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Background Impact on 3D CXDI reconstruction of single particles.

Coherent X-ray diffractive imaging (CXDI) of single particles at X-ray free-electron lasers (XFEL) is a method to determine structure. Single particles are injected sequentially at unknown, random orientations into the intense XFEL beam and noisy diffraction patterns are measured, known as diffraction before destruction.[1] We orient these patterns using the expand, maximize and compress (EMC) algorithm, resulting in a three-dimensional diffraction intensity map.[2] The goal of the method is to reconstruct the structure of the sample, but for this we also need to recover the phases which is possible by iteratively applying constraints in real space, a positive density in a restricted volume, and fourier space where we constrain the intensities using our result from EMC.

The samples are injected and aerosolized by electrospray and launched into the XFEL beam, but the carrier gas contributes to the diffraction patterns as background. [3] We want to help plan experiments to see if they are feasible given expected signal and background levels with regards to EMC and phase retrieval.

To test this we used background measurements from an electrospray injector at the European XFEL combined with simulated signal diffraction patterns of phytochrome. We tested the performance of the EMC algorithm with various amounts of background and signal photons in the diffraction patterns. After subtracting the background of the final models we could perform phase retrieval, solving the structure for many of the cases. Finally we could compare the results from the different combinations for EMC and phase retrieval.

We found by running EMC multiple times for the same combinations of signal and background that successful EMC convergence is insensitive to the random initial conditions. Using the phase retrieval transfer function (PRTF) [4] method of calculating the resolution of the reconstruction we can see how the resolution deteriorates as we increase the background.

[1] Chapman, H. N. (2019). X-Ray Free-Electron Lasers for the Structure and Dynamics of Macromolecules. Annual Review of Biochemistry, 88(1), 35–58.
[2] Loh, N. T. D., & Elser, V. (2009). Reconstruction algorithm for single-particle diffraction imaging experiments. Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, 80(2), 1–20.
[3] Bielecki, J., Hantke, M. F., Daurer, B. J., et al. (2019). Electrospray sample injection for single-particle imaging with x-ray lasers. Science Advances, 5(5).
[4] Chapman, H. N., Barty, A., Marchesini, S., Noy, A., Cui, C., Howells, M. R., Rosen, R., He, H., Spence, J. C. H., Weierstall, U., Beetz, T., Jacobsen, C., & Shapiro, D. (2005). High-resolution ab initio three-dimensional X-ray diffraction microscopy.

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