PlasmaPy: initial development of an open source core Python package for plasma physics

Nicholas A. Murphy,[1] Andrew J. Leonard,[2] Dominik Stańczak,[3] Colby C. Haggerty,[4] Tulasi N. Parashar,[4] Yi-Min Huang,[5] and the PlasmaPy Community

[1]Harvard-Smithsonian Center for Astrophysics, [2]Aperio Software, [3]Warsaw University of Technology, [4]University of Delaware, [5]Princeton University

59th Annual Meeting of the APS Division of Plasma Physics
Milwaukee, Wisconsin, USA
October 23–27, 2017

Link to this poster:
http://q-r.to/baoaBr

Introduction

- In recent years, researchers in several different subfields of physics and astronomy have collaboratively developed core Python packages such as Astropy[1] and SunPy[2]
- These packages provide core functionality, common frameworks for data analysis and visualization, and educational tools
- A similar open source package for plasma physics would greatly benefit our field
- **We have begun open development of PlasmaPy, which will be a community-developed and community-driven core Python package for plasma physics**

[1] Astropy Collaboration (2013, A&A, 558, 833)
[2] SunPy Community (2015, CS&D, 8, 014009)

Current status of scientific programming in plasma physics

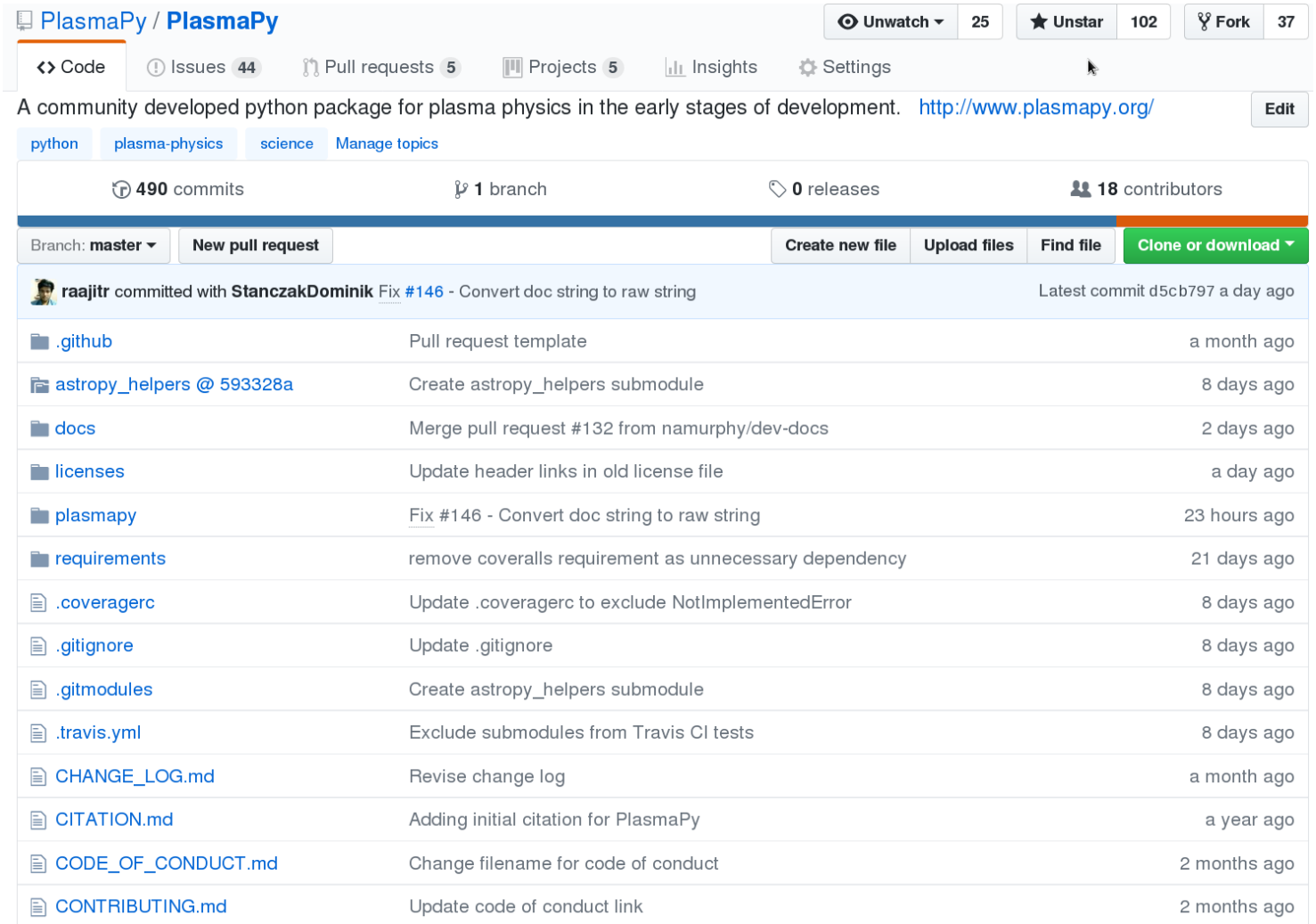
- Major codes often use low-level languages such as Fortran
- Programmers are often self-taught
- Code is often difficult to read
- Compiling and installing codes is difficult and time-consuming
- Different codes lack interoperability
- Documentation is usually inadequate
- Access to major codes is often restricted in some way
- Somewhat unusual to share code
- Many versions of software do essentially the same thing
- Research is difficult to reproduce

There is a considerable need for open, general-purpose shared software for plasma physics using modern best practices for scientific programming.

Why choose Python?

- Free and open source
- High-level, interpreted language
- Programming style emphasizes readability
- Can "glue" together software written in different languages
- Can reach near-compiled speeds using packages such as Numba and Cython, or by calling compiled routines
- Well-developed numerical and scientific analysis packages
- Active user community
- Can learn from and collaborate with ongoing highly successful projects such as Astropy and SunPy
- Will help students learn programming skills that will be useful in finding employment outside of plasma physics

PlasmaPy is an open source Python 3.6+ package for plasma physics in the early stages of development



The long-term goal of the PlasmaPy community is to facilitate a fully open source Python ecosystem for plasma physics.

PlasmaPy is open source for open and reproducible science

- Some software packages in plasma physics are described as open source, but do not meet the definition[3] set by the Open Source Initiative (OSI) or use an OSI-approved license[4]
- PlasmaPy is under the permissive **BSD 3-clause license** with OSI-approved language to protect against software patents
  - Using a permissive license maximizes compatibility with software under different licenses
  - Permissively licensed code may be incorporated into both proprietary and copyleft software
- Creative works besides source code are usually under Creative Commons licenses
  - The **CC BY 4.0** license allows works to be shared and adapted as long as attribution is given to the original work
  - The **CC BY-SA 4.0** license allows works to be shared and adapted with attribution if derivative works are shared under the same license

[3] Open source definition: https://opensource.org/osd

[4] OSI-approved licenses: https://opensource.org/licenses

PlasmaPy is using best practices for scientific computing[6] to ensure that code is easy-to-use and maintainable

- Simple and intuitive application program interface (API)
- Readable and consistent style (PEP 8 standard)
- Embed documentation in code
- Use modular, object-oriented programming
- Version control with git with useful commit messages
- Avoid prematurely optimizing code
- Use semantic versioning
- Use open Matrix/Gitter channel for real-time communication
- Continuous integration testing with coverage checks
- Issue tracking and code review using GitHub
- Adopt a code of conduct[5] and work toward a welcoming and inclusive community

[5] See CODE_OF_CONDUCT.md in the PlasmaPy repository

[6] Many of these practices are described by G. Wilson et al., "Best Practices for Scientific Computing," PLOS Biology **12**, e1001745 (2014)

Organizational development in 2017

- Create organizational infrastructure
  - Set up team communication channels
  - Write vision statement and contribution guide
  - Adopt a code of conduct
  - Appoint the Coordinating Committee
  - Start the PlasmaPy Enhancement Proposals repository
  - Choose license and versioning scheme
  - Begin development roadmap
- Set up documentation structure
  - Enable builds of online documentation using Sphinx that are hosted on Read the Docs
  - Create initial website using Nikola and GitHub Pages
- Plan for release of version `0.1.0` as a prototype and developer's preview in early 2018.[7]

[7] The API of the `0.*.*` development releases should be considered unstable. Beginning with version `1.0.0`, the API will maintain backward compatibility until the next major release.

Code development began in earnest in April 2017

- Implemented continuous integration testing with Travis CI and coverage testing with Coveralls to find code not covered by tests 

- Began development of core data structures (`Plasma` class)
- Created `atomic` subpackage for easy access to atomic data
- Began `physics` subpackage for calculating plasma parameters and transport coefficients
- Began `math` subpackage for plasma dispersion function, etc.
- Began development of plasma simulation capabilities
- Implemented a particle pusher

PlasmaPy's entire code development history is openly available on our GitHub repository.

PlasmaPy uses the `astropy.units` package for units

This package creates `Quantity` objects with attached units.

```
>>> from astropy import units
>>> distance = 44*units.imperial.mile
>>> time = 30*units.minute
>>> distance/time
<Quantity 88.0 mi / h>
>>> (distance/time).to(units.m/units.s)
<Quantity 39.33952 m / s>
>>> (1.21*units.GW).cgs
<Quantity 1.21e+16 erg / s>
>>> 2*units.m/units.s + 4*units.m/units.s**2
UnitConversionError: Can only apply 'add' function to quantities
with compatible dimensions
```

Built-in equivalencies can handle non-standard unit conversions commonly used in plasma physics:[8]

```
>>> kT = 1.2*units.keV
>>> kT.to(units.K, equivalencies=units.temperature_energy())
<Quantity 13925426.47248121 K>
```

[8] Code inside PlasmaPy strictly uses SI units to avoid confusion and for consistency with established international practices.

Review of PlasmaPy: "Your code has documentation."

```
def plasma_dispersion_func(zeta):
    r"""Calculate the plasma dispersion function

    Parameters
    ----------
    zeta : complex, float, ndarray, or Quantity
        Argument of plasma dispersion function.

    Returns
    -------
    Z : complex, float, or ndarray
        Value of plasma dispersion function.

    Raises
    ------
    TypeError
        If the argument is invalid.
    UnitsError
        If the argument is a Quantity but is
        not dimensionless
    ValueError
        If the argument is not entirely finite

    Notes
    -----
    The plasma dispersion function is defined as:

    .. math::
        Z(\zeta) = \sqrt{\pi}\int_{-\infty}^{+\infty}dx
                   \frac{e^{-x^2}}{x-\zeta}

    where the argument is a complex number
    [fried.conte-1961].

    In plasma wave theory, the plasma dispersion
    function appears frequently when the
    background medium has a Maxwellian distribution
    function.  The argument of this function then
    refers to the ratio of a wave's phase velocity
    to a thermal velocity.

    References
    ----------
    .. [fried.conte-1961]
    Fried, Burton D. and Samuel D. Conte. 1961.
    The Plasma Dispersion Function: The Hilbert
    Transformation of the Gaussian.

    Examples
    --------
    >>> plasma_dispersion_func(1j)
    0.7578721561413119 7j
    >>> plasma_dispersion_func(-1.52+0.47j)
    (0.6088888957234255 3+0.33494583882874029j)
    """
```

- We use the numpydoc docstring format and sometimes put more effort into writing documentation than writing code.

What does PlasmaPy need to succeed?

- Open development
  - Low barrier to entry
  - Inviting new contributors
  - Open data policies for major experiments
- A welcoming and inclusive environment
  - Provide a culture of appreciation for contributors to PlasmaPy
  - Use a code of conduct
- A sustainable funding model[9]
  - Astropy development is mostly a volunteer, grassroots effort
  - Most work on Astropy has been done by graduate students and postdocs, with little direct funding support
  - There is a need for funding agencies and large institutions to support open development of general purpose software

[9] This issue is described thoroughly by D. Muna et al. in *The Astropy Problem* (arXiv:1610.03159)

Summary

- **We have begun open development of PlasmaPy, which will be a community-developed and community-driven core Python package for plasma physics**
- Our goals for the next year include:
  - Release prototype version `0.1.0` in early 2018
  - Add fluid and particle simulation capabilities
  - Develop analysis tools for experimental and space data
  - Expand core functionality (e.g., a Grad-Shafranov solver, a dispersion solver, and topology analysis tools)
  - Join NumFOCUS and organize Software Carpentry workshops
- New contributors are welcome and can become involved by:
  - Joining our email list and conversation on Matrix
  - Raising issues on GitHub with new ideas for code development
  - Contributing code, such as those labeled **Good first contribution**
  - Contributing documentation
  - Becoming an early adopter and providing feedback

PlasmaPy Websites

- PlasmaPy's **GitHub repository** is:

  https://github.com/PlasmaPy/plasmapy

- Our **Matrix channel** for real-time communication is:

  https://riot.im/app/#/room/#plasmapy:matrix.org

- Sign up for the **PlasmaPy email list** at:

  https://groups.google.com/d/forum/plasmapy

- We are developing **online documentation** at:

  http://plasmapy.readthedocs.io/en/latest/

- We are developing our **webpage** at:

  http://www.plasmapy.org/