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Molecular (and lattice) dynamics to analyze neutron scattering experiments – MDANSE2018

The school on *Molecular (and Lattice) Dynamics to Analyse Neutron Scattering Experiments – MDANSE2018* was held on the picturesque island of Tenerife, Spain, September 24–28, 2018. This was the fourth school in this series. It was held at ILL, France in 2012 and 2014 and at ISIS, UK in 2016. This time, the event was jointly organized by Institut Laue-Langevin (ILL) (Grenoble, France), Technical University of Denmark (DTU) (Kgs. Lyngby, Denmark), the Data Management and Software Centre, European Spallation Source ERIC (ESS) (Copenhagen, Denmark) and ISIS at the Rutherford Appleton Laboratory (Harwell, UK). This was a perfect occasion to integrate ESS with other major neutron facilities, namely LLB, ILL and ISIS, along with DTU, and demonstrate the capability of next-generation software for simulations and analysis of neutron experiments. The school focused on simulation of inelastic neutron scattering using McStas and molecular dynamics models. It was generously supported by SINE2020 (www.sine2020.eu), ILL, ESS, DTU and ISIS. With 30 international participants across the globe, including Europe, India and China, the school was packed with hands-on tutorials and lessons given by leading experts in the field.

The weeklong meeting focused on showing how computational simulations can be applied to the calculation of experimental spectra. The two main computational methodologies, Molecular Dynamics (MD) and Lattice Dynamics (LD), were used to perform computer simulations of full virtual experiments of neutron scattering spectrometers that produced realistic simulated data for inelastic and quasi-elastic neutron scattering intensities. Both methods, MD and LD, were introduced by formal lectures on the morning of day one. Hands-on practicals (Figure 1) started from the afternoon of the same day. USB sticks were distributed to students with relevant software and data files. Hard copies of tutorial documents were also provided.

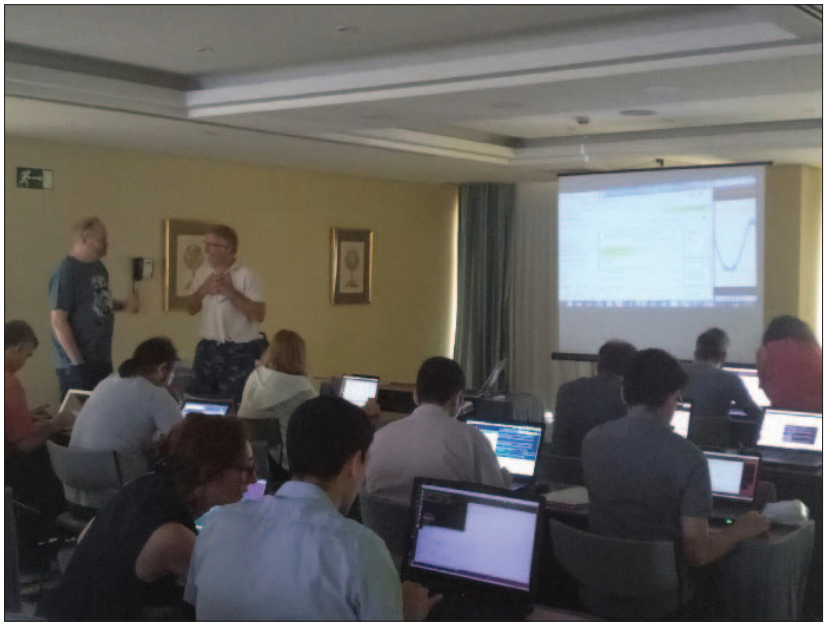

Figure 1. Students working attentively during a hands-on lesson during MDANSE 2018 (Image credit: Miguel A. Gonzalez).

Emmanuel Farhi (ILL) started the meeting by welcoming all delegates and highlighting the critical importance of virtual experiments for neutron spectroscopy. He was followed by Miguel González (ILL), who gave a concise introduction about the history of this school. Miguel started the first lecture of the school by giving a useful talk on MD simulation and its application in analyzing quasi elastic neutron scattering (QENS) spectroscopy. He was followed by Sanghamitra Mukhopadhyay (ISIS), who introduced electronic-structure methods and lattice dynamics. In the afternoon session, the students got their first opportunity to apply these theoretical lessons in a hands-on practical in which they compared their simulated results with experimental data to get a better idea of how simulations can help to analyze neutron experiments.

The second day started with lessons delivered by Sylvain Petit

(LLB) on spin-waves in magnetic materials, which was followed by practical sessions on using simulations to determine the exchange couplings and anisotropies in magnetic materials. Thomas Holm Rod (ESS) introduced the students to the Atomic Simulation Environment (ASE) in a hands-on tutorial in which it was demonstrated how ASE can be used to manipulate atomic structures and as a uniform interface to several different programs for performing MD and LD simulations. The practical was an introduction to using a *jupyter* notebook to undertake simulations. The second half of the day was devoted to instrument simulations using McStas. Peter K. Willendrup (DTU) gave a clear introduction about McStas instrument simulations methodology and its concept of components and classes, and was followed by Erik Knudsen (DTU), who explained how to build the several types of time-of-flight spectrometers that exist in different facilities. An intense day of hands-on practical sessions was enriched by lively discussions. Students learned how to build a Laue camera, i.e., a neutron diffractometer. Example instruments were DMC from PSI, TOPAZ from SNS and SENJU from JPARC. A hands-on practical of building a simple triple-axis spectrometer was also provided. These tutorials also laid the foundation for simulations of virtual experiments—the main scope of this school.

The third day started with practical sessions on building time-of-flight instruments. Example instruments were TOSCA and OSIRIS from ISIS and IN4 from ILL. How to use Mantid, a modern data reduction and analysis software package, to handle output from McStas was also discussed in this practical session. On this morning, students also got the opportunity to analyze QENS data using MD simulations. Students were free during the second half of the day to explore the beautiful island of Tenerife (Figure 2). A prebooked bus took delegates to visit the top of the volcanic mountain Teide to experience a breathtaking panoramic view of the whole island and the Atlantic Ocean.

Figure 2. Group photo of MDANSE 2018 participants (Image credit: Emmanuel Farhi).

The fourth day was packed with hands-on tutorials on virtual experiments. Emmanuel Farhi gave an illuminating lesson on this topic followed by very interactive practical sessions. Erik Knudsen introduced McStas samples and advanced samples, and explained the concepts of incoherent, coherent, and multiple scattering in terms of McStas components. Single crystal, powder and liquid samples were discussed, showing the full methodology to produce virtual spectra by going from the instrument design to the sample scattering, and passing by the use of computer simulations to calculate the sample response.

The final day of the school was dedicated to more advanced techniques on simulations of virtual experiments. Emmanuel explained, followed by a hands-on tutorial, how to simulate inelastic spectra mixing phonons, spin-waves, incoherent scattering, multi-phonons and multiple scattering contributions in the direct geometry instrument IN4 at ILL. Students were excited to discover the power of simulations. In the last tutorial of the school, Sanghamitra and Peter jointly demonstrated the simulation of INS spectra from TOSCA instruments at ISIS. Students got the opportunity to compare the real-life INS from the same instrument to those derived from the virtual experiments. The next-generation technique of virtual experiment was a timely way to conclude the school for this year, projecting a bright future of simulations of neutron scattering. The final wrap-up was given by Emmanuel.

In conclusion, we thank all participants, students, teachers and organizers, for the great atmosphere and discussions during the school. This school opened up a new chapter in virtual experiments to train the next generation of neutron scientists. More information about the school can be found at http://mdanse2018.esswork shop.org/ and https://www.isis.stfc.ac.uk/Pages/MDANSE-2018.aspx. All data used in tutorials will be available at https://edata.stfc.ac.uk/handle/edata/12. With great feedback from participants, the school was a big success.

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