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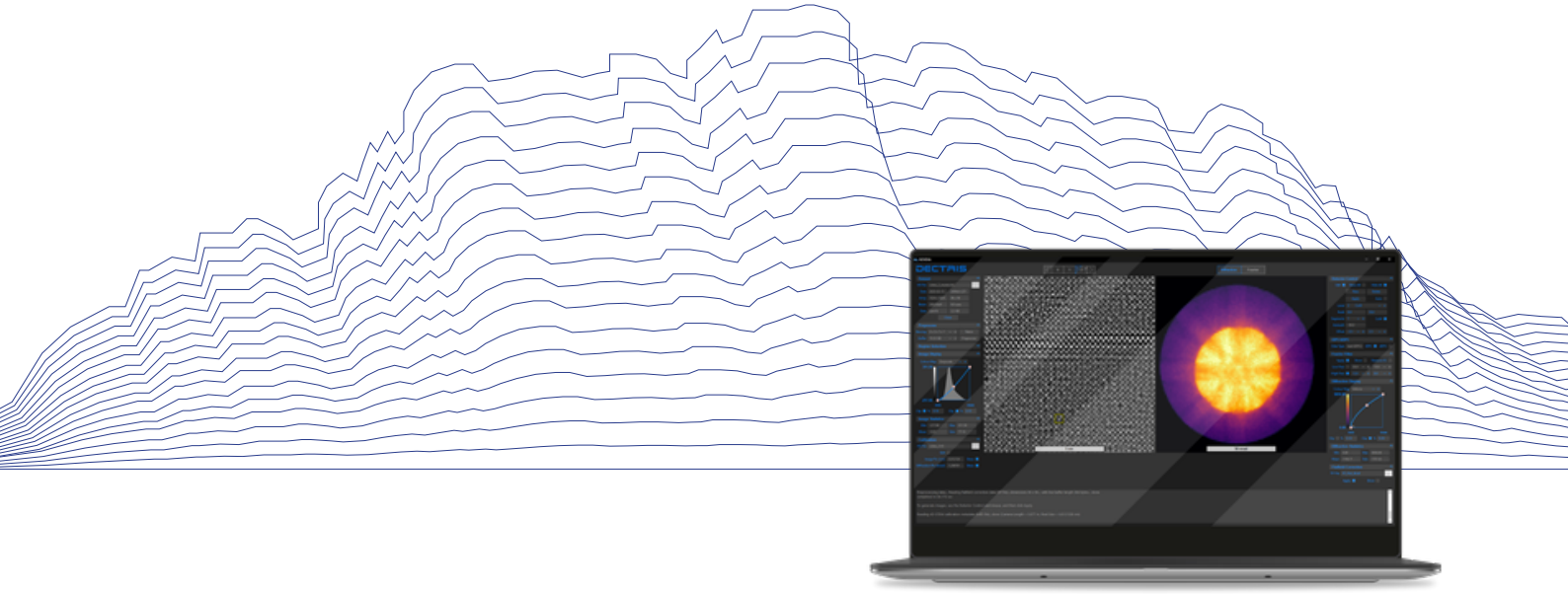

# User Manual
## DECTRIS NOVENA® Analyse


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# CONTENT

# 1. GENERAL INFORMATION

## 1.1. Contact and Support


| | | | |
|---|---|---|---|
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Should you have questions concerning the system or its use, please contact us via telephone, e-mail or fax.

## 1.2. Explanation of Symbols

### 1.2.1. Symbols in the Manual

| Information | #0 |
|---|---|
| Information blocks are used to highlight important information. | |

# 2. INTRODUCTION TO NOVENA ANALYSE

## 2.1. Overview

NOVENA Analyse is designed to efficiently visualize and analyze 4D Scanning Transmission Electron Microscopy (STEM) datasets from DECTRIS detectors. The functionality includes:

- Simultaneous view of image and diffraction space
- Virtual STEM image calculation and visualization
- Center-of-mass (CoM) image calculation and visualization

## 2.2. System Requirements

**Table 2.1:** System Requirements

| | |
|---|---|
| Operating System | Windows 10 / 11 (x64) |
| Processor | Intel Core i5 or equivalent (i7 and higher recommended) |
| Memory | 16 GB RAM (32 GB or more recommended) |
| Data Storage | SSD drive (internal[1]) |
| Monitor | Large monitor |
| Input | Keyboard and Mouse (2 buttons and wheel[2]) |

## 2.3. Installation instructions

NOVENA Analyse is provided as a standalone executeable and therefore, no installation is required. To run the software we recommend the following procedure:

- Download and install Microsoft Visual C++ Redistributable 2015-2022 (x64) (if not done already)
- Unzip the zip file and save the executable (.exe) in a convenient location on your computer which can be accessed by all relevant users
- Double-click the executable to run NOVENA Analyse
- Right-click on the software icon on the Windows taskbar and select “pin to taskbar” for easy future access (optional)

**Information** #1

If you cannot execute the file the most likely reason is:

- Windows “trust” issue: Windows needs to trust the software executable in order to run it
- Missing DLL files: Re-install Microsoft Visual C++ Redistributable 2015-2022 (x64)

You may need to adjust your computer display setting to produce a good compromise between the workspace area and the readability of the controls. Typically, a good value is between “100%” and “150%”, with smaller

1 use of external hard drives for reading and writing data can be very slow
2 touchpad is also supported

sizes being appropriate for smaller monitors. Note, that it will be necessary to close and reopen the software each time when the display setting is changed. Ultimately, the layout should appear similar to that shown in figure 2.1.

## 2.4. User Interface

The user interface of NOVENA Analyse before any dataset is imported is shown in figure 2.1. Real space is on the left, and the controls on the left generally referring to that space. Similarly diffraction space and its controls are on the right. Both spaces can be panned by holding down the left mouse button. Both spaces can be zoomed using the mouse wheel (or touchpad double stroke). A right-click on one of the spaces will open a menu where you can enable to show pixel values (entry `Show Values`). If this is enabled individual pixel values will be displayed when zoomed in the dataset. Real space and diffraction space each have their own contrast settings and colour map. The lower grey panel within the software window supplies basic instructions.

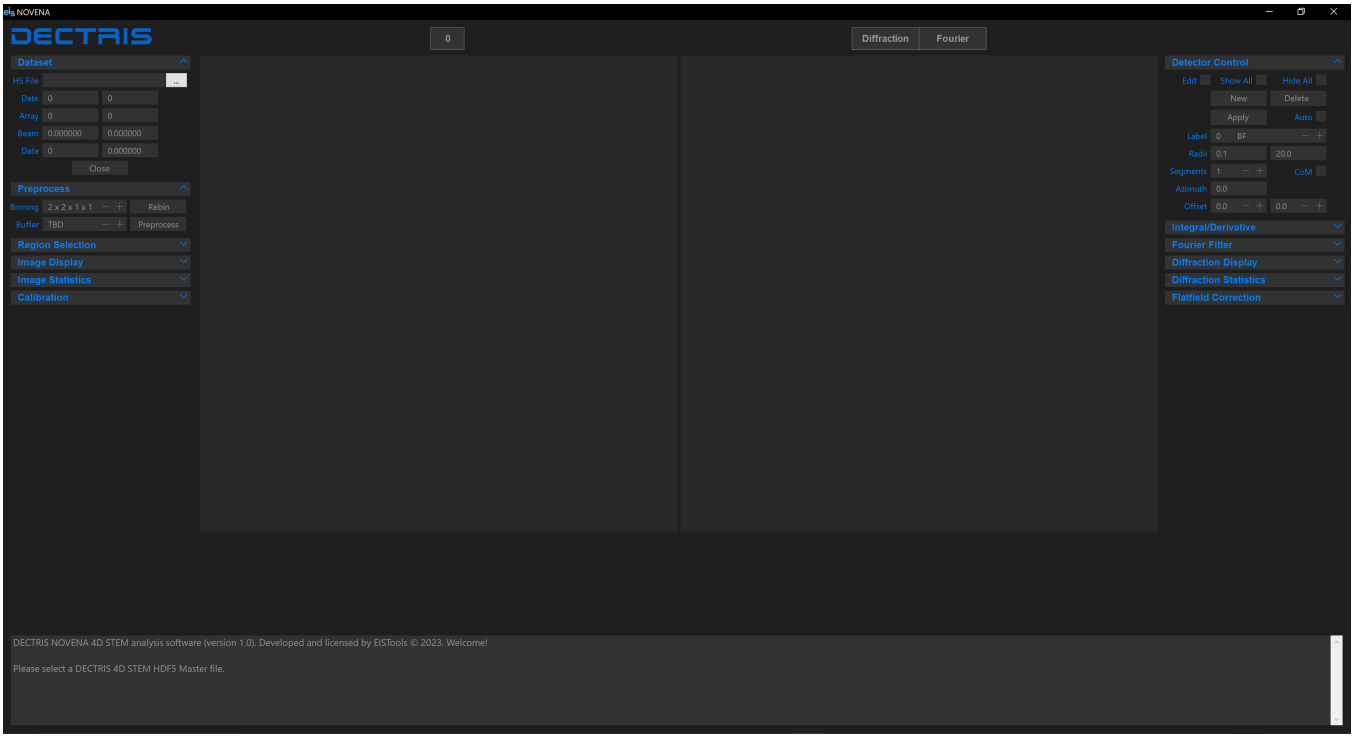


**Figure 2.1:** The NOVENA Analyse 4D STEM software (before data loading).

## 2.5. Memory usage versus speed

NOVENA Analyse is designed to save memory, and it does so at some cost of speed (typically, there is always a sacrifice between memory used and speed). Depending on your computer, certain image processing operations can take 5–10 seconds. Those processes are generally ones where a large number of pixels are selected. Note that certain options, such as interpolation and displaying pixel values, can sometime cause a noticeable slowing of the diffraction display refresh rate.

## 2.6. Coordinate system used

The Cartesian coordinate systems used for real space and diffraction space are extitleft-handed systems in which the $x$ axis points to the right and the $y$ axis points extitdownwards. This system is arguably most consistent with the raster motion of the STEM probe used to collect 4D STEM data. Likewise the Argand (complex number) plane relevant to the calculation of complex images (calculated using segmented or CoM detectors) has the real part increasing to the right and the imaginary part increasing extitdownwards (and thus the complex phase angle increases from the real axis in a extitclockwise sense). Notwithstanding this, in the case of complex images, an overall minus sign is applied to the image at the final calculation step (which compensates for the negative charge of the beam electrons and produces an image representing the diverging transverse electric field in the case of atomic columns).

# 3. GENERAL USAGE OF NOVENA ANALYSE

## 3.1. Open 4D STEM Dataset

### Files in a 4D STEM Dataset

DECTRIS 4D STEM datasets are made up of HDF5 (*.h5) and TIFF (*.tif) files:

- Master file containing detector-specific and dataset-specific metadata

  `*_master.h5`

- Multiple data files containing the image data chunks, named

  `*_000001.h5, *_000002.h5, ....`

- Optional file containing flatfield correction data

  `FF*.tif`

- Optional file containing 4D STEM calibration data

  `*.h5`

### Open Master File

Under Dataset (top left), use the filepicker tool to select an HDF5 _master file. The loading process usually takes 5–10 seconds. (Note that reading from an external drive can be up to 10 times slower, even if it is a solid-state drive.) Once the 4D STEM HDF5 data is loaded, the text fields under Dataset will display some details, the diffraction pattern corresponding to the center pixel of real space is shown, and the real space image will remain blank. At this point it is possible to select and view diffraction data (see below).

### Selecting/Viewing Diffraction Data

Use the keyboard and mouse within the (possibly blank) real space image to view diffraction data from any desired position. Rick-click on real space allows to change the size of the selected region, and right-click again fixes the region size. (Right-click also shows a little menu, but just move the mouse away from it and it will disappear). The selected region can be controlled precisely with the Region Selection controls, or by zooming in on real space using the mouse wheel (or touchpad double stroke).

### Preprocessing the Data

Before preprocessing the data (see next paragraph), you can optionally rebin the dataset to reduce its size. This is especially useful for larger datasets, as it makes the speed of operators faster. There are three rebinning options: $2\times2\times1\times1$, $1\times1\times2\times2$ and $2\times2\times2\times2$, corresponding, respectively, to rebinning real space, rebinning diffraction space, and rebinning both spaces. There are also three further rebinning options, which are similar to those mentioned but are marked `2*bd`. These options double the bit depth of 8-bit and 16-bit data, and they should be used only when it is suspected that rebinning will cause numerical overflow. If used, 8-bit data is rebinned at 16-bit, and 16-bit data is rebinned at 32-bit (note that currently the bit depth of 32-bit data cannot be increased). To rebin the data, select the desired Binning and then click Rebin. Note that rebinning is optional, but if it is desired it must be performed before the preprocessing step.
A data preprocessing step is required before you can generate images. Preprocessing requires a memory buffer. Under Preprocessing, the Buffer Size can be selected, or you can simply use the initial (default) setting. Once you have chosen the Buffer Size, click Preprocess to begin the process. It typically takes 30–60 seconds (example benchmarks are shown in section 4.1). It is possible to continue selecting/viewing the diffraction data while preprocessing takes place (only the speed will be slowed).
After the dataset is processed, images can be generated as shown in figure 3.1. How to generate images is described from section 3.3.1 onwards.

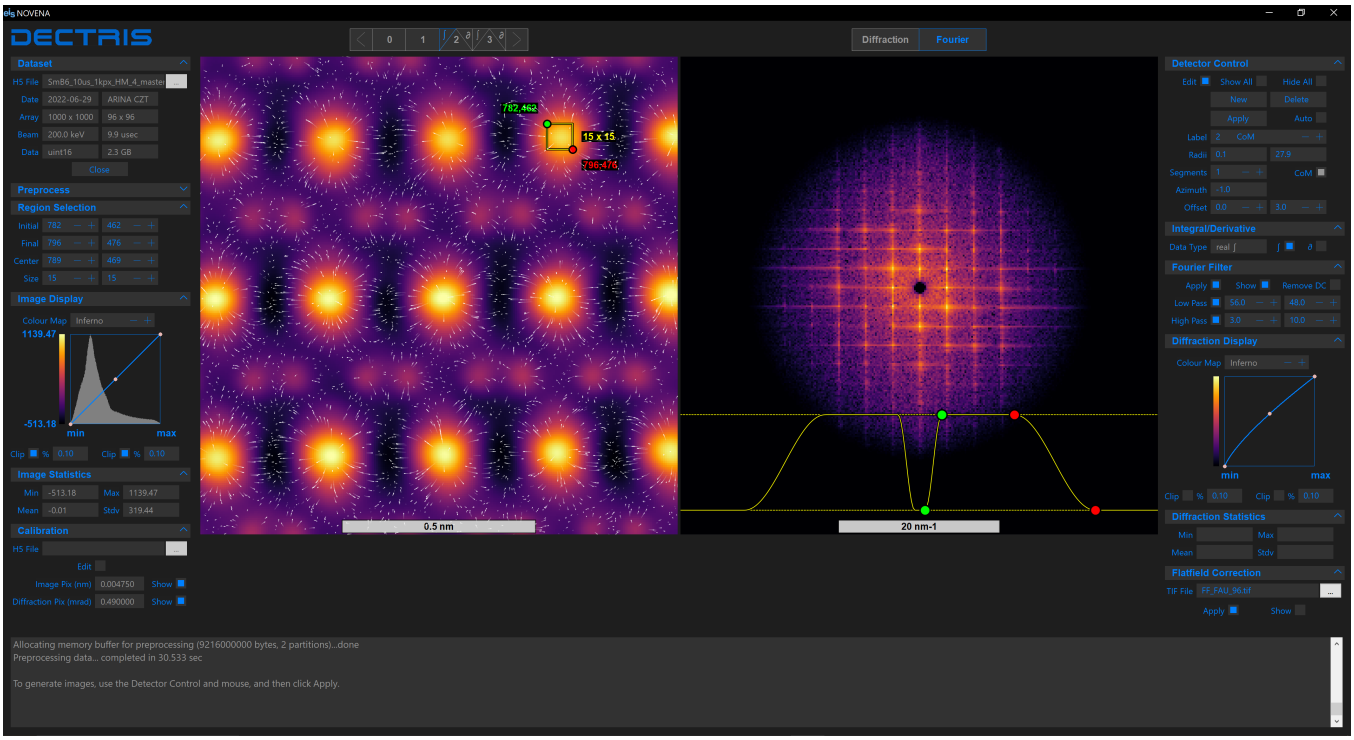


**Figure 3.1:** NOVENA Analyse 4D STEM software with data loaded.

## 3.2. Calibration

Data needed to calibrate the length scale of real space and the angular scale of diffraction space are contained in the HDF5 calibration file. Under Calibration, select Edit and then use the filepicker tool to select the appropriate file (one that matches the dataset). Deselect Edit to protect the calibration data read from the file. If no calibration file is available, or if the data in the calibration file appears invalid, then calibration can be performed manually with the aid of the calibration tools. To use the tools, under Calibration select Edit. The calibration tools will appear in real space and diffraction space. Use the tools to measure the length in pixels of a known feature such as an atomic spacing in real space or the diameter of the central disk in diffraction space. For real space, use the measurement to calculate the pixel size in nm (i.e., the known length in nm divided by the measured length in pixels) and enter the value into the appropriate field under Calibration. For diffraction space, the operation is similar except that the units are mrad. Deselect `Edit` to protect the calibration data.
Once the correct calibration data is loaded or entered, click Show to display the corresponding scale bars. Exported SVG images will contain these scale bars. How to export images is described in section 3.6.

## 3.3. Generating Virtual Images

Under Detector Control, select Edit and use the mouse and/or controls (Radii, Offset, etc.) to configure a virtual detector. Then click Apply to generate the corresponding image. A double-click on diffraction space will set the detector Offset to that position. Grabbing the "top half" of a detector allows you to move it, while grabbing the "bottom half" allows you to resize it. If you make further changes to a virtual detector, then you should click Apply again to update the corresponding image.
Click New to add a new detector. Up to 10 virtual detectors (and their corresponding images) are possible. Detectors can be given a name for convenience. Clicking `Delete` will remove the detector and its corresponding image. Deselecting Edit will protect the detector settings.

### 3.3.1. Virtual BF, DF, ABF and ADF

If a virtual detector has just one (1) Segments and is not a CoM type, then the corresponding image data type is "real." This applies to bright-field (BF), dark-field (DF), annular BF (ABF), and annular DF (ADF) detectors/images. For BF or DF, set the inner radius to $\leq 0.5$ (treated as zero). For ABF or ADF, use an inner radius greater than 0.5 and the outer radius must always be greater than the inner radius. It is possible to set the radii to be larger than the diffraction space by using the Radii control. A pixel in diffraction space contributes to the corresponding image only if the extitcenter of the pixel is included by the virtual detector. Note that, in addition to being "real", BF, DF, ABF and ADF images are always positive (or possibly zero) because they are generated by summing intensities in diffraction space.

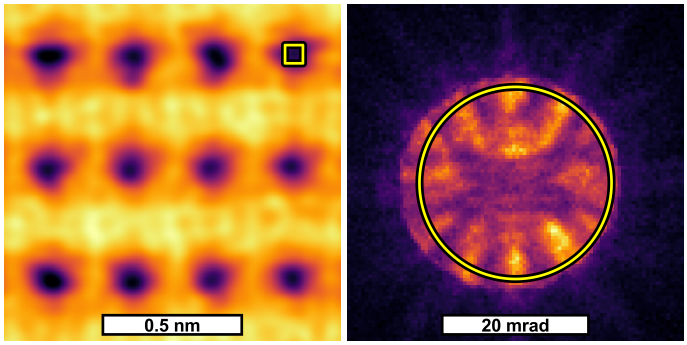


**Figure 3.2:** BF image of $[110]$ $SmB_6$ (left) with selected diffraction data and corresponding virtual detector (right).

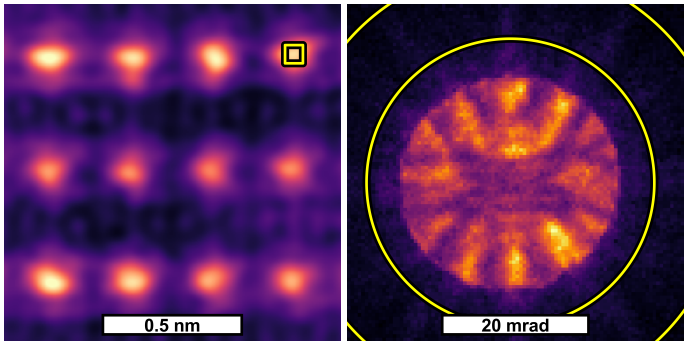


**Figure 3.3:** ADF image of $[110]$ $SmB_6$ (left) with selected diffraction data and corresponding virtual detector (right).

### 3.3.2. Complex (CoM/DPC-type) Images

If a virtual detector is a CoM type or it has two or more Segments, then the corresponding image data type is "complex." This applies to differential phase-contrast (DPC) images and center-of-mass (CoM) images. For a segmented detector, during image generation, a phase angle (in the sense of a complex number) is associated with each detector segment according to the angular position of the segment's midpoint. This produces a

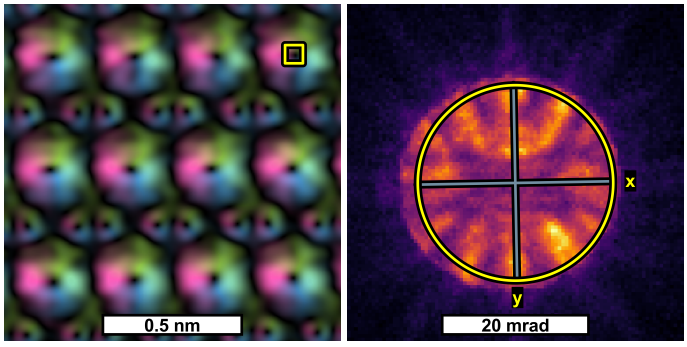


**Figure 3.4:** CoM image of $[110]$ $SmB_6$ (left) with selected diffraction data and corresponding virtual detector (right).

complex-valued image (where the value of every pixel is a complex number). A complex-valued image can also be regarded as a 2D vector-valued image (where the complex phase gives the direction of the vector and the complex modulus gives the magnitude of the vector). For a CoM detector, a 2D vector is associated with every pixel in diffraction space, where the vector points from the center of the detector to the given pixel. This produces a 2D vector-valued image (or complex-valued image).
For non-magnetic samples, under favorable experimental conditions, the 2D vector/complex number at each image pixel is proportional to the 2D (projected) electric field of the sample convoluted with the STEM probe's intensity distribution. Note that an overall minus sign is applied to complex images at the final calculation step, which compensates for the negative charge of the beam electrons and produces an image representing the diverging transverse electric field in the case of atomic columns. In the case of magnetic samples, under favorable experimental conditions, and for samples of sufficient uniformity, the 2D vector/complex number at each image pixel is proportional to the 2D (projected) magnetic field convoluted with the STEM probe's intensity distribution.
In order for a complex image to represent the sample's electric or magnetic field, it is vital that the virtual detector is rotated using the Azimuth control to achieve rotational alignment of the image and diffraction spaces. (Note that the data does not appear rotated in the software, rather the virtual detector is rotated.) Generally, this requires some a priori information about the sample's electric/magnetic field. For example, for electric fields, and for atomically-resolved data, the rotational alignment can be checked in two ways: (1) If the atomic columns are well resolved, then it is possible to adjust the Azimuth such that the diffracted intensity "moves to the opposite side" of an atomic column, in the sense described in figure 3.5. (2) When rotational alignment is achieved, the phases of the complex values in the vicinity of an atomic column will coincide with the appearance of the phase color wheel in the Image Display panel. For magnetic fields circulating in the $x$-$y$ plane of the sample, the phases of the complex values will appear rotated by 90 degrees relative to the phase color wheel.

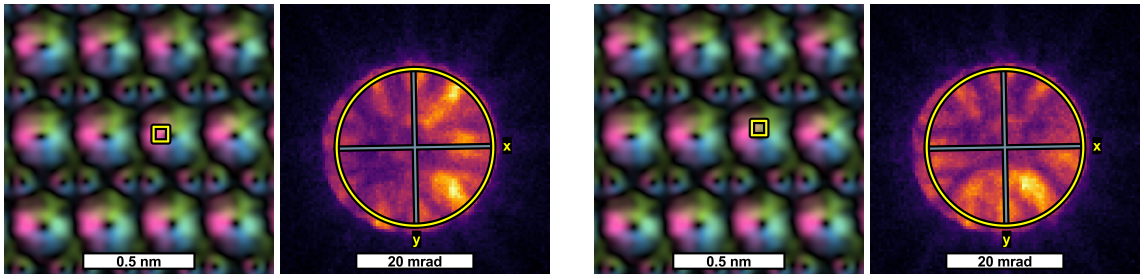


**Figure 3.5:** The CoM detector has been rotated such that the diffraction pattern from a small region displaced in the image $-x$ direction (relative to an atomic column center) exhibits intensity shifted in the virtual detector's $+x$ direction. Analogously, a region displaced along image $-y$ will give diffracted intensity shifted along the virtual detector's $+y$. Note that in this example, the required rotation of the virtual detector was only 1°.

### Integrated and Differentiated Images

In the case of complex images, that is, DPC and CoM images, an integration or differentiation (divergence) operation can be performed. To generate such an image, begin with a complex image, and then under Integral/Derivative select either "$\int$" or "$\partial$". Integrated and differentiated images are real-valued, but unlike BF, DF, ABF and ADF images, they contain negative pixel values. Moreover, they often require Fourier filtering to obtain good results (see below).
For non-magnetic samples, under Detector Control select "E". Then, with the Azimuth set correctly (see above), under favorable experimental conditions, the pixel values in an Integrated image are proportional to the (projected) electrostatic potential of the sample (convoluted with the STEM probe intensity distribution). Similarly, under favorable experimental conditions, the pixel values in a Differentiated image are proportional to the (projected) electrostatic charge density of the sample (convoluted with the STEM probe intensity distribution).
For magnetic samples, under Detector Control select "B". Then, under the requirements stated above, the pixel values in an Integrated image are proportional to the (projected) $z$ component of the magnetic vector potential, and those in a Differentiated image are proportional the $z$ component of the current.

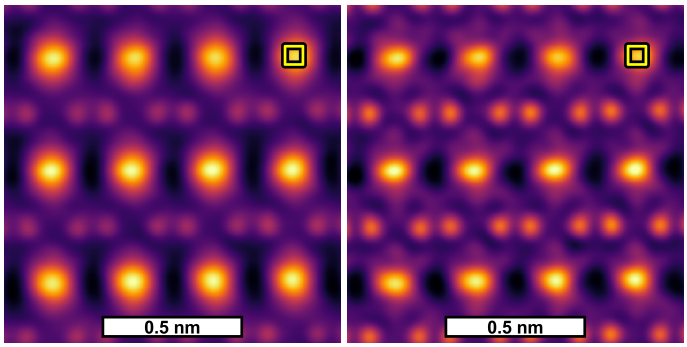


**Figure 3.6:** Integrated (left) and Differentiated (right) images of [110] $SmB_6$, both derived from the CoM image in figure 3.4, and with Fourier filtering applied.

## 3.4. Fourier Filtering

Fourier filtering can be applied to any image via the Fourier Filter controls. Each image has its own filter (which must be set appropriately by the user). Select View to view the Fourier transform of the current image, then select Apply to view (and apply) the filter. The filter is configured using the High Pass and Low Pass controls. Remove DC sets the pixel at the origin of Fourier space to zero (its effect can be seen directly only in the case of complex images).
Fourier filtering should always be done with care as overuse will introduce artifacts. Low Pass filtering can be an excellent way of removing "counting noise" and "scan noise". High Pass filtering can be useful in removing "slowly varying" components of an image. Integrated images often contain exaggerated low spatial frequency components, and so they usually benefit from High Pass filtering. Similarly, Differentiated images contain exaggerated high spatial frequency noise, and so Low Pass filtering is almost always required.

## 3.5. Flatfield Correction

When a 4D STEM dataset is loaded (by choosing an HDF5 master file, section 3.1), the software attempts to find the corresponding flatfield correction TIFF file in the same directory as the master file. If the file is not found, or if the data size in the file does not match the 4D STEM dataset, a warning is given and the software will default to reading a flatfield correction from the HDF5 master file, which, however, is likely to be extitinvalid. Therefore, if the flatfield correction TIFF is not found, you should find an appropriate file manually using the filepicker under Flatfield Correction.
The flatfield correction is necessary to make the 4D STEM data quantitatively valid. Hence, for quantitative accuracy, the valid flatfield correction should always be applied by selecting Apply (the default). To judge the validity of the flatfield correction, you can compare the diffraction data with and without Apply selected. The flatfield correction itself can be viewed by selecting View. For an explanation of the use of flatfields with DECTRIS detectors, refer to the user manual of our electron microscopy detectors [1].

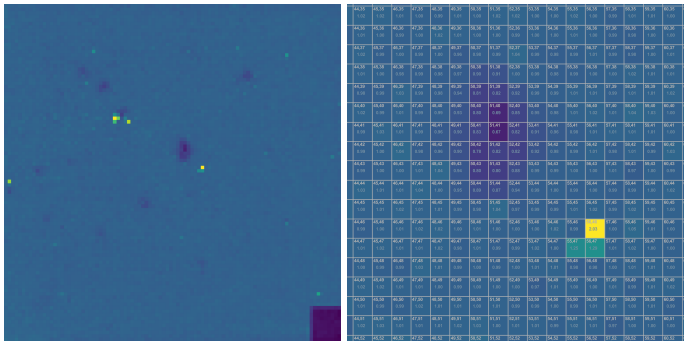

**Figure 3.7:** Example of a $96 \times 96$ flatfield correction (left), and a magnified view of center region showing pixel values.

[1] https://www.dectris.com/dectris-support/detector-manuals/electron-detectors/

## 3.6. Exporting Images

On real space or diffraction space, right-click, choose Export Image, and choose an appropriate filename. The software will save a set of images:

- a TIFF containing the entire image/diffraction pattern
- a binary file containing the entire image/diffraction pattern
- an SVG file containing the current view of the image/diffraction pattern with complete annotation
- an SVG file containing the current view with selected annotation drawn with thicker lines and larger fonts appropriate for publication

SVG files of the latter type were used to create the above figure 3.2–figure 3.6. Note that it is possible to edit all of the font/line sizes and font/line colours in an SVG file using a program such as Inkscape or even most web browsers.

## 3.7. Closing Datasets

Under Dataset, click Close.

| Information | #2 |
|---|---|

The active dataset has to be closed before a new dataset can be loaded.

## 3.8. Exiting NOVENA Analyse

Under Dataset, click Close (if a dataset is open). Then click X at top-right.

# 4. APPENDIX

## 4.1. Benchmark Example

**Table 4.1:** Benchmark System Hardware Configuration

| | |
|---|---|
| Operating System | Windows 10 Pro |
| Processor | i7-10750H CPU @ 2.60GHz, 6 Cores, 12 Logical Processors |
| Memory | 32 GB RAM |
| Data Storage | 1 TB Toshiba KXG6AZNV1TO2 SSD |

**$SmB_6$ Dataset**

- Scan size: 1000 x 1000
- Frame size: 96 x 96 @ uint16
- File size (hdf5, compressed): 2.3 GB
- File size (uncompressed): 18.4 GB
- Data load time: 3.3 s

**Table 4.2:** Preprocess times $SmB_6$ dataset

| Buffer size | Time |
|---|---|
| 1.15 GB | 66.3 s |
| 1.54 GB | 55.0 s |
| 2.30 GB | 43.7 s |
| 3.07 GB | 39.0 s |
| 4.61 GB | 34.4 s |
| 6.14 GB | 31.2 s |
| 9.22 GB | 29.5 s (fastest) |
| 18.43 GB | 42.7 s |

**BTO Dataset**

- Scan size: 1024 x 1024
- Frame size: 96 x 96 @ uint16
- File size (hdf5, compressed): 2.2 GB
- File size (uncompressed): 19.3 GB
- Data load time: 4.1 s

**Table 4.3:** Preprocess times BTO dataset

| Buffer size | Time |
|---|---|
| 1.61 GB | 92.3 s |
| 2.42 GB | 66.8 s |
| 3.22 GB | 51.3 s |
| 4.83 GB | 45.4 s (fastest) |
| 6.44 GB | 56.8 s |
| 9.66 GB | 68.5 s |
| 19.33 GB | 84.0 s |

### STO Dataset

- Scan size: 1000 x 1000
- Frame size: 96 x 96 @ uint32
- File size (hdf5, compressed): 0.7 GB
- File size (uncompressed): 36.8 GB
- Data load time: 2.9 s

**Table 4.4:** Preprocess times STO dataset

| Buffer size | Time |
|---|---|
| 4.61 GB | 74.2 s |
| 6.14 GB | 60.7 s |
| 9.22 GB | 48.6 s |
| 12.3 GB | 42.5 s |
| 18.4 GB | 38.8 s (fastest) |
| 36.8 GB | not possible |

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