Contribution ID: **69**   Type: **On-site planned, but remote also possible**

Merging 3D reciprocal space from individual diffraction patterns

The measurements of diffraction are usually performed using a 2D detector and the actually measured diffraction pattern corresponds to a spherical cut through the reciprocal space. By collecting many of such patterns, corresponding to different orientations of a measured sample, one can reconstruct a full 3D reciprocal space of the measured object. This is very useful for the accurate analysis of the internal structure of the measured sample.

Our group (group leader H.N.Chapman) has a lot of experience in performing experiments at the most advanced x-ray sources in the world (LCLS, eXFEL, Petra3, APS, ESRF). And we are performing diffraction experiments in different fields: from material science to structural biology. Also, we are analyzing the measured data and developing new methods for structure determination. Therefore, we have several Pb of measured diffraction patterns that can be further analyzed using the developed program.

The development of the new program for 3D merging was started last year and a lot of progress have been achieved already. But the development of the GUI was just started. Further development is needed together with the successful demonstration of application to the experimental data.

Field

A6: Theory and computing

DESY Place

Hamburg

DESY Division

FS

DESY Group

CFEL-FS1

Special Qualifications:

Python and some knowlege of C++

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