

PLUG-IN-BASED PTYCHOGRAPHY & CDI RECONSTRUCTION USER INTERFACE DEVELOPMENT

Sang-Woo Kim*, Kyung-Hyun Ku, Woul-Woo Lee
Pohang Accelerator Laboratory, Pohang, South Korea

Abstract

Synchrotron beamlines have a wide range of fields, and accordingly, various open source and commercial softwares are being used for data analysis. Inevitable, the user interface differs between programs and there is little shared part, so the user had to spend a lot of effort to perform a new experimental analysis and learn how to use the program newly.

In order to overcome these shortcomings, the same user interface was maintained using the Xi-cam framework [1], and different analysis algorithms for each field were introduced in a plugin method. In this presentation, user interfaces designed for ptychography and cdi reconstruction will be introduced.

INTRODUCTION

With the development of technology, the amount of data from detectors used for synchrotron radiation facilities is rapidly increasing. Diverse programs for processing the massive data are being developed individually at synchrotrons and universities with various languages such as python, matlab, labview, etc. In this situation, Xi-cam [1] proposed to jointly develop data analysis software with standardized framework and to utilize the developed program in other research institutes. Analysis programs using standardized framework have the advantage of being able to easily add necessary functions by loading plugins while maintaining a unified user interface. In addition, since the Xi-cam program handles GUI and analysis code execution, it is possible to focus on the implementation of core functionality. For this reason, we created a ptychography and cdi data processing program using Xi-cam's framework.

Ptychography and CDI are two types of coherent X-ray imaging techniques. As the focused and coherent X-rays pass through the sample, an interference pattern is created and this pattern is recorded by the detector. By using the interference pattern, the wavefunction of the probe, the density distribution of the sample, and the strain information could be obtained. The method estimates the wave function of the probe and the distribution of the sample at the beginning, and repeats the process of updating the probe and sample information to match the measured interference pattern while repeating propagation and backward propagation to obtain a value close to the actual probe and sample. Propagation is mathematically equivalent to a Fourier transformation. When CPU is used to repeatedly perform FFT and inverse FFT of large image data, it takes a long time to obtain a result,

whereas GPU could significantly reduce operation time because multiple cores can operate in parallel.

Ptychography and CDI operations were performed using the PyNX [2] developed by ESRF. PyNX was chosen because it is designed to increase the operation speed by using CUDA cores of GPU and is designed based on mathematical operators so that the user can modify the application of the algorithms to suit their data. Although PyNX provides a script that can apply the reconstruction algorithm from the command line, a graphical user interface was created so that general users who are not familiar with command-line can utilize it.

PTYCHOGRAPHY

Figure 1 shows the initial screen of Xi-cam. A list of installed plugins is displayed in the upper right corner. Currently, ptychography and cdi plugins are displayed, and plugins can be added on demand. Figure 2 is the screen displayed when the Ptychography plugin is selected. Tabs are arranged in the order of data processing, Preprocessing, STXM Viewer, Reconstruction, and Result Viewer. Similarly, CDI plugin (Fig. 6) consists of Preprocessing, Reconstruction, and Result Viewer.

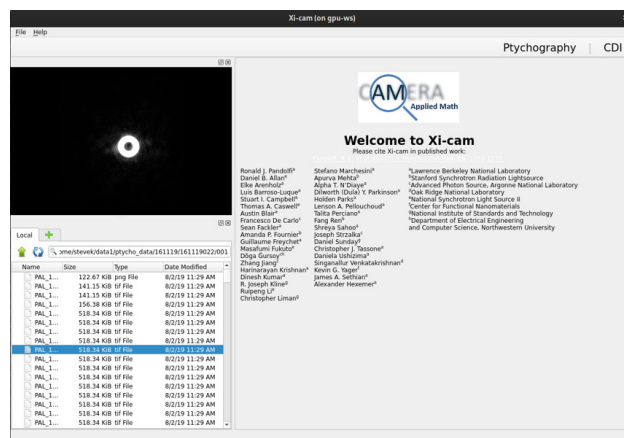


Figure 1: The initial screen of the Xi-cam. Installed plugins can be selected from the upper right corner.

Preprocessing

In preprocessing, meta data such as energy and the distance between the sample and the detector is read from the header file and average, background, subtraction, crop, resize, denoising, etc. are performed and then saved as a cxi file. The cxi file format [3] is used as a standard in the field of coherent X-ray imaging and is supported by many programs. Thousands of images are compressed and stored in a single

* physwkim@postech.ac.kr

file, so the efficiency of management and data transmission is increased.

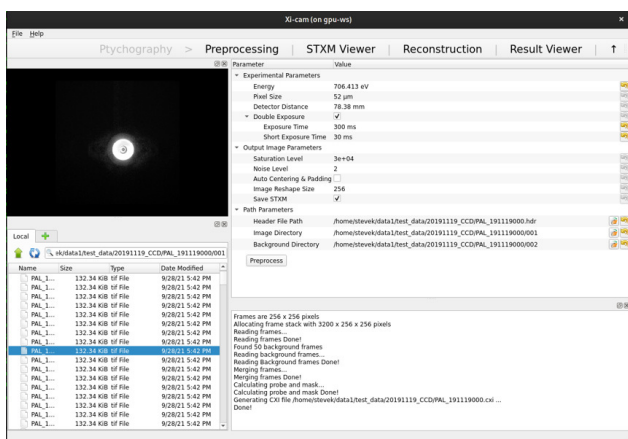


Figure 2: The first screen displayed when the Ptychography plugin is selected. The tabs are arranged in the order of Preprocessing, STXM Viewer, Reconstruction, and Result Viewer workflow.

Reconstruction

In the Reconstruction tab (Fig. 3), the initial probe size and shape are determined, and reconstruction is performed by combining algorithms to be applied. Reconstruction may not work well depending on the direction in which the camera is mounted. In this case, it is possible to find the condition for good reconstruction when the image is transposed or flipped. On the right side, there is a window that updates the amplitude and phase of the sample and the amplitude and phase of the probe while the calculation is in progress. The black square box displayed on the object indicates the area where the actual scan was made. In the lower right log window, the name of the currently running algorithm, the error value, the elapsed time, and the size of the probe finally obtained are displayed.

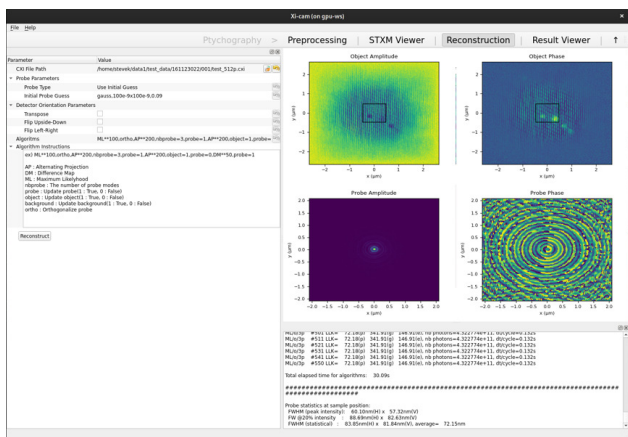


Figure 3: Ptychography reconstruction panel is shown. In the left setting window, the initial probe size, and reconstruction algorithm could be changed.

Since the wave function of the probe can be obtained through the ptychography, it has the advantage of accurately grasping the size and shape of the beam. In addition, if this data is applied to the next operation, a good reconstruction result could be obtained with much fewer operations.

Result Viewer

Figure 4 shows the Result Viewer tab. In this tab, the reconstruction results can be immediately checked and exported or captured. The left panel shows the hierarchy of a cxi file. Not only the reconstruction result, but also meta data such as pixel size and energy and the wave function of the probe could be accessed. The right panel shows the amplitude of the reconstructed sample. The black square box indicates the area where the actual scan was made.

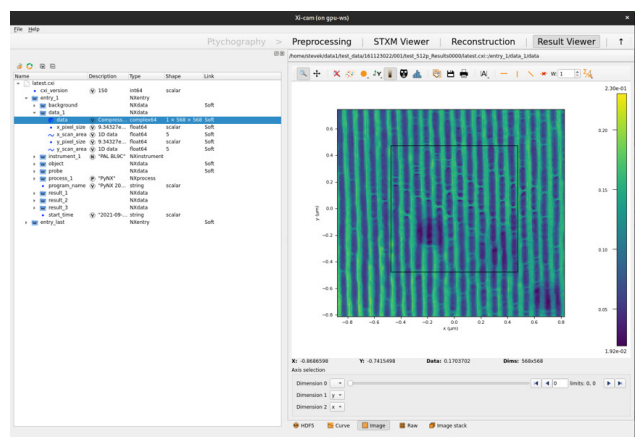


Figure 4: The Result Viewer tab of the Ptychography Plugin. The hierarchy of the CXI file resulting from the reconstruction is shown on the left, and the operation result image is shown on the right. The black box indicates the scan area.

Figure 5 shows the STXM (a) and Ptychography reconstruction results (b) of measuring a zoneplate with defects. STXM data were measured in 50 nm steps when the beam size was 60 nm (FWHM). In the reconstruction result, the pixel size was reduced from 50 nm to 9.3 nm, and the noise seen in the STXM data was also greatly reduced in the result. Since the image quality can be improved through the reconstruction, it has many advantages when performing 2D XANES and Tomography experiments using the STXM technique. The soft X-ray beamline 10A1 and the hard X-ray beamline 9C are using the Ptychography plugin.

CDI

Unlike the case of ptychography, the wavefunction of the probe cannot be obtained through CDI reconstruction. Instead, designate an arbitrary support area that is slightly larger than the actual sample and perform the reconstruction until it approaches the actual sample while narrowing or increasing the support area. Through this support update, when the boundary of the actual sample and that of the support match, the error is minimized and the information of the sample could be obtained.

Content from this work may be used under the terms of the CC BY 3.0 license (© 2022). Any distribution of this work must maintain attribution to the author(s), title of the work, publisher, and DOI

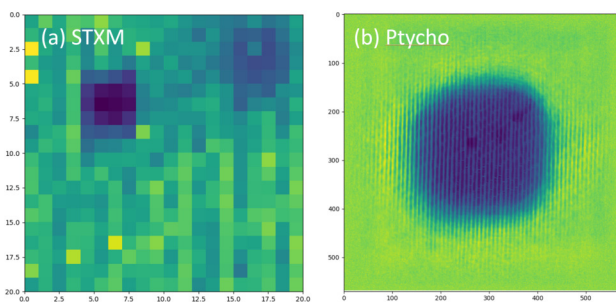


Figure 5: The result of measuring the zoneplate at PLS-II 10A1 beamline is shown. The left (a) is the data measured by typical STXM, and the right (b) is the result obtained after performing the Ptychography reconstruction. The pixel size of (a) is 50 nm, and the pixel size of (b) is 9.3 nm.

The Bragg CDI technique can obtain the 3 dimensional characteristics of the sample in real space by using the interference pattern obtained from the rocking curves around the diffraction peak. The images obtained through rocking measurement is converted into q-space during preprocessing to obtain diffraction patterns in reciprocal space.

Reconstruction

Figure 6 shows the reconstruction tab of the CDI plugin. The parameters of support type and size and reconstruction algorithm setting screen are located on the left. On the right screen, the amplitude and phase of the sample, the reconstructed interference pattern and the measured interference pattern are shown. The sample distribution in real space was revealed through CDI reconstruction of interference patterns in 3D q-space.

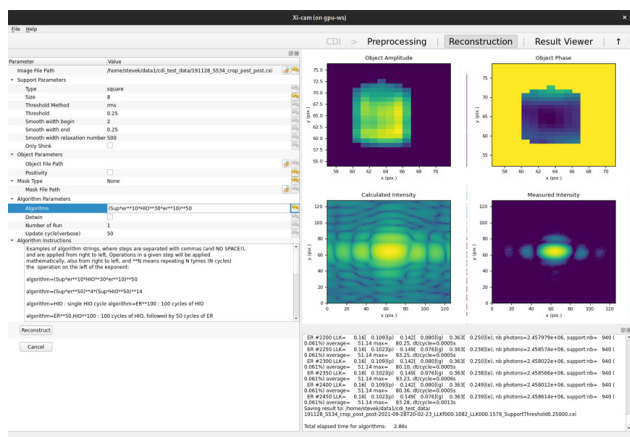


Figure 6: The reconstruction tab of the CDI plugin. Setting parameters and status results are displayed.

Result Viewer

Figure 7 shows the result viewer tab where the CDI reconstruction result can be viewed as a 3D image. The 3D

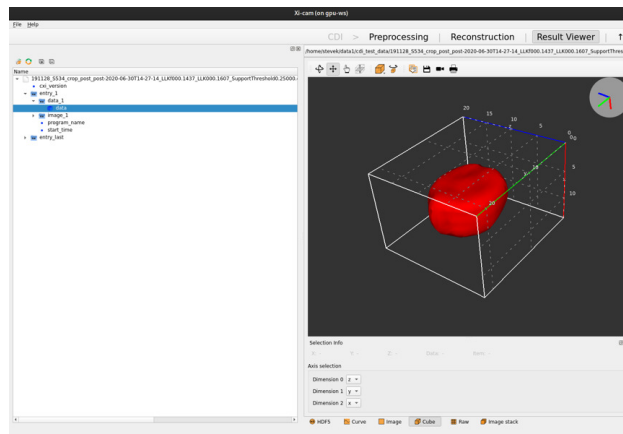


Figure 7: Result Viewer tab of CDI plugin. A three-dimensional image of the reconstructed sample is displayed.

image was displayed using the image viewer of silx [4], and the cross-sectional image of the sample can be displayed.

CONCLUSION

Using Xi-cam as a standard framework for data analysis, Ptychography [5] and CDI [6] plugins were made. The unity of the user interface has been increased, and the efficiency has also been increased as it is possible to focus only on the production of core functionalities.

The Ptychography and Bragg CDI plugins were applied to the hard X-ray and soft X-ray beamlines. It is confirmed that image quality can be improved with ptychography compared to stxm and 3D sample information could be obtained through Bragg CDI.

REFERENCES

- [1] R. J. Pandolfi *et al.*, “Xi-cam: a versatile interface for data visualization and analysis”, *J. Synchrotron Radiat.*, vol. 25, Part 4, p. 1261, Jul. 2018.
- [2] V. Favre-Nicolin *et al.*, “PyNX: high-performance computing toolkit for coherent X-ray imaging based on operators”, *J. Appl. Cryst.*, vol. 53, p. 1404, Aug. 2020.
- [3] Maia, F. R. N. C., “The Coherent X-ray Imaging Data Bank”, *Nat. Methods*, vol. 9, pp. 854–855, 2012.
- [4] Thomas VINCENT *et al.*, “silx-kit/silx: v0.11.0: 03/07/2019”, *Zenodo*, 03-Jul-2019.
- [5] <https://bitbucket.org/physwkim/ptychography/src/pls/>.
- [6] <https://bitbucket.org/physwkim/xicam.cdi/src/master/>.