MDANSE2018
(Molecular Dynamics and Lattice Dynamics to Analyse Neutron Scattering Experiments)
Materials and Neutron Scattering Instrument Modelling.

Sept 23rd-29th 2018 - Puerto de la Cruz, Tenerife

Scope:

Simulation of Inelastic Neutron Scattering using McStas and material dynamics models

The neutron scattering technique is a perfect tool to measure the density of states, the intra-molecular and dispersion relations in materials, complementary to x-rays due to different interaction cross sections. Given the increasing complexity of the materials studied nowadays, the use of computational tools has become essential to complement and help in the understanding of the experimental data. In particular, DFT and MD calculations are indispensable to interpret measured neutron vibrational density of states or phonon dispersion curves. Therefore the school will be focused on showing how computational codes can be applied to calculate experimental spectra. As such this school is at the interface between computational and experimental scientists and we intend to bring together both communities. The expected attendees will be either scientists with a strong computational background and collaborating with experimental groups (in particular neutron scattering users) or experimentalists with some previous knowledge of electronic-structure calculations and/or force-field based simulations. Both will learn how to use existing modern tools to compute the measured signal (including instrument effects) starting from an initial structure, down to the neutron scattering intensity, helping to bridge the gap between experiment and simulation.

The MDANSE 2018 school intends to train neutron scientists to better design new instruments, but also to make better use of the allocated beam time. It has specialized scope (inelastic scattering, material modelling) and covers many existing or planned neutron scattering instruments. The school will not focus on the data analysis, but rather on all aspects of simulation, from materials to instruments, and present an integrated pipeline.

The MDANSE 2018 is focused on the calculation of materials dynamics, e.g. dynamic structure factor S(q,w) vibrational properties, using both DFT and classical MD codes. This calculation will then be forwarded to full virtual experiments of neutron scattering spectrometers in order to produce realistic simulated data, such as inelastic and quasi-elastic neutron scattering intensity. A set of representative spectrometer descriptions will be proposed to attendees, together with the so-called scattering kernels which model the neutron-matter interaction.

This school is the continuation of the MDANSE 2012 and 2014 at the ILL, and 2016 in ISIS <https://www.isis.stfc.ac.uk/Pages/MDANSE-2016.aspx> series. It also relates to previous neutron scattering instrument simulation McStas schools/workshops in 2006-2016 (<http://www.essworkshop.org/>).

The school targets scientists with confirmed knowledge in inelastic scattering and/or materials modelling, whereas previous such schools were more oriented towards beginners. It will consist mainly in practicals and hands-on sessions.

This MDANSE event will build a bridge between the two communities: materials and neutron scattering instrument modelling.

Programme:

Preparing data for neutron scattering virtual experiments:

- *Initial input: atomic configuration (CIF, PDB, data bases, ...)*
- *Phonons in single crystals (lattice dynamics, ASE, PhonoPy, VASP, QE, ...)*
- *Vibrational modes in powders and liquids (MD trajectories, nMoldyn/MDANSE)*
- *Magnons (SpinW)*
- *Cross sections from simple models (S(a,b), ENDF, Nuclear data bases)*

McStas inelastic neutron scattering spectrometers models:

- *Triple-Axis Spectrometers and multiplexed versions*
- *Time of Flight Spectrometers*
- *Molecular spectroscopy*
- *QENS*

McStas scattering kernels:

- *Incoherent scatterer*
- *Liquids/Powders (Isotropic Sqw)*
- *Single crystal inelastic scattering*
- *Single crystal mixed with other kernel*
- *Structure (diffraction: powder, single crystal)*

Full simulation pipeline:

- *DFT/MD → McStas format → Virtual experiment*
- *Data treatment can be done using Mantid and similar tools*

Date and Venue:

The school will take place in Hotel Be.Live Orotava, Puerto de la Cruz, Tenerife from Sept. 23rd to 29th.

Registration:

Before May 15th 2018 at <http://www.isis.stfc.ac.uk/Pages/MDANSE_2018.aspx>. Registration cost will be 125 euros, which includes a full accommodation, teaching materials, smiles and sun. Maximum audience: 25.

Organizers and Contacts:

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