`

- Base classes to represent different plasmas

`plasmapy.utils`

- Helpful tools for the rest of the package

`plasmapy.addons`

- Entry point for affiliated packages to be put in PlasmaPy namespace

Biggest challenges for PlasmaPy

- Changing the culture
  - Community-wide software development
- Building community
  - Supporting new contributors
- Lack of a community-wide portal for experimental data
- Lack of open metadata standards 🙀

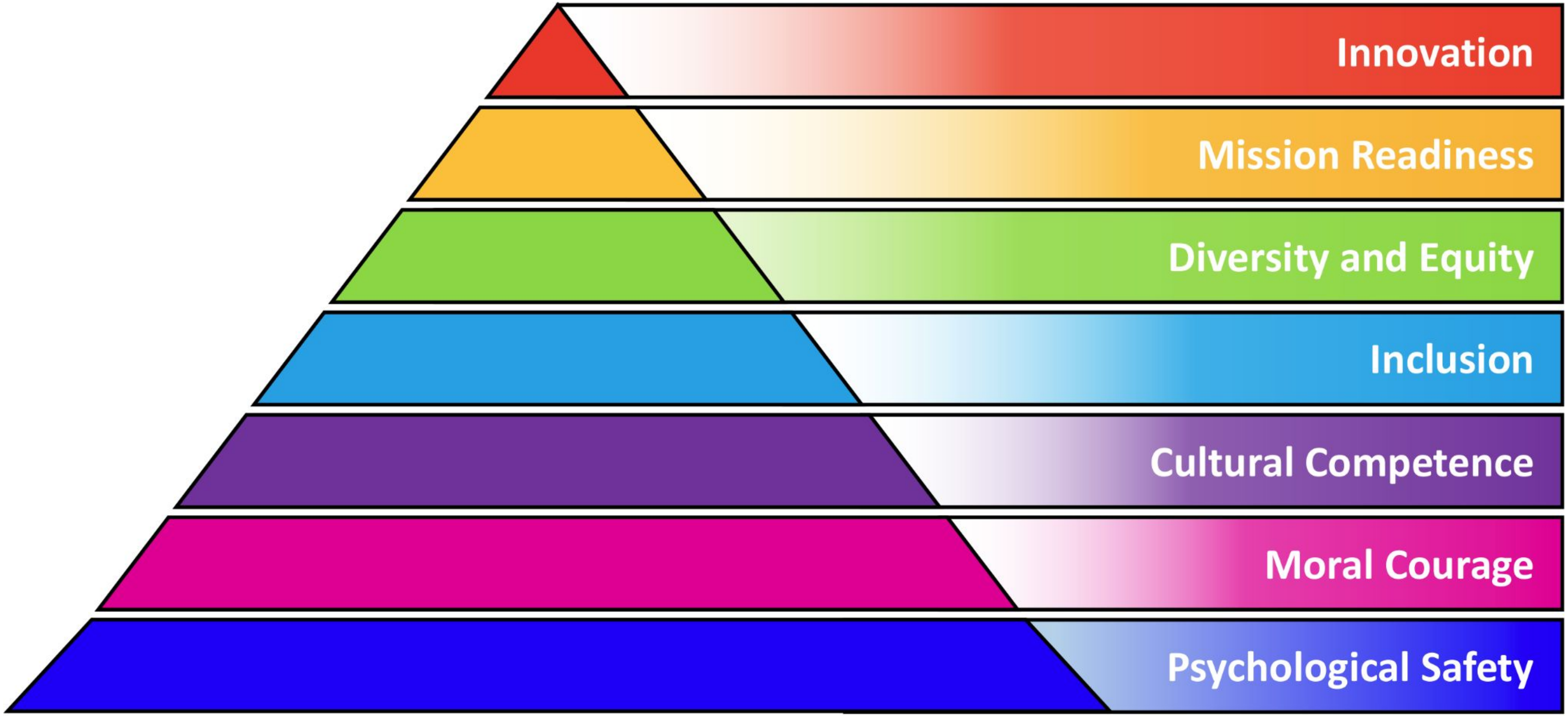
Plasma Hack Week 2021 (28 June – 2 July)

- Mix of a summer school and a hackathon
- Tutorials for research software engineering
  - How to contribute to open source projects
  - Writing clean scientific code
  - Testing scientific software
- Tutorials for different plasma packages
  - PlasmaPy, OMFIT, BOUT++, Gkeyll, etc.
- Videos to be posted online soon
- Expected to be annual event

The nascent field of research software engineering

- Research software engineers (RSEs) include
  - Researchers who spend most of their time programming
  - Software engineers developing scientific software
  - Everyone in between
- The term “research software engineer” was coined in ~2012
- Problems
  - Unclear career paths for RSEs
  - Insufficient training for scientists to become RSEs
- University courses on research software engineering?

Building a healthy and innovative workforce



Developed by Dr. Kimberly Young-McLear, U.S. Coast Guard Academy [1]

Psychological safety is necessary for open science

- Members of the plasma community should be able to:
  - Be their authentic selves;
  - Share their perspectives and make mistakes;
  - Without fear of bullying, retribution, or discrimination
- Psychological safety is foundational for diversity, equity, and inclusion
- Diversity, equity, and inclusion are foundational for open science

Reference: *Beyond Buzzwords and Bystanders: A Framework for Systematically Developing a Diverse, Mission Ready, and Innovative Coast Guard Workforce* by K. Young-McLear, S. Zelmanowitz, R. W. James, D. Brunswick, & T. W. DeNucci.

Codes of conduct

- All collaborative software projects need a code of conduct
  - Describe unacceptable behaviors (e.g., harassment)
  - Promote positive behaviors (e.g., demonstrating empathy)
- Each code of conduct should have an enforcement policy
- Example: Contributor Covenant Code of Conduct

Summary

- Fusion energy & plasma sciences are becoming more open
- Open science requires cultural change, institutional change, and technical infrastructure
- Scientific data should be findable, accessible, interoperable, and reusable
- Work has begun on an open source software ecosystem for plasma research and education