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Scientific computing support for neutron scattering experiments at ANSTO

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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 both ACNS dedicated cores and ANSTO shared ones, with jobs managed by PBS. We give a brief overview of all of the above capabilities and an example of a typical calculation/analysis.

Level of Expertise

Experienced Researcher

Presenter Gender

Man

Pronouns

Which facility did you use for your research

Australian Centre for Neutron Scattering

Students Only - Are you interested in AINSE student funding

Do you wish to take part in the Student Poster Slam

Condition of submission

Yes

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