Preface

The neutron is a chargeless particle and its interaction with the electrons of a non-magnetic condensed matter system can in general be neglected. Instead the neutron is scattered by atomic nuclei via a weak interaction, the corresponding scattering cross-sections being known precisely for all nuclei. Once, therefore, atomic trajectories have been determined, the full spectral profile $S(Q,\omega)$ can be calculated and compared directly with measurement, the combination of numerical and experimental data giving detailed insight into the structure and dynamics of ever more complex systems. The way in which experimentalists can use modern simulation tools to better understand their experimental data was the theme of the summer school of the JDN18 held in Rémuzat in the Drôme Provençale in June 2010 and the articles in this collection have been produced following the school.

Atomic trajectories can be obtained from total energy calculations which give the forces and therefore accelerations acting on atoms, allowing equations of motion to be integrated. The simplest calculations of this kind are based on analytical expressions (force fields) for the inter-atomic interactions which evoke a picture of springs between bonded atoms and electrostatic and Van der Waals' interactions at longer range. With force field methods, hundreds of thousands of atoms can be handled on computational clusters that are commonly found in research departments and the time scale can extend up to the microsecond, if a trade-off is made between system size and the number of simulation steps. These time and length scales are almost perfectly matched to those available on neutron scattering instruments. Only the larger systems, studied for example by small angle scattering, go beyond these scales in which case, anyway, the atomistic detail becomes less relevant. In these cases, simpler, so-called "coarse-grain" models have to be developed almost on a system-by-system basis.

When a more accurate description of inter-atomic interactions is required, for example when studying phonon dispersion in hard condensed matter systems, the electronic structure of the system has to be taken into account. Density functional theory (DFT) based methods give the best compromise between speed and accuracy but time and length scales are limited significantly to hundreds of picoseconds and atoms respectively. Electronic structure methods are also required to study numerically the magnetism of the electrons in condensed matter systems which are probed experimentally by the magnetic moment of the neutron.

Many standard codes are available for force field and DFT based simulations and they are referred to in many of the articles in this collection. While codes can be used as tool boxes giving rapid access to simulations, the way these codes, for example, solve Schrödinger's equation, implement the thermodynamic principles underlying molecular dynamics or allow the dynamical matrix underpinning normal mode analysis to be determined, must be understood. These issues are addressed in the introductory articles. Of key importance to experimentalists is the ability to use the output from standard packages to calculate neutron scattering observables and two of the articles concern particularly useful software in this respect: the PHONON code and the nMoldyn code. A number of articles illustrates how the techniques and codes are applied to different systems, ranging from magnetic systems where highest numerical precision is required to polymeric systems where time and length scales impose the most approximate methods. Finally, in virtual experiments, simulations of samples are combined with simulated neutron trajectories in neutron scattering instruments, giving insight into experimental artefacts like multiple scattering, including scattering from the sample environment. In the future, a "neutron scattering experiment simulator" will allow real experiment strategies to be tested in advance, optimising the use of beamtime.

N. Malikova, M. Plazanet, M. Johnson