

A resilient feature extractor in SAXS images

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Research on the application of small-angle x-ray scattering (SAXS) method, using x-ray free-electron laser (XFEL) images, utilizes normalizing flows for the inversion of experimental X-ray scattering images. One of the main challenges lies in the inversion of such experimental scattering images, which contain various artifacts such as parasitic scattering, slit scattering, beamstop, and detector background. These artifacts pose a significant domain shift for the neural network used in the inversion process. Parasitic scattering typically appears as a Gaussian-shaped cluster around the primary beam, accompanied by scattered photons in the vicinity. Slit scattering manifests as streaks around the primary beam, while the beamstop obstructs the main beam entirely, resulting in a lack of signal. The detector background refers to an offset with some underlying structure. Currently, the simulated dataset is being modified to incorporate these artifacts. However, this approach may not be sustainable in the future, as the exact characteristics of the artifacts are unknown in advance, and there is limited time to model them during the experiment. Hence, the intention is to collaborate in developing a resilient feature extractor capable of extracting features from both simulated and experimental data, even in the presence of unknown artifacts. These extracted features will subsequently be utilized for the inference process in the primary neural network responsible for inversion.

We aim to address the problem by using contemporary deep learning techniques. At present, we are exploring two potential approaches: one involves learning representation through β -VAE, while the other entails utilizing image-to-image translation methods such as CycleGAN and pix2pix.

Primary authors: EREN, Engin (IT (Research and Innovation in Scientific Co)); THIESENHUSEN, Erik (Eur.UPEX); HUANG, Lingen (Eur.UPEX); HEUSER, Philipp (DESY/Helmholtz Imaging)

Presenter: EREN, Engin (IT (Research and Innovation in Scientific Co))

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