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## Toward three-dimensional structure using X-ray free-electron laser

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X-ray free electron laser (XFEL) is an exciting new technology that could significantly extend our structural knowledge of biological systems. One of the experimental approaches currently pursued is “single particle analysis,” in which intense laser light from XFEL is used to observe single molecular complexes. Since it does not require crystallization, various systems could be studied under different physiological conditions. However, applications to biological systems are still challenging due to their low diffraction power and require further developments of experimental as well as computational analysis techniques.

Therefore, we have been developing programs to perform three-dimensional reconstruction from a data set of diffraction patterns by adopting algorithms used in cryo-EM 3D reconstruction to handle XFEL diffraction patterns. This approach was successfully tested with X-ray tomography experimental data. Using synthetic data, we have estimated the experimental conditions necessary to achieve sub-nanometer resolutions for molecules such as the ribosome. In addition, we have investigated the molecular size dependence on the achievable resolution. Finally, after processing nanoparticles’ experimental diffraction patterns to reduce background noise, we obtained a 3D shape consistent with scanning electron microscope images.

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