MS046.O03

Virus structures recovered from correlations in scattered XFEL pulses

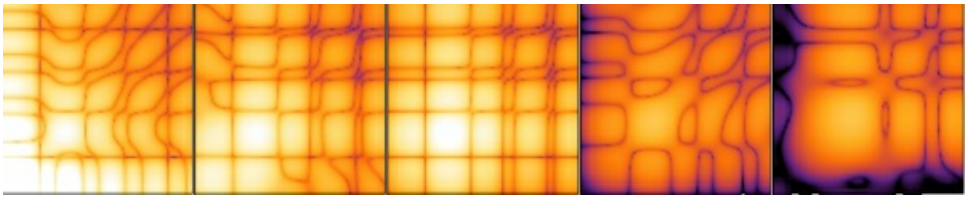
Ruslan Kurta[1], Jeffrey Donatelli[2], Chun Yoon[3], Andrew Aquila[3], Peter Zwart[4], Adrian Mancuso[1]
[1]European XFEL, Schenefeld, Germany, [2]Mathematics Department, Lawrence Berkeley National Laboratory and Center for Advanced Mathematics for Energy Research Applications, Berkeley, United States, [3]SLAC National Accelerator Laboratory, Menlo Park, United States, [4]Molecular Biophysics and Integrated Bioimaging, Lawrence Berkeley National Laboratory and Center for Advanced Mathematics for Energy Research Applications, Berkeley, United States
E-mail: ruslan.kurta@xfel.eu

Serial femtosecond crystallography (SFX) at x-ray free electron lasers (XFELs) offers outstanding possibilities for structure determination of complex biological macromolecules which can form crystals. For those structures which cannot be easily crystallized an alternative technique of single particle coherent diffraction imaging (SPI) has been proposed. It was predicted that diffraction patterns from single particles, for instance macromolecules or viruses, can be measured in "destruction before diffraction" experiments at XFELs before the sample is destroyed by intense radiation, and hence their damage-free structure identified. Substantial technical and algorithmic achievements have now made it possible to perform such measurements. However, the limited resolution of the reconstructed biological samples demonstrated so far demands further theoretical and experimental efforts to establish SPI techniques at XFELs [1]. Therefore, alternative methods for structural characterization of nanoscale objects at XFELs are of great interest.

Here we apply the fluctuation x-ray scattering (FXS) technique, which is based on the analysis of angular cross-correlation functions from scattered x-ray pulses, to XFEL diffraction data. In the most general case, FXS aims to recover the structure of a single particle from a translationally and rotationally disordered ensemble of many reproducible particles [2]. Therefore, FXS is expected to be especially advantageous for weakly scattering objects, for which crystalline samples cannot be generated, and could potentially close the gap between conventional SPI and SFX techniques.

We employed FXS to recover the three-dimensional (3D) structure of free-flying virus particles measured with the Linac Coherent Light Source (LCLS) [3]. We determined 2D correlation maps, which comprise a complex fingerprint of the whole 3D structure of a virus (see figure). Our results of model-based structural analysis and ab-initio structure recovery reveal deviations of the virus structures from the expected icosahedral shape. Our findings demonstrate substantial potential of FXS for the future studies of structure and dynamics of biological materials with an XFEL.

[1] Aquila, A. et al. (2015). Structural Dynamics 2, 041701.
[2] Donatelli, J. J. et al. (2015). Proc. Nat. Acad. Sci. 112, 10286.
[3] Kurta, R. P. et al. (2017) in preparation



Keywords: single particle imaging, fluctuation x-ray scattering, x-ray free electron lasers