

## Toward a digital twin at the NeXus file level

Here, we report on our approach to establish a durable, rigid connection between the Aquarius beamline at synchrotron source Bessy II and its digital counterpart build in the simulation software Ray-UI [1]. While simulations play a crucial role in the instrument design as a digital precursor of the real-world object and contain a comprehensive description of the setup, usually the digital representation is neglected once the real instrument is fully commissioned.

To preserve the symbiosis of simulated and real-world instrument beyond commissioning and approach the digital twin concept we combine the two worlds at the NeXus file level [2]. For this purpose, the instrument section of the NeXus file is enriched by detailed simulation parameters where the current state of the instrument is reflected by including real motor positions, e. g. to incorporate the actual aperture of a slit system. As a result, on one hand, the enriched instrument description increases the reusability of experimental data in sense of the FAIR principles [3] and, on the other hand, allows to perform simulations of a measurement from the NeXus file, ready to be exploited by machine-learning techniques, e. g. for predictive maintenance.

[1] P. Baumgärtel, P. Grundmann, T. Zeschke, A. Erko, J. Viefhaus, F. Schäfers, and H. Schirmacher, RAY-UI: New Features and Extensions, AIP Con. Proc. 2054, 060034 (2019).

[2] <https://manual.nexusformat.org/index.html>

[3] Wilkinson, M., Dumontier, M., Aalbersberg, I. et al. The FAIR Guiding Principles for scientific data management and stewardship. Sci Data 3, 160018 (2016). <https://doi.org/10.1038/sdata.2016.18>

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Digital Twin, Simulation, NeXus, Instrumentation

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