Exploration on Data Software for Small Angle Neutron Scattering and Reflectometry

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Abstract

The Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR) are neutron producing facilities. SNS is a set of accelerators that shoots near lightspeed protons at liquid mercury to scatter neutrons off of it by spallation [6]. HFIR is a nuclear reactor that uses fission to release neutrons that are slowed and then guided to the instruments [2]. These are user facilities that help outside users measure nanoscale material properties with the neutrons. The neutrons are sent down to beamlines that connect to one or two instruments [6]. These instruments measure a selected sample by receiving information from the neutrons after it has passed through the sample [6]. Providing user-friendly data reduction and analysis software for neutron science is a necessary part of maintaining an effective user facility. The different scattering technique data requires varying levels of adjustments, which makes the software landscape complex and diverse. I focused on the software for the neutron scattering techniques of small angle neutron scattering (SANS) and reflectometry. The data reduction software needs to be able to eliminate unnecessary information called instrument artifacts, and analysis software has to be able to extract structural information out of reduced data [9]. Throughout my internship, we had informal discussions with instrument scientists about the software used and how the instrument scientists interact with the data and users. We scoured the internet for supporting material on the software including, technical documents, user guides, source locations, and papers. We organized the information and arranged each software based on the data processing type (data reduction and data analysis), instrument facility (SNS and HFIR), and neutron scattering technique (SANS and reflectometry). We have collected information and resources to understand how users reduce and analyze their data and what are the users' experience using the various software to achieve that.

Introduction

The complexities of the neutron scattering data reduction and analysis processing procedure led us to explore what software is used and what publicly available resources exist to help enable users' experiments. Neutron scattering provides insight into the structure and properties of materials [3]. The Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFIR) are user facilities that harness neutrons to perform neutron scattering experiments. The three neutron scattering techniques that we investigated were Small Angle Neutron Scattering (SANS), reflectometry, and spectroscopy. SANS measures the structures of nanoscale materials using one of four instruments General Purpose Small-Angle Neutron Scattering Diffractometer (GP-SANS) and Biological Small-Angle Neutron Scattering Instrument (BIO-SANS) at HFIR and Extended Q-Range Small-Angle Neutron Scattering Diffractometer (EQ-SANS) and Ultra-Small-Angle Neutron Scattering Instrument (USANS) at SNS [5]. Reflectometry probes thin structures through the use of neutrons' refractive properties and can help identify the composition of the sample [4]. Spectroscopy measures energy changes in materials for use in fields focused on a multitude of materials [7]. User Experience is how users interact with a given computer program [1]. When studying User experience, you study who uses the program, why they use it, and how they use it [1]. In our project, we studied which technique groups use which software. There were two main types of software we focused on, data reduction and data analysis. Data reduction software focuses on the removal of unnecessary information called artifacts so that substance specific data is left, while data analysis for neutron science reveals insights into the structure and properties of a sample [9].

Goals and Motivation

The motivation of the project was to help enable users to perform neutron scattering science. To achieve this, we gathered data to inform users about the various data reduction and analysis software and their resources. My goal was to focus on the SANS and Reflectometry instruments, while some additional material is included.

Progress

Data software for SANS and reflectometry is used by Computational Instrument Scientists (CIS) and users. Throughout the project, we had informal discussions with several CISs from SANS, reflectometry, and spectroscopy investigating the data reduction and analysis software used throughout the neutron scattering data processing procedure. We also investigated various publicly available materials on the internet. During the informal discussions, we talked to the CISs about the software that is used by their technique and more specifically their instrument and about difficulties experienced throughout the CIS-User interactions. We interviewed six CIS and investigated thirty-six software tools for publicly available materials.

Informal Discussions

Our first discussion was with Yingrui Shang (Computational Instrument Scientist). He gave us a broad overview of all the SANS data reduction and analysis software procedure. He is the CIS for USANS and uses a software called USANSDATA that is able to perform both data reduction and analysis. USANSRED is a data reduction script branched off from USANSDATA. This is a package in parallel with drtSANS which is used for all of SANS. There is a legacy software that is used for data analysis named Irena which has a graphical user interface (GUI). It is used by few people, and because it is an Igor pro licensed software, we were unable to use it. SasView is the newer data analysis software that is commonly being used.

When we talked with Gergely Nagy (Senior SANS Instrument Scientist) about EQ-SANS, he talked about how he personally often performs a majority of the data reduction. Some EQ-SANS users use scripts and are able to complete the reduction on their own. He talked about GRASP being a good application for reducing small amounts of data at other SANS instruments with instant results but becomes time inefficient when using large amounts of data. When he is working on data reduction, he sometimes needs to change variables, and this becomes inconvenient with how long reduction takes. A single set of samples may contain ten samples which take 1-1.5 minutes each to process. Version updates may cause various problems to arise in the code.

When talking with Wellington Leite (Neutron Scattering Scientist), he told us about BIO-SANS's data reduction and analysis. Most of the users ask for a GUI to work with compared to using scripts. Users are uncomfortable using the scripts because they lack the experience to know if they are doing the work correctly. Including dropdown choices could help simplify the process. When there is more data, the time to process increases exponentially. Since there is only one Jupyter file, there is no concern for errors that arise from updates. There are only problems when Jupyter itself is down. There is talk of incorporating AI into the experimentation and data process.

Talking with Mathieu Doucet (Senior R&D Staff) gave us insight into reflectometry. He told us about how both instruments have auto reduction script to help with data reduction, but it is not exclusively used. There is a reduction software for each instrument to use in place of the script. The manual reduction software are named QUICKNXS (Magnetic Reflectometry) and REFRED (Liquid Reflectometry). REFL1D is the main choice for analysis for both magnetic and liquid reflectometry instruments. There is a project in progress called WebView to add a GUI to REFL1D. He told us that data take up to six months to finalize for users.

Talking with Andrei T. Savici (Neutron scattering scientist) showed us insight into the data software for spectroscopy. The reduction is mostly done automatically with a script or by the user through Shiver. Shiver helps to visualize the data into an up to four-dimensional graph called a histogram. For analysis there are many software, and each is used by a specific scientist. Sunny.jl, Inspire, Dave, Horace, and Graffiti are some of the spectroscopy data analysis software that he told us about.

Yongqiang Cheng (Senior Staff Scientist) explained that there are three types of spectrometers: direct geometry, indirect geometry (chemical spectroscopy), and triple axis. Triple axis does not involve specific reduction. Chemical spectroscopy uses Mantid to reduce the data. Scripts are heavily used, but they are setup, so the users just change certain sections for their experiment. Jscatter is used to help with the Neutron Spin Echo Spectrometer by fitting the reduced data (by DrSPINE) with various models. Oclimax simulates neutron scattering spectra from a structural model to compare with experiments. He talked about how AI is in the early stages of being used to prepare spectra approximations for substances.

Publicly Available Materials

Using the names of software given to us by the CIS, we searched for publicly available materials on the various software used at ORNL. We searched for technical documentation, user guides, source locations, papers, examples, code language, and other information. We found GitHub repositories for twenty-two out of the thirty-six software. Some of these repositories had links to guides and technical documentation, but all the repositories had the code language.

Results

We compiled the information from our exploration into a spreadsheet. We separated the information by software. The first column of the spreadsheet was for indicating whether the software was data reduction or analysis, and the second and third column for which facility and technique. Each successive column was about the instrument name, how the software is typically used as, technical documentation, user guide, source code/location, paper, coding language, examples, input data, input file type, output data, and output file type. Here in Table 1 is a reduced version of the spreadsheet focused specifically on my areas of SANS and Reflectometry.

Data Reduction	Software	Instrument	Documentation	User Guide	Source Location	Paper	Coding Language
All	Mantid		Yes	Yes	Yes	Yes	Python, C++
SANS	DRT-SANS	All SANS	Yes	Yes	No	Yes	Jupyter, Python
	USANSDATA/USANSRED	USANS	Yes	Yes	Yes	No	Python
	Grasp	EQ-SANS	No	Yes	Yes	Yes	Matlab
Reflectometry	mr_reduction (autoreduction)	MAGREF	Yes	No	Yes	No	Python
	QUICKNXS	MAGREF	No	Yes	Yes	No	Python
	lr_reduction (autoreduction)	LIQREF	No	No	Yes	No	Jupyter, Python
	REFRED	LIQREF	No	No	Yes	No	Python
Data Analysis	Software	Instrument	Documentation	User Guide	Source Location	Paper	Coding Language
SANS	RAW	BIO-SANS	Yes	Yes	Yes	Yes	Python
	IRENA	GP-SANS, BIO-SANS	Yes	Yes	Yes	Yes	Igor pro
	SASVIEW	GP-SANS, BIO-SANS, EQ-SANS	Yes	Yes	Yes	No	Python, C++
	USANSDATA	USANS	Yes	Yes	Yes	No	Python
	Origin	EQ-SANS	Yes	Yes	Yes	No	
Reflectometry	Refl1d	MAGREF, LIQREF	Yes	Yes	Yes	No	Python, C++
	REFNX		Yes	Yes	Yes	No	Jupyter, Python
	Genx	MAGREF	Yes	Yes	Yes	No	Jupyter, Python

Table of data reduction and analysis software and their resources (Table1)

Future work

We will try to make the gathered information available to users to aid in their reduction and analysis. We also plan on trying to do some user experience testing on the software and data we have access to. We listened to a talk on data curation by the department of energy data

curation group, and I became interested in trying to place a finalized version of the software and resources table in the new database that was mentioned.

Impact

Through our work, we have been able to aid ORNL's mission which is "primarily for open research. ... Many of its facilities are user facilities, which means that they are available to researchers from other national labs, academia and industry" [8]. We have helped create a resource for the users of SNS and HFIR to help smooth out the data reduction and analysis process. This work was supported in part by the U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists (WDTS) under the Community College Internships program.

Conclusions

With this project, we compiled a list of software used by SANS, reflectometry, and spectroscopy and their resources. Through this we saw how little standardization there is in style and location between the resources for the software. Some resource styles we have seen are video tutorial, pdfs, docx, software specific websites, and GitHub wikis. Some software store their resources in their GitHub repositories, software specific websites, and even comments within the code walking the user through the process. Now, we can continue to improve the CIS-User experience by updating the spreadsheet and in house resources to keep up with the ever-changing landscape of software.

References

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Appendix

Participants-

Name	Institution	Role
Patrick Angelino	Pellissippi Community College	Intern
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Yingrui Shang	Oak Ridge National Laboratory	Interviewee, Computational Instrument Scientist
Mathieu Doucet	Oak Ridge National Laboratory	Interviewee, Senior R&D Staff
Andrei T. Savici	Oak Ridge National Laboratory	Interviewee, Neutron scattering scientist
Gergely Nagy	Oak Ridge National Laboratory	Interviewee, Senior SANS Instrument Scientist
Wellington Leite	Oak Ridge National Laboratory	Interviewee, Neutron Scattering Scientist
Yongqiang Cheng	Oak Ridge National Laboratory	Interviewee, Senior Staff Scientist

Scientific Facilities -SNS and HFIR

Notable Outcomes-
Poster presentation at ORNL Software and Data Expo 2024
Exploration of Data Software for Small Angle Neutron Scattering and Reflectometry

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