Contribution ID: 3

## Modifications to the EMC algorithm for orientation recovery in Single Particle Imaging experiments on X-ray free electron lasers

Tuesday, June 9, 2020 12:00 PM (15 minutes)

The emergence of super-bright light sources - X-ray free electron lasers(XFELs) combined with Single Particle Imaging(SPI) method, makes it possible to obtain nanometer resolution 3D structure of biological particles such as proteins or viruses without needing to freeze them. SPI relies on the "diffraction before destruction" principle, meaning that each sample only produces a single diffraction image before being destroyed by an X-ray pulse. The orientation of the particle in the beam is random for each shot. This gives rise to the problem of orientation recovery, in which an array of 2D diffraction images has to be combined into a single 3D image, necessary for the reconstruction of 3D structure of the studied particle. The orientation recovery problem is most commonly solved by the EMC algorithm[1], which is the most computationally expensive part of data analysis for SPI experiments. In this work we introduce several modifications to the EMC algorithm aimed at improving the quality of reconstruction and/or increasing the algorithm's speed of convergence. We analyse the effectiveness of these modifications using simulated diffraction data. Loh, N. D. & Elser, V. (2009). Phys. Rev. E, 80, 026705.

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