Scientific Computing Support for Neutron Scattering Experiments at ANSTO

Hardware and Software Capabilities for Atomistic Modelling Calculations

Ramzi Kutteh, ACNS

The purpose of the scientific computing support at ACNS/ANSTO is to aid in the interpretation of both structural and dynamical data from the neutron scattering instruments using various atomistic modelling calculations. To accomplish this aim the computing support exploits a number of scientific software packages and tools installed on a local cluster.

Software support

In order to help instrument scientists and users at ANSTO analyze and interpret their experimental data, in-house scientific computing software support comprises two aspects. First, software support at a basic level provides installation service on our local cluster (and occasionally off-site clusters) of various popular scientific software packages for performing atomistic modelling calculations. Most of these packages are DFT-based, such as VASP, WIEN2K, ABINIT, SIESTA, PHONON, and QUANTUM ESPRESSO, but some rely on empirical force fields, such as LAMMPS, DL_POLY, NAMD, and GULP. In addition to these packages, analysis and visualization tools are also installed, such as VMD, NMOLDYN, XCRYSDEN, and ISAACS. Furthermore, local analysis software is occasionally coded on a per need basis. This basic level of software support also provides where possible introductory tutoring and tips in using the foregoing packages and tools, aimed at getting the user up and running in a short time.

Where users are uncomfortable carrying out their own calculations and analysis, either due to their time restrictions or because doing so entails an undesirably steep learning curve, we are able to offer greater involvement in a second more advanced level of software support. This level of support includes performing some or all required calculations/analysis for the user as well as contributing to the writing of the resulting publication(s), and is necessarily more scientifically imbued than the first more basic and purely technical level of support. As such, this second level of support is offered only on a collaborative or joint-project basis.

Hardware support

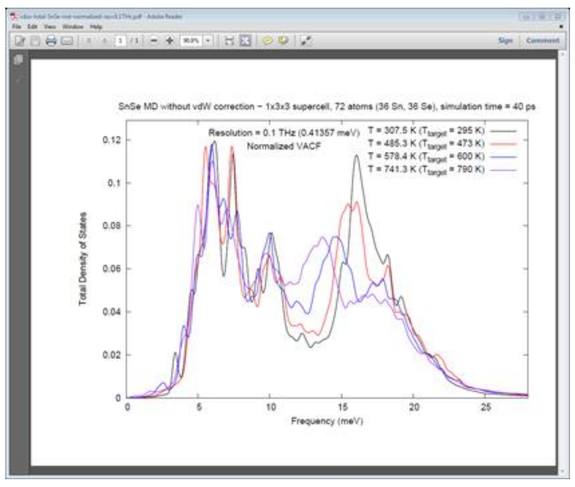
Hardware support for the above scientific software packages and tools is mainly in the form of a local computing cluster with the following attributes:

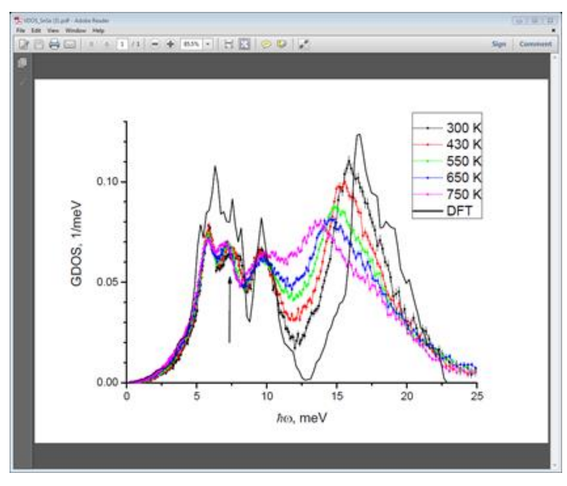
- ❑ Heterogeneous Linux cluster comprising 624 ACNS-dedicated cores and 1416 cores shared by all ANSTO cluster users.
- ❑ Jobs on the cluster are managed by PBS and can be submitted to a variety of queues, depending on the nature of the job and the user specific affiliation within ANSTO.
- ❑ Because they are CPU-intensive, most jobs on the cluster run in parallel using OpenMPI.
- ❑ Most scientific software packages for ACNS are built with the more robust PGI suite, although the faster Intel suite is also available and sometimes used.
- ❑ There are no limitations on the wall clock time of jobs running on the local cluster, in contrast to most supercomputing centres. This attribute is crucial for the computationally demanding jobs typically required to support analysis and interpretation of neutron scattering data from the instruments.

Although some ANSTO users do run their calculations on external clusters, it is important to appreciate the drawbacks of such a strategy. First, on external clusters such as in supercomputing centres with typically large numbers of installed packages, it is not feasible for the support staff to test carefully each package to ensure that it generates the correct numbers. Wrong numbers are often the result of over-optimization in the compilation stage of a code and are quite commonly encountered when running packages compiled in supercomputing centres. Second, almost all supercomputing facilities impose strict limits on wall clock times for running jobs on their queues, presenting a major obstacle for running the types of demanding jobs we need to support interpretation of neutron scattering data.

Example calculation/analysis

A common calculation done to aid in the interpretation of dynamical data from neutron scattering instruments is the computation of the vibrational density of states (DOS) of a material. This quantity can be computed by different approaches, one of which is molecular dynamics (MD) simulation as illustrated in the figure on the left for SnSe at four temperatures. This VASP calculation took several months to complete on 32 cores of the local cluster. The figure on the right shows the experimental DOS measured on PELICAN by Dr. Sergey Danilkin. Matching of the two sets of data provides an initial validation of the computational model used to generate the figure on the left. With this validation in hand one can confidently proceed to draw conclusions based on this model using various analysis tools to interpret the figure on the right.





+61 2 9717 3111 enquiries@ansto.gov.au www.ansto.gov.au