

Project synopsis

The aim is to deliver an open source software package to allow fast analysis of area detector images at the GEMS beamlines as well as off-line by user groups.

- Simplify the data processing step both to speed up processing for experienced users and to attract new user groups.
- Enable fast analysis during experiments, allowing users to optimize their decision during beamtime, for example during *in situ* experiments.

However, the open architecture of pydidas is designed to allow using pydidas over a wide range of applications and not limited to its primary use case.

pydidas features

Pydidas aims to provide a user interface which gives users all the necessary tools to work with their diffraction data:

- Data browsing (including hdf5 files)
- Detector calibration (using pyFAI calibration tools)
- Definition of experiment and scan
- Workflow assembly
- Testing workflows and tweaking processing parameters
- Running workflows (using parallelization)
- Result visualization
- Result export

All of pydidas' processing functionality can also be run from the command line, for example on clusters.

Availability

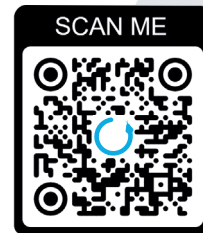
Pydidas is developed as open source project and freely available:

- The source code is available on Github
- A standalone Windows distribution including embedded python is available upon request
- Pydidas is available via the module system on the DESY Maxwell cluster

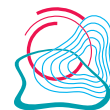


Contact

- Direct contact via email: malte.storm@hereon.de
- A feedback / contact form is available on the pydidas website <https://ms.hereon.de/pydidas>
- Via the github project page <https://github.com/hereon-GEMS/pydidas>



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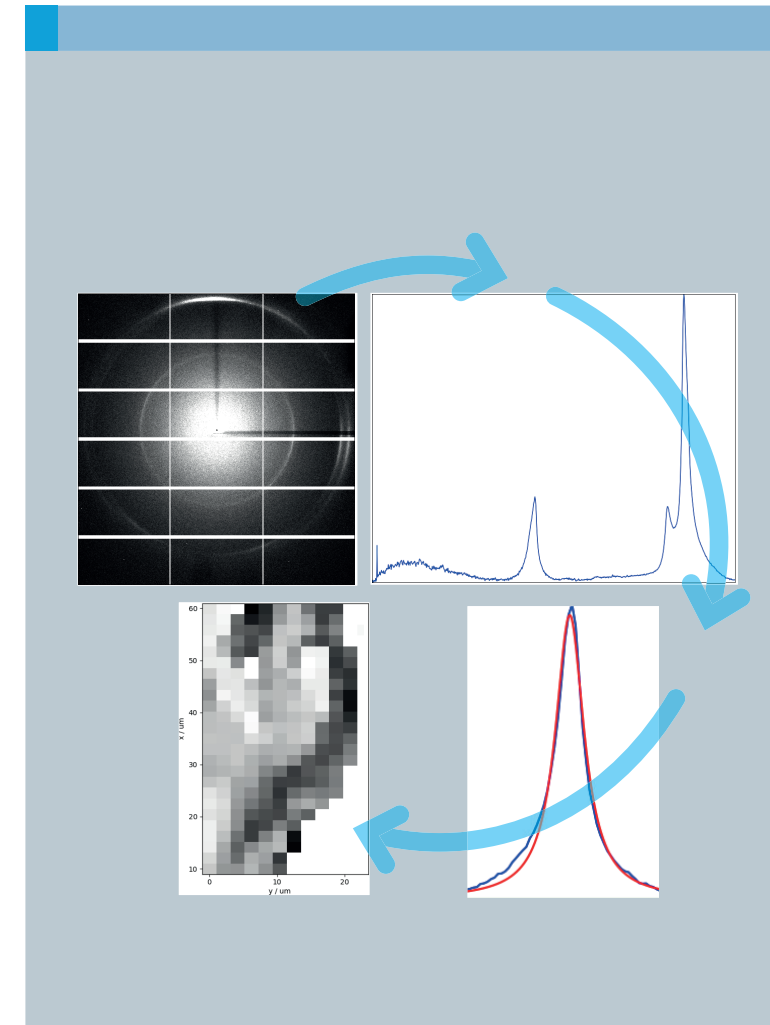
Helmholtz-Zentrum Hereon
Max-Planck-Straße 1
21502 Geesthacht
www.hereon.de

Helmholtz-Zentrum Hereon

pydidas



A user-friendly python software suite for the analysis of X-ray diffraction data using the pyFAI engine.

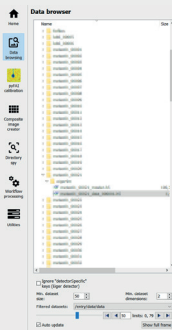


Status: Jan 2023



Data browsing

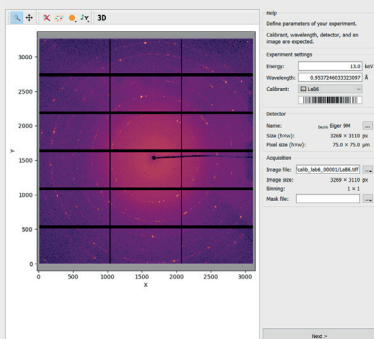
- Browse through the full file system
- Visualize image data with a single click
- Support for hdf5 files:
- Select different hdf5 datasets
- View individual frames



Detector calibration

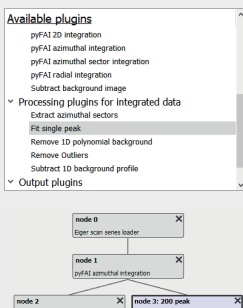
Use the pyFAI calib2 tool conveniently from within pydidas

- Allows export of calibration results
- Calibration results can be used further in pydidas directly without the need to export a file



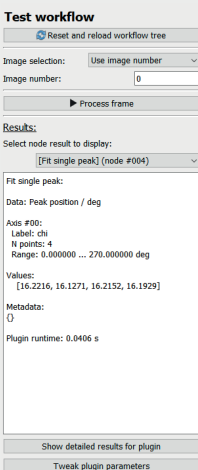
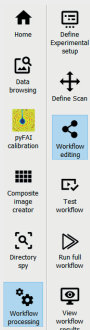
Workflow editing interface

- Browse through all available plugins (and show detailed information for all plugins)
- Add and configure plugins
- Re-arrange the workflow tree



Pydidas data processing

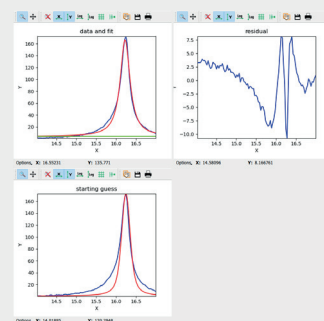
- Required information separated in three segments which can each be easily reused:
 - **Experiment** defines X-ray energy, detector, geometry
 - **Workflow** configures the data processing steps
 - **Scan** defines file names, data paths and scan points
- All configurations can be exported from and re-imported into pydidas
- Workflows are defined from individual plugins for each step for high flexibility.
- Pydidas supports branching workflows
- Pydidas plugins are simple to write and users can add their own plugins for specialized analysis features.



Testing workflows

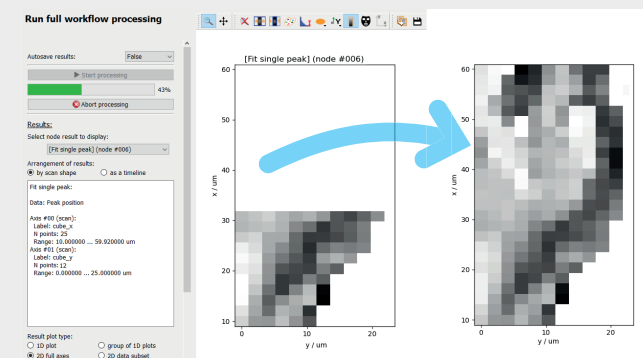
Pydidas includes an interface to test the workflow on a single data point:

- Access all intermediate results
- Inspect individual plugins
- Tweak plugin parameters and check their impact on results



Running workflows

- Workflows can be run from the GUI using multiple background processes for parallelization
- Processing can also be started from the command line, for example on clusters
- Results can be visualized in real time as the processing progresses:
 - Any result (subset) can be plotted as 1d or 2d image
- All scan dimensions can be squeezed to a scan timeline for visualization



Additional tools

Pydidas includes additional convenience tools to facilitate data processing:

- Process image series (sum / average)
- Load and edit detector masks (ESRF silx)
- Directory spy to display the latest data file in the selected directory
- Composite creator to tile individual images

Pydidas is still under development and this flyer describes an early version.

If you are missing features, please get in touch (see contact on the back) to describe your needs and discuss how these could be implemented in pydidas.