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Start-to-End XFEL experiment simulation:A framework and coherent imaging example

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The advent of newer, brighter, and more coherent X-ray sources, such as X-ray Free Electron Lasers (XFELs), represents a tremendous growth in the potential to apply coherent X-rays to determine the structure of materials from the micron-scale down to the Angstrom-scale. We present a framework for Start-to-End (S2E) simulations of a coherent X-ray experiment, including source parameters, propagation of the coherent X-rays though optical elements, interaction of the photons with matter, and their subsequent detection and analysis. To demonstrate this framework, we show a single-particle structure determination example using parameters of the Single Particles, Clusters and Biomolecules (SPB) instrument [1] at the under-construction European XFEL [2, 3]. We use cross platform wave optics software [4] for the propagation of the coherent beams, a molecular dynamics treatment of real space dynamics of atoms, ions and free electrons to account for radiation damage [5], and the Expansion-Maximization-Compression (EMC) algorithm [6] for assembling the simulated data before subsequent phasing and structure determination. It is hoped such simulations can provide an insight into the critical regions of parameter space for the single-particle imaging problem, and hence direct efforts to best utilize these next generation light sources.

[1] *A. P. Mancuso, et al, Technical Design Report: Scientific Instrument Single Particles, Clusters, and Biomolecules (SPB), http://dx.doi.org/10.3204/XFEL.EU/TR-2013-004, (2013,* ***[2]*** *L. Samoylova, et al, Proc. of SPIE Vol. 8141, 81410A1-10 (2011),* ***[3]*** *N.-T. D. Loh and V. Elser, Phys. Rev. E 80, 026705 (2009).*

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