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#1-46 Harnessing Digital Twins and Simulation for Advancing Neutron Experimentation

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Data from virtual experiments are becoming a valuable asset for research infrastructures: to develop and optimise current and future instruments, to train in the usage of the instrument control system, to study quantifying and reducing instrumental effects on acquired data. Furthermore large sets of simulated data are also a necessary ingredient for the development of surrogate models (supervised learning) for faster and more accurate simulation, data reduction and analysis. So far, the production and usage of data from virtual experiments have been mostly reserved to simulation experts. In this work, we present how at ILL data from virtual experiments are made available to the general users.

The presented framework wraps in a digital twin of the facility instruments, the knowledge of its physical description, the simulation software and the high performing computing setup. The twin presented in this paper has been developed at the ILL in the framework of the PANOSC European project in close collaboration with other research facilities (ESS and EuXFel) for some of its essential components. An overview of the core simulation software (McStas), its Python API (McStasScript), the public instrument description repository and the instrument control system (NOMAD) are given. The choices on the communication patterns, based on ZMQ, and interaction between the different components are also detailed. A flavour of advanced features like collision prediction will also be provided.

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