Poster

Parameter optimization for serial diffraction data analysis

A. B. Fonjallaz[1*], G. Hofer[1], P. Hager[1], L. Pacoste[1], L. Wang[1], X. Zou[1]

[1]*Department of Materials and Environmental Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, SE-106 91, Sweden*

alexisbenjamin.bjorkstenfonjallaz@mmk.su.se

Serial X-ray diffraction (XRD) using free-electron lasers and synchrotron sources has shown great advantages in studying the structure of microcrystals and time resolved structure changes. Recently, serial electron diffraction has also been developed, which shows promise for studying microcrystals, complementing both XRD and 3D electron diffraction methods. Common to all serial diffraction is the necessity to index individual diffraction patterns and to accurately integrate the reflection intensities amidst background noise. Currently, CrystFEL is widely used for the entire serial diffraction data processing pipeline. In order to increase the rate of indexing and quality of integration, optimisation of a large number of parameters is required.

Here we explore automated scripts for the iterative use of fast indexing, as well as integration parameter optimization. For indexing, our group has used the fast XGANDALF algorithm, and the more precise PinkIndexer algorithm. Using XGANDALF, we found that iterative runs with fast indexing settings over small parameter variations outperform slower indexing settings in indexing rate. Furthermore, we present an automated Python script for optimizing integration parameters, thereby enhancing data quality with minimal manual intervention. This script iteratively adjusts integration settings to identify optimal settings tailored to specific datasets. The application of these improvements to serial XRD is explored and assessed.

Given the significant costs and effort associated with serial diffraction data collection, the implementation of automated techniques to refine and optimize processing parameters is a cheap way to improve data quality.

[1] Schriber, E. A., Paley, D. W., Bolotovsky, R., Rosenberg, D. J., Sierra, R. G., Aquila, A., ... & Hohman, J. N. (2022). Chemical crystallography by serial femtosecond X-ray diffraction. Nature, 601(7893), 360-365.

[2] Smeets, S., Zou, X., & Wan, W. (2018). Serial electron crystallography for structure determination and phase analysis of nanocrystalline materials. Journal of applied crystallography, 51(5), 1262-1273.

[3] Bücker, R., Hogan-Lamarre, P., Mehrabi, P., Schulz, E. C., Bultema, L. A., Gevorkov, Y., ... & Dwayne Miller, R. J. (2020). Serial protein crystallography in an electron microscope. Nature communications, 11(1), 996.

[4] Gevorkov, Y., Yefanov, O., Barty, A., White, T. A., Mariani, V., Brehm, W., ... & Chapman, H. N. (2019). XGANDALF–extended gradient descent algorithm for lattice finding. Acta Crystallographica Section A: Foundations and Advances, 75(5), 694-704.

[5] Gevorkov, Y., Barty, A., Brehm, W., White, T. A., Tolstikova, A., Wiedorn, M. O., ... & Yefanov, O. (2020). pinkIndexer–a universal indexer for pink-beam X-ray and electron diffraction snapshots. Acta Crystallographica Section A: Foundations and Advances, 76(2), 121-131.