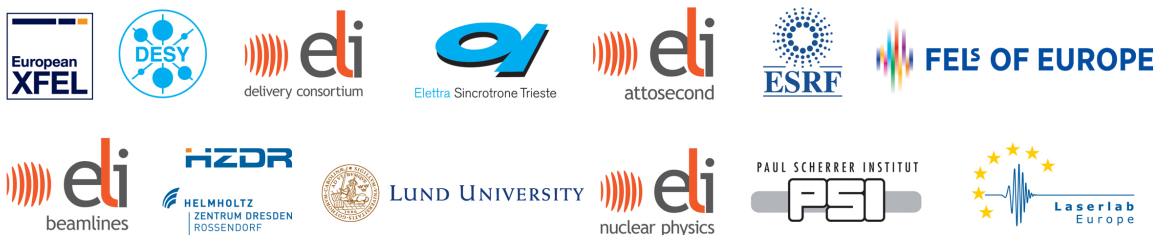


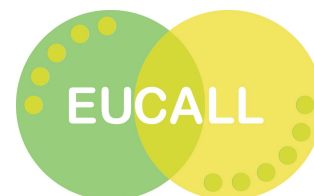
WP 4 – SIMEX

Milestone M4.2: Demonstration of a first example simulation

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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 us 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 are published in Ref. [1]. In addition, we published the individual datasets resulting from the simulations on the [EUCALL Data Repository](#) hosted on [Zenodo](#). We note in passing that the deposition of diffraction data from a non-plasma sample [5] partially fulfills SIMEX Deliverable D4.4. Coherent diffraction data from a plasma sample was accomplished in Milestone M4.3 (Interoperability of simulations) [3].

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 [4].

Newer simulations, studying proteins embedded in a solvent (water) were recently presented at the Optics and Photonics Conference 2017 [2].

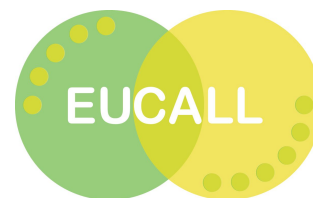
2 Supporting material

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

Articles

1. Fortmann-Grote, C., Buzmakov, A., Jurek, Z., Loh, N.-T. D., Samoylova, L., Santra, R., Schneidermiller, E. A., Tschentscher, T., Yakubov, S., Yoon, C. H., Yurkov, M. V., Ziaja-Motyka, B., and Mancuso, A. P., *Start-to-end simulation of single-particle imaging using ultra-short pulses at the European X-ray Free-Electron Laser*, *IUCr* **4**, 560–568 (2017).





2. Fortmann-Grote, C., Bielecki, J., Jurek, Z., Santra, R., Ziaja-Motyka, B., and Mancuso, A. P., *Simulations of single-particle imaging of hydrated proteins with x-ray free-electron lasers*, in *Advances in Computational Methods for X-Ray Optics IV*, SPIE Optical Engineering + Applications, **10388**, (International Society for Optics and Photonics, 2017), 103880M, doi:[10.1117/12.2275274](https://doi.org/10.1117/12.2275274).

Project Reports

3. Fortmann-Grote, C., Andreev, A., Sharma, A., Briggs, R., Garten, M., Huebl, A., Grund, A., Kluge, T., Yakubov, S., Bussmann, M., and Mancuso, A. P., *Milestone M4.3, Demonstration of interoperable simulations*, Project Milestone report, (European Cluster of Advanced Laser Lightsources (EUCALL), 2017), doi:[10.5281/zenodo.897650](https://doi.org/10.5281/zenodo.897650), <<https://dx.doi.org/10.5281/zenodo.897650>>.
4. Fortmann-Grote, C., Andreev, A., Briggs, R., Bussmann, M., Huebl, A., Kluge, T., Pascarelli, S., Sharma, A., and Mancuso, A. P., *Milestone M4.1, Delivery of individual simulation modules and common interfaces for interoperability*, Project Milestone report, (European Cluster of Advanced Laser Lightsources (EUCALL), 2016), doi:[10.5281/zenodo.896329](https://doi.org/10.5281/zenodo.896329), <<https://dx.doi.org/10.5281/zenodo.896329>>.

Datasets

5. Fortmann-Grote, C., *Simulated coherent diffraction from 2NIP (SPB-SFX instrument, 3 fs, 4.96 keV European XFEL pulses)*, European Cluster of Advanced Laser Lightsources (EUCALL), <<https://dx.doi.org/10.5281/zenodo.886087>> (2017).

