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Three-dimensional reconstruction of the Melbournevirus from experimental coherent diffractive imaging data

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Diffraction before destruction using x-ray free-electron lasers (XFELs) has the capability to determine radiation damage-free structures without the need for crystallization. In this poster we present the 3D reconstruction of the Melbournevirus from single-particle x-ray diffraction patterns collected at the LINAC Coherent Light Source (LCLS) and use reconstructions from simulated data to explore the limitations of experimental sources of noise. [1] The reconstruction from experimental data suffers from a strong artifact in the center of the particle, which could be reproduced with simulated data by adding experimental background to the diffraction patterns. In the simulations, the relative density of the artifact increases linearly with background strength. This indicates that the artifact originates from the Fourier transform of the relatively flat background, concentrating all power in a central feature of limited extent. In addition to background scattering, large amounts of blurring in the diffraction patterns were found to introduce diffuse artifacts that could easily be mistaken as biologically relevant features. Sample heterogeneity and variation of pulse energy did not significantly affect the quality of the reconstructions. We anticipate that these artifacts can be minimized by the recent inauguration of high repetition-rate XFELs, which would allow for larger data volumes that could increase the signal-to-background ratio, and the development of background-aware 3D Fourier volume assembly algorithms, which would maximize the use of existing data.

References

[1] I. V. Lundholm et al., submitted to IUCrJ (2018).

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