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PyPLUTO: a Data Analysis Python Package for the PLUTO Code

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Summary

In recent years, numerical simulations have become indispensable for addressing complex astrophysical problems. The so-called magnetohydrodynamics (MHD) framework represents a key tool for investigating the dynamical evolution of astrophysical plasmas, which are described as a set of partial differential equations (Chiuderi & Velli, 2015) that enforce the conservation of mass, momentum, and energy, along with Maxwell's equation for the evolution of the electromagnetic fields. Due to the high nonlinearity of the MHD equations (regardless of their specifications, e.g., classical/relativistic or ideal/resistive), a general analytical solution is not possible, making the numerical approach crucial. Numerical simulations usually end up producing large sets of data files and their scientific analysis relies on dedicated software tools designed for data visualization (Ahrens et al., 2005; Childs et al., 2012). However, in order to encompass all of the code output features, specialized tools focusing on the numerical code may represent a more versatile and integrated solution. Here, we present PyPLUTO, a Python package tailored for efficient loading, manipulation, and visualization of outputs produced with the PLUTO code (Mignone et al., 2007; Mignone, Zanni, et al., 2012). PyPLUTO uses memory mapping to optimize data loading and provides general routines for data manipulation and visualization. PyPLUTO also supports the particle modules of the PLUTO code, enabling users to load and visualize particles, such as cosmic rays (Mignone et al., 2018), Lagrangian (Vaidya et al., 2018), or dust (Mignone et al., 2019) particles, from hybrid simulations. A dedicated Graphical User Interface (GUI, shown in Fig. 1) simplifies the generation of single-subplot figures, making PyPLUTO a powerful yet user-friendly toolkit for astrophysical data analysis.

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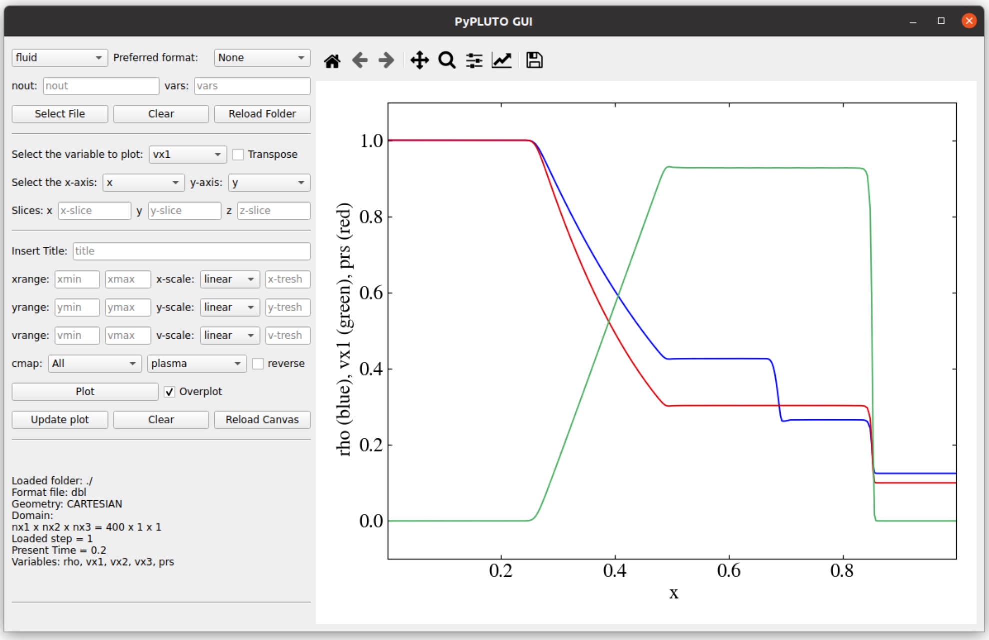

Figure 1: Interactive visualization of shock tube test results (i.e., density, pressure, and velocity profiles) with the GUI.

Statement of Need

The PLUTO code (Mignone et al., 2007) is a widely used, freely distributed computational fluid dynamics code designed to solve the classical and (special) relativistic MHD equations in different geometries and spatial dimensions. The original code is written in C (while the upcoming GPU version provides a full C++ rewrite) and it contains several numerical methods adaptable to different contexts. Data post-processing is a crucial step in analyzing the results of any numerical simulation. Other packages addressing related needs (e.g., plutoplot), provide valuable functionality for working with PLUTO data, including loading and visualization. However, they may not support all data formats or offer integration for tasks like data manipulation and advanced plotting. In this work, we present PyPLUTO v1.1, a Python package designed to load, manipulate and visualize efficiently the output from the PLUTO code. While a previous version of PyPLUTO is available, PyPLUTO v1.1, is a complete rewrite hosted at a new repository. The package retains its core strengths while offering user-friendly methods for generating publication-quality plots with high customization. In addition to its enhanced flexibility, PyPLUTO offers strong computational efficiency, enabling the rapid handling of large datasets typical of state-of-the-art numerical simulations. Through this balance between customization, performance, and ease of use, PyPLUTO represents a key tool to effectively communicate scientific results while minimizing the effort required for post-processing.

Main Features

PyPLUTO is a package written in Python (version $\geq$ 3.10) with the additions of NumPy (Harris et al., 2020), Matplotlib (Hunter, 2007), SciPy (Virtanen et al., 2020), pandas (team, 2020), h5py (Collette, 2013) and PyQT6 (although the last two are optional). The package, which can be installed through pip, primarily consists of three main classes:

- The `Load` class loads and manipulates the PLUTO output files containing fluid-related quantities.
- The `LoadPart` class loads and manipulates the PLUTO output files containing particle-related quantities.
- The `Image` class produces and handles the graphical windows and the plotting procedures.

Additionally, a separate `PyPLUTOApp` class launches a GUI able to load and plot 1D and 2D data in a single set of axes. PyPLUTO has been implemented to be supported by Windows, MacOS, and Linux, through both standard scripts and more interactive tools (e.g., IPython or Jupyter). The style guidelines follow the PEP8 conventions for Python codes (enforced through the Black package (Langa & Black, 2020)) and focus on clarity and code readability. Finally, by leveraging the capabilities of the sphinx package, PyPLUTO features extensive docstrings, serving the dual purpose of creating extensive and consistent documentation and providing a useful reference for future users and developers.

Benchmark Examples

PyPLUTO provides a set of benchmarks immediately accessible after installing the package. These consist of test problems that can be applied to relevant astrophysical applications and showcase the full range of PyPLUTO's features. Here we report two key examples demonstrating the package's capabilities.

Disk-planet Interaction

This test simulates the interaction of a planet embedded in a disk (Mignone, Flock, et al., 2012) and represents an ideal scenario for understanding the formation and evolution of planetary systems. In particular, the formation of spiral density waves and disk gaps represent some key observational signatures of planet formation and planet-disk interaction (Melon Fuksman et al., 2021; Muley et al., 2024). In the left panel of Fig. 2, we show an adaptation of Figure 10 of (Mignone, Flock, et al., 2012), featuring two separate zoom-ins around the planet's location.

- The first zoom (upper-right subplot) shows an enlarged view of the density distribution using the same color map and logarithmic scale as the global plot.
- The second zoom (upper-left subplot) highlights the changes in toroidal velocity due to the presence of the planet by employing a different color map (to enhance the sign change) and a linear color scale.

These zoomed views offer deeper insights into the physical processes at play and demonstrate the utility of PyPLUTO for analyzing complex astrophysical systems.

Particles Accelerated near an X-point

This test problem examines particle acceleration near an X-type magnetic reconnection region (Puzzoni et al., 2021). In the last decades, magnetic reconnection (Bugli et al., 2024; G. Mattia et al., 2023) has proven to be a key physical process to explain the population of non-thermal particles in solar flares, relativistic outflows, and neutron star magnetospheres. This sort of test provides valuable insights into particle acceleration mechanisms in high-energy astrophysical environments by enabling the investigation of particle trajectories and energy distribution near the X-point.

In the right panel of Fig. 2 we show an adaptation of the top panel of Figure 13-14 from (Mignone et al., 2018). The main plot displays the distribution of test particles, color-coded by their velocity magnitudes, with magnetic field lines overlaid as solid and dashed lines. The inset panel shows the energy spectrum at the initial ($t = 0$, in blue) and final ($t = 100$, in red) time. In this scenario, the absence of a guide field ($\vec{E} \cdot \vec{B} = 0$), results in a symmetric distribution along the y-axis from the combined effects of the gradient, curvature, and $\vec{E} \times \vec{B}$ drifts in the vicinity of the X-point, where the electric field is the strongest. This plot provides a clear visual representation of particle motion and energy changes, demonstrating how PyPLUTO can be used to investigate complex systems such as particle acceleration in astrophysical sources.

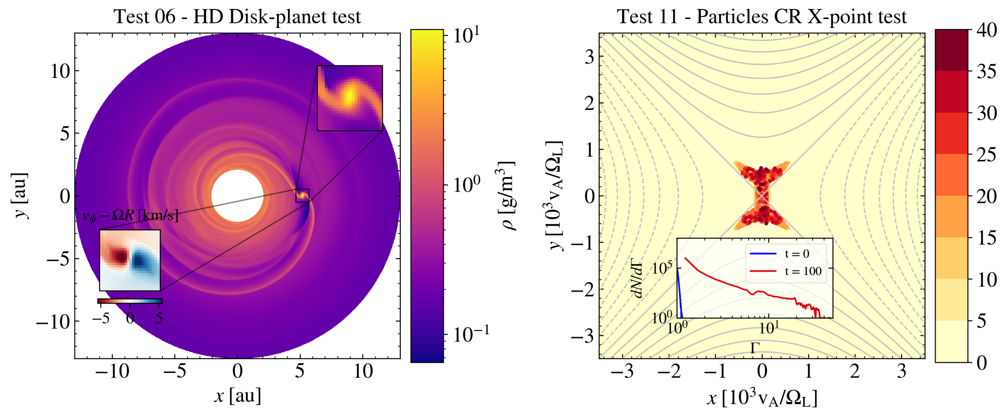

Figure 2: Left panel: Example of inset zooms of the planet region of the disk-planet test problem. The main plot and the right zoom show the density on a logarithmic scale, while the left zoom highlights the toroidal velocity on a linear scale. Right panel: Example of an X-point region with magnetic field lines overlaid (as contour lines of the vector potential, solid lines). The main plot shows the test-particle distribution, color-coded by velocity magnitudes, while the inset plot displays the particle energy spectrum at the beginning (in blue) and end (in red) of the simulation.

Ongoing research using PyPLUTO

Research applicable with PyPLUTO includes the development of numerical algorithms (Berta et al., 2024; G. Mattia & Mignone, 2022) and numerical simulations of astrophysical objects, such as jets (G. Mattia et al., 2023; Giancarlo Mattia et al., 2024; Giancarlo Mattia & Fendt, 2022) and protoplanetary disks (Melon Fuksman et al., 2024a, 2024b), as well as physical processes, such as particle acceleration (Wang et al., 2024) and magnetic reconnection (Bugli et al., 2024).

Conclusion and Future Perspectives

The PyPLUTO package is designed as a powerful yet flexible tool to facilitate the data analysis and visualization of the output from PLUTO simulations, focusing on user-friendliness while allowing the necessary customization to produce publication- quality figures. To overcome current limitations and further enhance the package's capabilities, particular focus will be devoted to:

- introducing specific routines for rendering 3D data to provide users with tools for visualizing volumetric data;
- supporting interactive visualization and comparison of multiple simulation outputs, allowing the users to track temporal evolution directly with the GUI;
- expanding the graphical interface to support particle data, including dynamic visualization of particle distributions and trajectories;

Alongside these improvements, the PyPLUTO development will focus on encompassing the latest features of the PLUTO code, such as new Adaptive Mesh Refinement strategies and extensions to more general metric tensors. PyPLUTO is a public package that can be downloaded alongside the CPU and GPU versions of the PLUTO code. Regular updates will be released with improvements and bug fixes. Additionally, a repository containing the PyPLUTO development versions will be available for users who wish to exploit the code's latest features in advance.

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