PadTools User Manual

PadTools IDL electron microscopy 4D STEM Tools

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1 Getting Started

1.1 Installation

System Requirements

The compiled version of PadTools requires the presence of the IDL virtual machine v8.8 or higher. The IDL virtual machine itself is freely available from the IDL website. IDL is a cross-plattform application and can be installed on the following operating systems: MAC OS X, Windows, PC-Unix (LinuX) and Unix.

Download and Installation of PadTools

Visit the PadTools download page and get the latest PadTools build. It comes as a compressed file. Unpack the archive and copy the PadTools folder into an appropriate installation directory. On Windows this is preferably the system-wide 'Program Files' folder, on Mac OS X the system-wide 'Applications' folder.

On other Unix variants there a are a few more steps to take: copy the PadTools folder to an installation directory of your choice (e.g. '/usr/local' and Create a script named "PadTools" containing the following line:

idl -vm=/INSTDIR/PadTools/PadTools.sav

where INSTDIR is the installation path.

Make the script executable (´sudo chmod a+x PadTools´) and copy it to a binary directory, e.g. '/usr/ local/bin'.

Download and Installation of HDF5 libraries and HDF5 plugins

DECTRIS file data comes in HDF5 containers, in addition the frame data is compressed. To load DECTRIS data PadTools, i.e. IDL, accesses the HDF5 system library. HDF5 plugins are required for deflating the data. You'll need to install the HDF5 libraries and the plugins from hdfgroup.org. Make sure to set the environment variable 'HDF5_ROOT' and 'HDF5_PLUGIN_PATH'. For details see here and under 'Troubleshooting' below. Currently, PadTools is tested against version 1.14 of the HDF5 libraries on the Windows platform. Note that at present, the decompression fails on the Apple Silicon architecture due to an issue with the HDF5 plugins.

1.2 Preference Files

PadTools stores parameters in a preference file named PadTools.pref. E.g. recently visited directories are stored in this file. On a multiuser system each user can have his own preference file, located in the HOME directory. On unix systems, the HOME directory is defined and the value, i.e. the actual directory, can be retrieved from the $HOME environment variable. On Windows, this environment variable does not exist by default. Please follow the steps below to set your $HOME environment variable under Windows.

Once you have a $HOME directory set, copy the system-wide preferences file, which is located in the installation directory of PadTools, to the HOME directory and restart PadTools. It should launch without an error

message. The user preference file will be updated upon closing the program, the file needs to be writeable.

Microscope and detector calibration data are stored in a file MicroscopeCalibrationDB.pref. Copy the default file from the PadTools installation directory in your HOME directory. MicroscopeCalibrationDB.pref contains JSON-encoded information for the calibration data. Currently there is no user interface for editing the data, please use a standard JSON editor to edit the file according to your system calibrations.

1.3 Program Start

On Windows systems: Double-click on the file PadTools.sav.

On Mac OS X: Double-click on the supplied application icon. You can drag the icon onto the dock to keep it in the dock.

On Other Unix systems: first check the DISPLAY environment variable and the access permissions to the client X-server, then type´PadTools´ on the command line.

1.4 User Interface

PadTools offers an easy-to-use graphical user interface. The user interface consists of a command menu, control windows and four dialog windows (Fig. 1.2.1):

The PadTools command menu or '*Menu Bar'* is used to call a command in order to perform an action on a data set.

The menu items are sorted according to the following considerations:

• File - Input/Output operations for the import and export of data sets.

• Transformations - Transformations of the 4D volume data to perform all sorts of corrections, like frame alignment, masking, hot pixel correction, scaling, averaging over various dimensions etc.

• Analysis - Analysis of the 4D-STEM data: Virtual Detectors, Orientation mapping, DPC, Peak Finding etc.

• Tools - Helpful functions, e.g for cyclic color map display.

• Windows - Access to GUI control windows.

• Macros - Automated batch jobs, pre-compiled

An important control window is the *'Data Inspector'* that is used for the administration of the list of data sets. Context-based menus are available for changing e.g. display options.

With the 'Data Inspector' you take control of the list of currently managed data sets. The 'Data Inspector' window is organized into three tabs named '3D Data', 'XY Graphs', and 'Tables'. The tab '3D Data' contains a list of data sets, which can be either a 4D STEM data set represented as a series of frames, a 3D data set or a single image. All these data items are connected to one display output window,

Each tab contains scrollable frames. The upper frame lists all entries in the list of data sets that are available. This upper frame is mainly used in order to set the focus onto a certain data set on which any command subsequently selected from the 'Menu Bar' will be performed: A left mouse button click on a label string will highlight the data set and focus this data set for operations that you select from the command menu. (Note that you cannot focus on a data set just by clicking on the graphical output window associated with the data set, there is no interaction between the window manager and the list manager!) The lower frame in the tab presents informational text about the selected data set.

The scrollbars below the information window give you access to individual frames in a 4D STEM or 3D data set. The lower scrollbar is used to average over neighboring frames, for display purposes.

The list frames of the tabs are associated with a context-sensitive menu. A simple click on the right mouse button will activate this menu.

The 'Console' GUI window shows informational program output, that can also be saved as a text file.

The ‘Contrast Inspector’ gives control over the contrast cut-off levels for the image display. Clicking the right mouse button on the histogram data window will open a context menu, giving access to e.g. auto contrast routines.

Additional dialog windows are used by processing routines to interact with the user and to read parameters. They are displayed when a user invokes a function from the ‘Menu Bar’ or a context menu command in the ‘Data Inspector’.

2 Troubleshooting

How to set the HOME environment variable in Windows

Open the Start Search, type in “env”, and choose “Edit the system environment variables”:

Click the “Environment Variables…” button.

Set the environment variables as needed.

- The New button adds an additional variable
- The Edit button modifies the selected variable
- The Delete button deletes the selected variable