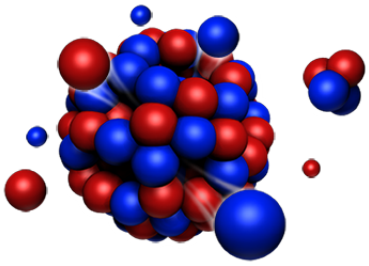

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ICE-MAN and VirtuES, the Integrated Computational Environment-Modeling & Analysis for Neutrons at ORNL

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ICE-MAN is a modeling and analysis workbench for multi-modal studies, specifically design with neutron science in mind. The integrated and extensible environment will provide scientists with a common interface to a suite of tools, and developers with a common API to seamlessly add new functionality. This project aims to reduce the barrier to analyze and interpret neutron scattering experiments in combination with other multi-technique research studies. It will streamline the workflow between different experimental techniques, computer modeling, and databases and reduce the time and learning curve needed to access them thus making a holistic approach to data interpretation more amenable and efficient as well as multi-model studies more accessible.
1) ICE-MAN overcomes the limitation of an individual's expertise to utilize different atomistic modeling techniques and to quickly compare simulated and experimental data.
2) ICE is fully HPC integrated it will expose the methods to an HPC environment. It is a step towards the realization of a vision of routine "on-the-fly"computer modeling, analysis and interpretation in multi-modal neutron experiments. 3) At the SNS, ICE-MAN will provide tools that can be used in 14 instruments.
ICEMAN runs as a virtual machine in VirtualBox and uses Docker containers. At present, it has two main modules, OClimax and QClimax. There are several small modules to generate input files and read output files. OClimax software can model phonon and vibrational spectra on VISION (BL-16B) as well as other inelastic neutron scattering instruments and can be used to rigurously model both polycrystalline and single crystal spectra. Currently, OClimax is principally used on VISION (BL-16B) but can also be used to analyze data from the direct geometry or triple-axis spectrometers.
A necessary step in analyzing data with OClimax is performing DFT calculations. On the VirtuES cluster, calculations can be performed using CASTEP, VASP, Quantum Espresso, Gaussian, CP2K, etc. The ICEMAN project aims to simplify this step in the analysis procedure, allowing for fast setup of initial files and running scripts for different DFT packages. Maintaining this software stack, so it is ready for users requires significant effort, especially as these codes use specialized packages.
The focused resources applied to data analysis on VISION (BL-16B) have contributed to it being the world leader in neutron vibrational spectroscopy measurements. The scientific output of the spectrometer is roughly 80% dependent on these analysis capabilities and have significantly improved the scientific impact of the instrument.
QClimax, on the other hand, provides users with a flexible, straightforward environment to enable fitting to complex user-defined functions. It allows fits to be performed to data from multiple Q values simultaneously and provides global fitting parameters. This allows both the energy and wave vector response to be modeled at once utilizing the statistical power of the full data set. It represents a significant step forward in the analysis of quasielastic neutron scattering data. QClimax can be used to analyze QENS data from any quasielastic spectrometer, including BASIS (BL-2), DCS (NIST), and CNCS (BL-5). The ICEMAN project is still under active development, and the QENS analysis capabilities of QClimax are being refined with feedback from instrument staff and users.

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