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Scientific computing support for neutron scattering experiments at ANSTO

The purpose of the scientific computing support at ANSTO is to aid in the interpretation of both structural and dynamical data from the neutron scattering instruments using atomistic modelling calculations. Most of these calculations are done with ab initio scientific software packages based on Density Functional Theory, including VASP, WIEN2K, ABINIT, SIESTA, PHONON, and QUANTUM ESPRESSO, although some are performed with packages based on classical force
fields, such as LAMMPS, DL_POLY, NAMD, and GULP. Analysis of the results of these calculations exploits tools such as VMD, NMOLDYN, XCRYSDEN, and ISAACS, in addition to in-house code. Calculations and analysis are carried out locally on a scientific computing Linux cluster comprising 624 ACNS dedicated cores and 1416 ANSTO shared cores, with jobs managed by PBS. We give a brief overview of all of the above capabilities and an example of a typical calculation/analysis.

Topic

Neutron Facilities

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