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MONTE CARLO RAY TRACING OF SCANNING COHERENT DIFFRACTION IMAGING

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INTRODUCTION: Coherent diffractive imaging (CDI) techniques have gained significant momentum in recent years, and most synchrotrons have dedicated beamlines for CDI techniques, with full-field CDI and ptychography among the most commonly applied. Simulations of CDI experiments can assist in interpretation of data by helping to distinguish signal from noise, or allow design of experiments that minimize X-ray dose. Several factors are however hampering simulations in a ray tracing framework, and so far only simplified test-cases have been reported.

EXPERIMENTAL: We implemented strategies for correct and efficient simulation of diffraction, i.e. enacting Huygens principle by a Monte Carlo process that maximizes yield of computational effort. The sample is specified in terms of its transfer function as a 2D mask of refractive indices. Some meaningful test cases are considered, and the validity of the diffraction patterns then obtained is examined by comparison to expected theoretical expressions, or by inspection of the reconstructions.

RESULTS AND DISCUSSION: We show that diffraction patterns of gratings are properly computed and closely follow the expected theoretical trends; the full-field CDI patterns can be Fourier transformed yielding a noisy version of the initial object; the ptychographical data-set produced by McXtrace (Figure) can be effectively reconstructed by a standard phase retrieval algorithm (ePIE[1], difference map[2]).

CONCLUSIONS: We detail and discuss the new CDI simulation capabilities of McXtrace[3], with a particular focus on ptychography. Ongoing work aims at assessing the signal to noise ratio (SNR) of simulated diffraction patterns of a volume of refractive indices, representing realistic volumetric samples.

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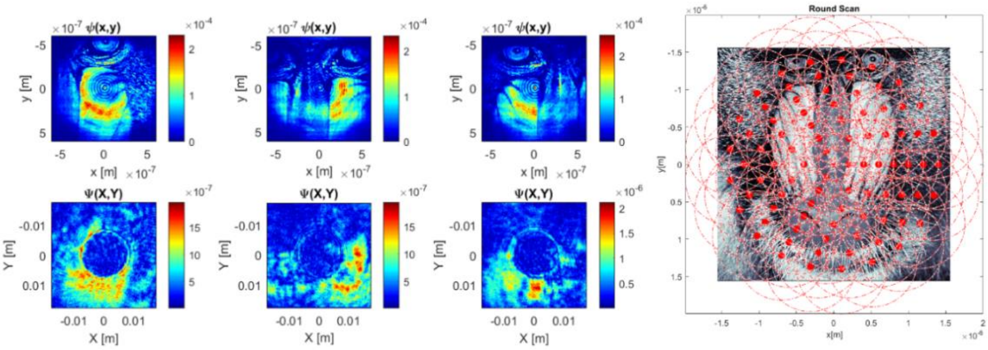

Transmission images (top) and diffraction patterns (bottom) from the ptychographical dataset of a simulated concentrical raster scan (right).