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Integrated Computational Workflows for the MIRACLES Backscattering Spectrometer at ESS

Among the instrument suite which is currently constructed at the European Spallation Source (ESS), the time-of-flight backscattering spectrometer Miracles [1] will provide the highest energy resolution permitting diverse studies of molecular dynamics.

This poster contribution is focusing on the computational aspects of the spectrometer.

To support efficient and reproducible research, MIRACLES integrates a robust computational pipeline covering both the data reduction and scientific analysis.

Following data collection, mimicked by McStas simulations [2] of the instrument, Scipp [3] enables flexible, performant reduction of event-based neutron data, leveraging Python workflows tailored to MIRACLES' needs. The workflow further supports advanced analysis via the easy science software package [4].

By combining simulation, reduction, and analysis, the MIRACLES computational environment fosters rapid, transparent scientific insight and user engagement. We present an overview of these tools, illustrate typical workflows, and show how computational integration at ESS accelerates both instrument development and experimental science.

[1] Félix J. Villacorta et al, Rev. Sci. Instrum. 96, 045101 (2025)

[2] P. Willendrup, and K. Lefmann, Journal of Neutron Research, vol. 23, 2021

[3] Simon Heybrock, et al, Scipp, doi.org/10.5281/zenodo.17513273

[4] <https://app.easyscience.software/>

Session

Instrumentation

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