EUCALL

WP 4 – SIMEX

Milestone M4.3: Simulations interoperable

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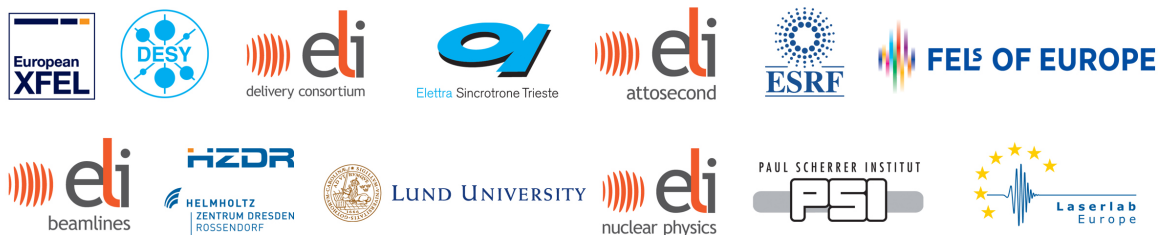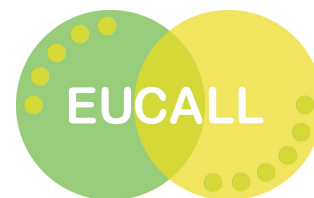
1 Summary

Simulations in SIMEX are now interoperable. The simulation platform *simex_platform* [1, 2, 3], publicly available from https://www.github.com/eucall-software/simex_platform under the conditions of the open source license GPL-v3 [4], enables start–to–end simulations of various types of photon experiments using different sources (X–ray free electron lasers, synchrotrons, optical lasers), different means of photon propagation from the source to the sample (coherent wavefront propagation, x–ray tracing), various types of photon matter interaction (particle–in–cell, radiation–hydrodynamics, molecular dynamics, continuum plasma theory), signal generation (coherent diffraction from plasma and non–plasma samples, inelastic scattering, x–ray absorption spectroscopy) and detector simulations.

Details and use cases, demonstrating how the various simulation modules can be used in an interoperable and interchangeable way are given in the Milestone document M4.2 [5] and Deliverable Report D4.3 [6]. In particular, use of custom as well as generic metadata standards and data formats facilitate the transfer of simulation data between modules, which fulfills the requirement of "interoperability".

Modules are interchangeable, e.g. a coherent diffraction imaging experiment for a molecular sample can be altered into a diffraction experiment for a crystalline sample by switching just one simulation module, the signal generator. These and other applications are also demonstrated in online tutorials, located on the wiki pages of *simex_platform* at https://www.github.com/eucall-software/simex_platform/wiki.

The release of version 0.3.3 of *simex_platform* [7] marks the project milestone M4.3.

References

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2. Fortmann-Grote, C., Andreev, A. A., Appel, K., Branco, J., Briggs, R., Bussmann, M., Buzmakov, A., Garten, M., Grund, A., Huebl, A., Jurek, Z., Loh, N. D., Nakatsutsumi, M., Samoylova, L., Santra, R., Schneidmiller, E. A., Sharma, A., Steiniger, K., Yakubov, S., Yoon, C. H., Yurkov, M. V., Zastrau, U., Ziaja-Motyka, B., and Mancuso, A. P., *Simulations of ultrafast x–ray laser experiments*, in *Advances in X-ray Free-Electron Lasers Instrumentation IV*, SPIE Optics + Optoelectronics, **10237**, (International Society for Optics and Photonics, 2017), 102370S, doi:`10.1117/12.2270552`.

3. *The github repository for simex_platform*, <`https://github.com/eucall-software/simex_platform`>.

4. *GNU General Public License*, version 3, Free Software Foundation, <`http://www.gnu.org/licenses/gpl.html`> (2007).

5. Fortmann-Grote, C., *Milestone M4.2, First example simulation*, Project Milestone report, (European Cluster of Advanced Laser Lightsources (EUCALL), 2017), doi:`10.5281/zenodo.998696`, <`https://dx.doi.org/10.5281/zenodo.998696`>.
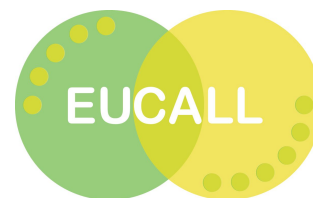
6. Fortmann-Grote, C., Andreev, A., Sharma, A., Briggs, R., Garten, M., Huebl, A., Grund, A., Kluge, T., Yakubov, S., Bussmann, M., and Mancuso, A. P., *Deliverable D4.3, Interoperability of simulation workflows*, Project Deliverable report, (European Cluster of Advanced Laser Lightsources (EU-CALL), 2017), doi:`10.5281/zenodo.998647`, <`https://dx.doi.org/10.5281/zenodo.998647`>.

7. Fortmann-Grote, C., *simex_platform version 0.3.3*, European Cluster of Advanced Laser Light-sources (EUCALL), <`https://github.com/eucall-software/simex_platform/releases/tag/v0.3.3`> (2017).