Contribution ID: **4** Type: **not specified**

A review of methods of resolution estimation for 3D reconstructions for nanoscale biological objects from experiments data on super-bright X-ray free electron lasers (XFELs)

Tuesday, June 9, 2020 11:45 AM (15 minutes)

The ability to investigate 3D structure of biomolecules, such as proteins and viruses, is essential in biology and medicine. With the invention of super-bright X-ray free electron lasers (XFELs) the Single Particle Imaging (SPI) approach allows to reconstruct 3D structures from many 2D diffraction images produced in the experiment by X-rays scattered on the biomolecule exposed in different orientations. Nowadays the Fourier shell correlation (FSC) [1] is the most common metric for estimating global resolution of the obtained 3D structures in SPI experiments, where the resolution is defined as the spatial frequency at which the correlation between two independently reconstructed structures is equal to some given threshold value. The choice of a threshold value is currently a controversial issue. In addition, this approach can't account fact that the quality of reconstruction can be uneven and depend on the specific area of the biomolecule. Thus, the issue of effective resolution estimation methods remains open. In this way we considered various alternative approaches to the resolution estimation from related scientific fields, such as cryogenic electron microscopy (local resolution estimation methods) and optics (digital camera resolution measurement), and analyzed the applicability of these approaches to resolution estimation in SPI experiments on XFELs. 1. Marin Van Heel and Michael Schatz (2005), Fourier shell correlation threshold criteria. Journal of Structural Biology 151(3): 25-262.

Presenter: Ms IKONNIKOVA, Kseniia (National Research Center «Kurchatov Institute»)

Session Classification: Session 4