User manual
DEVA

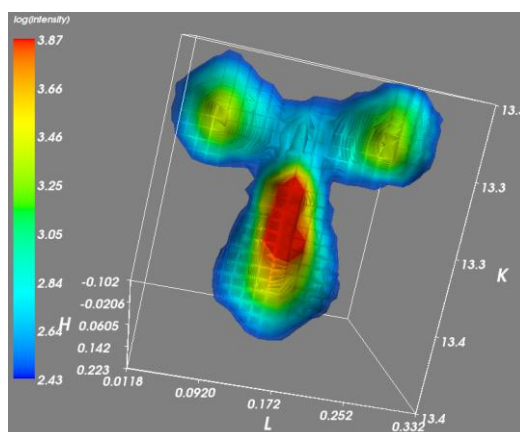**Version 2.0.4 (09/04/2015)**

Copy right: Thanh-Tra NGUYEN

Please feel free to inform me for bugs or your contribution

Thanhtra0104 [at] gmail.com

DEVA (D2AM EDF image Visualization and Analysis) is a software dedicated to treat X-ray diffraction data collected from XPAD area detectors (D1, D5 and S70 are supported for now). This software is used for data measured at the BM02 (or D2AM) beamline at the ESRF (http://www.esrf.fr/UsersAndScience/Experiments/CRG/BM02)

This software is fully written in Python language. The graphical user interface is written using GTK library. This software has been fully tested and used under Linux. Windows is also tested and run for some experiments. MAC OSX has in principle no problem to run this software.

The source scripts can be downloaded here: https://github.com/Traecp/DEVA

Please refer to the README file for installation. This manual describes briefly how to use it.

CONTENT

1) Main window:

Upon running the program by typing Deva.py in a terminal (or command prompt on Windows), the main window appears:
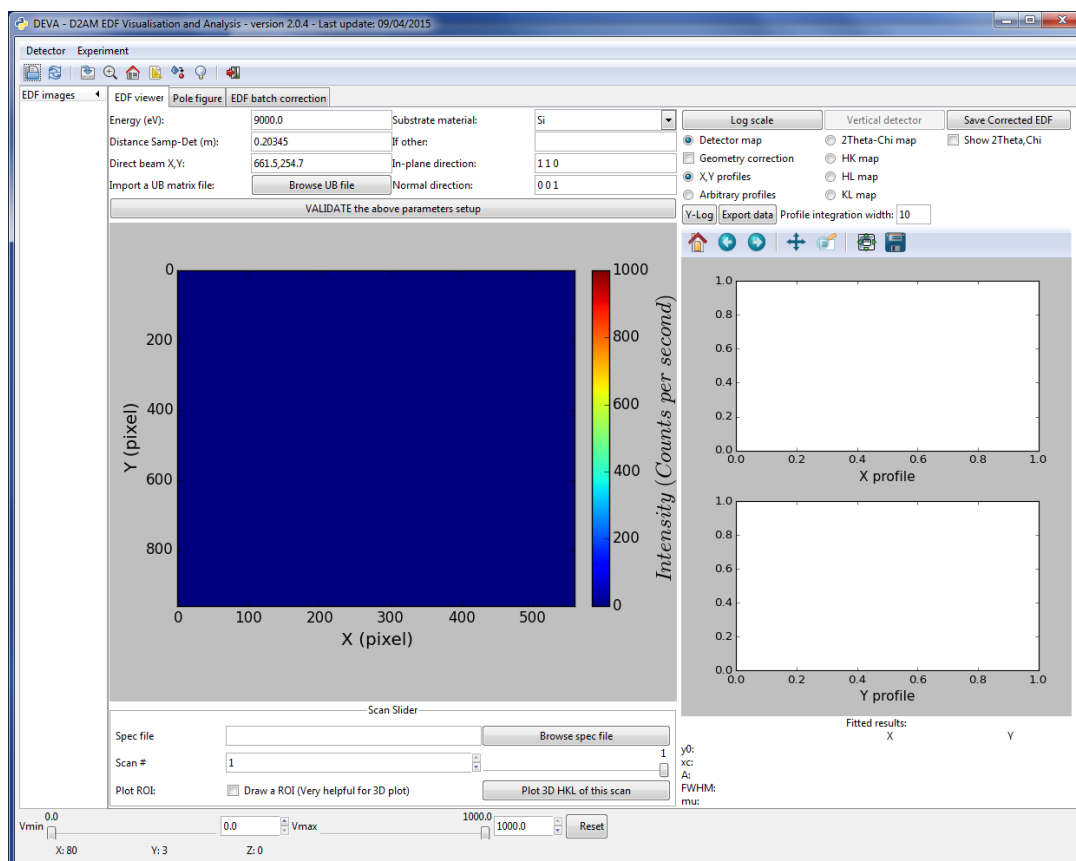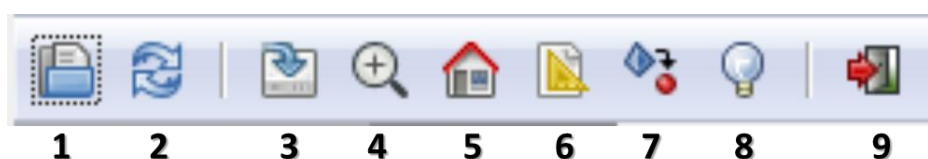

2) Menu bar:

Detector: Choose the detector used for your data acquisition (XPAD detectors D1, D5 and S70 are supported for now).

Experiment: Choose your experiment session (Gonio = Kappapsic, GISAXS)

+++ By default, the detector type is D5 and the experiment session is Kappapsic (Gonio).

3) Tool bar:

1: Open data folder

2: Refresh (update) data folder

3: Save current image as PNG or PDF

4: Zoom image (click to activate, click again to deactivate it)

5: Home = Reset the image to its initial scale

6: Ratio control = Click to change the aspect ratio of the image

7: Load a calibration file (a PONI file, generated by pyFAI). Poni file is a text file which contains the experimental geometry (X-ray wavelength, sample-detector distance, direct beam position, detector rotations …). This is useful for quantitative analysis.

8: Dark subtraction. Click this button to choose the current image as a dark image. Other images will be subtracted by this image. Click again to deactivate the dark image subtraction.

9: Quit the program.

4) Right panel buttons:

Log scale button: change to Log/Linear scale

Save Corrected EDF: after correcting the geometry of the XPAD detector image, you can save this EDF image for later use. The corrected image is saved in the same place where the raw image is found.

Geometry correction: Check this button to correct the geometry of the XPAD image. For example the two images below: left: raw image, right: corrected image.
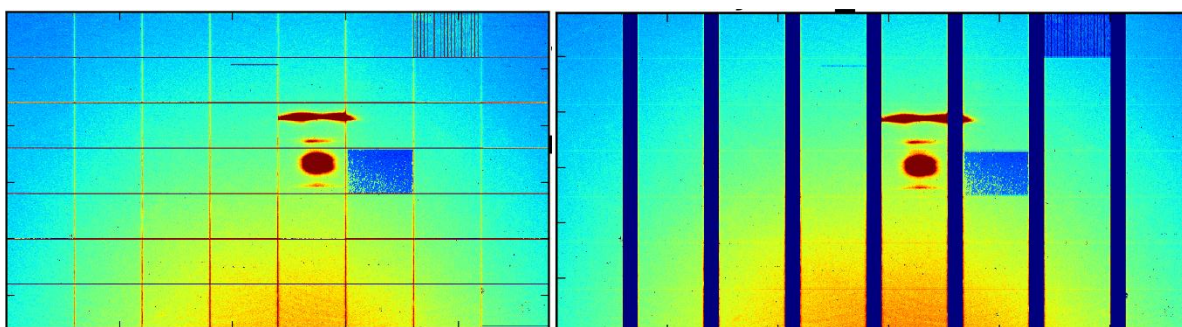
5) Load data folder
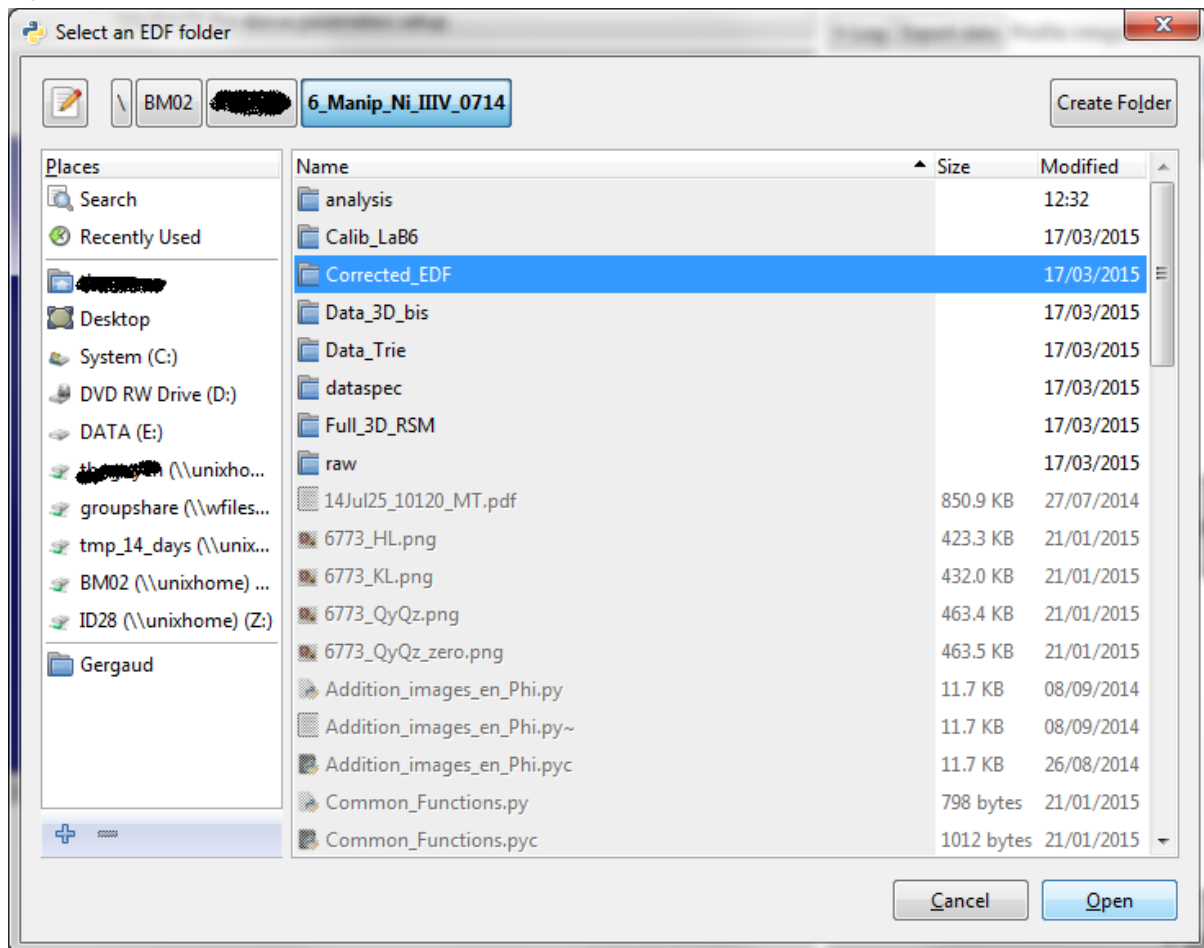
Choose the folder where all your data are stored. Click the folder to highlight it and click **Open**.

Please note that you have to name your data images as follow: prefix_imagenumber.edf

**For example: 12Jan15_0005.edf, SampleX_0125.edf.gz**

Please provide one underscore to separate the prefix and the image number. This will help so much for data management and data interaction with spec files.
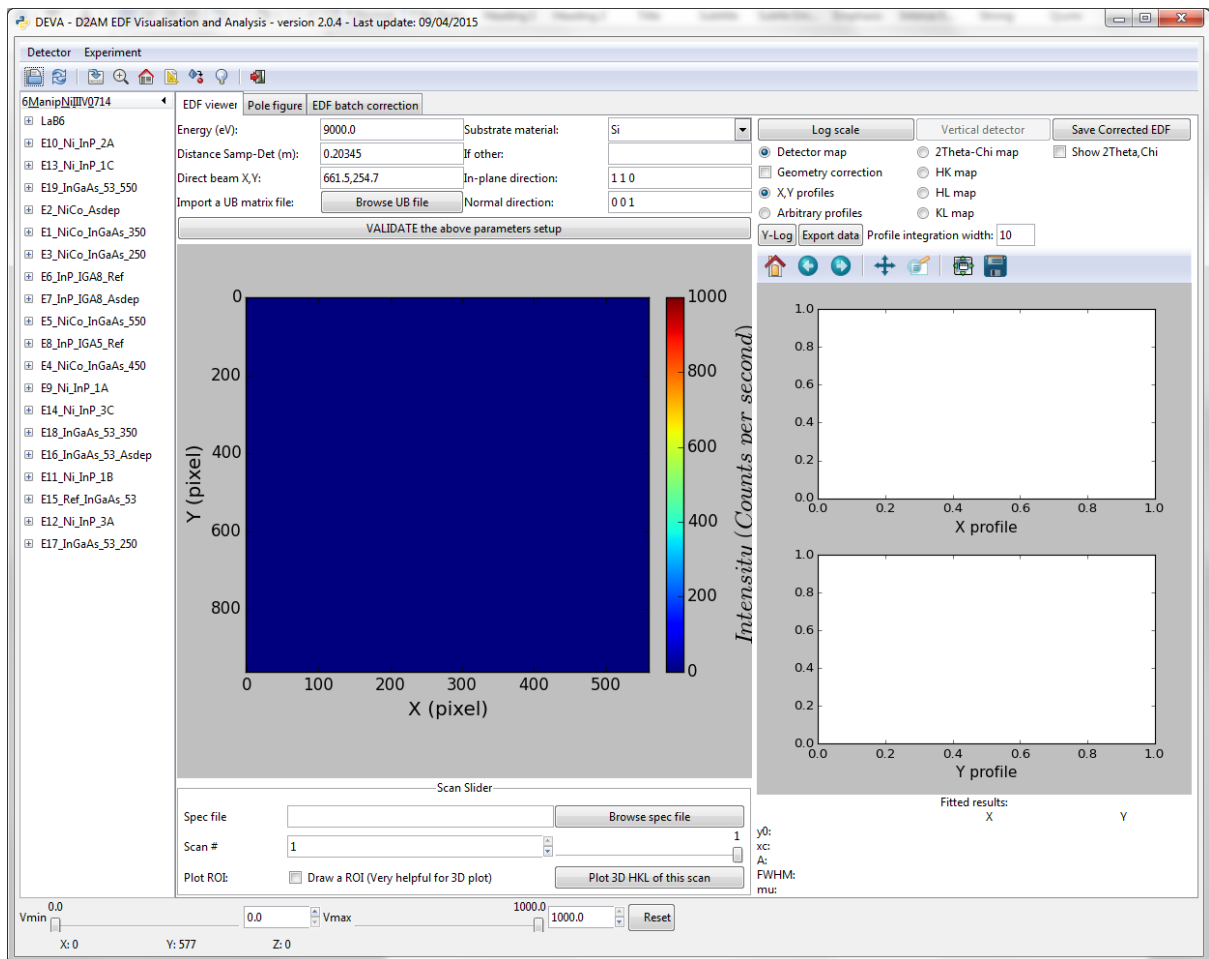
Note that you can reorder the data folder/data files by clicking on the Title of this small window. A small triangle on the right of the title means this field can be sorted.

6) Visualization of an image:

To view an image, just double click on the image name. In this example, I have chosen the image 14Jul25_12445.edf, then I clicked on the Graph's ratio button to change the image ratio.
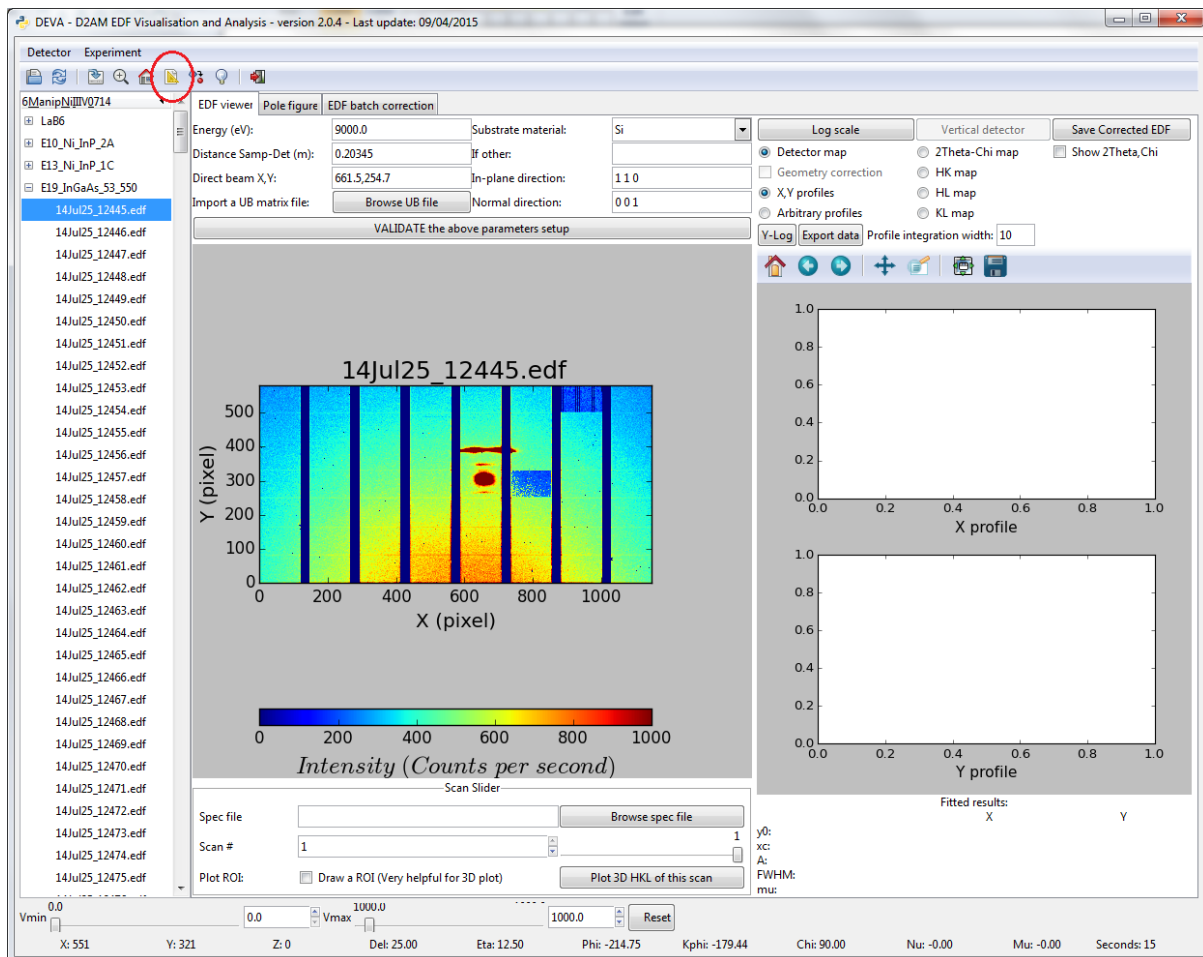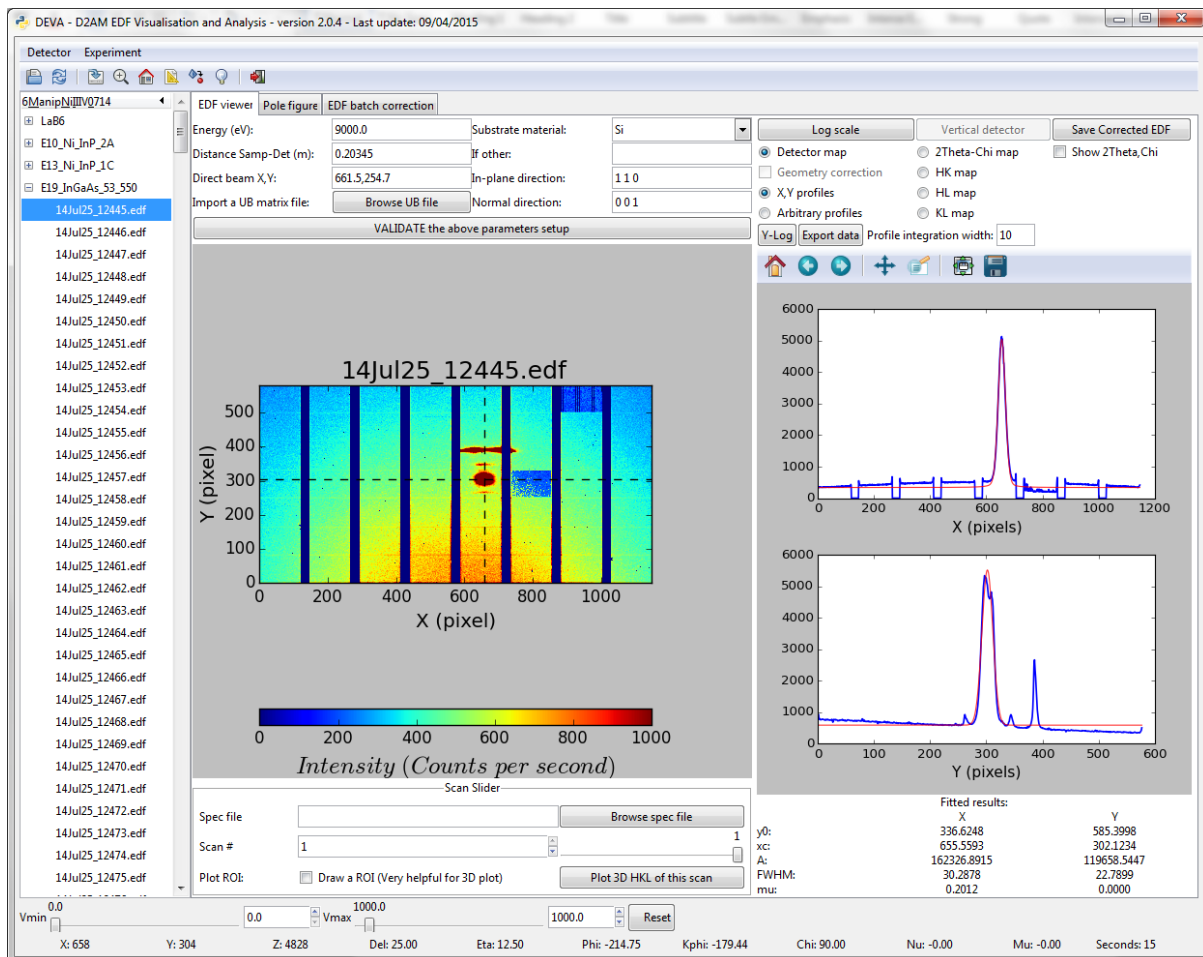
7) XY profiles and arbitrary profiles:

To extract the XY profile from the current image: **Right Click** on the position you want to extract. The X and Y profiles are plotted and fitted automatically using a Pseudo-Voigt function as shown below. The fitting parameters are also reported in the table underneath the profiles.

To clear out the cross line in the image: **Middle-Click**

Hint: in the profile graphs, we can measure the periodicity of the fringes if we have some periodic signal (like thickness fringes in epitaxial thin films). The steps to follow are:

++ **Right-Click** at the maxima/minima of the peaks to select the fringes

++ When selection done**: Left-Click** to plot the order of fringes as a function of fringes position. The slope of this plot tells us the period.

++ **Middle-Click** in the plot: make a Fast Fourier Transform of the profile.

An arbitrary profile can be extracted by firstly choosing the "**Arbitrary profile**" button (on the upper right window), then **Left-Click** on the two points which define the line that you want to extract.
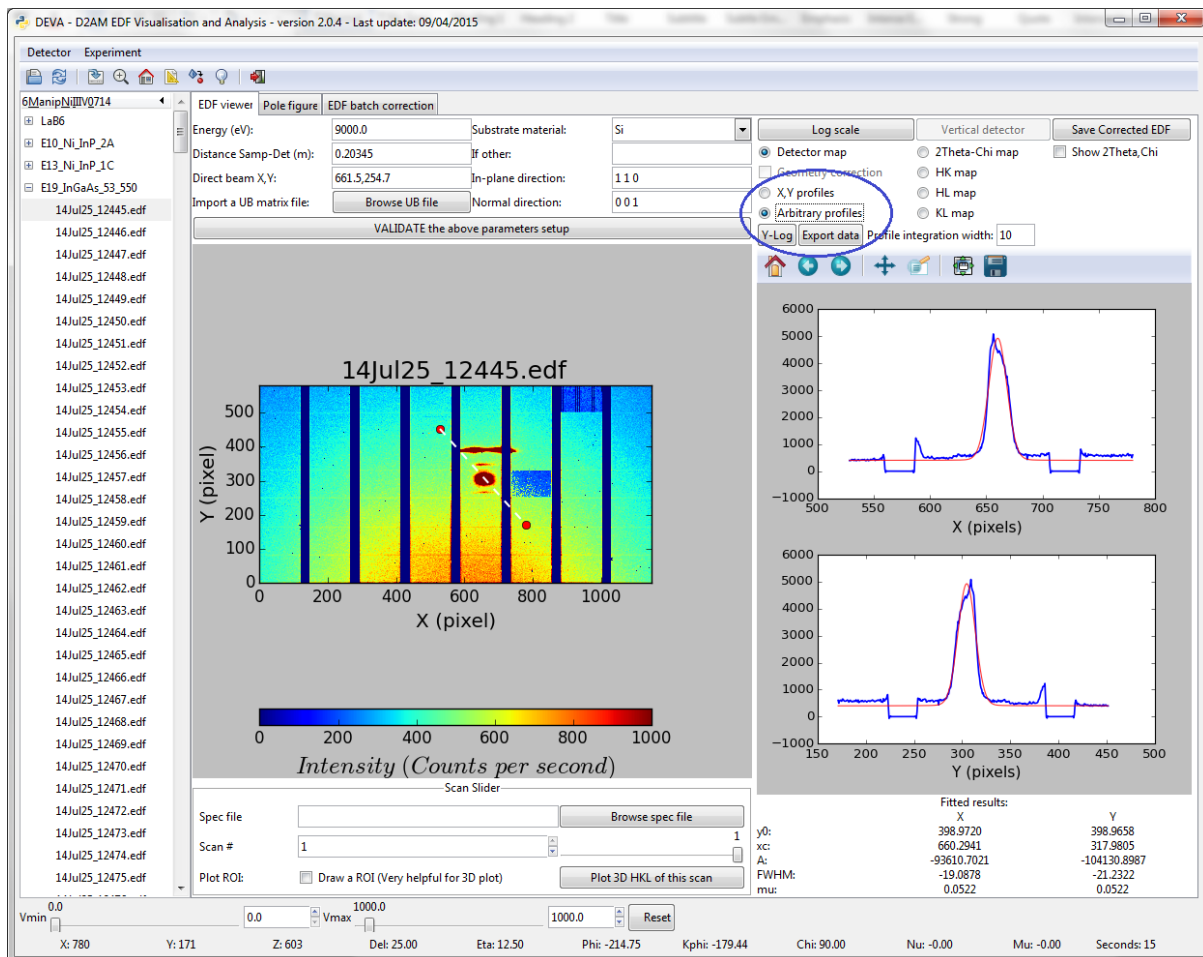
The profile scale can be switched to Log with the "**Y-Log**" button.

The "**Export data**" button is to export profile data to a text file.

The field "**Profile integration width**" can be adjusted to change the integration large of the profile. That means the number of pixels to be integrated when extracting a profile. This should be an even number (4, 6, 8, 10).
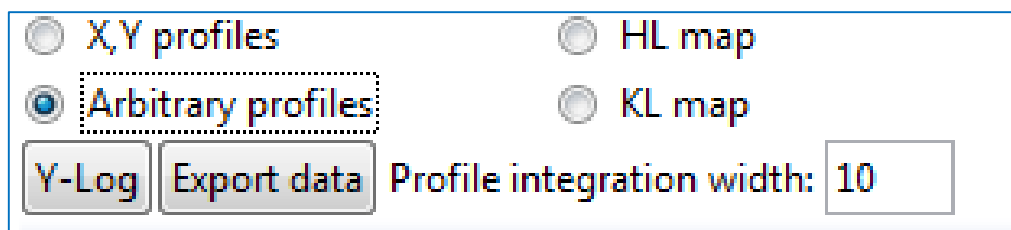
8) Coordinates transform (pixel to angular/reciprocal space)

Up to now we are working on the detector pixel coordinates. We can transform the detector coordinates into angular coordinates (2 theta, chi) or into reciprocal space coordinates. To do that, we have to provide the geometry information of the experiment, such as: X-ray energy (eV), sample to detector distance (m), direct beam position (X, Y position in pixel) when the detector and all of the motors are at zero. The first three fields are obligated to be filled. You can select the substrate and its orientation if you want, but this not obligated. If you want to use an orientation matrix UB, you can save the matrix in a text file (3 rows, 3 columns) and load it by clicking on the button "Browse UB file".

Finally, we have to click on the button "**VALIDATE the above parameters setup**" in order to take into account the experimental information. When we hit this button, all of these information will be saved to a text file "Geo_config.DEVA". This will be useful for your next run of the program. You don't need to re-enter the parameters, but you have to click on the **VALIDATE** button.

Now we can plot the image in the angular or reciprocal space. To see the plot, just click on the radio buttons: **2Theta-Chi map, HK map, HL map, KL map, Detector map**.

Note: The "**Show 2Theta, Chi**" button is useful when you want to know the 2Theta, Chi values of each pixel (when the image is in the detector coordinates):
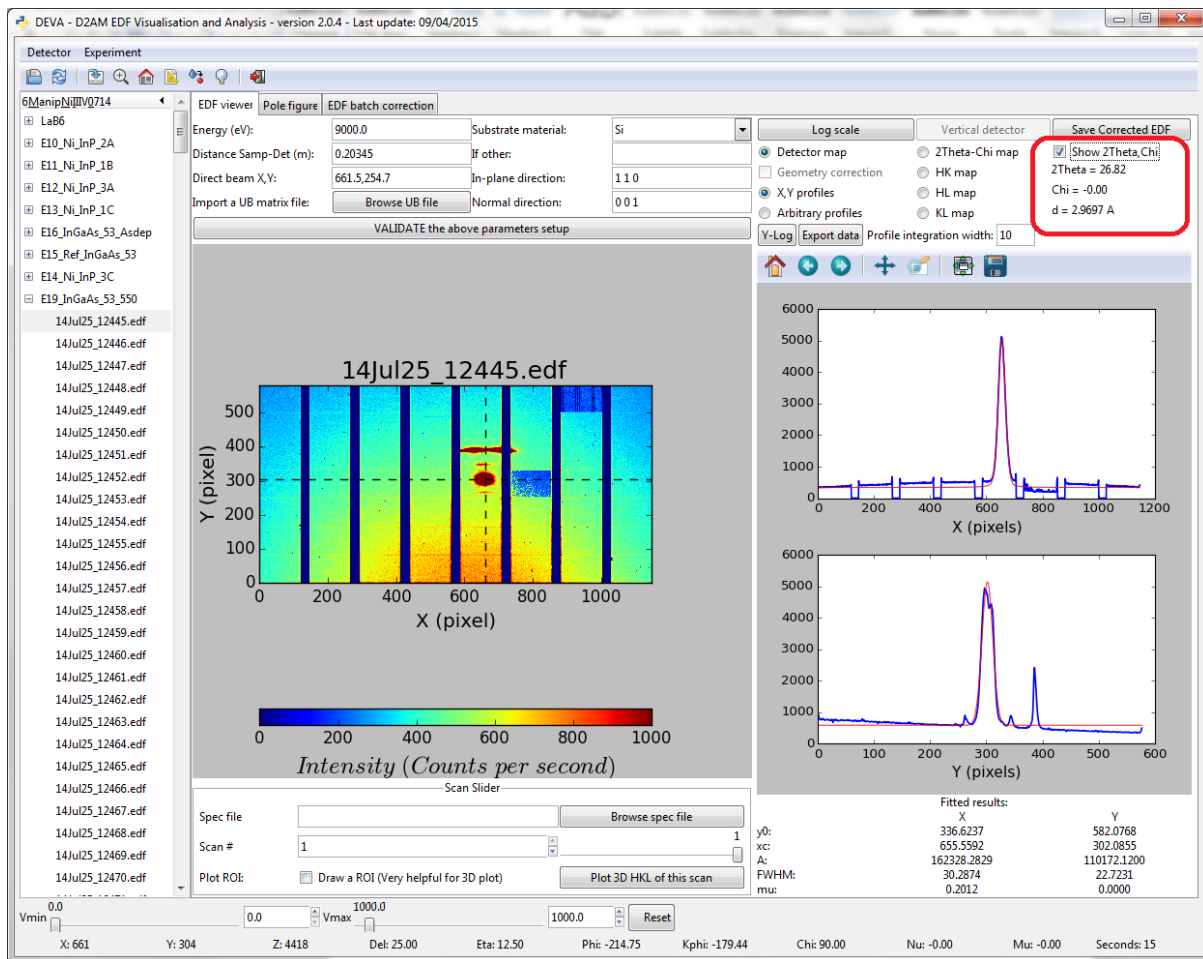
9) Scan Slider: access to SPEC file

The **Scan Slider** allows us to load a spec file (click on the "**Browse spec file**" button to select the spec file). The program will firstly explore all of data scans in the spec file, then it will find the right scan where your actual image is found. Every time you change the image, the program will re-find the scan corresponding. This scan number will be displayed in the "**Scan #**" field. The slider on the right allows the user to slide the data images in this scan. This is helpful if we want to quickly observe the data of this scan. You can check what happens in the console window.
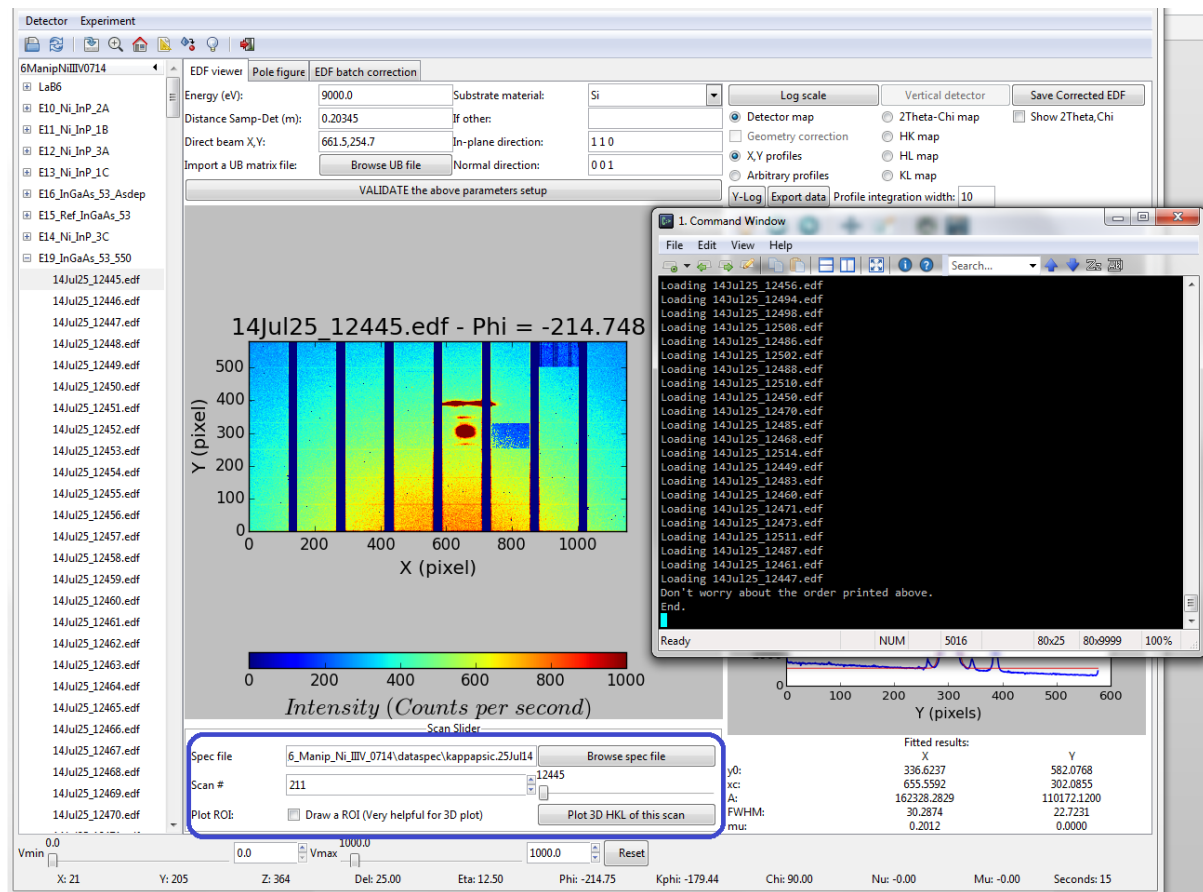
As you can see, all of data in this scan will be loaded to the memory for further use, such as sliding the data, 3D plotting, etc.

10)   Scan Slider: follow a ROI as a point detector

We can follow the evolution of the data in a specific zone (ROI – or Region Of Interest) during the scan. This can be done by checking the "**Draw a ROI**" button, then click and drag the mouse to draw a rectangular ROI. Finally slide the slider to plot the intensity v.s. scanning motor:

11
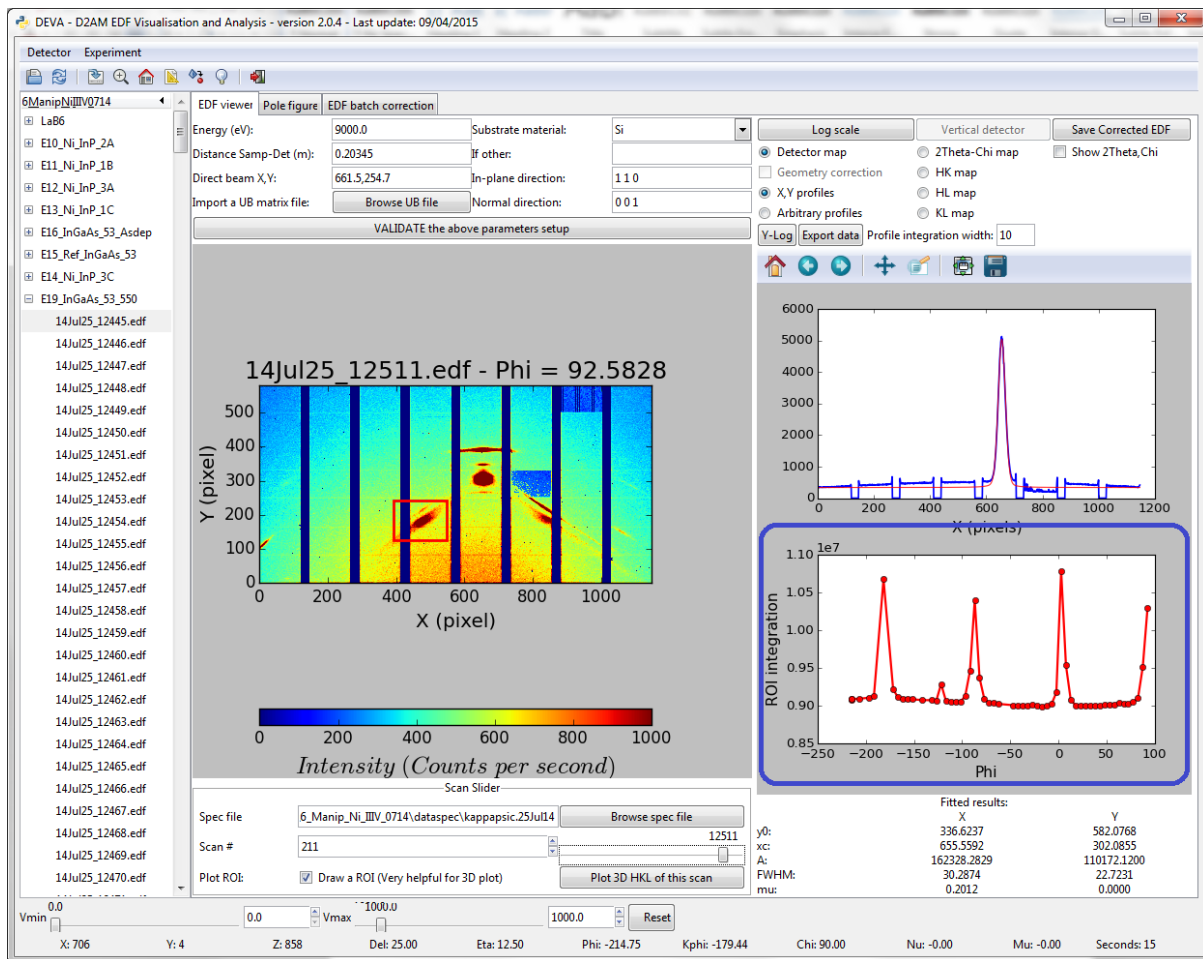
11) 3D plotting of the scan in the HKL space

Before plotting the 3D image, please make sure that you have VALIDATED the geometry information (See Section 8).

It is recommended to draw a ROI in which you want to plot the 3D image. This is very helpful for memory issues, because a big data matrix can halt the system.

After drawing a ROI on the image, click the "**Plot 3D HKL of this scan**" button to plot the 3D image. This image is plotted using mayavi.mlab library.
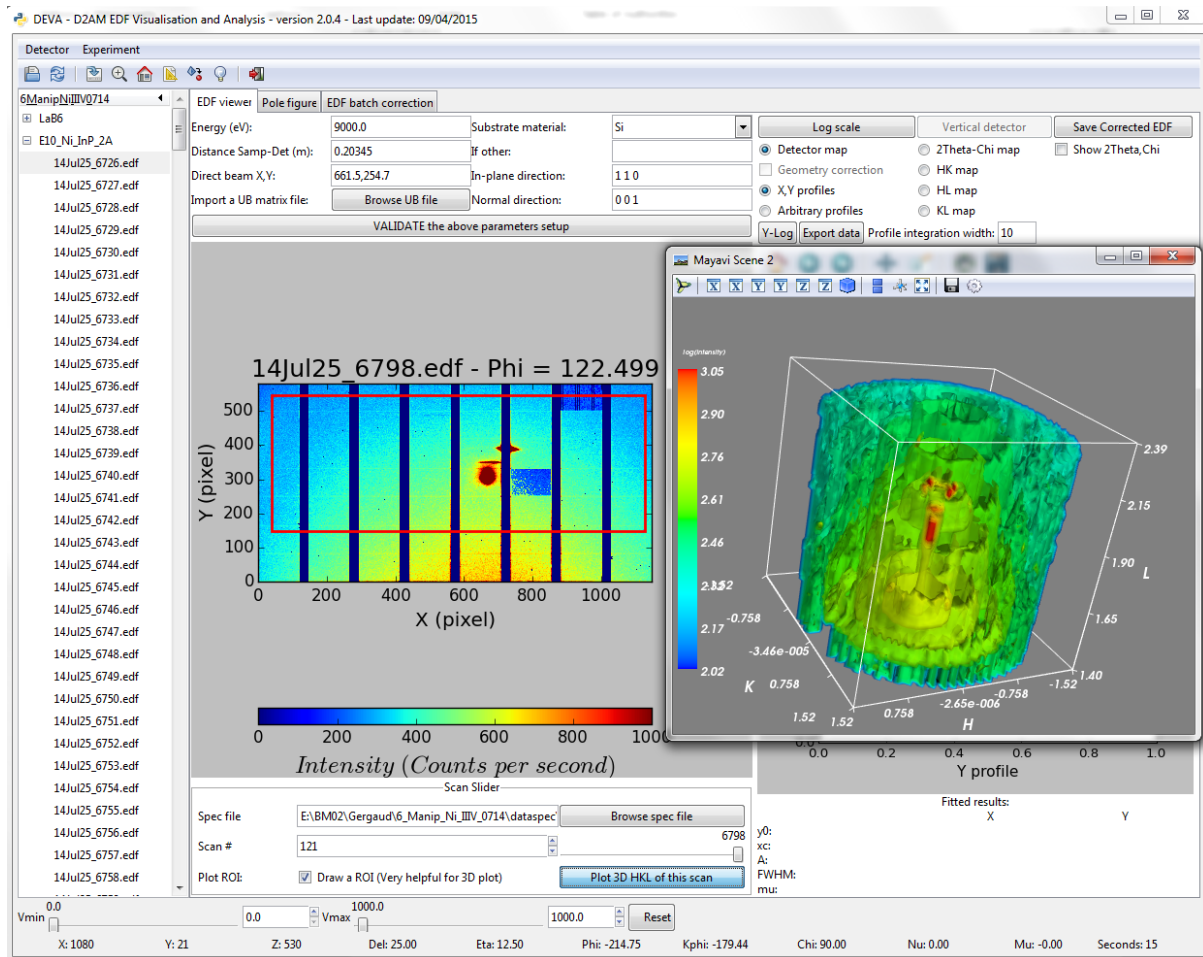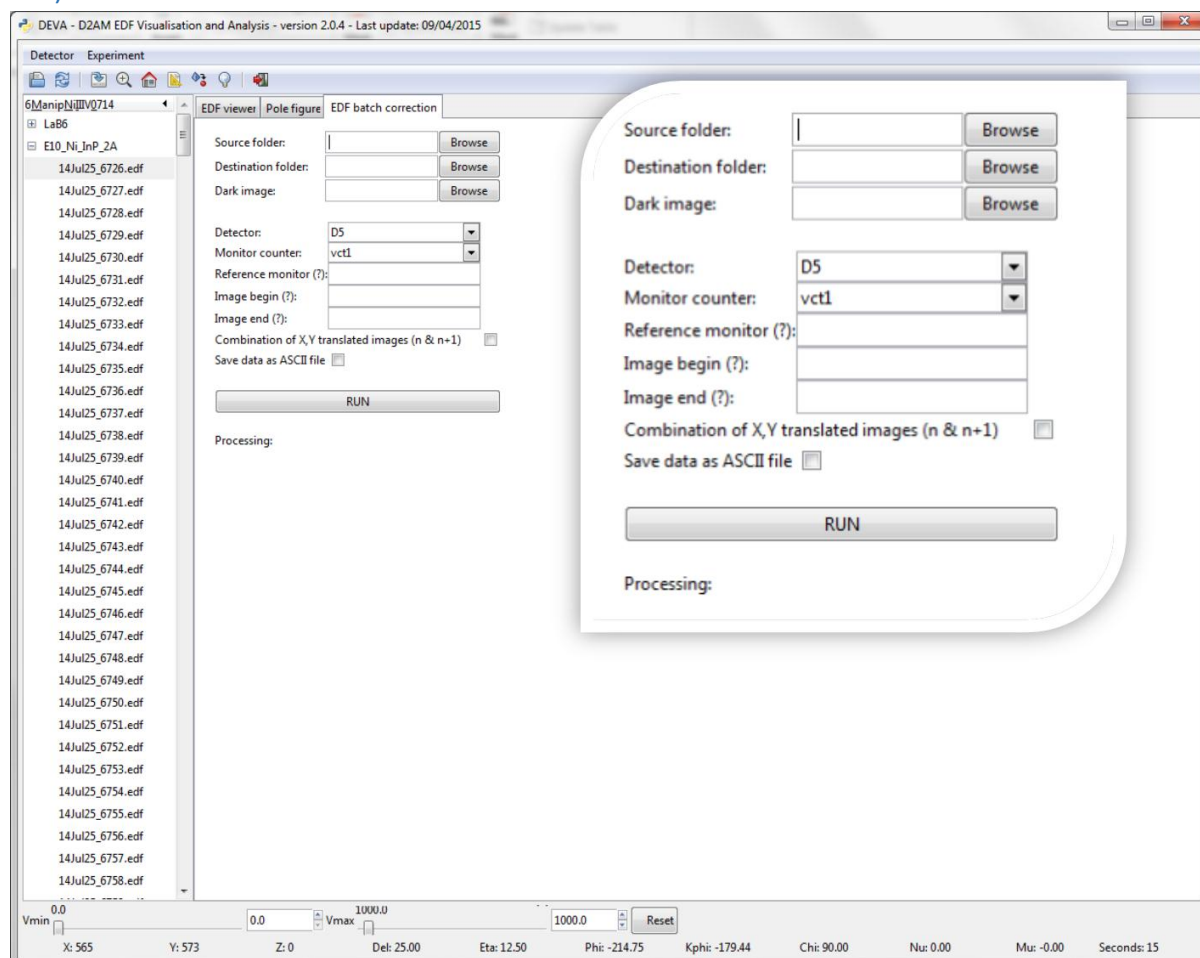
12) The Pole Figure tab

This tab is to plot the pole figures. A pole figure is plotted using an image range and a 2Theta value. The PHI motor can be Phi or Kphi (pseudo motor and real motor, respectively). Please make sure that you have VALIDATED the geometry parameters (see Section 8) before plotting the pole figures.
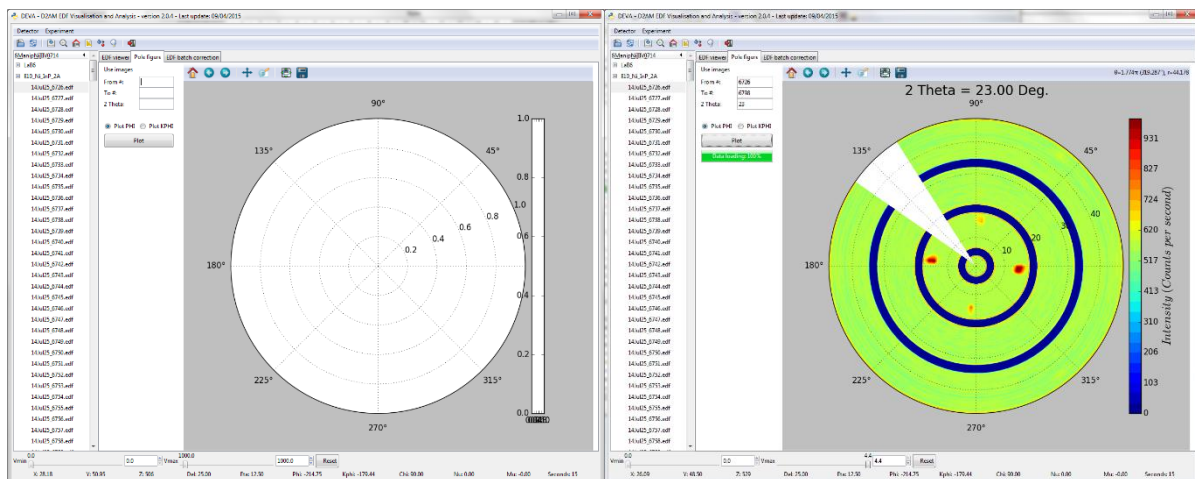
13) Batch correction

This Tab is used for batch corrections of raw data.

- **Source folder**: the folder where raw data are found
- **Destination folder**: the folder where the corrected data are stored
- **Dark image**: dark image for subtraction
- **Detector**: XPAD detector type (D1, D5, S70)

If the Detector is D1, the user has to specify the spec file, the direct beam center and the sample to detector distance. The correction of D1 detector is done using the program xpad3_geometry.py written by Jean-Francois Bérar.

- **Monitor counter**: the incident beam monitor counter name. This is served for data normalization.
- **Reference monitor**: The reference incident flux → for normalization.
- **Image begin, Image end**: the image numbers
- **Combination of X, Y translated images (n & n+1)**: as the XPAD detectors have large gaps between the modules, one might need to suppress these gaps by measuring 2 images at 2 X, Y position of the detector. These two images will be combined into one unique image where the gaps are suppressed.
- **Save data as ASCII file**: if the user is not familiar with EDF format, he/she can adapt text format for further data treatment. By checking this button, the corrected data will be saved as text files.
- Finally the **RUN** button starts the job.