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PIVA: Photoemission Interface for Visualization and Analysis

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Summary

Angle-resolved photoemission spectroscopy (ARPES) is a powerful probe for elucidating the electronic structures of quantum materials. As the technique's throughput continues to increase, there is a pressing need for specialized tools that enable rapid and intuitive data inspection and analysis. The PIVA package introduced in this work addresses this need by providing an interactive interface specifically designed for the efficient visualization and examination of large volumes of multidimensional datasets. It integrates image-processing methods, measurement tools, and a comprehensive suite of analysis routines within an intuitive environment. Together, these capabilities offer a robust framework for conducting detailed ARPES investigations, significantly enhancing the efficiency and depth of data exploration.

Statement of need

Over the past few decades, our ability to collect data has rapidly outpaced our capacity to process it efficiently and extract meaningful insights. This trend is evident not only in the broad field of data science but also across many areas of experimental research, where specialized tools are essential to manage the ever-increasing speed and scale of data acquisition.

The challenges of analyzing large amounts of complex data certainly arise for physicists utilizing angle-resolved photoemission spectroscopy (ARPES), a technique that directly probes the electronic band structure of crystal materials (Sobota et al., 2021). The overall significance of ARPES in the field of condensed matter physics can hardly be exaggerated, as it has provided vital insights into numerous important topics, like unconventional superconductivity (Damascelli et al., 2003), topological states of matter (Dil, 2019), and novel forms of magnetism (Krempaský et al., 2024). These scientific discoveries would not have been possible without significant advancements in instrumentation and technical capabilities (Koralek et al., 2007; Strocov et al., 2014; Wannberg, 2009; Zhou et al., 2018), each setting a milestone in data acquisition efficiency.

The increasing speed of the measurement process brings, however, unique challenges to data handling and analysis in ARPES investigations. Namely, researchers require flexible tools to quickly glean insights from the data during an ongoing, dynamic experiment, as well as to perform deeper data exploration and analysis later on. PIVA is a package specifically designed to meet these needs. In comparison to other available solutions (*ARPES Python Tools*, 2024; Rotenberg et al., 2021; Stansbury & Lanzara, 2020), its primary objective is to enhance the efficiency of ARPES data inspection and analysis by offering interactive and intuitive tools tailored to manage large amounts of multidimensional datasets simultaneously—all without relying on proprietary environments. While the content of this manuscript describes

PIVA's implementation and structure, more details and examples can be found in the project's documentation (*PIVA - Documentation*, 2024).

Software description

The PIVA package is an open-source, Python-based software. Its data handling and analysis components utilize standard numerical and scientific libraries, including NumPy, SciPy, Pandas, Matplotlib, and Numba (Harris et al., 2020; Hunter, 2007; Lam et al., 2015; The pandas development team, 2020; Virtanen et al., 2020). The GUI applications are built with the PyQt5 and pyqtgraph toolkits (*The PyQt Project*, 2024; *The PyQtGraph Project*, 2024). Figure 1 depicts PIVA's general structure and its individual components.

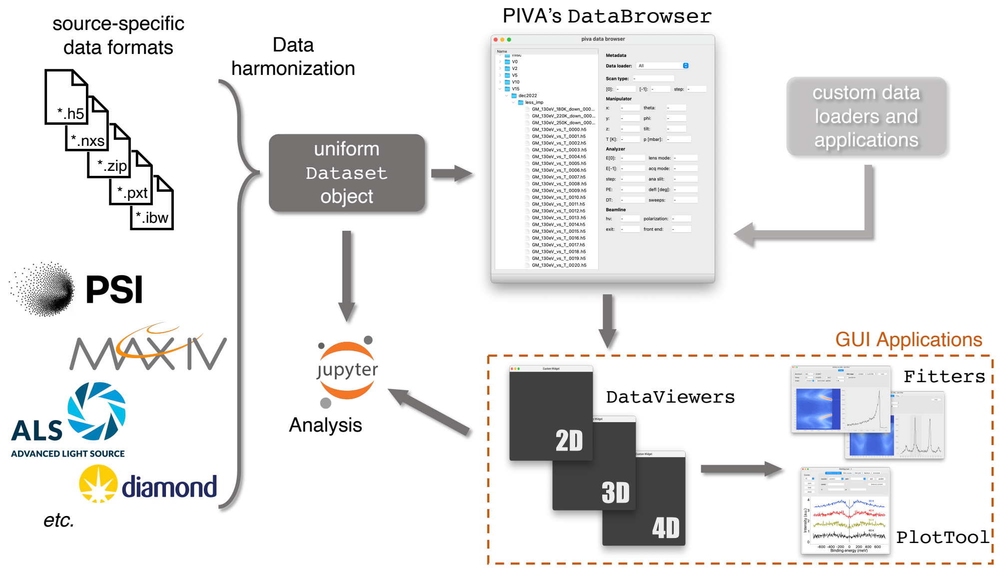

Figure 1: Schematic of the PIVA package showing its components and workflow within the software.

The package consists of two main components. The first part is a graphical user interface (GUI) application designed for quick data visualization and inspection during time-critical measurements. The GUI utilizes interactive graphics tools based on the `data-slicer` package (Kramer & Chang, 2021). It allows one to navigate through the acquired data files, open selected data files in interactive applications, conveniently browse through multidimensional datasets, and carry out preliminary analysis. In the next steps, the users can take advantage of PIVA's collection of analysis methods and conduct the second part—detailed scrutiny of the recorded spectra. This can be performed within an environment of the user's choice or by using built-in tools to transfer the workspace to a Jupyter notebook.

Data handling

While handling the acquired data, in the first step, raw files need to be read and loaded into a uniform format. Since data formats used by various experimental setups differ from lab to lab, dedicated file-loading scripts are required for each system. Within PIVA, this task is handled by the `data_loader` module, which imports the data and metadata into a uniform `Dataset` object, inheriting from the `Namespace` class (*The Argparse Module*, 2024). The package includes specific `Dataloader` classes already implemented for numerous synchrotron sources around the world, which can also be easily imported outside the interactive environment and used to run custom analysis routines. Consequently, adopting a single, standardized format facilitates convenient transfer of loaded datasets between other PIVA modules and utilities and significantly simplifies data handling when manual processing is required.

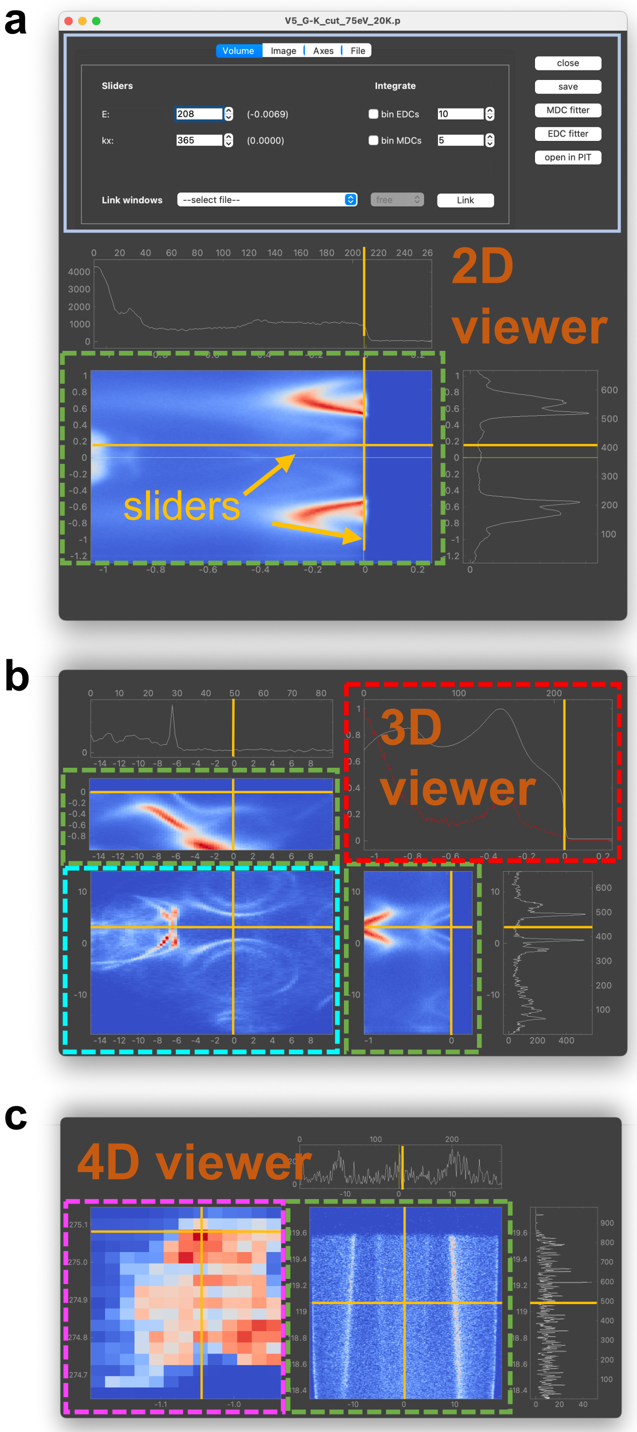

Figure 2: Overview of the `DataViewers`. **a-c** Appearance of the 2D, 3D and 4D `DataViewer`, respectively. Interactive sliders are marked with yellow lines. The main graphical components are highlighted with dashed lines as follows: angle-energy detector image (green), constant energy map (cyan), energy slider for the constant energy map (red), and manipulator raster scan (magenta). The utilities panel, displayed only in the case of the 2D viewer (panel **a**), is highlighted with a solid light-blue box.

Interactive tools

The main visualization applications are three `DataViewers`, designed to handle 2-, 3- and 4-dimensional datasets, depending on the scan mode in which they were acquired. Their main components and layout are presented in Figure 2. All three `DataViewers` consist of a set of plotting panels and the utilities panel. The former consists of image/curve plots (depending on the dimensionality of the extracted cut) and draggable sliders that allow one to freely browse through datasets and display slices along the corresponding directions. The utilities panel contains numerous functionalities for data exploration and visualization including, *e.g.*, averaging over selected direction and range, normalizing along specific axes, and applying experimental corrections.

Additional interactive tools include the `EDCFitter` and the `MDCFitter`, suitable for scrutinizing 1D energy or momentum distribution curves, respectively, and `PlotTool`, a convenient utility that allows the creation of customized figures by means of combining different plots.

Analysis modules

Unlike many other experimental techniques, ARPES data and analysis can vary widely depending on the system under investigation and the information to be extracted. As a result, deep analysis necessitates meticulous and highly specialized data handling, which would be significantly limited when encapsulated within a purely graphical interface. For that reason, apart from interactive applications, PIVA provides an extensive library of functions and procedures that can easily be imported into an environment of the user's choice. (As a recommended option, the package includes tools for exporting datasets to Jupyter notebooks.) There, users can conduct detailed fitting and more sophisticated analysis using various methods already implemented within the analysis module or apply their own routines, requiring hands-on scripting.

Modularity

PIVA contains built-in procedures for importing modules and plugins written by users. This includes data-loading scripts (for file formats not implemented within the package), GUI applications to elevate interactive data processing capabilities or any other utilities that one might want to incorporate. Once implemented, the extensions are automatically loaded and ready to be used at the beginning of each session. A comprehensive description and examples of how to implement and configure such extensions are provided in the documentation (*PIVA - Documentation*, 2024). Notably, while the current functionalities are primarily designed for ARPES, custom plugins can be developed to manage and visualize various other types of data, thereby expanding PIVA's applicability to a wide range of experimental techniques that produce image-like results.

Conclusions and outlook

In conclusion, PIVA was developed to address bottlenecks in users' ability to process ARPES data. The `DataViewers` enable efficient visualization and preliminary analysis of a broad range of multidimensional datasets. Further detailed analysis can be performed using dedicated interactive `Fitters` or by utilizing implemented analysis methods. Furthermore, the package addresses an essential aspect of data format inhomogeneity arising from varying conventions across sources and instruments, by introducing a standardized `Dataset` object. Thanks to these advantages, PIVA has been utilized by external users and staff members of the SIS beamline at the Swiss Light Source and employed in numerous experiments, some of which have already been documented in published works (Hu et al., 2023; Pudelko et al., 2024; Soh et al., 2024; Wang et al., 2022).

Although PIVA's combination of features fulfills most of the everyday needs of ARPES experimenters, further developments are planned to expand its capabilities. Foreseen improvements include implementing data loading scripts for additional beamlines and instruments, expanding the library of postprocessing methods with analysis routines and machine learning algorithms for noise reduction, and developing new interactive applications tailored for other variants of ARPES, such as spin-resolved measurements.

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