Development of Calculator Code for Optimization of MFX Transfocator

SLAC NATIONAL ACCELERATOR LABORATORY

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Introduction

In the MFX experimentation hutch, the Transfocator is a tunable apparatus that focuses X-rays through the application of compound refractive Beryllium lenses. The application and removal of these lenses allow for a wide range of energies and focal lengths for use in the hutch's macromolecular crystallography experiments.

Keywords: Transfocator, Beryllium Lenses, Python, MFX, LCLS II

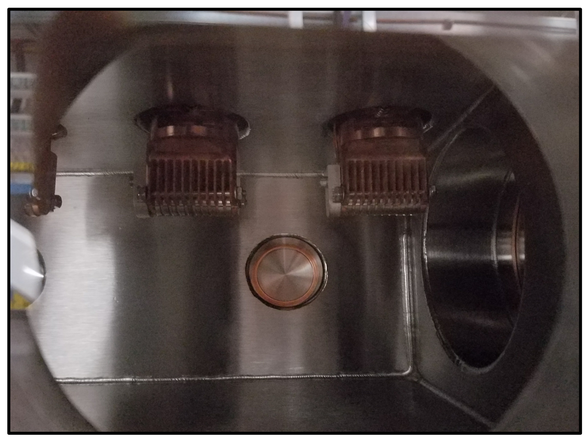
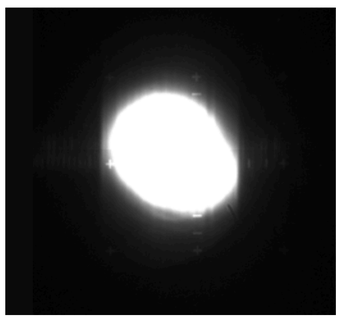
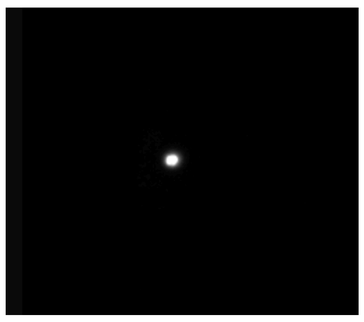


Figure 2: Motor-driven Beryllium lens arrays used to focus the LCLS X-rays located inside the Transfocator.





Figures 3 & 4: LCLS beam before (left) and after (right) focusing via lenses in the Transfocator.

Problem Statement

Because the Transfocator system is not automated, users and scientists must manually calculate the optimal focal length and apply the correct lenses. This process requires multiple iterations to accurately complete and costs users valuable time. With the approaching launch of LCLS II and the resulting influx of users, it is necessary to streamline the experimental setup of the Transfocator so that users may capitalize on their allotted time.

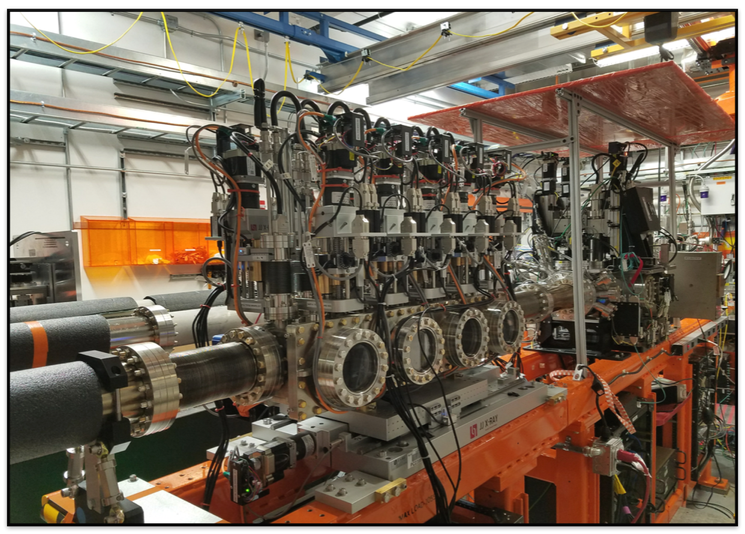


Figure 1: The Transfocator located in the MFX experimentation hutch

Development Process

To begin development of the Transfocator Calculator code, I learned Unix Shell, Git, and Python. Additionally, I learned basic optics.

Coding for the Transfocator followed an iterative design process. For each new segment of the project, I worked with Teddy to define the attributes and functionality within the overall project. I would then write and test the code iteratively in terminal and document my code using Github and Sphinx. All tests were written either by myself or Teddy.

The Transfocator code is composed primarily of 3 primary classes: Lens, LensConnect, and Transfocator.

Classes and Functions

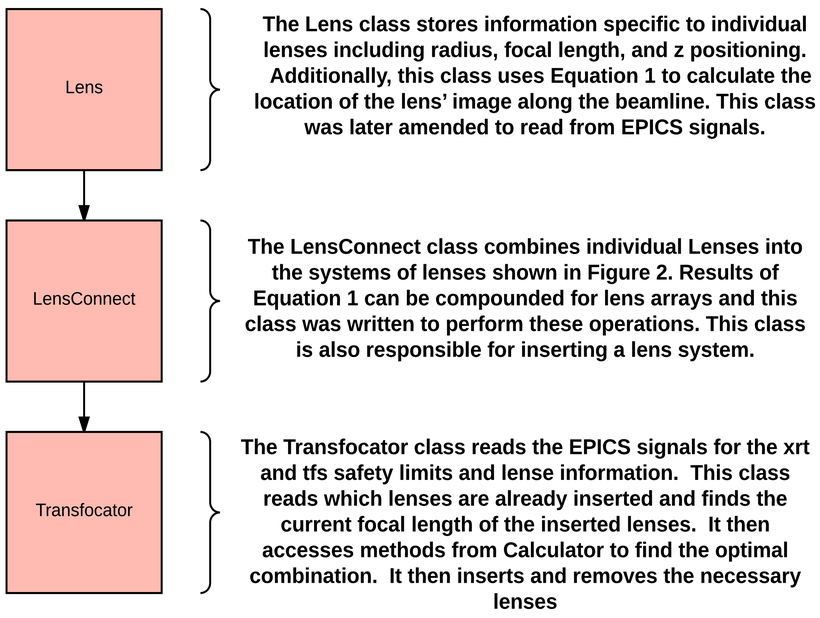


Figure 5: Outline and description of primary classes in Transfocator code.

$$\frac{1}{i} = \frac{1}{o} + \frac{1}{f}$$

Equation 1: The thin lens equation for a single lens. The equation is iterated to calculate the image distance for a system of lenses.

Relevance

Several properties of the code contribute to the relevance at LCLS and LCLS II:

- Optimizes the experimental set up for MFX
- Automates delivery of beam to MFX
- Code is flexible and extensible so that it can be used for any hutch that focuses with Beryllium lenses
- Code is easily applied on the beamline
- Provides a framework for similar projects
- Automatically factors in safety limits, partially removing human error from MFX beam calibration
- Allows user with no knowledge of Transfocator to calibrate the machine

Future Development

The Transfocator Calculator code is near completion and the next step in its development is addition scanning scripts to reach a level accuracy not possible with models alone. Although the program has performed very well, passing ~55 tests, there remain several aspects that warrant further development.

Possible future developments include:

- Implementation of Bluesky scans to increase the accuracy of the focal point by using the feedback from a live camera
- Creation of iterative function that finds another solution is Bluesky shows the initial one is inaccurate
- Creation of an introduction and user how to guide in Sphinx documentation (ongoing)
- Utilization of Calculator code for Beryllium lenses in other hutches

The Transfocator Calculator code is available on SLAC Github for general viewing and use.

Purpose and Novelty

The purpose of this project was to optimize the calculation and implementation of Transfocator Beryllium lens combinations with a "Transfocator Calculator" code.

Novel attributes of the code include:

- Calculation of correct combination of prefocus and Transfocator lenses based solely on sample position regardless of user knowledge of previous Transfocator settings.
- Automated delivery of beam to MFX by calculating the optimal lens combination and applying necessary lenses within hutch safety constraints

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