Testing and Documentation of Integrated Spectral Analysis Workbench (ISAW)

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Abstract

ISAW software developed by Drs. Dennis and Ruth Mickelson is an Integrated Spectral Analysis Workbench used by researchers at the Spallation Neutron Source (SNS). ISAW was started to create a network based, browser oriented, and platform-independent system for instrumentation control, data reduction, and data visualization. It is able to read, manipulate, view, and save neutron scattering data. It reads data from IPNS run files or Nexus files used by SNS and can merge and sort data from separate measurements. The aim of this assignment is to analyze codes within ISAW and execute existing example currently active in the ISAW User Manuel. Using ISAW software from the subversion repository, building the latest version to testing, and develops scripts written for SNS instruments. Testing different scripts developed for the ISAW software and updating a log daily that is available to the ISAW developers in subversion will better equip researchers to manage different codes on ISAW.

Introduction

The Integrated Spectral Analysis Workbench (ISAW) ISAW software developed by Drs. Dennis and Ruth Mickelson is an Integrated Spectral Analysis Workbench used by researchers at the Spallation Neutron Source (SNS). The single-crystal diffractometer (TOPAZ) is part of the SNS Instruments Next Generation Project (SING), for which commissioning began in September 2009. TOPAZ will address problems and greatly expand the range of materials explored in chemistry, earth sciences, materials science and engineering, solid-state physics, and biology. The Integrated Spectral Analysis Workbench (SNAP) diffractometer allows studies of a variety of powdered and single-crystal samples under extreme conditions of pressure and temperature.

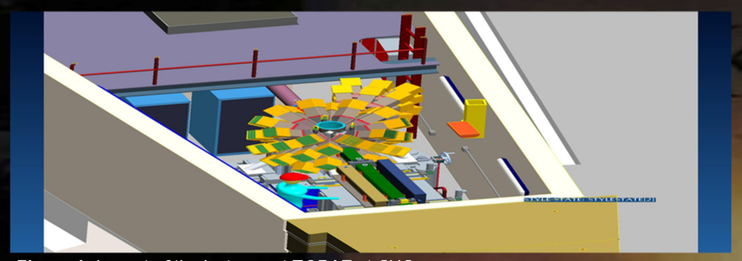

Figure 1. Layout of the instrument TOPAZ at SNS.

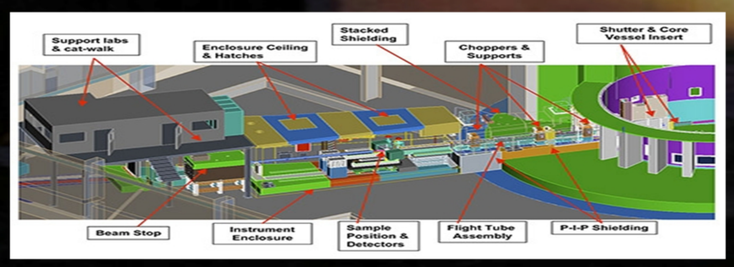

Figure 2. Layout of the instrument SNAP at SNS.

Research objectives

- Verify and clarification of ISAW software
- Ensure ISAW runs smoothly
- Document any errors that may come up while testing
- Ensure results are the same
- Resolve ISAW problems including updates automatic testing of ISAW

Methods

- Read the user manual
- Download latest version from subversion repository
- Build ISAW on a daily basis
- Test sample data on EV Viewer and Daily Peeks Wizard daily
- Event file used as input to IsawEV (*SNAP_240_neutron_event.dat*)

IsawEV

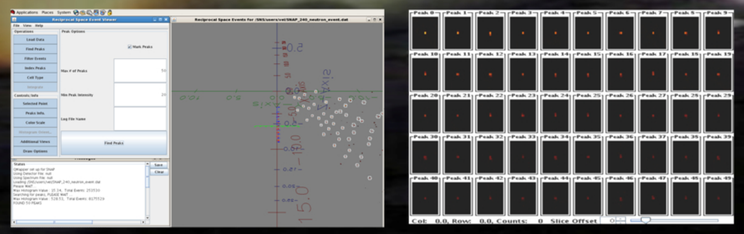

Figure 3. screenshots of IsawEv peaks from SNAP results.

Results

ISAW is a large software package that change daily. Users of SNS instruments depend on ISAW to analyze and view results. Software testing is very important to ensure that everything runs smoothly. No problems were found with daily testing of updated software. Tests and results were logged daily.

Daily Peeks Wizard

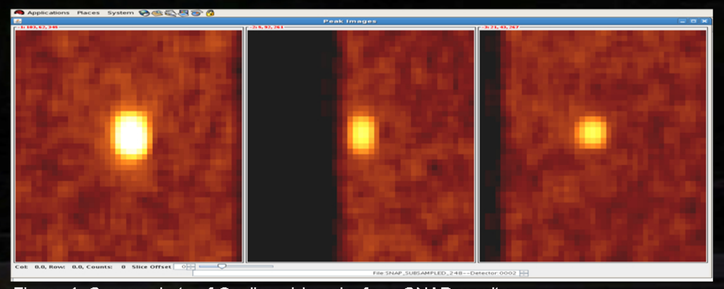

Figure 4. Screen shots of Oxalic acid peaks from SNAP results.

Future research

- Resolve ISAW problems including updates
- Design new and creative ways to make ISAW more user friendly
- Revise user manual

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