Contribution ID: **372** Type: **Talk (17 + 3 min)**

AI-assisted neutron spectroscopy - Log-Gaussian processes for TAS

Wednesday, March 22, 2023 12:10 PM (20 minutes)

Three-axes spectroscopy (TAS) is a well-established method that has not substantially changed in the past decades of its use. Nowadays, with increasing demand and limited availability of TAS, application of AI methods is one option to increase their efficiency. From an AI perspective, TAS experiments collect noisy observations of a 2D intensity function to investigate a material of interest. If the intensity distribution is unknown, experimenters usually decide manually where to place measurements for a rapid overview. AI methods can assist this process by avoiding measurements in the background but preferring more informative regions of signal while taking instrument costs into account. Our method for discovering regions of signal is based on Gaussian Process Regression as a technique for probabilistic approximations of log-intensity functions. It handles noise and background and respects weak as well as strong intensities to avoid loss of information. For example, for simple dispersions like intensity-modulated phonons, full information can be achieved only within a reasonably short amount of experimental time. The algorithm was tested on simulated intensity functions (e.g., CEF, phonon, SDW) and experimentally on EIGER/PSI. In order to quantify the benefit of our approach, we present results of a benchmarking procedure that we have developed as a cost-benefit analysis in a synthetic but still representative setting.

Author: Dr TEIXEIRA PARENTE, Mario (JCNS at MLZ, Forschungszentrum Jülich)

Co-authors: Mr BRANDL, Georg (JCNS at MLZ, Forschungszentrum Jülich); Dr FRANZ, Christian (JCNS at MLZ, Forschungszentrum Jülich); Dr STUHR, Uwe (Paul Scherrer Institute); Dr GANEVA, Marina (JCNS at MLZ, Forschungszentrum Jülich); Dr SCHNEIDEWIND, Astrid (JCNS at MLZ, Forschungszentrum Jülich)

Presenter: Dr TEIXEIRA PARENTE, Mario (JCNS at MLZ, Forschungszentrum Jülich)

Session Classification: Data Evaluation & Software 2

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