Neutrons and Numerical Methods

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Abstract

The neutron is a charge-less particle and its interaction with the electrons of a system of atoms can, to a first approximation, be neglected. Instead the neutron is scattered by the atomic nuclei via a rather weak interaction, the corresponding scattering cross-sections being known precisely for all nuclei. Once the atomic trajectories have been obtained from an atomistic model and a description of inter-atomic interactions (total energy calculations), it is possible to directly calculate the full spectral profile and compare this with measurement. The time-dependent, atomistic model leads to greatly improved understanding of dynamics in condensed matter. Structural information is obtained from the time-average of the atomic trajectories or, at low temperature, by finding the structures that minimise the potential energy. However, the neutron-electron interaction allows experimental measurement of magnetic structure and excitations, which can be investigated numerically by calculating the spin density and total energy of different spin structures.

Recent examples of work at ILL will be given, showing how total energy calculations have been used to help understand neutron scattering data. Empirical, force field-based methods have been used to study the adsorbtion of small molecules in carbon nanotube bundles. Solid state quantum chemistry methods have been used to calculate molecular vibrations and phonons in bio-polymers and, most recently, by retaining the spin information, magnetic structures in battery materials and molecular magnets. The complementarity of neutron scattering and numerical modelling will be highlighted and the current limitations of the computational methods will be discussed.