An Exploration on the Data Reduction and Analysis Software Used for Spectroscopy at Spallation Neutron Source and High Flux Isotope Reactor

Paul Kim,[1] Patrick Angelino,[2] Maria Patrou,[3] Marie Backman[3]

[1]Arizona State University, Tempe, AZ 85287

[2]Pellissippi State Community College, Knoxville, TN 37932

[3]Oak Ridge National Laboratory, Oak Ridge, TN 37830

Contents

I. Abstract

Neutron scattering today is a research tool that anybody can apply for, and its availability has attracted many users that may not be familiar with the complex software ecosystem. Data acquisition, data reduction and data analysis are the main processes in the data lifecycle for neutron sciences at ORNL, and for the spectroscopy technique, data acquisition and reduction are mostly the responsibility of the facility, and analysis is up to the user. However, in practice, users often manage their own data reduction, which can create inefficiencies. Additionally, some users require further assistance with data analysis, indicating that better familiarity with the software tools would aid them with research. This research report aims to facilitate the understanding of the complex ecosystem of software that is mostly being used for the Spectroscopy technique at SNS and HFIR when reducing and analyzing the data. We include information about the software used for data reduction and data analysis from discussions with Computational Instrument Scientists who work directly with users to process their data. Overall, we discuss our findings 1) on a general level to provide understanding of the complex software-ecosystem and 2) on a granular level to examine the software characteristics and user experience by collecting information from instrument scientists and our own investigation.

II. Introduction

The origins of neutron scattering dates back to the 1940s when a scientist named Ernest Wollan who was working on the Manhattan project first requested funding for neutron experiments [1]. Since its inception, neutron scattering has evolved significantly, with advances in technology and methodology propelling the field forward. Software tools and processes have also become more powerful, enabling unprecedented scale, capabilities, and accessibility of neutron scattering, especially for the scientific community as an analytical tool. In 2006, the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, a 1.5 billion dollar investment commissioned by the DOE, became operational and it attracts hundreds of scientists across the globe each year who have helped contribute to more than 5,000 publications in the areas of materials science, condensed matter physics, nuclear physics, energy, chemistry, biology, and more. The SNS produces pulsed neutron-beams and houses at least 20 instruments to detect neutrons varying in their capabilities and use-cases. In addition to the SNS, the High Flux Isotope Reactor (HFIR), which provides one of the highest steady-state neutron fluxes in the world through steady-state neutron streams, also houses at least 13 instruments [2]. The instruments produce about 100 terabytes of data each year that needs to be reduced, curated, analyzed, and visualized [3]. Users then have the option to transform or reduce and analyze the data in various ways.

The scientific techniques at SNS and HFIR can be categorized into 5 major categories:

- Diffraction

- Imaging
- Reflectometry – *discussions included
- Small Angle Neutron Scattering (SANS) – *discussions included
- **Spectroscopy – main focus**

Below is a list of the instruments for each group within the spectroscopy technique.

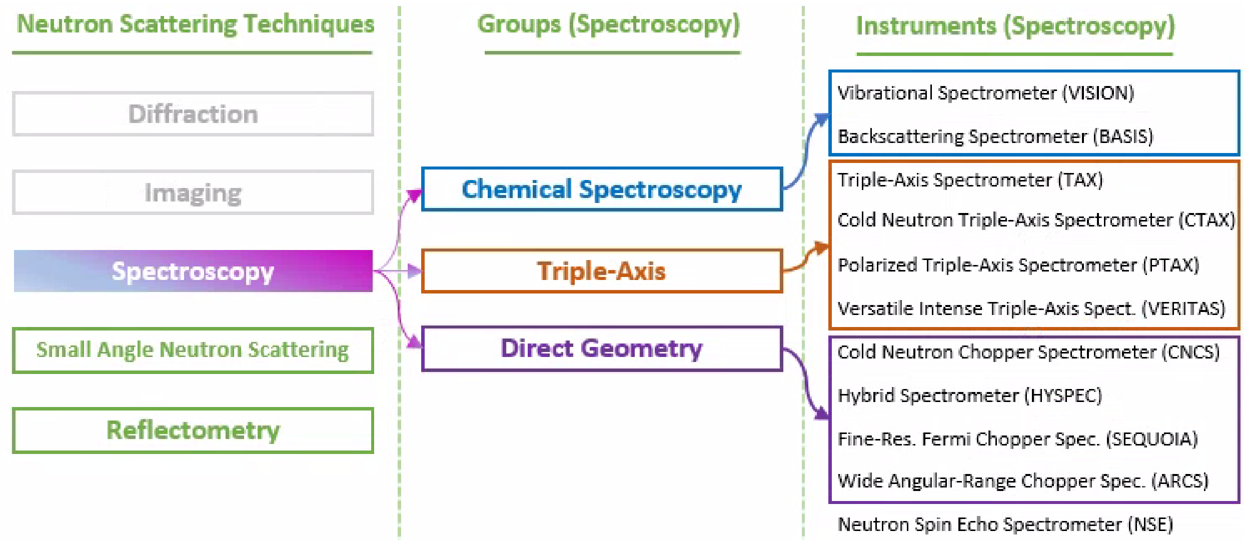

Figure 1: List of the neutron scattering techniques, and the subdivisions of the spectroscopy technique and their associated instruments

The scope of this paper is focused on Spectroscopy but includes interviews with for Reflectometry and SANS instrument scientists.

A. Overview of the Data Reduction and Analysis for Spectroscopy at SNS and HFIR

1. What is Data Reduction?

The overall purpose of Data Reduction is to remove instrument-specific artifacts. Another definition is "the transformation of a dataset collected from an instrument into a dataset in physical units" [4]. A way to think about raw data and reduced data is that "raw data is instrument-specific (requires knowledge of detector geometry, motor positions, etc.)" while "reduced data is proportional to the neutron scattering cross-section from the sample expressed in terms of physically meaningful variables (e.g., momentum transfer, energy)" [5]. For spectroscopy, although the format and organization of spectroscopy data are generally dependent on the instrument, "the goal of reduction is to produce a quantity (the double differential scattering cross section) which is (almost) independent of the instrument [6]. Other considerations that are made are the "sample itself and on the strength of the interactions between the neutrons and the sample's constituent elements" [6].

Definitions of Data Reduction are also defined by each instrument category at ORNL below:

Spectroscopy Groups	Data Reduction process
Direct Geometry (CNCS, HYSPEC, SEQUOIA, ARCS)	"For direct geometry spectrometers and BASIS, data reduction transforms collected data from time-of-flight events into S(Q,ω)… The four direct geometry spectrometers use Mantid to perform mostly automatic reduction to S(detector,ω) – the transformation to S(Q,ω) is performed manually in either MSlice, Horace, or Mantid. " [7]
Triple-Axis (CTAX, PTAX, TAX, & VERITAS)	"For the triple-axis spectrometers, the data collected is already in the appropriate S(Q,ω) form assuming counts were collected to a fixed incident beam monitor and only small, simple corrections are required (like accounting for higher order contamination in the beam monitor)." [7]
Chemical Spectroscopy (VISION, BASIS)	"For VISION, the double-focusing analyzers integrate the intensity over a range of scattering angle (or Q), thus the product of reduction is S(ω)… The automatic reduction at BASIS uses Mantid to directly obtain S(Q,ω) with default Q and energy binning. At VISION, two S(ω) spectra corresponding to the backscattering banks (120-150 degree) and forward scattering banks (30-60 degree) are automatically produced with Mantid." [7]
Spin Echo (NSE)	"DrSPINE (Data Reduction for SPIN Echo experiments) enables the reduction of neutron spin echo data produced at both reactor and pulsed neutron sources." [7]

2. What is Data Analysis?

Analysis is the process of understanding the physics of the materials. Data analysis is often described as much more complex and the insights from analysis are articulated in publications. One good resource to find instrument-specific publications is through the PuSH database (https://snsapp1.sns.ornl.gov/xprod_ro/f?p=134:32).

III. Related Work

There is a publicly available 2020 tri-annual review by the Department of Energy that delves into the details of the instruments being used at ORNL including an overview of the instruments, scientific focus, analytical capabilities, data and computing capabilities, and more [8]. Additionally, the Data Management section in ORNL's neutron sciences website describes the overall process and lists out available software [9].

IV. Methodology

A. Informal Interviews

We informally interviewed 6 computational instrument scientists (CIS), liaisons between the instrument and user, about the data reduction/analysis process. 3 out of 5 of the neutron scattering scientific techniques were interviewed for – spectroscopy, reflectometry, and small angle neutron scattering (SANS). The discussions below are paraphrases of in-person, informal discussions.

B. Online Literature Review

We conducted a thorough search of the ORNL web page and relevant literature that refers to data reduction, data analysis, and the software being used.

V. Results

A. Discussion with Andrei Savici (Spectroscopy – Direct Geometry & Triple-Axis Group)

Andrei Savici is a Computational Instrument Scientist who works on direct geometry spectrometry and triple axis spectrometers. He also develops reduction and analysis software for neutron scattering experiments and is a developer for Mantid software. He is one of the contacts for the TAX instrument [10].

1. Who are the users for the Direct Geometry and Triple-Axis Instrument Group Instruments?

For spectroscopy, users are usually more advanced, especially for Direct Geometry. Very few people come and do one experiment, they usually return for multiple experiments. These users are usually accustomed to their set of tools that they use.

2. How is data reduced for the Direct Geometry and Triple-Axis Group?

For direct geometry instruments (CNCS, HYSPEC, SEQUIOA, ARCS), data is reduced using auto-reduction. These are scripts using mantid. These custom scripts live in the instrument computer, where everyone has access to them.

For triple-axis (CTAX, PTAX, TAX, VERITAS), data is already reduced. The program to visualize these results is Graffiti, which is a part of Spice. Graffiti's underlying software is Labview. Dave, Shiver, Horace are all used for reduction or visualization. Visualization is important for single crystal, 3D structure.

Reduction/Visualization Software	Description	Useful Links and Resources
Dave	"The main objective of DAVE is to provide a user friendly tool for scientists involved in neutron scattering research to quickly reduce, visualize and interpret their data" [11]	The Dave website includes links to user manuals, paper, documentation, course notes, downloads, features, screenshots, changelogs, and more.
Shiver	"Tool (desktop application) for allowing the examination of Time of Flight (ToF) inelastic neutron data, from single crystal, direct geometry experiments." [12]	User documentation, developer documentation, source code. Can also be accessed by the command 'shiver' on the analysis cluster.
Horace	"Horace is a suite of programs for the visualization and analysis of large datasets from time-of-flight neutron	User documentation, developer documentation, source code, examples, local installation. To use in the analysis

	inelastic scattering spectrometers." [13]	cluster, open Matlab, then type 'horace' in the command line.

3. How is data analyzed?

Spectroscopy investigates interactions, while, for example, Diffraction investigates how atoms are arranged. Interactions are more complicated than structure and, for example, a magnetism perspective may be relevant.

4. What are some software that is being used for data analysis?

To analyze magnetic properties, you can use the SpinW software (which can be used in matlab), or Sunny. There is also a package called Phonopy, GSAS2, Spice/Graffiti and a very new one called Inspire, where the backend is developed by Yongqiang Cheng (an instrument scientist also in the Spectroscopy group).

Analysis Software	Description	Useful Links and Resources
SpinW	"SpinW is a MATLAB, Python, and C++ library that can plot and numerically simulate magnetic structures and excitations of given spin Hamiltonian using classical Monte Carlo simulation and linear spin wave theory." [14]	Source code, official documentation. The SpinW website also includes documentation, installation instructions, tutorials, publications, presentations, and more.
Sunny	"Sunny is a Julia package for modeling atomic-scale magnetism. It provides powerful tools to study equilibrium and non-equilibrium magnetic phenomena. In particular, it allows estimation of dynamical structure factor intensities, S(q,w), to support quantitative modeling of experimental scattering data." [15]	Documentation, github
Phonopy	"Phono3py is another open source package for phonon-phonon interaction and lattice thermal conductivity calculations." [16]	The Phonopy website includes guides, documentation, features, and more.
GSAS-II	"GSAS-II is used to analyze all types of x-ray and neutron diffraction data, including single-crystal, powder, constant-wavelength, pink-beam and time-of-flight, lab, synchrotron, spallation and reactor sources, including Rietveld analysis." [17]	The GSAS-II website includes developer documentation, tutorials, and source code.
Spice/Graffiti	"SPICE is a LabVIEW based program designed for control of neutron scattering instruments. Currently, SPICE is being used on the HB1 and HB3 triple-axis spectrometers at the High Flux Isotope Reactor at Oak Ridge National Laboratory." [18]	The Spice website includes introductions, user guides, downloads, and more.
multiphonon	"Powder spectra measured by inelastic neutron spectrometers provide information such as phonon density of states (DOS), a fundamental property of a solid. The measured spectra, however, are two-dimensional in axes of Q (momentum transfer) and E (energy transfer). This code converts a S(Q,E) INS spectrum to DOS." [19]	Documentation, github, examples

B. Discussion with Yongqiang Cheng (Spectroscopy – Chemical Spectroscopy Group)

Yonqiang Cheng is a Senior Staff Scientist at the Spallation Neutron Source. He is one of the contacts for the VISION instrument [20].

1. **Who are the users for the Chemical Spectroscopy Group Instruments (VISION & BASIS)?**

   The subject matter for the Chemical Spectroscopy Group is vibrational or diffusive dynamics, which often attracts scientists with a biology or chemistry background. However, technically, what the two instruments (VISION & BASIS) measure are very different, and consequently the data analysis workflows are also different.

2. **How is data reduced for the Chemical Spectroscopy Group?**

   At BASIS, most users are assisted by the instrument scientists to reduce the data. There are existing algorithms in Mantid and experienced users can easily reduce the data by themselves.

   At VISION, all data is reduced automatically. These are python scripts that are view for anyone to inspect at analysis.sns.gov. Some of the post-reduction operations include merging the data that is saved hour by hour and smoothing.

   For the NSE instrument (part of the SANS & Spin Echo Group), which is a very different technique than all the other instruments, the reduction software that is used is DrSpine.

Reduction Software	Description	Useful Links and Resources
Mantid	"The Mantid project provides a framework that supports high-performance computing and visualization of scientific data. Mantid has been created to manipulate and analyze Neutron and Muon scattering data but could be applied to many other techniques." [21]	The Mantid website includes downloads, tutorials, user documentation, developer documentation, and more.
DrSPINE	"DrSPINE is a software package that performs data reduction and analysis for reactor and pulsed source based Neutron Spin Echo experiments." [22]	The gitlab includes manuals, guides, source code, and papers.

3. **How is the data analyzed?**

   There are lots of software packages that can be used, it is ultimately the user's choice. The data is usually a 1-dimensional spectrum. Oclimax is one example of software that is being used. Some of the main functions include analyzing lattice dynamics, phonon calculations. Dr. Cheng works on Density Functional Theory simulations. Another software package is jscatter for NSE.

Analysis Software	Description	Useful Links and Resources
Oclimax	"A program for the calculation of inelastic nuclear scattering." [23]	Website. An introduction, examples, and installation can be found in this presentation.
JScatter	"Jscatter is a python package that provides useful models for neutron and X-ray scattering form factors, structure factors, and dynamic models (quasi elastic neutron scattering) and other topics." [24]	The website includes guides, documentation, examples, installation, and more.

C. Discussion with Gergely Nagy (Small Angle Neutron Scattering – EQ-SANS Instrument)

Gergely Nagy is a Senior SANS Instrument Scientist. He is the one of the contacts for the EQ-SANS instrument [25].

1. How is data reduced for the EQ-SANS instrument?

Data reduction is performed in various ways: entirely by the instrument scientists, jointly with users, or independently by users after an initial demonstration.

Data is reduced mainly using scripts. The software package that is used is typically DRT-SANS.

Reduction Software	Description	Useful Links and Resources
drt-sans	"Instrument scientists can calibrate instruments and reduce large quantities of datasets. Users can correct the collected data with dark current subtraction and normalization by neutron flux, detector sensitivity, solid angle subtended by the detectors, and scaling to absolute units. Lastly, conversion from time-of-flight and/or wavelength to 1D or 2D momentum to prepare for analysis." [26]	Documentation, paper, source code.

2. How is data analyzed for the EQ-SANS instrument?

SasView, RAW, Igor Pro, and customer software are typically used to analyze the data. He will occasionally use Jupyter notebooks or Origin. He used to use Grasp, as it has a reputation for being intuitive, capable, and easy to use.

Analysis Software	Description	Useful Links and Resources
SasView	"The aim of the SasView project is to provide open source, collaboratively developed software for the analysis of any small angle scattering data." [27]	Github. The SasView website includes documentation, about, downloads, tutorials.
BioXTAS RAW	"BioXTAS RAW is a GUI based, free, open-source Python program for reduction and analysis of small-angle X-ray solution scattering (SAXS) data. The software is designed for biological SAXS data." [28]	The BioXTAS website has installation, tutorials, manuals, documentation, and more.
IgorPro	"IgorPro is an interactive software environment for experimentation with scientific and engineering data. Igor provides many analysis capabilities, including curve fitting, peak analysis, signal processing and statistics, and much more." [29]	The WaveMetrics website includes downloads, case studies, manuals, and more.
Origin/OriginPro	"Origin is a powerful data analysis and publication-quality graphing software, tailored to the needs of scientists and engineers. OriginPro offers features such as Peak Fitting, Surface Fitting, Statistics, Signal Processing and Image Handling." [30]	The OriginLab website includes links to tutorials, list of apps, showcase, documentation, and more.
Grasp	"'GRASP' is a Matlab script application designed for the graphical inspection, analysis and reduction of multi-detector data produced by the Small-Angle Neutron Scattering (SANS) instruments of the Institut Laue-Langevin (ILL)." [31]	The ILL website includes key features, downloads, documentation, example data, and more.

3. What are some difficulties that you have encountered with data reduction?

- Going to next versions of software is a source of anxiety.

- Reduction workflow is slow. Typically, a batch of 10 samples will be reduced which takes about 1-1.5 minutes per sample for a total of over 10 minutes.
- Currently, there is development going on in the area of anisotropic distortions.

D. Discussion with Wellington Leite (Small Angle Neutron Scattering – BIO-SANS Instrument)

Wellington Leite is a SANS instrument scientist in the Center of Structural and Molecular Biology and the Neutron Scattering Division. He is one of the contacts for the BIO-SANS instrument, but the main contact point is Sai Venkatash "Venky" Pingali [32].

1. Who are the users of the BIO-SANS instrument?

Bio-SANS users are focused on Biology and biomaterials.

2. How is data reduced for the BIO-SANS instrument?

They currently use jupyter scripts. They would prefer a GUI. Mantid is another way to do the reduction. The staff at ORNL use DRT-SANS to reduce the data.

Reduction Software	Description	Useful Links and Resources
Mantid	"The Mantid project provides a framework that supports high-performance computing and visualization of scientific data. Mantid has been created to manipulate and analyze Neutron and Muon scattering data but could be applied to many other techniques." [21]	The Mantid website includes downloads, tutorials, user documentation, developer documentation, and more.
drt-sans	"Instrument scientists can calibrate instruments and reduce large quantities of datasets. Users can correct the collected data with dark current subtraction and normalization by neutron flux, detector sensitivity, solid angle subtended by the detectors, and scaling to absolute units." [26]	Documentation, paper, source code.

3. How is data analyzed for the BIO-SANS instrument?

A large proportion of users are dependent on the instrument scientists to do the analysis for them. There are a lot of software that can be used. A few examples are ATSAS, BioXTAS RAW, SasView, and Igor. ATSAS is a biological databank. BIOXTAS RAW can do Guinier analysis. SasView is used for shape-dependent analysis. Igor has a higher learning curve but is well-established in the field.

Analysis Software	Description	Useful Links and Resources
ATSAS	"The ATSAS software suite encompasses a number of programs for the processing, visualization, analysis and modelling of small-angle scattering data, with a focus on the data measured from biological macromolecules." [33]	The EMBL Hamburg website has downloads, tutorials, manuals, a paper, and more.
BioXTAS RAW	"BioXTAS RAW is a GUI based, free, open-source Python program for reduction and analysis of small-angle X-ray solution scattering (SAXS) data. The software is designed for biological SAXS data." [28]	The BioXTAS website has installation, tutorials, manuals, documentation, and more.
SasView	"The aim of the SasView project is to provide open source, collaboratively developed software for the analysis of any small angle scattering data." [27]	Github. The SasView website includes documentation, about, downloads, tutorials.

IgorPro	"IgorPro is an interactive software environment for experimentation with scientific and engineering data. Igor provides many analysis capabilities, including curve fitting, peak analysis, signal processing and statistics, and much more." [29]	The WaveMetrics website includes downloads, case studies, manuals, and more.

4. What are some difficulties that you have encountered with data reduction/analysis?

- When loading the data using ONCat, it is very easy to get lost. It would be very helpful to have a dropdown of experiments in the data reduction.
- If users are remote, they have to use FileZilla to transfer files across machines which introduces considerable delays.
- 1 curve takes 30 seconds but when 3 or 4 samples are inputted, then it takes minutes, which suggests that there is not any type of parallelization built in.

E. Discussion with Yingrui Shang (Small Angle Neutron Scattering – USANS Instrument)

Yingrui is a Computational Instrument Scientist for the SANS group. He is one of the contacts for the USANS instrument [34].

1. How is data reduced for the USANS instrument?

For USANS, there is the USANS data reduction package. DRT-SANS can also be used.

Reduction Software	**Description**	**Useful Links and Resources**
USANSRED	This is the Python script for USANS data reduction / analysis.	Documentation, github, ORNL source code
drt-sans	"Instrument scientists can calibrate instruments and reduce large quantities of datasets. Users can correct the collected data with dark current subtraction and normalization by neutron flux, detector sensitivity, solid angle subtended by the detectors, and scaling to absolute units. Lastly, conversion from time-of-flight and/or wavelength to 1D or 2D momentum to prepare for analysis." [26]	Documentation, paper, source code.

2. How is data analyzed for the USANS instrument?

There is software that is reaching the end of its lifecycle such IRENA, which is a suite of Igor Pro. However, SASView is the industry standard for data analysis with SANS instruments. You can hook SASView with Tensorflow or Pytorch, but there is no known documentation on this.

Analysis Software	**Description**	**Useful Links and Resources**
SasView	"The aim of the SasView project is to provide open source, collaboratively developed software for the analysis of any small angle scattering data." [27]	Github. The SasView website includes documentation, about, downloads, tutorials.
Irena	"Irena is data manipulations and analysis toolbox for small-angle scattering (SAXS, SANS, USAXS, USANS) data. It is mostly used for analysis of data in materials science, chemistry, polymers, metallurgy, physics, and other systems of typically solid or liquid samples. It addresses complex	The AGL website includes downloads, documentation, user info, source code, video tutorials, and more.

	systems with size distributions, hierarchical structures, diffraction peaks, etc." [35]	

3. What are some difficulties that you have encountered with data reduction/analysis?

In terms of feeding data, it is slow. The user interface could use a lot of improvement. Fitting more than 1 curve slows the performance down. They have an optimizer that is developed in-house called "dumps" that could use improvement.

F. Discussion with Mathieu Doucet (Reflectometry – LIQREF Instrument)

Mathieu Doucet is a neutron scattering scientist in the Neutron Reflectometry group. He is one of the contacts for the LIQREF instrument [36].

1. How is data reduced for the Reflectometry Group?

Each of these instruments have their own reduction software. For MAGREF, the software is QuickNXS and for LIQREF, the software is RefRed.

Reduction Software	Description	Useful Links and Resources
RefRed	"Data Reduction Software for the Liquids Reflectometer at the Spallation Neutron Source at Oak Ridge National Laboratory" [37]	Source code.

2. How is data analyzed for the Reflectometry group?

Refl1D can process data for both instruments. GenX is a versatile fitting software for x-ray and neutron reflectivity. Another software being used is refnx, which is a software for curve fitting analysis, but it is not used very often at the laboratory.

Analysis Software	Description	Useful Links and Resources
Refl1D	"Refl1D is a program for analyzing 1D reflectometry measurements made with X-ray and neutron beamlines. The 1-D models give the depth profile for material scattering density composed of a mixture of flat and continuously varying freeform layers. With polarized neutron measurements, scientists can study the sub-surface structure of magnetic samples. The architecture supports the addition of specialized layer types such as models for the density distribution of polymer brushes, and volume space modeling for proteins in bio-membranes." [38]	Github, the documentation includes getting started, tutorials, user guide, and documentation.
GenX	"GenX is a versatile program using the differential evolution algorithm for fitting, primarily, X-ray and neutron reflectivity data, lately also surface x-ray diffraction data." [39]	The GenX website includes source code, downloads, publications, how to, and more.
refnx	"refnx is a flexible, powerful, Python package for generalised curvefitting analysis, specifically neutron and X-ray reflectometry data." [40]	The refnx website includes installation, getting started, examples, API reference, and source code.

3. What are some difficulties that you have encountered?

Once the computational instrument scientists give the users their data, it can take six months to fit data and discuss the real meaning of the data. This is typically domain-specific and complex enough to write a paper about the topic, often together.

VI. Conclusion

The overall process of reducing data is generally very well-established. Additionally, the computational instrument scientists, research software engineers, and many other contributors allow for users to be able to perform the analysis that they would like. There is room for improvement, such as a more consistent practice across all instruments, a more streamlined software process, and software features that would make both user and instrument scientist's job easier.

VII. Future Work

We would like to conduct more informal interviews with users from outside of ORNL to better understand their motivations, pain points, etc. to build a better set of feature and product roadmaps that would ultimately increase the usage of the facility and enable more world-class analysis into the community's hands. We would also like to explore user interface heuristics as a discussion template to enable deeper insight into the exact need of the user.

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We extend our sincere thanks to our colleague, Patrick Angelino, for his invaluable collaboration and support. We are deeply grateful to our mentors, Maria Patrou and Marie Backman, for their guidance and insightful feedback, which have been instrumental in shaping this research. We also appreciate the insights provided by Gergely Nagy, Yingrui Shang, Yongqiang Cheng, Andrei Savici, Matthieu Doucet, and Wellington Leite during our interviews. Their expertise has greatly enriched this study.

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