CDCS
CENTER FOR DATA AND COMPUTING
IN NATURAL SCIENCES

OPENING SYMPOSIUM 2022

Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

DESY.

TUHH

Contribution ID: **124** Type: **Poster**

Phase Retrieval from Crystals with Rotational Displacement

To date the application of X-ray crystallography has resulted in the largest amount of resolved protein structures. With novel and upcoming sources of radiation, like XFELs, the range of measurable biological molecules increases everyday. Conventional crystallography relies on refining the structure against a set of observed Bragg peaks from the crystallized molecule. However, the given information is usually not enough to reconstruct the structure ab initio. The new X-ray sources allow the measurement of imperfect crystals which create a second, observable diffraction pattern. This so-called continuous diffraction is generated by the random translational and rotational displacement of individual molecules compared to the crystal packing. It allows for reconstruction of the electron density without any prior knowledge.
The goal of this work is to develop a novel iterative phasing algorithm which incorporates information about the rotational molecular displacement. Instead of handling the blurring effect of the displacement separately as an inverse problem, the displacement is handled in parallel to the phase retrieval. Currently the algorithm is validated on simulated data.

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Session Classification: Poster session with buffet

Track Classification: CDL2 (Photon Science)