

15th International Conference on Muon Spin Rotation, Relaxation and Resonance



Contribution ID: 177

Type: Oral

MuSpinSim: spin dynamics calculations for muon science.

Wednesday, 31 August 2022 10:40 (20 minutes)

MuSpinSim is a Python software to simulate muon (μ SR) experiments. In particular, it simulates the spin dynamics of a system of a muon plus other spins such as electrons and atomic nuclei. MuSpinSim can simulate various common experimental setups used in μ SR, such as zero, transverse and longitudinal field experiments; and it can simulate μ SR experiments that are resolved in time, field, or temperature. Furthermore, MuSpinSim can account for the effects of hyperfine, dipolar, quadrupolar and Zeeman couplings, as well as simulate quantum systems exchanging energy with the environment with the Lindblad master equation. Finally, MuSpinSim can be used to fit experimental μ SR data with simulations that use all of the capabilities described above. The fittings can be run in parallel on multiple cores, which significantly reduces the computational cost of the most expensive tasks. In this work, we present the Python package MuSpinSim with all the utilities it provides to facilitate simulations of μ SR experiments, demonstrate the effectiveness of the method with some chosen example systems and show a prototype application of MuonGalaxy, a web-based implementation of MuSpinSim that is based on the Galaxy platform.

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Session Classification: Oral contributions

Track Classification: Site calculations