

Analysis of 3D structure resolution limits in single particle imaging with limited data

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Abstract

The ability to discover three-dimensional structure of biomolecules, like proteins and viruses, is crucial in biology and medicine. With the invention of super-bright X-ray free electron lasers (XFELs), scientists can now collect diffraction images from individual particles, but there are still challenging problems in reconstruction of high-resolution 3D structures of biomolecules from XFEL experimental data.

In real experiments the diffraction intensity from biological molecules is often weak, a small number of photon is registered at the detector, especially at high wavenumber pixels. Also experiment setup, sample preparation and injection are still challenging problems resulting in a limited number of quality diffraction patterns obtained during the experiment. Thus an important problem arises as how the amount and quality of diffraction patterns affect the result and resolution of the final 3D structure.

In the framework of the study, a single-particle experiment was simulated using the Dragonfly software [1] and it was determined how the number of diffraction images and the number of diffracted photons affects the resolution and what is the threshold values of these parameters when it is possible to make a three-dimensional reconstruction.

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1. Ayer, K., Lan, T. Y., Elser, V., & Loh, N. D. (2016). Dragonfly: an implementation of the expand-maximize-compress algorithm for single-particle imaging. *Journal of applied crystallography*, 49(4), 1320-1335.