

MDANSE – school: Molecular Dynamics (and Lattice Dynamics) to Analyse Neutron Scattering Experiments

9-10 May 2014, Grenoble (France)

Organizers: Miguel A. Gonzalez and Mark R. Johnson

This school aims to train the participants in the use of modern simulation tools in the context of analyzing and interpreting experimental, neutron scattering data. It will be focused mainly on practical training, so the number of participants is limited to 30. Taking into account the QENS2014 and WINS 2014 conferences in the nearby location of Autrans from May 11 to May 16 (<http://www.ill.eu/news-events/events/qens-2014-wins-2014/>), the school will be a satellite event. Therefore the school will be focused on the use of Molecular Dynamics simulations to explore diffusive processes on the time scales covered by quasielastic neutron scattering spectrometers and Lattice Dynamics to study phonon dispersion curves and vibrational densities of states that are typically measured with inelastic neutron scattering spectrometers.

The goal of this school is therefore to show how widely-available simulation tools can be applied to the analysis and interpretation of neutron scattering data. The school will last 2 days and will concern mainly the practical aspects of running and analyzing simulations so that, firstly, numerical and experimental data can be directly compared and, secondly, simulations can then be investigated in atomic detail. A range of simulation codes allowing electronically complex materials, molecular and polymer systems, porous media and bio-molecules to be handled, will be made available to participants on the cluster at ILL. Simulation analysis will focus on using the nMoldyn code. McStas will be used to incorporate the instrument response in a virtual experiment. Model analysis and fitting tools applicable both to simulated and experimental data will also be presented. Lectures on the fundamental aspects of running and analyzing simulations will be complemented by hands-on tutorials.

In view of the practical nature of the school, a maximum of 30 participants will be accepted. In view of the close link with the QENS and WINS 2014 conference, any conference participant wanting to attend the school will be given priority. Scientists may attend the school and not the conference. In order to select candidates in case of over-demand, we ask applicants to state briefly their scientific fields of interest, why they would like to attend the school and previous experience with computer simulations.

Fees: A single fee of 100 € is requested. This fee includes the accommodation (3 nights from 8 to 11th May 2014 in the guesthouse), the meals in the canteen at midday and the school dinner.

Registration and deadlines: A web site (www.ill.eu/mdanse2014) will be open early January providing additional details and allowing registration for the school. The registration deadline is expected to be February 28 2014.

Provisional programme:

May 9: Introduction to molecular dynamics, force fields and analysis followed by practical session

May 10: Introduction to density functional theory and lattice dynamics followed by practical session

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