Contribution ID: **32** Type: **not specified**

ML-driven Reconstruction of X-ray Scattering Data

Wednesday 12 May 2021 15:50 (10 minutes)

Recent developments in photon science enable the investigation of structures and fundamental dynamics at nanometer and femtosecond scales. The corresponding imaging techniques such as Small Angle X-Ray Scattering (SAXS) at Grazing Incidence (GI-SAXS) or Ptychography produce imaging data at unprecedented spatial and temporal resolution. However, the reconstruction of relevant properties from the acquired incomplete X-ray intensities of SAXS, GI-SAXS or Ptychography requires to solve an ill-posed inverse problem which is commonly approached by Iterative reconstruction schemes that are typically time-consuming and require manual tuning of hyperparameters. Additionally, imaging of non-equilibrium processes prone to perturbations due to e.g. non-planar wavefronts hamper the usage of these methods even further and emphasise the need for very fast & automatic feedback systems. In this talk, we are introducing novel data-driven approaches for fast and reliable reconstruction of X-ray scattering data. The approaches can be seen as a combination of traditional data-driven methods, Bayesian statistics and optimisation resulting in reliable means for very fast reconstruction of known structures as well as robust reconstruction methods of previously unknown structures.

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Session Classification: Machine Learning