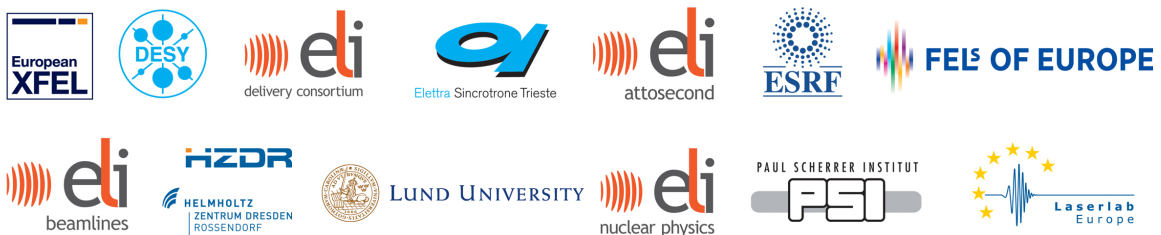


## WP 4 – SIMEX

# 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 controlled through the machine parameters of the FEL, in particular the electron bunch charge.

The results of this study analysis 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	<a href="#">10.5281/zenodo.855301</a>	<a href="#">Manual Video</a>	<a href="#">Manual</a>
Propagation	<a href="#">10.5281/zenodo.884873</a>	<a href="#">Manual</a>	<a href="#">Manual</a>
Interaction	<a href="#">10.5281/zenodo.886061</a>	<a href="#">Manual</a>	<a href="#">Manual</a>
Diffraction	<a href="#">10.5281/zenodo.886087</a>	<a href="#">Manual</a>	<a href="#">Manual</a>