WP 4 – SIMEX

Milestone M4.2: Demonstration of a first example simulation

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Contents

1 Summary

Milestone M4.2 (as detailed in **Task 4.2.1**) of the SIMEX workpackage in EUCALL is the demonstration of a first example simulation. In this example, we simulate a single–particle imaging experiment at the European X–ray Free Electron Laser. FEL pulses of 3 fs, 9 fs and 30 fs pulse duration and 4.96 keV photon energy are propagated through the SASE 1 beamline and the focusing optics of the SPB-SFX scientific instrument. In the focus, the photons interact with the 2NIP molecule and scatter into a pixel area detector situated 13 cm behind the sample. We save each simulated diffraction pattern and feed the patterns into the orientation reconstruction algorithm EMC. Statistical analysis of oriented 3D diffraction datasets allows to assess the data quality of our simulated data as a function of the pulse duration, which is is controlled through the machine parameters of the FEL, in particular the electron bunch charge.

The results of this study analyis of the simulated diffraction patterns are published in Ref. [**Fortmann-Grote2017**], a copy is attached to this report. In addition, we published the individual datasets resulting from the simulation modules on the EUCALL Data Repository hosted on Zenodo.

Tutorials for the individual simulation steps can be found on the SIMEX wiki and on the EUCALL youtube channel. Finally, the reference manual of the simulation environment simex_platform contains a description of the data formats of all relevant simulation datasets, see also Milestone M4.1.

2 Supporting material

Module	Dataset	Usage instruction	Data format
FEL source	10.5281/zenodo.855301	Manual Video	Manual
Propagation	10.5281/zenodo.884873	Manual	Manual
Interaction	10.5281/zenodo.886061	Manual	Manual
Diffraction	10.5281/zenodo.886087	Manual	Manual

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