



Magnetic Analysis and Reconstruction of Tomographies App (MARTApp)

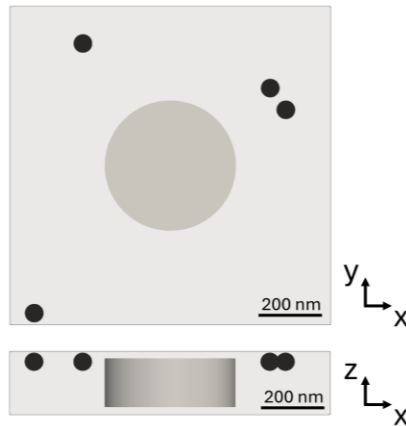
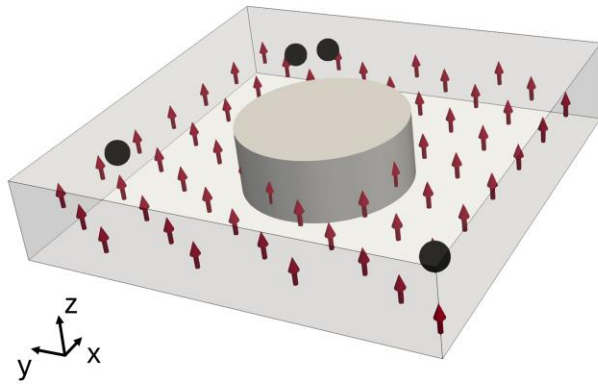
User guide

References:

- MARTApp's article: A.E. Herguedas-Alonso, J. Gómez Sánchez, et al. doi.org/10.48550/arXiv.2501.13127
- Magnetic reconstruction of 2D samples algorithm article: A.E. Herguedas-Alonso, et al. Sci. Rep. 13, 9639 (2023). doi.org/10.1038/s41598-023-36803-z
- Magnetic reconstruction of 3D samples algorithm article: A. Hierro-Rodriguez, et al. J. Synchrotron Radiat. 25, 1144-1152 (2018) doi.org/10.1107/S1600577518005829

Links:

- MARTApp download and documentation: <https://github.com/ALBA-Synchrotron/MARTApp>



Magnetic hopfion within a continuous film:

- The hopfion is computed/simulated in a cylinder surrounded by an out-of-plane magnetization. Sample is considered a 3D sample.
- Spheres were added to simulate Au fiducial markers for the alignment.
- Gray box represents the simulation space where hopfion is.

To convert raw data (.xrm) into normalized stacks (.hdf5)

To obtain the XMCD image of each tilt series

Manual alignment of images


3D reconstruction of the magnetization vector for 2D samples

3D reconstruction of absorbance for 3D samples

3D reconstruction of magnetization vector of 3D samples

MARTApp

Magnetic Analysis & Reconstruction of Tomographies App



Tilt Series 1 Tilt Series 2

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Raw data directory path



Preprocessing

Convert .xrm files in .hdf5 files and to obtain normalized and averaged stacks (using FFs and backgrounds (optional)) for each polarization.

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Preprocessing

Path

/beamlines/bl09/sdm/shared/HopfionDataset/TS1

Select path

Input

Folder

File .txt

Name pattern

Database .json

Delete previous execution

Select

Select

Alignment

Method

pyStackReg

Sub-pixel

Outlier threshold

0.70

Normalization

Flat-field

Background**

Interpolate Flat-field *

Output

Crop stack

Save all in a single file (stack, flat-field, background)

Delete intermediate processing HDF5 files

GO!

Visualization

Created stacks:

Individual images to stacks took 0.352994441986084 seconds ---

magnetism preprocessing took 1 seconds

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Close

Creates two separate stacks for each polarization:

- sample_1.0_FF_norm_stack.hdf5
- sample_-1.0_FF_norm_stack.hdf5

"Folder" option is sufficient ff files follow the filename standard (date_sample_polarization_angle_[FF/BG]_repetition.xrm). If not, "File .txt" option may be used to set se acquisition script, or a specific name patter can be specified using "Name pattern" option.

Different available alignment algorithms to align repetitions before averaging them.

* Activate *Interpolate FF* if flat-fields were measured for every angle adquisition.

** Activate background correction if there is a Dark Field region in the sample.

Opens a visualization window for the generated .hdf5 files

Select Dataset@hpcinteractive01

2DAlignedNegativeStack

2DAlignedPositiveStack

Absorption2DAligned

Angles

MagneticSignal2DAligned

OriginalNegativeStack

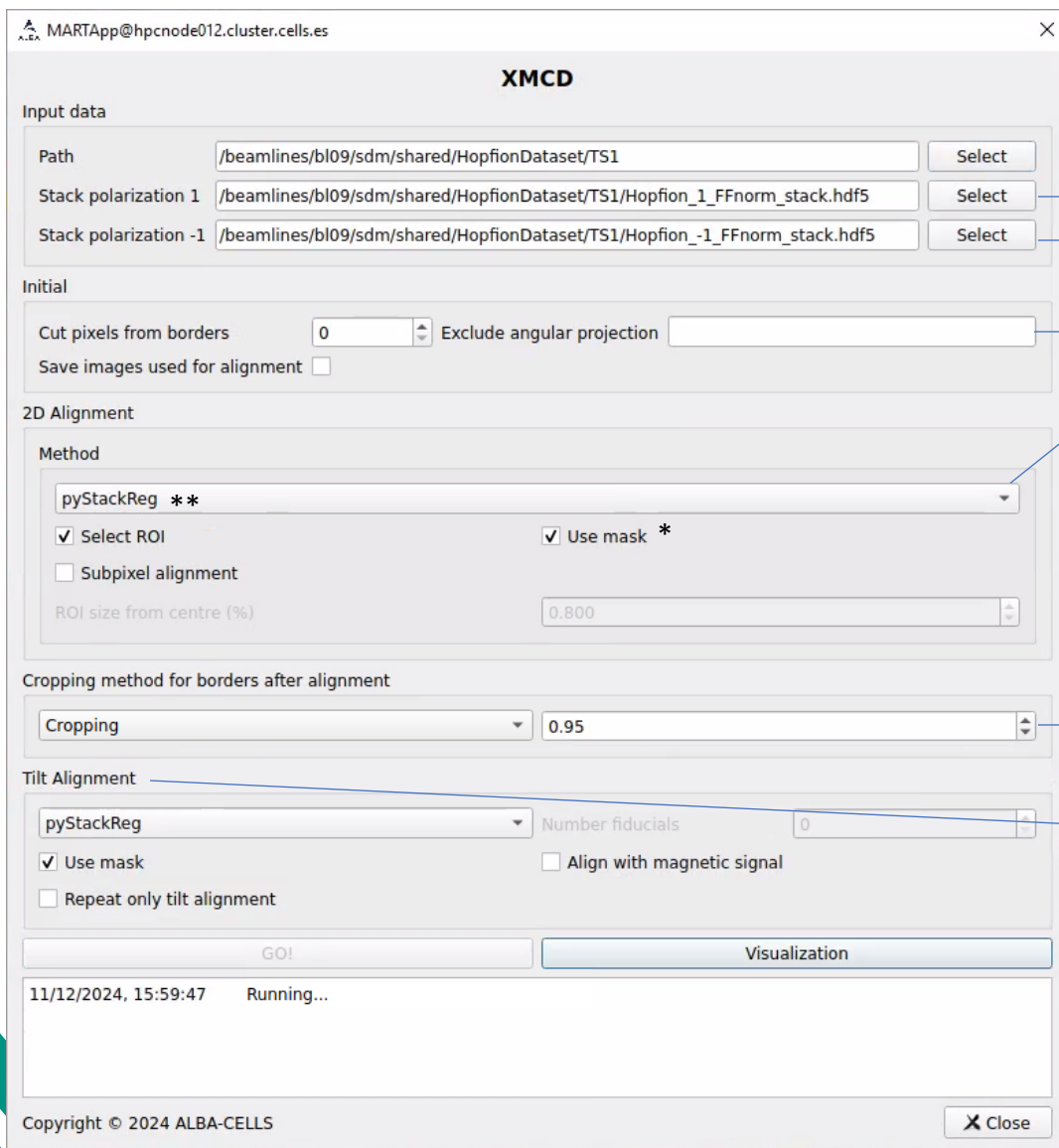
OriginalPositiveStack

Open Napari

Open Matplotlib

(Almost always) best option: Open Matplotlib
Alternative: Fiji

To calculate the XMCD image of each angle. Results are saved in **sample_xmcd.hdf5**. The XMCD images of each angle in the stack are not aligned with respect to each other.



The screenshot shows the MARTApp XMCD interface with the following sections:

- Input data:**
 - Path: /beamlines/bl09/sdm/shared/HopfionDataset/TS1
 - Stack polarization 1: /beamlines/bl09/sdm/shared/HopfionDataset/TS1/Hopfion_1_FFnorm_stack.hdf5
 - Stack polarization -1: /beamlines/bl09/sdm/shared/HopfionDataset/TS1/Hopfion_-1_FFnorm_stack.hdf5
- Initial:**
 - Cut pixels from borders: 0
 - Exclude angular projection: (empty)
 - Save images used for alignment: ☐
- 2D Alignment:**
 - Method: pyStackReg **
 - ☒ Select ROI
 - ☒ Use mask *
 - ☐ Subpixel alignment
 - ROI size from centre (%): 0.800
- Cropping method for borders after alignment:**
 - Cropping: 0.95
- Tilt Alignment:**
 - Method: pyStackReg
 - Number fiducials: 0
 - ☒ Use mask
 - ☐ Align with magnetic signal
 - ☐ Repeat only tilt alignment
- Buttons:** GO!, Visualization
- Status:** 11/12/2024, 15:59:47 Running...
- Footer:** Copyright © 2024 ALBA-CELLS

Select **sample_1.0_FF_norm_stack.hdf5**

Select **sample_-1.0_FF_norm_stack.hdf5**

The index in the stack (starting from 1) must be specified, not the angle. **

Select the appropriate alignment method. Recommendations (to be improved):

- Structures with sharp edges: cross correlation or cross correlation in Fourier space
- Fiducials or beads: cross correlation in Fourier space

* Mask is used to remove the magnetic contribution during the alignment. It is possible to do the alignment without mask nor ROI.

** In case of choosing Optical Flow a “Sample center for 2D alignment” will be opened. Then, select a rectangle taking the sample edge.

This value has to be the same for both Tilt Series. It helps removing alignment drifts in borders. They can also be filled with background values.

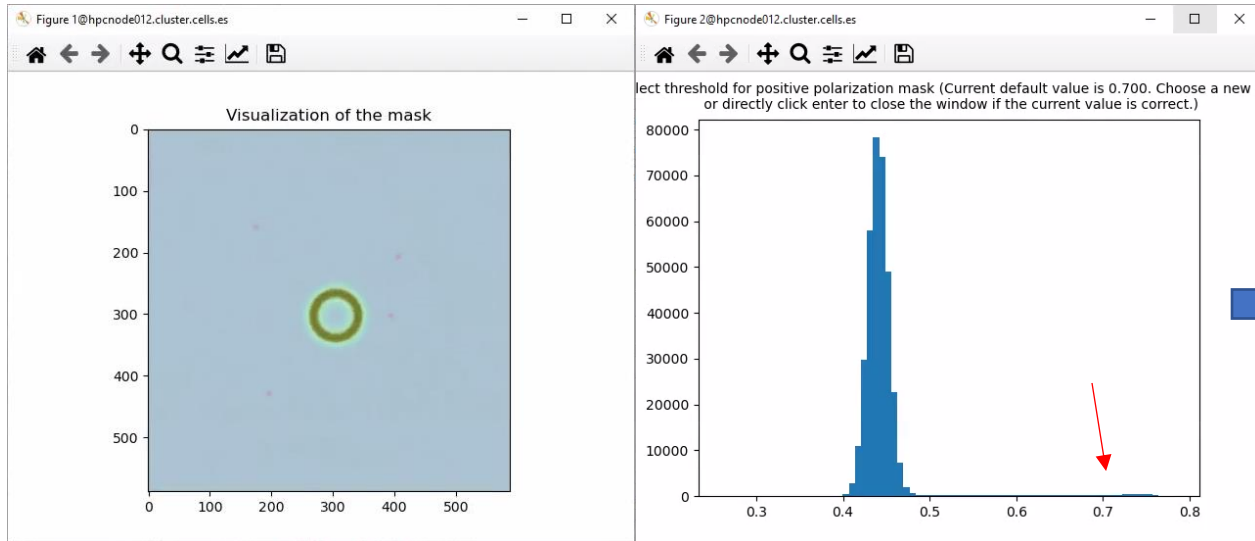
To align the XMCD images of different angles with respect to the same rotation axis. Only needed for reconstruction of the magnetization in 3D samples.

** If any of the angular projections is removed from one tilt series, (i.e. proj. 48 in TS1) it should also be removed when doing the XMCD in the TS2, to avoid problems in the magnetic reconstruction.

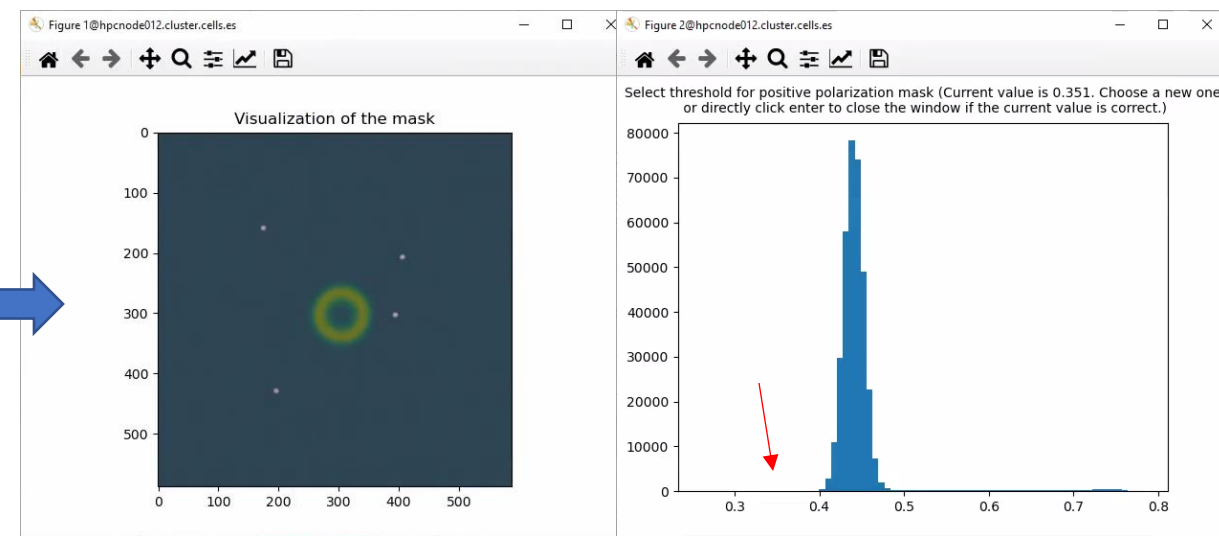
XMCD – Alignment using a mask

1. A mask to remove the magnetic contribution and help aligning images using real features is applied. Select the proper mask parameters to remove magnetic signal in the image. There is one mask for each polarization set of data.

Example of wrong mask (overlayed with original image). To correct it, change the threshold value by clicking on the histogram and press *Enter*.

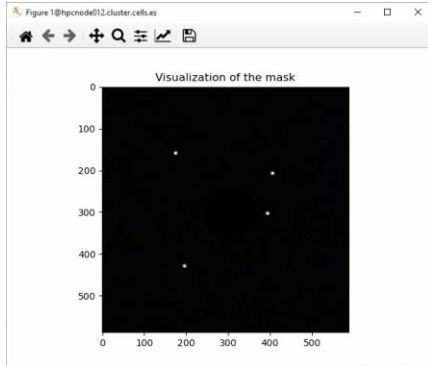


Now mask is correct (fiducials are visible and magnetic signal is not).



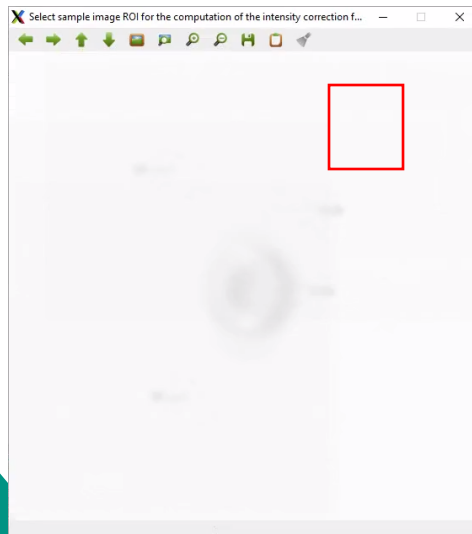


Visualization of the mask and preview of the stack:



This screen is showing an average of the images of sample_1_FF.hdf5

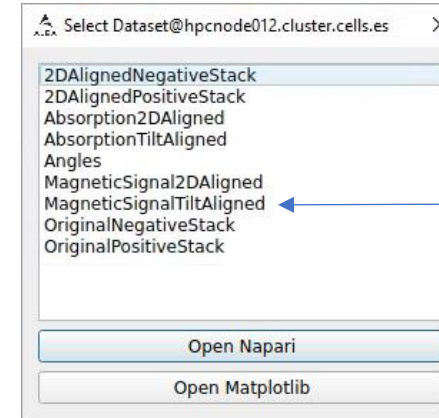
2. Select a ROI for the computation of the intensity between both polarizations and press “enter”:



If there is not FF in the image (i.e. thin films) select the entire image to have an average of the intensity.

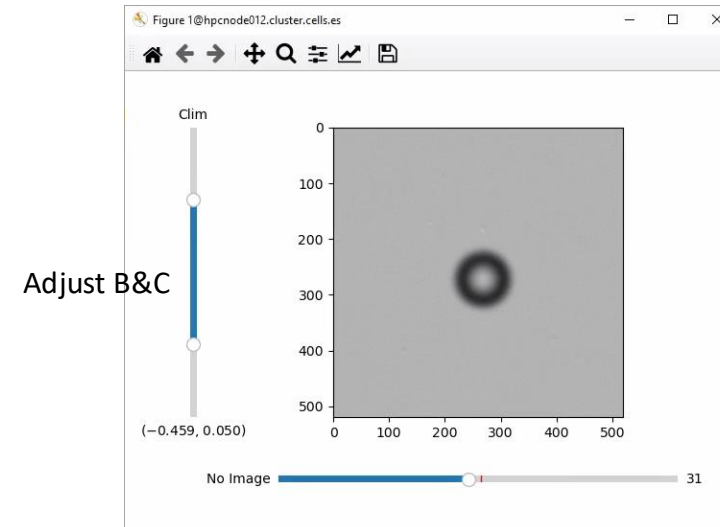
XMCD– Alignment using a mask

3. A file **sample_xmcd.hdf5** is created which contains the following stacks:



In case of having selected the tilt alignment

4. Visualization of the **sample_xmcd.hdf5** stack using Matplotlib:



* Depending on the selected alignment procedure (Cross Correlation, CC in Fourier, CT align or Optical Flow), there can be extra steps, in that case, follow the instructions.



Magnetic reconstruction of 2D samples

* The hopfion is a 3D sample, here is used just as an example.

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Magnetic reconstruction of 2D samples

Input data

Path

Tilt Series 1

Tilt Series 2 (rotated)

Distance between magnetic layer and fiducials [in pixels]:

Rotation axis

Cosine Stretching Alignment

Tilt Series 1 ☒ Select ROI ☐ Select points for initial transformation

Tilt Series 2 ☒ Select ROI ☐ Select points for initial transformation

Join Tilt Series

☒ Select ROI ☐ Select points for initial transformation

Initial angle

Reconstruction

Attenuation length (m)

Thickness (m)

Dichroic coefficient

Repeat step

Path to save the 2D reconstruction data.

Select the .hdf5 files containing the xmcd images for each polarization.

In case of magnetic 2D layers, if fiducials are used as alignment marks.

Cosine stretching correction between images of the same tilt series.

Correction of rotation angle between tilt series 1 and tilt series 2.

Select the sample parameters for the reconstruction.
If there are some unknown values, leave the value 1.

For know values, the result is the normalized magnetization.

In the case the repetition of any step of a previous execution is needed, select here.

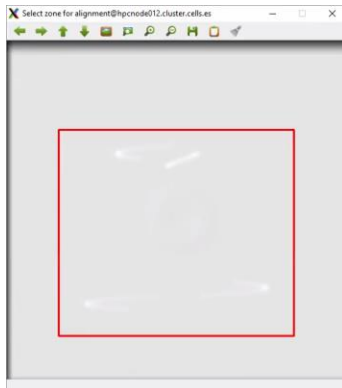


Cosine stretching using ROI.

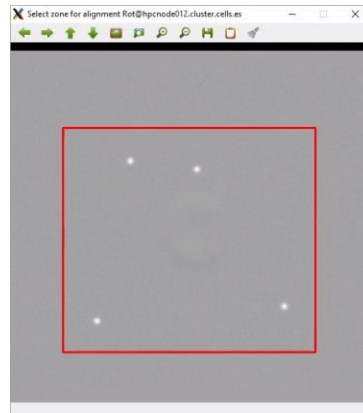
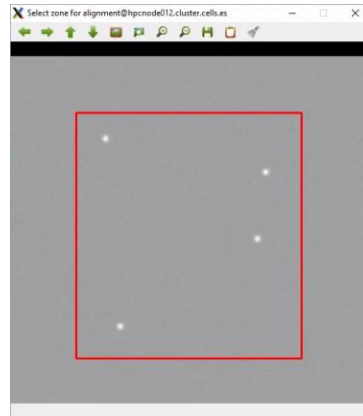
1. This window shows the average image of the TS1 stack. Select the region of interest and press enter.



Same window will appear with data from TS2 to be aligned:

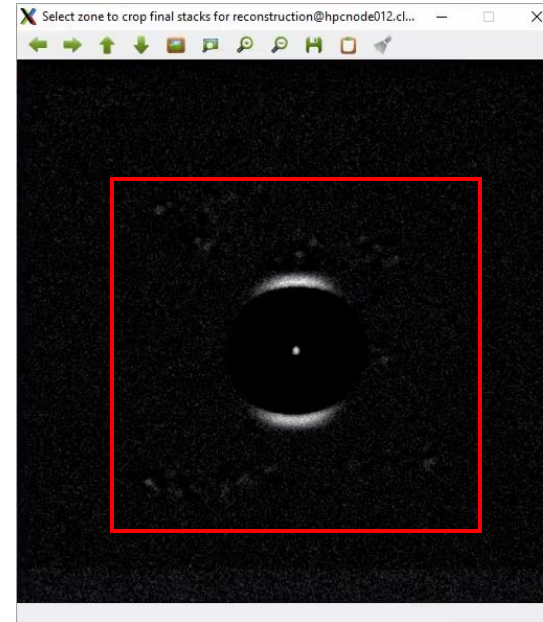


2. Correction of the rotation angle between TS1 and TS2. Select the region of interest for both tilt series and press "enter":

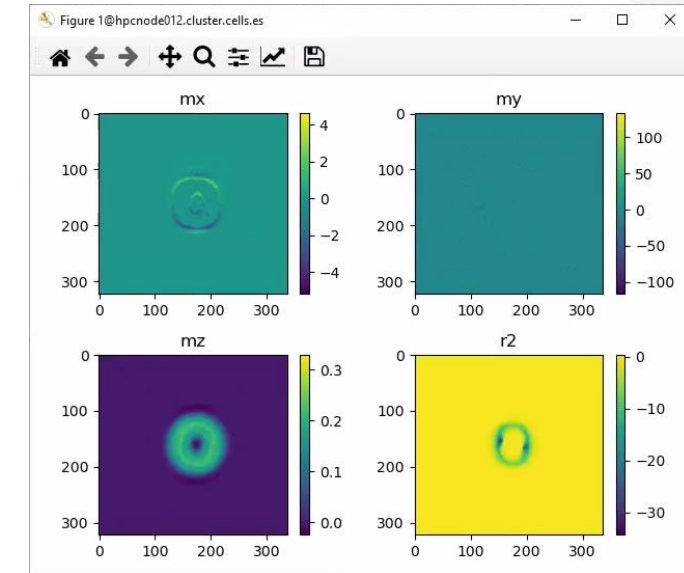


Magnetic reconstruction of 2D samples

3. Select the region of interest for the reconstruction and press "enter":



4. Preview of the 2D reconstruction



Generated files:

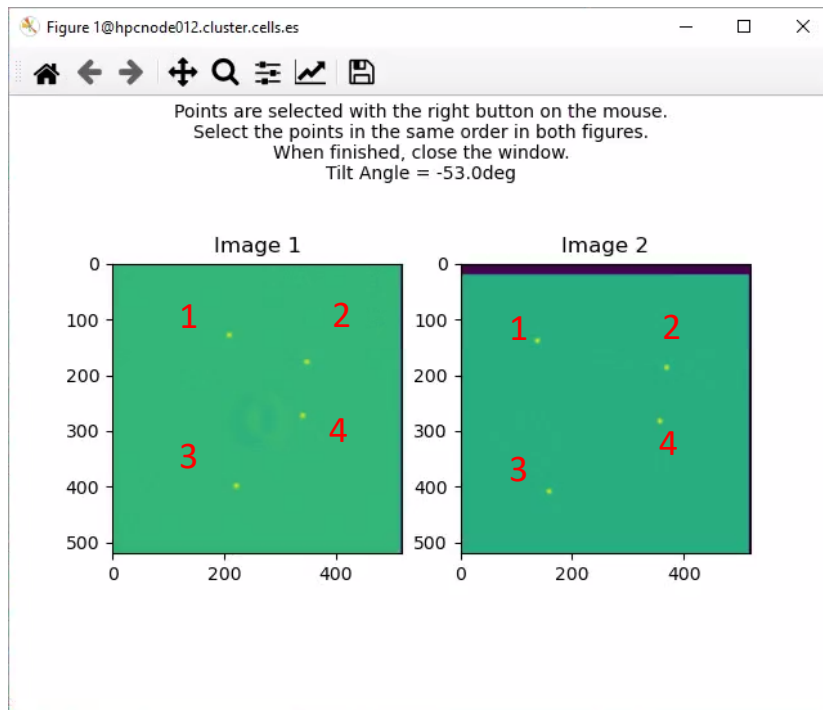
- **cos_stretching.hdf5** : Tilt series 1
- **cos_stretching_rotated.hdf5** : Tilt series 2 oriented as Tilt series 1
- **join_tilt_series.hdf5** : both series together
- **Reconstruction.hdf5** : reconstructed mx, my, mz and r2. (r2: reconstruction error)

Magnetic reconstruction of 2D samples

Cosine stretching by selecting points

1. Select points for the initial transformation.

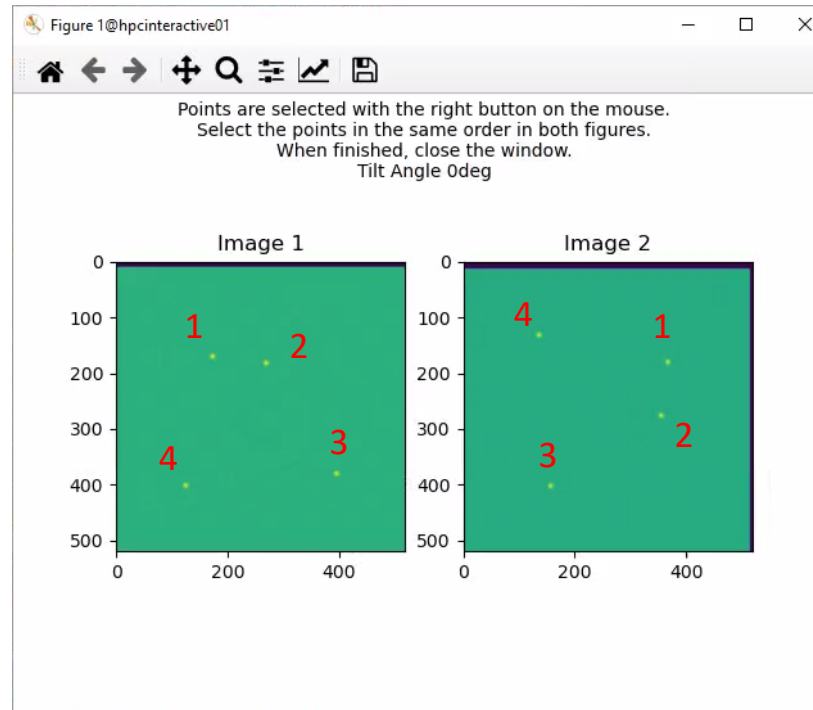
Important! Select the points in same order for both images



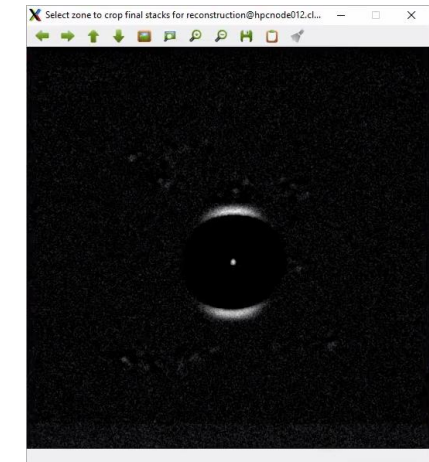
You will be asked to select points in all the angular projections contained in the xmcd.hdf5

ROI and point selection can be combined

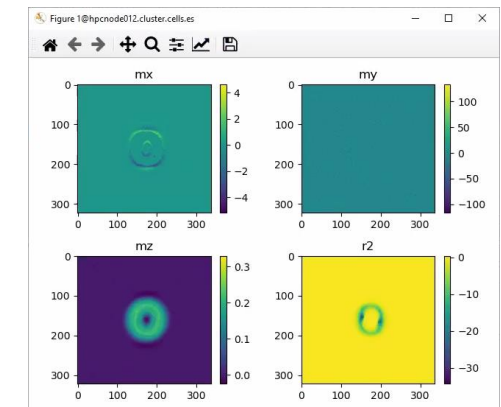
2. Select points for the correction of the rotation angle between TS1 and TS2.



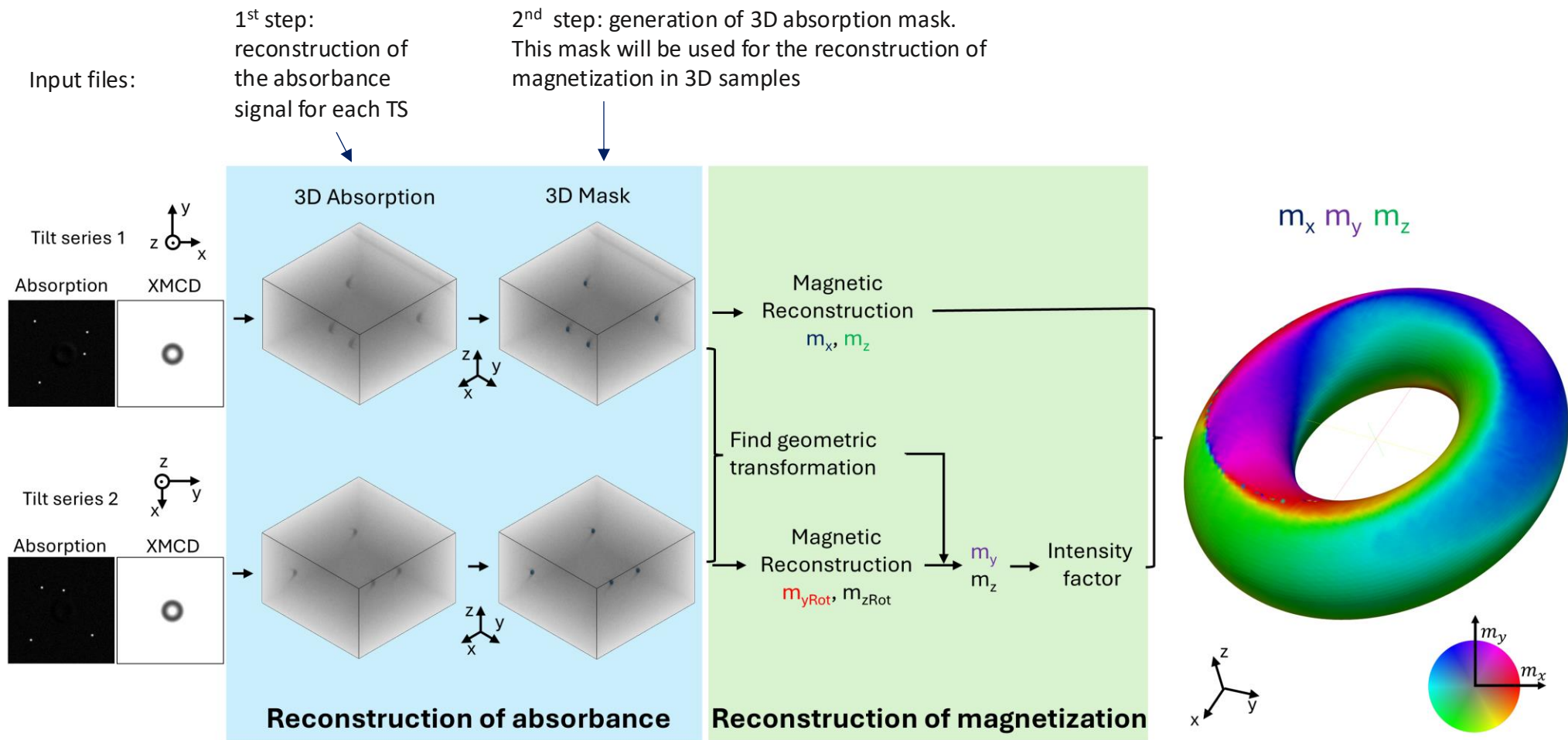
3. Select the region of interest for the reconstruction and press “enter”:



4. Preview of the 2D reconstruction



Absorbance & magnetic reconstruction of 3D samples



Absorbance reconstruction of 3D samples

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Absorption reconstruction of 3D samples

	Tomo	Tomo Rot
HDF5 file	ared/HopfionDataset/TS1/Hopfion_xmcd.hdf5	d/HopfionDataset/TS2/HopfionRot_xmcd.hdf5
Dataset Absorption 3DAligned	AbsorptionTiltAligned	AbsorptionTiltAligned
Dataset Angles	Angles	Angles
Output path	09/sdm/shared/HopfionDataset/3DAbsRecons	09/sdm/shared/HopfionDataset/3DAbsRecons
Output filename	Hopfion_AbsorptionReconstruction.hdf5	HopfionRot_AbsorptionReconstruction.hdf5
Segmentation mode	Threshold	Threshold
Threshold value	Manual	Manual
Negative mask	<input type="checkbox"/>	<input type="checkbox"/>
	Reconstruction+Segmentation	Reconstruction+Segmentation
	Only Segmentation	Only Segmentation
	Visualization	Visualization
Number of cells	X 520 Y 520 Z 200	
Pixel size (nm)	10.00	
Number iterations	20	
Continuous film	<input type="checkbox"/>	
Reconstruction Axis	YTilt	
Simultaneous Slices	10	
GPU	<input type="checkbox"/>	
Save Projection Matrices	<input type="checkbox"/>	
Use Projection Matrices	<input type="checkbox"/>	

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→ .hdf5 files containing the tilt aligned XMCD images

→ Select the tilt aligned absorption stack

→ Select the angle dataset

→ Output folder. It is recommended to create a new folder (i.e. 3DAbsRecons) to save these data.

→ Write the output name of the files

→ Available segmentation modes:

- Threshold
- 2D symmetry: for materials with 2D symmetry
- Continuous films

→ The selection of the threshold value can be chosen manually or using different algorithms (Otsu, Triangle, Huang, Max Entropy)

→ Number of cells in Z must be higher than the thickness of the sample to avoid edge effects in the reconstruction.

→ Mark this in case of using GPU

→ Mark this to save x-ray projection matrix.

→ Mark to use saved x-ray projection matrix. (i.e. repetition of the reconstruction with different number of iterations, it affords computation time).

Absorbance reconstruction of 3D samples

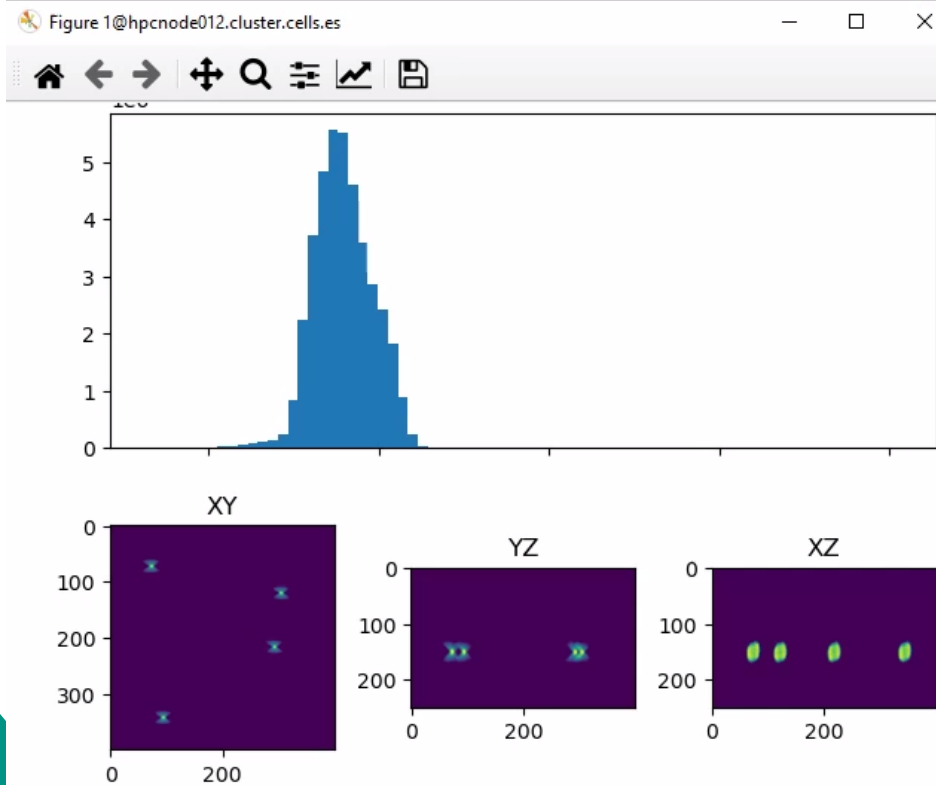
For the segmentation, three modes are available:

- Threshold
- 2D symmetry
- Thin films

Generated files: sample_name_AbsorptionReconstruction.hdf5

- **Absorption3D**
- **Mask3D**
- **Mask3DRegistration**

Threshold: if manual value is selected, choose the value on the histogram (yellow areas are the ones that are going to be considered for the segmentation)



Select (in yellow) the positions that you want to be considered as “material” in z axis. It will fill with materials all the layers in yz projection which contain yellow pixels. Second threshold: select mask in xy (in yellow). The points of this mask are going to fill the z projection selected before.

XY, YZ and XZ views of the mask. An average of all the projections in the stack “absorption tilt alignment” of the XMCD HDF5 file is shown.

Magnetic reconstruction of 3D samples

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Magnetic reconstruction of 3D samples

	Tomo	Tomo Rot
HDF5 file	<input type="text" value="red/HopfionDataset/TS1/Hopfion_xmcd.hdf5"/> ...	<input type="text" value="/HopfionDataset/TS2/HopfionRot_xmcd.hdf5"/> ...
Dataset XMCD 3DAligned	<input type="text" value="MagneticSignalTiltAligned"/>	<input type="text" value="MagneticSignalTiltAligned"/>
Dataset Angles	<input type="text" value="Angles"/>	<input type="text" value="Angles"/>
HDF5 mask	<input type="text" value="ons/Hopfion_AbsorptionReconstruction.hdf5"/> ...	<input type="text" value="s/HopfionRot_AbsorptionReconstruction.hdf5"/> ...
Dataset Mask (reconstruction)	<input type="text" value="Mask3D"/>	<input type="text" value="None"/>
Dataset Mask (registration)	<input type="text" value="Mask3DRegistration"/>	<input type="text" value="Absorption3D"/>
Output filename	<input type="text" value="Hopfion"/> _MagneticReconstruction.hdf5	<input type="text" value="HopfionRot"/> _MagneticReconstruction.hdf5
Output path	<input type="text" value="/beamlines/bl09/sdm/shared/HopfionDataset/3DMagRecons"/> ...	
Number of cells	X <input type="text" value="520"/>	Y <input type="text" value="520"/> Z <input type="text" value="200"/>
Pixel size (nm)	<input type="text" value="10.00"/>	
Number iterations	<input type="text" value="20"/>	
Continuous film	<input type="checkbox"/>	
Reconstruction Axis	<input type="text" value="YTilt"/>	
Simultaneous Slices	<input type="text" value="10"/>	
GPU	<input checked="" type="checkbox"/>	
Save Projection Matrices	<input checked="" type="checkbox"/>	
Use Projection Matrices	<input type="checkbox"/>	
<input type="button" value="Reconstruction+Registration"/> <input type="button" value="Only registration"/> <input type="button" value="Visualization"/>		

Select the sample_xmcd.hdf5 which contains the tilt aligned xmcd data.

Select "MagneticSignalTiltAligned"

Select the .hdf5 which contains the absorption 3D reconstruction

Select the Mask3D obtained from absorption reconstruction

Select Mask3DRegistration data

Do not choose the same name for both files

Voxel size

Select in case the sample is a continuous film

Mark this in case of using GPU.

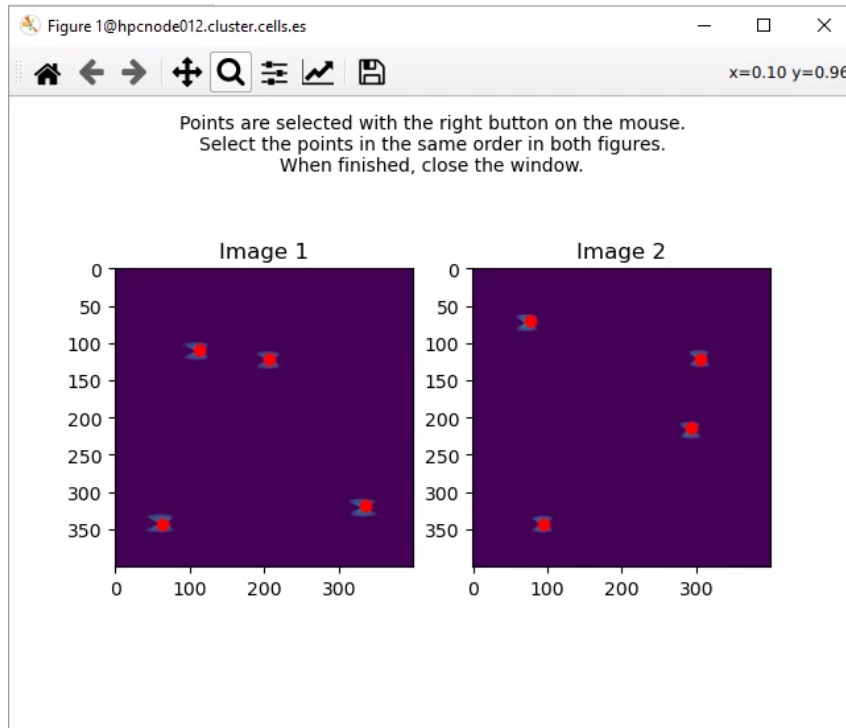
Mark this to save x-ray projection matrix.

Mark to use saved x-ray projection matrix. (i.e. repetition of the reconstruction with different number of iterations, it affords computation time).

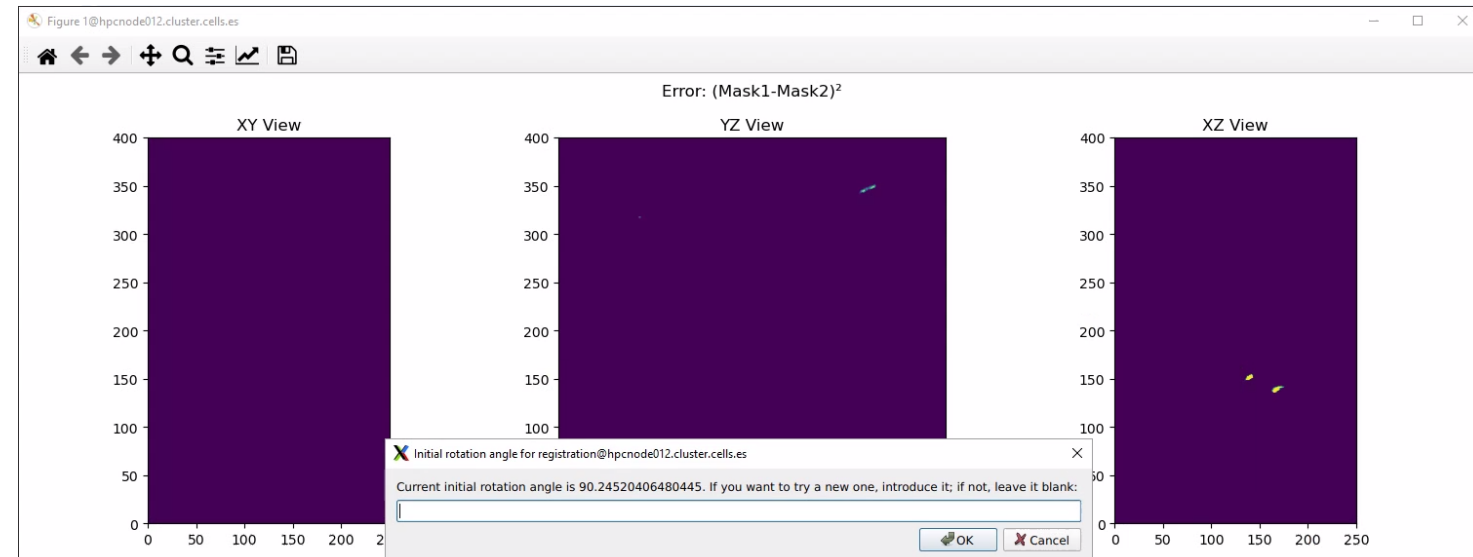


Magnetic reconstruction of 3D samples

Look for initial transformation matrix.
Select the same points in the same order for both images.



Visualization of the transformation error:



Generated files: sample_name_MagneticReconstruction.hdf5

- MagneticReconstruction/M1
- MagneticReconstruction/M2



References, resources and help

If you use MARTApp for your experiment, please cite the following articles:

- MARTApp's article: A.E. Herguedas-Alonso, J. Gómez Sánchez, et al. doi.org/10.48550/arXiv.2501.13127
- If you reconstruct a 2D material: A.E. Herguedas-Alonso, et al. Sci. Rep. 13, 9639 (2023). doi.org/10.1038/s41598-023-36803-z
- If you reconstruct a 2D material: A. Hierro-Rodriguez, et al. J. Synchrotron Radiat. 25, 1144-1152 (2018) doi.org/10.1107/S1600577518005829

If you want to use MARTApp in your machine, you can download it and find more information in the GitHub repository:

<https://github.com/ALBA-Synchrotron/MARTApp>

If you need help using MARTApp, you should contact your Local Contact (only if you are an ALBA user). Otherwise, you can open an issue in GitHub or send an email to [jgsanchez \(at\) cells.es](mailto:jgsanchez@cells.es).