Contribution ID: **86** Type: **Poster**

MDMC: a new program to refine force field parameters against experimental data

Monday, 20 March 2023 16:00 (2 hours)

We present a newly developed program that combines molecular dynamics (MD) simulations with an optimisation protocol. e.g. using Monte Carlo (MC) methods, in order to determine the force field parameters values that lead to the best agreement with experimental data. The program is currently focussed on classical MD simulations and quasi-elastic neutron scattering (QENS) data, such as dynamic structure factor measurements. However, the program is designed to be extensible to other simulation engines and measurable data types.

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Session Classification: Poster Session MONDAY

Track Classification: Neutron Instrumentation, Optics, Sample Environment, Detectors, and Software