European XFEL Theory Seminar

Thursday, 31 August 2017, 17:00
Campus Schenefeld, main building (XHQ) room E1.173

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Real-space local structure of disordered matter from fluctuation diffraction

Coherent diffraction from a disordered material is a seemingly random, continuous signal, which fluctuates as the beam is scanned across the sample. Statistical measures of these fluctuations contain significant information about local structure in the material. The widely used small-angle and wide-angle x-rays scattering methods (SAXS/WAXS) measure the mean signal that informs us about two-body real-space correlations, an effectively one dimensional data that gives limited information about 3D structure. The emerging cross-correlation methods aim to measure higher order statistics that contain multi-atom information. With electrons, this could be used to remedy the lack of knowledge about the local structure of amorphous materials, such as glasses. With x-ray free-electron lasers it is a potential route to determine the structures of non-crystalline proteins in an aqueous environment. The drawback is that cross-correlation data is difficult to interpret structurally. We have discovered a method of transforming cross-correlation data into a 3D real-space angular distribution function, which greatly facilitates direct structural interpretation. For amorphous matter, the real-space angular distributions contain a clear indication of the presence of medium range order (>5 Angstroms) and at the bond distance contain a symmetrised bond-angle distribution. For proteins and biological matter, the angular functions can provide greater sensitivity to protein conformation and inter-particle correlations than SAXS. Here we will present the background theory behind the technique and present some preliminary experimental results. We will discuss practical issues of experimental design such as resolution, the number of measurements required and expected signal-to-noise.

Host: Ruslan Kurta