OAK RIDGE National Laboratory

EQ-SANS: Extended Q-range Small-Angle Neutron Scattering Diffractometer

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Neutron Scattering Division
Feb 9, 2026

U.S. DEPARTMENT OF ENERGY

EQ-SANS Team

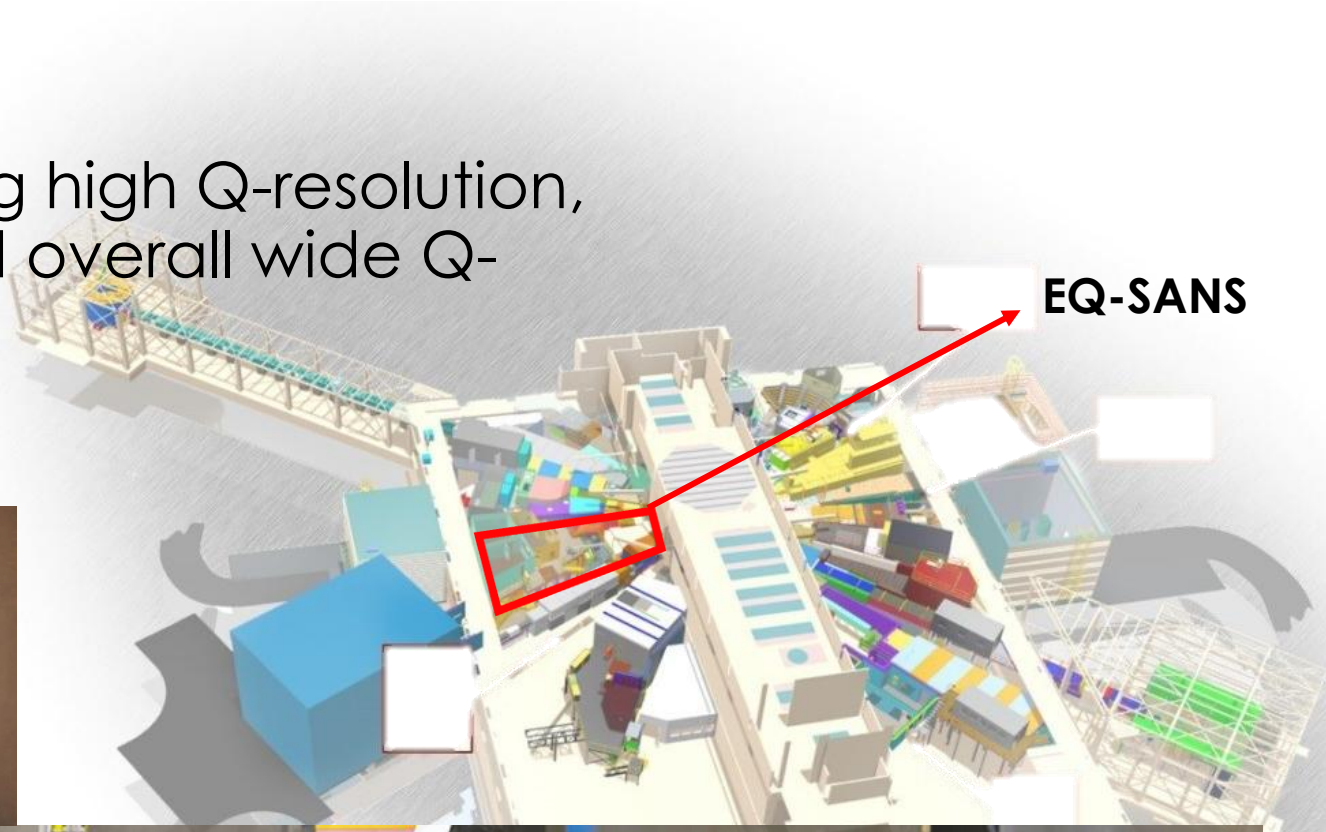



From the left,

Changwoo Do (IS), **William Heller** (IS), **Gergely Nagy** (IS), **Carrie Gao** (SA)

EQ-SANS Overview

- Beamline 6, SNS
- It is Time-of-Flight SANS offering high Q-resolution, broad dynamic Q-range, and overall wide Q-coverage.

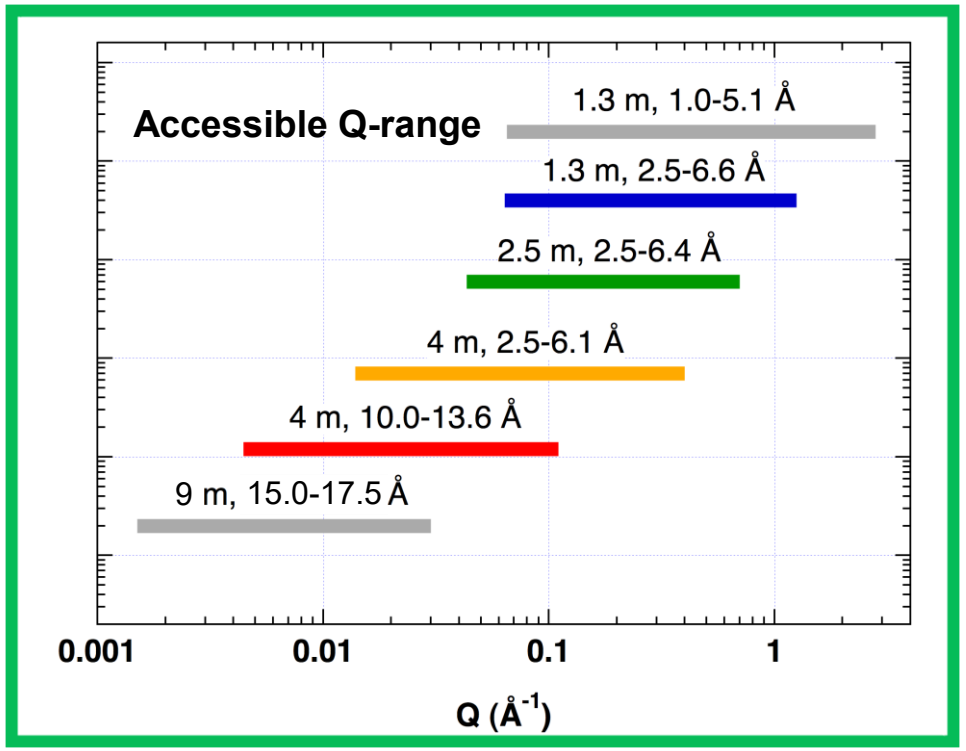


EQ-SANS Technical Capabilities and Global Positioning

TOF SANS with
- Wide simultaneous Q coverage (towards to high-Q)
- High Q-resolution ($1\% < \frac{\Delta\lambda}{\lambda} < 10\%$)

Strength
- Mid-Q to high-Q regime
- Time-resolved and kinetic studies

Moderator	Coupled supercritical hydrogen
Source-to-sample distance	14m
Sample –to-detector distance	1.3 ~ 9m
Detector size	1m x 1m
Bandwidth	3-4.3A
Integrated flux on sample	~ up to 10^7 n/cm^2/s/MW
Q range	0.002 < q < 3 A^{-1}
Detector resolution	5.5 x 4.3 mm



AI-Driven Leadership
- Efforts to integrate AI into the workflow (ESAC)
- Exploring ML-based data analysis framework

Response to 2020 EQ-SANS Suite Review (Summary)

2020 Recommendation	Status (2026 Feb)
Expand in situ sample environments to leverage TOF	Implemented (TOF rheo-SANS, TOF-tensile, Illumination)
Expand detector coverage	Proposal submitted
Continue sample environment development	Continues (new multi-position furnace, robot)
Develop data analysis capabilities	Ongoing Suite-wide
Maintain strong data reduction	Stable & mature
Optimize beamlines / reduce competition	Strength in kinetics study and mid-q range
Develop instrument complementarity	Complementary to NSE, USANS, BASIS, LREF
Strengthen EQ-SANS-USANS coupling	Implemented

Beam Time Use

General Operation

- ❑ General user program
- ❑ Discretionary beamtime (25% of available beamtime)

Specific to EQ-SANS

- ❑ Accessibility to provide complementary beamtime for USANS users.
  - ❑ Either specified in the original proposal or via proof of principle proposal
  - ❑ USANS and EQ-SANS use same type of sample cells.
- ❑ NSE flat cells can be used at EQ-SANS as well.
- ❑ Mail-in program (https://neutrons.ornl.gov/eqsans/mail-in)
  - ❑ Started as a pilot program, now became regular.

Day-to-Day Data Collection at EQ-SANS (Q3)

- Script-based experiment control (easy to use, flexibility)
- Programmable parametric studies
- Reliable, reproducible operation

Scan Monitor

ID	Created	Name	State
26332	2020-07-07 18:26:34.	runsample(S-2 1mm 25C 9m 15a, banjo, pc, 2, 8.0)	Logged
26331	2020-07-07 18:26:34.	runsample(S-1 1mm 25C 9m 15a, banjo, pc, 1, 8.0)	Logged
26330	2020-07-07 18:26:34.	openShutter()	Logged
26329	2020-07-07 18:26:34.	loadconf(conf_9000mm_15p0A_60Hz_scatt)	Logged
26328	2020-07-07 18:26:34.	closeShutter()	Logged
26327	2020-07-07 18:26:34.	runsample(T-18 1mm 25C 9m 15a, banjo, pc, 15, 0.05)	Logged
26326	2020-07-07 18:26:34.	runsample(T-17 1mm 25C 9m 15a, banjo, pc, 14, 0.05)	Logged

Example
Temperature variation experiment with multiple configuration

```
#switch IPTS
setipts(25934)

templist = [30, 40, 50, 60]
i=0
while i < 4:
    temp= templist[i]
    sethaaketemp(temp)

    loadconf('conf_4000mm_10p0A_60Hz_scatt')
    openShutter()
    runsample('S-1 peo-age 0.1-0 5mm ' + str(temp) + 'C 4m 10a','banjo', 'pc', 1, 2.0)
    runsample('S-2 peo-age 0.1-0.05 5mm ' + str(temp) + 'C 4m 10a','banjo', 'pc', 2, 2.0)
    runsample('S-3 peo-age 0.1-0.1 5mm ' + str(temp) + 'C 4m 10a','banjo', 'pc', 3, 2.0)
    closeShutter()

    loadconf('conf_2500mm_2p5A_60Hz_scatt')
    openShutter()
    runsample('S-1 peo-age 0.1-0 5mm ' + str(temp) + 'C 2.5m 2.5a','banjo', 'pc', 1, 0.7)
    runsample('S-2 peo-age 0.1-0.05 5mm ' + str(temp) + 'C 2.5m 2.5a','banjo', 'pc', 2, 0.7)
    runsample('S-3 peo-age 0.1-0.1 5mm ' + str(temp) + 'C 2.5m 2.5a','banjo', 'pc', 3, 0.7)
    closeShutter()
    i = i + 1
estimatetime(1.35)
```

Configuration 1

Configuration 2

Temperature loop

Day-to-Day Data Reduction at EQ-SANS (Q3)

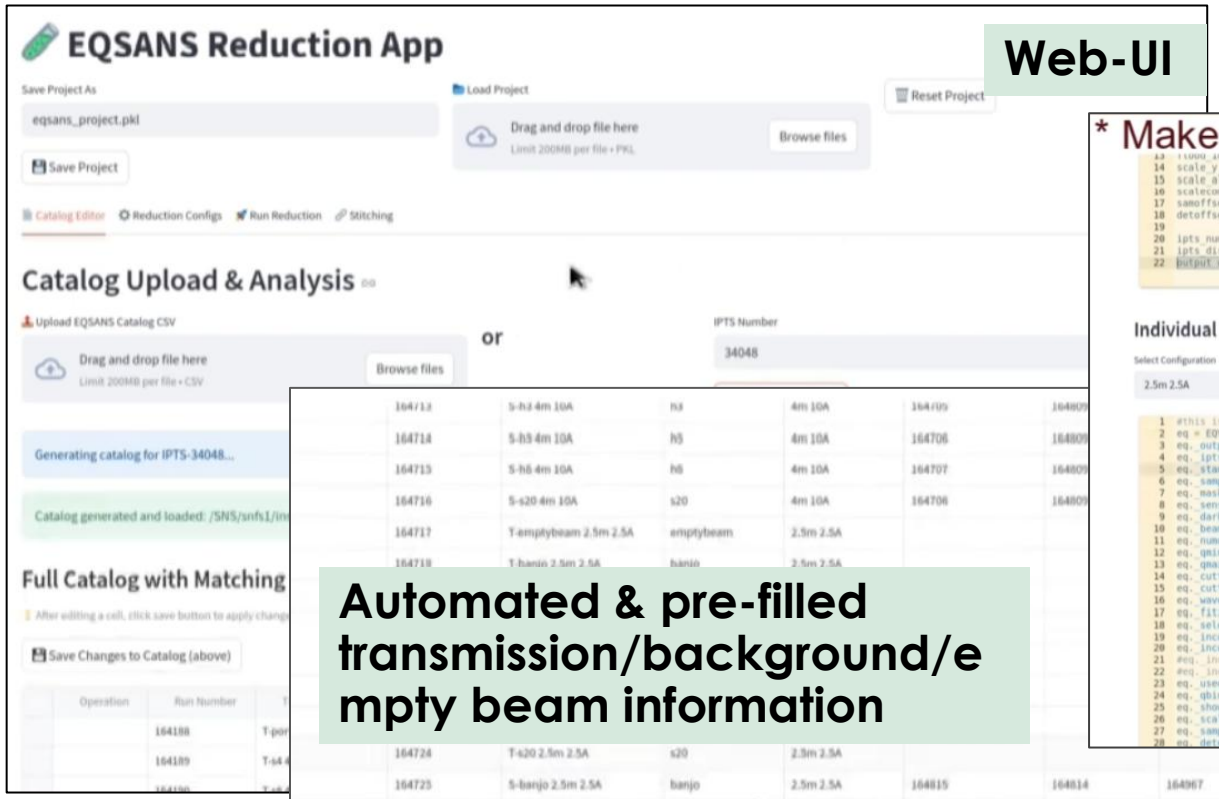
- Unified & Script-Based Reduction: Built on drtsans for centralized and standard workflows
- Reliable, reproducible operation
- EQ-SANS Custom Wrapper
  - Flexible Configurability: Tailored for both standard and complex reduction tasks
  - Provides multiple interfaces
    - **Script-based reduction**
    - **Table (spread sheet) reduction**
    - **Web-UI reduction**

Highly configurable

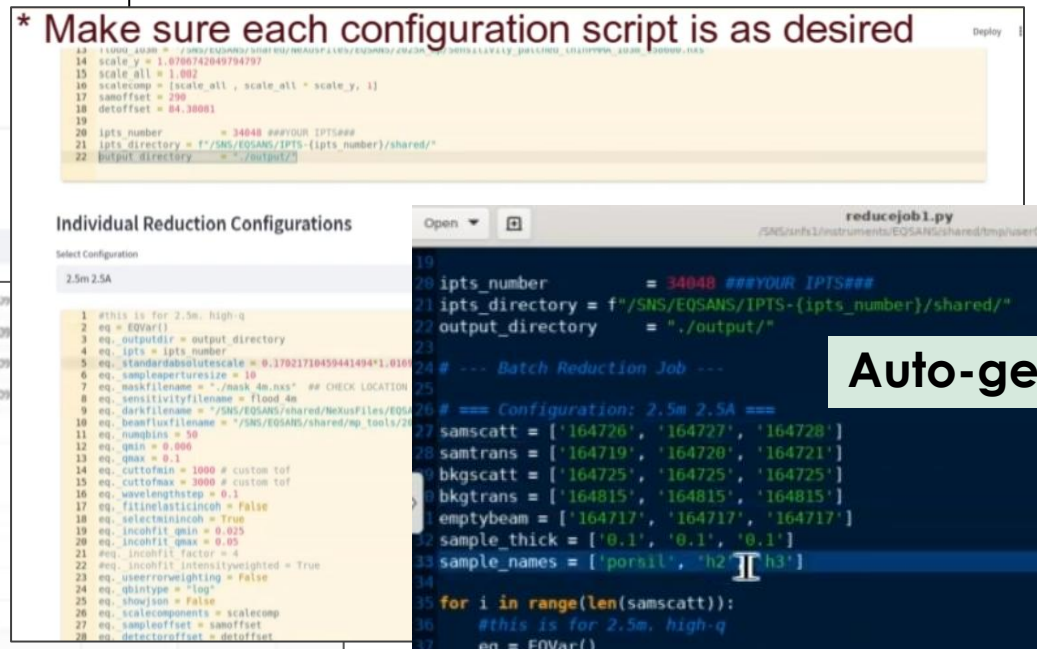
```
eq=EQVar('./4m.json')
eq._outputdir =  '/SNS/EQSANS/IPTS-12345/shared/output/'
eq._ipts = 12345
eq._standardabsolutescale = 1
eq._sampleaperturesize = 10
eq._maskfilename = '/SNS/EQSANS/IPTS-12345/shared/useThisMask.nxs'
eq._numqbins = 80
eq._empty = 10000
eq._thickness = 0.1
eq._bkgscatt = '10001'
eq._bkgtrans = '10002'
eq._samscatt = '10003'
eq._samtrans = '20003'
eq._filename = 'sample1'
reduceNow(eq)
```

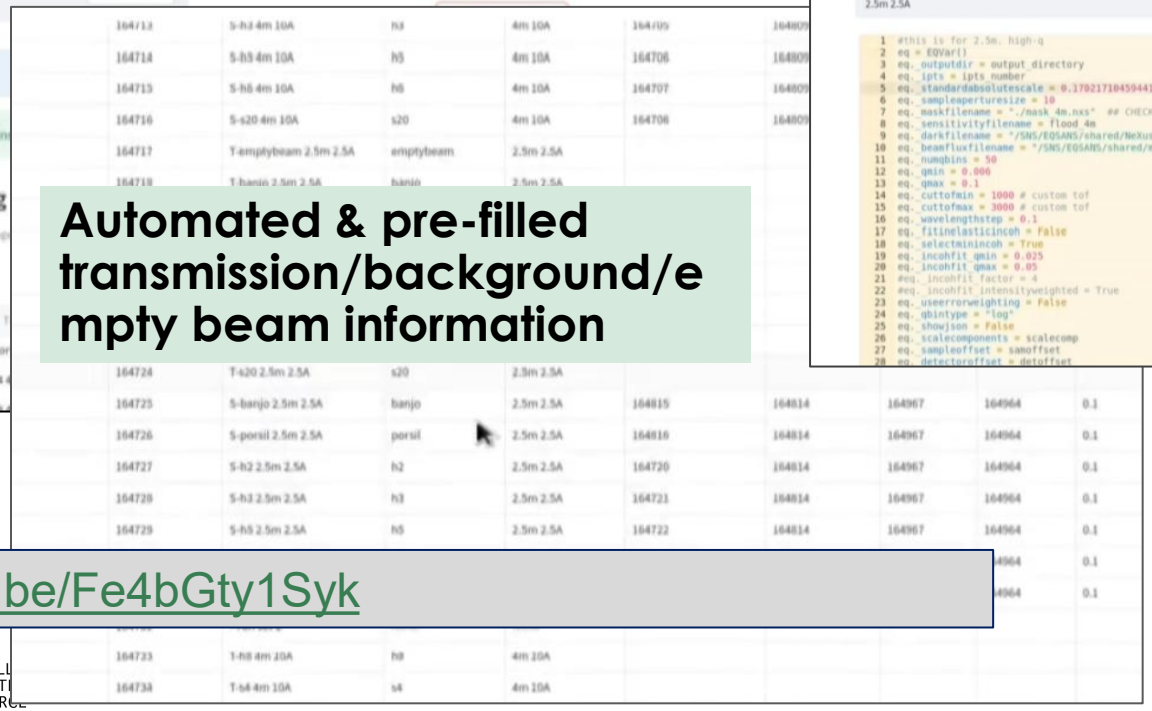
Day-to-Day Data Reduction at EQ-SANS (Q3)

- EQ-SANS Custom Wrapper enables different form of input with minimal efforts

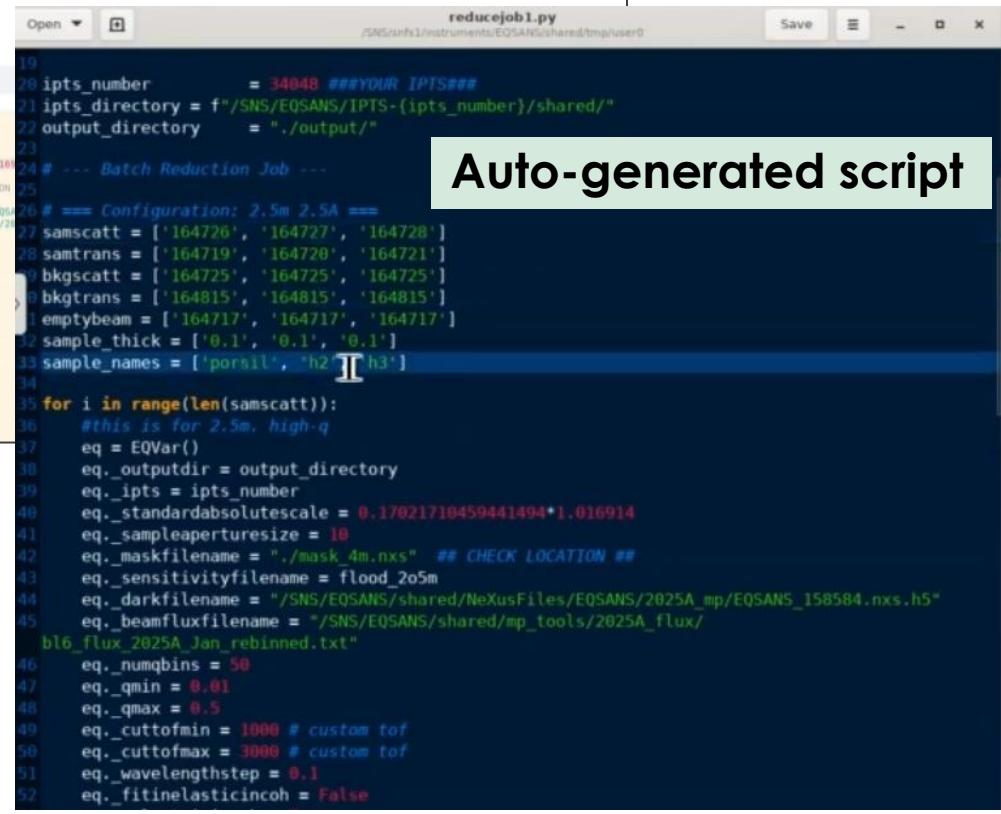


Web-UI





Automated & pre-filled transmission/background/empty beam information



Auto-generated script

https://youtu.be/Fe4bGty1Syk

Day-to-Day Data Reduction at EQ-SANS (Q3)

https://sites.google.com/view/eqsans

Data Reduction in a Nutshell

Useful Links

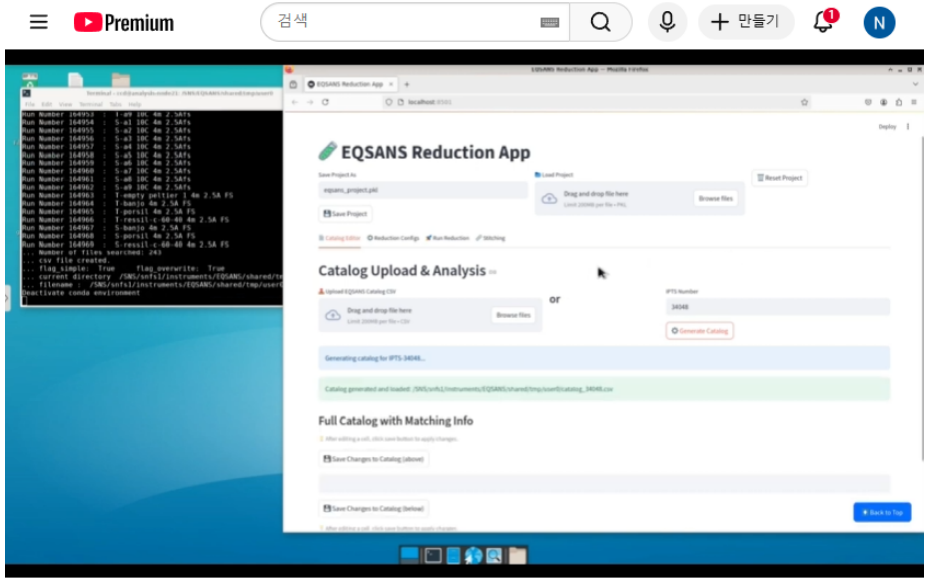
Data Reduction in a Nutshell

EQ-SANS data can be reduced in various environment and approaches.

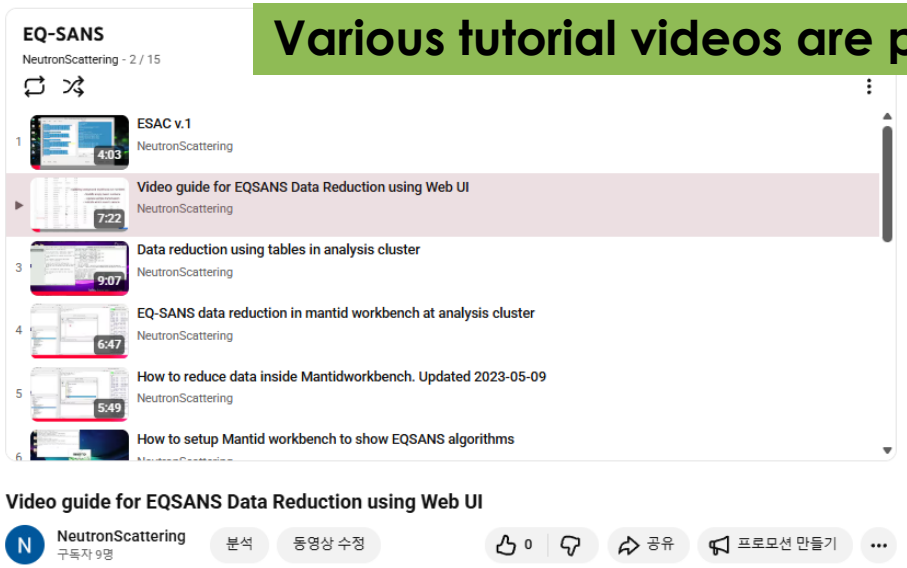
1. Python script based data reduction in the analysis cluster
2. Data reduction using an excel table in the analysis cluster
3. The script or table reduction can also be performed either in the termal window of the analysis cluster or in the mantidworkbench software of the analysis cluster.
4. Data reduction can also be performed in jupyter notebook in our jupyter.sns.gov server.

For more details, refer to the following pages

- Script-based Data Reduction
- Table-based Data Reduction
- Data Reduction in Mantid



Various tutorial videos are provided



Day-to-Day Data Reduction at EQ-SANS (Q3)

- We found a way to use the most amount of neutrons without introducing artifacts inherent to the TOF-SANS technique*,

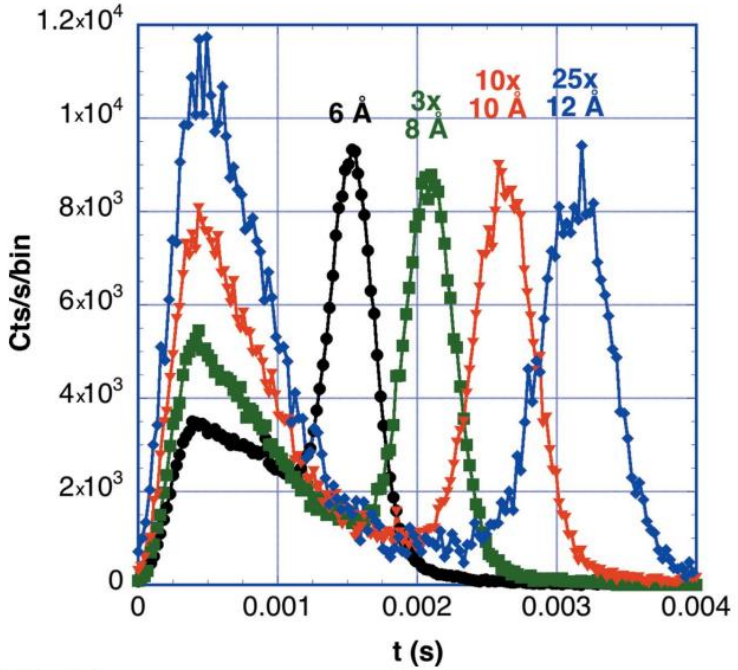


Figure 19
A plot of TOF data taken with a ^{3}He detector corrected for air background taken at L_2 = 2.0 m for a 1 mm-thick H_2O sample at wavelengths 6 Å (black), 8 Å (green), 10 Å (red) and 12 Å (blue). The vertical axis has the number of counts/bin, rescaled by values indicated in the figure captions. The counts were not corrected for the wavelength dependence of the ^{3}He detector efficiency.

Barker and Mildner • Background scattering in SANS 1069

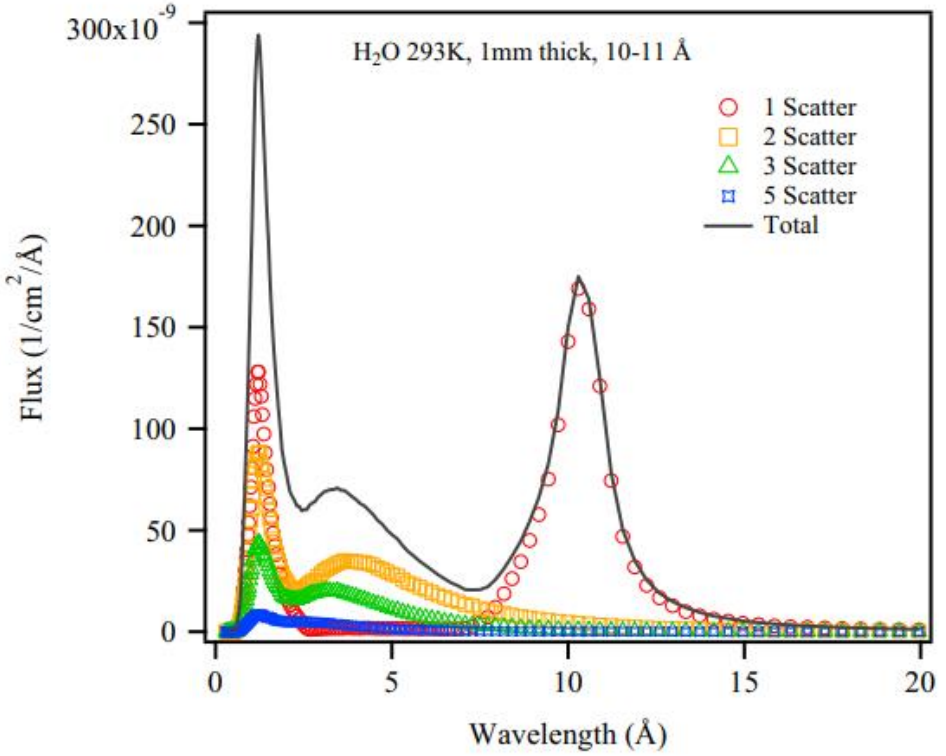


Fig. 6. Flux spectrum of simulated scattered neutrons from water with 10–11 Å neutrons. The fluxes of neutrons with different number of scattering events are summarized. The solid line is for the total flux spectrum from all the scattering events.

Do et al. Nucl. Instr. And Meth. In Phys. Res. A 737 42-46 (2014)

* Manuscript in preparation

Day-to-Day Data Reduction at EQ-SANS (Q3)

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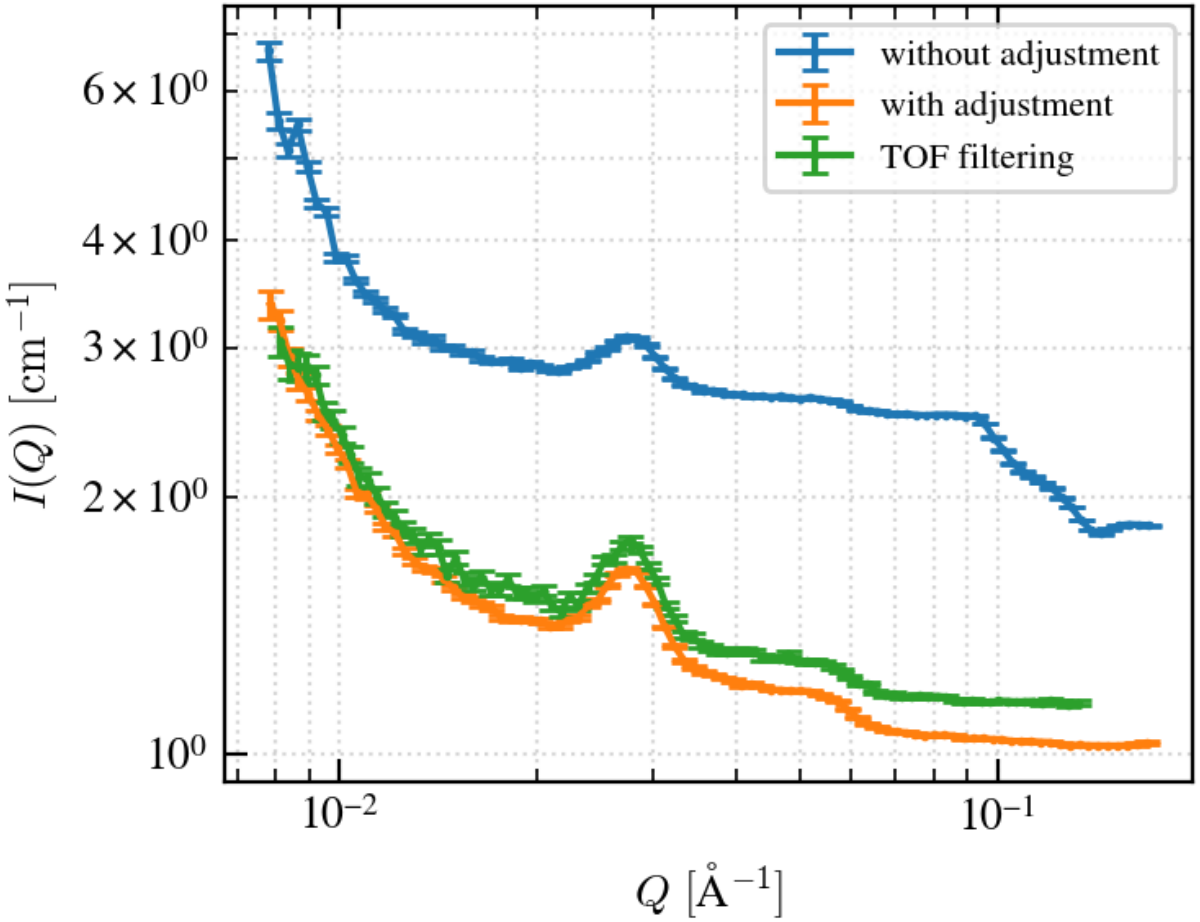
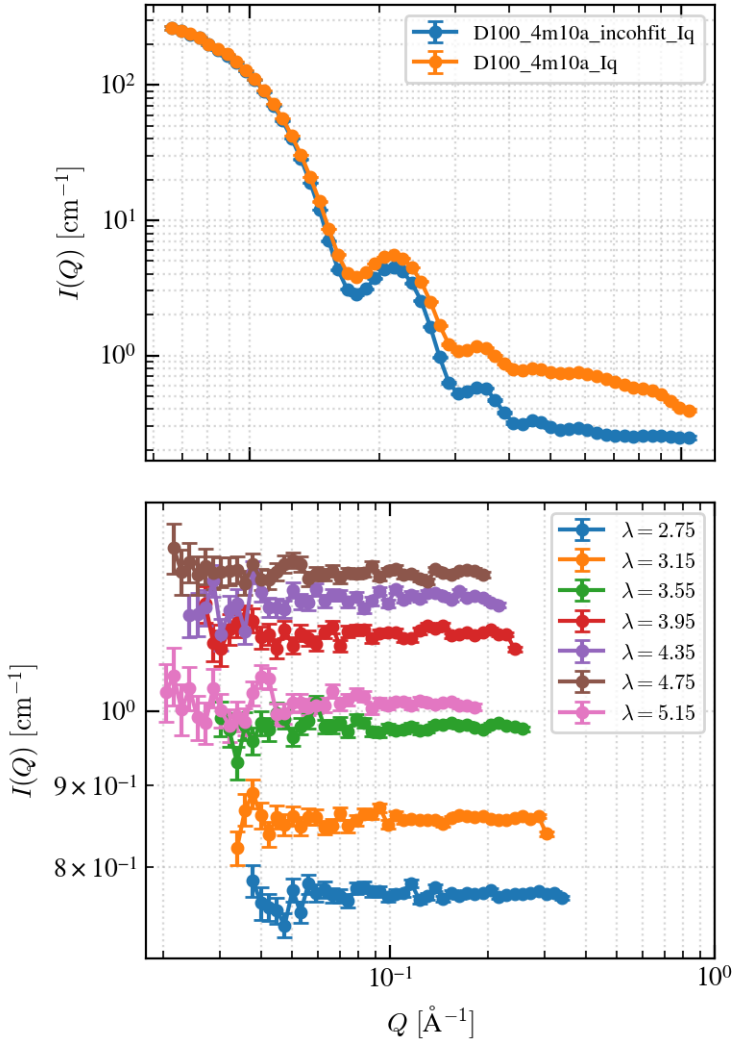
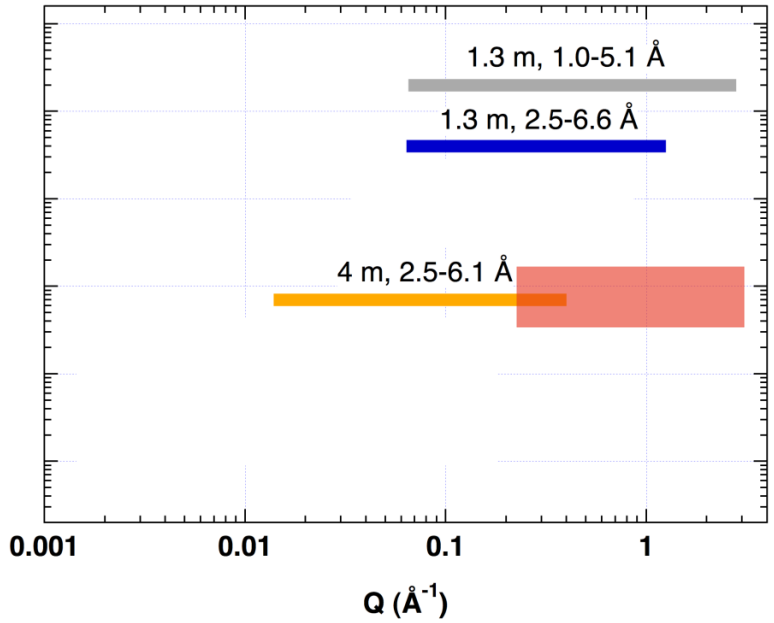




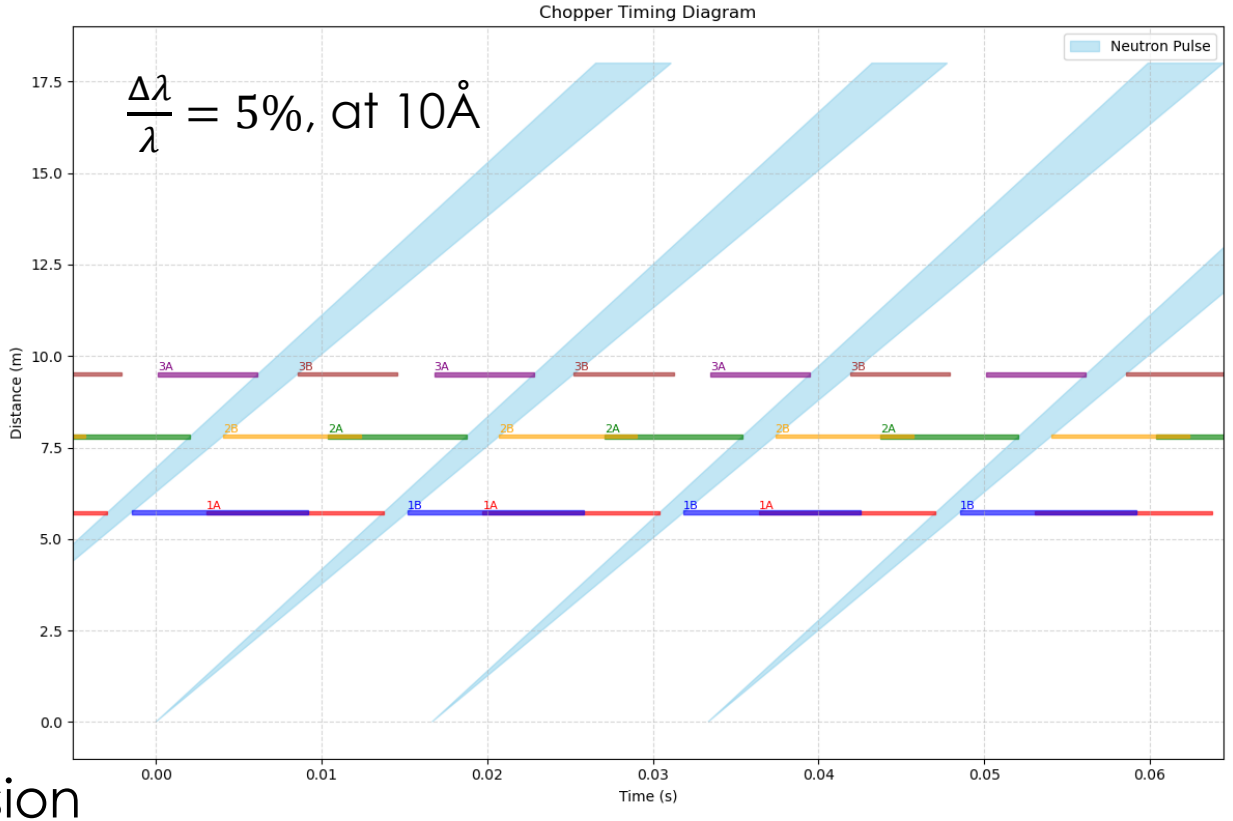
* Manuscript in preparation

EQ-SANS Development Roadmap (Q6)

- Proposal for adding wing-detectors is submitted



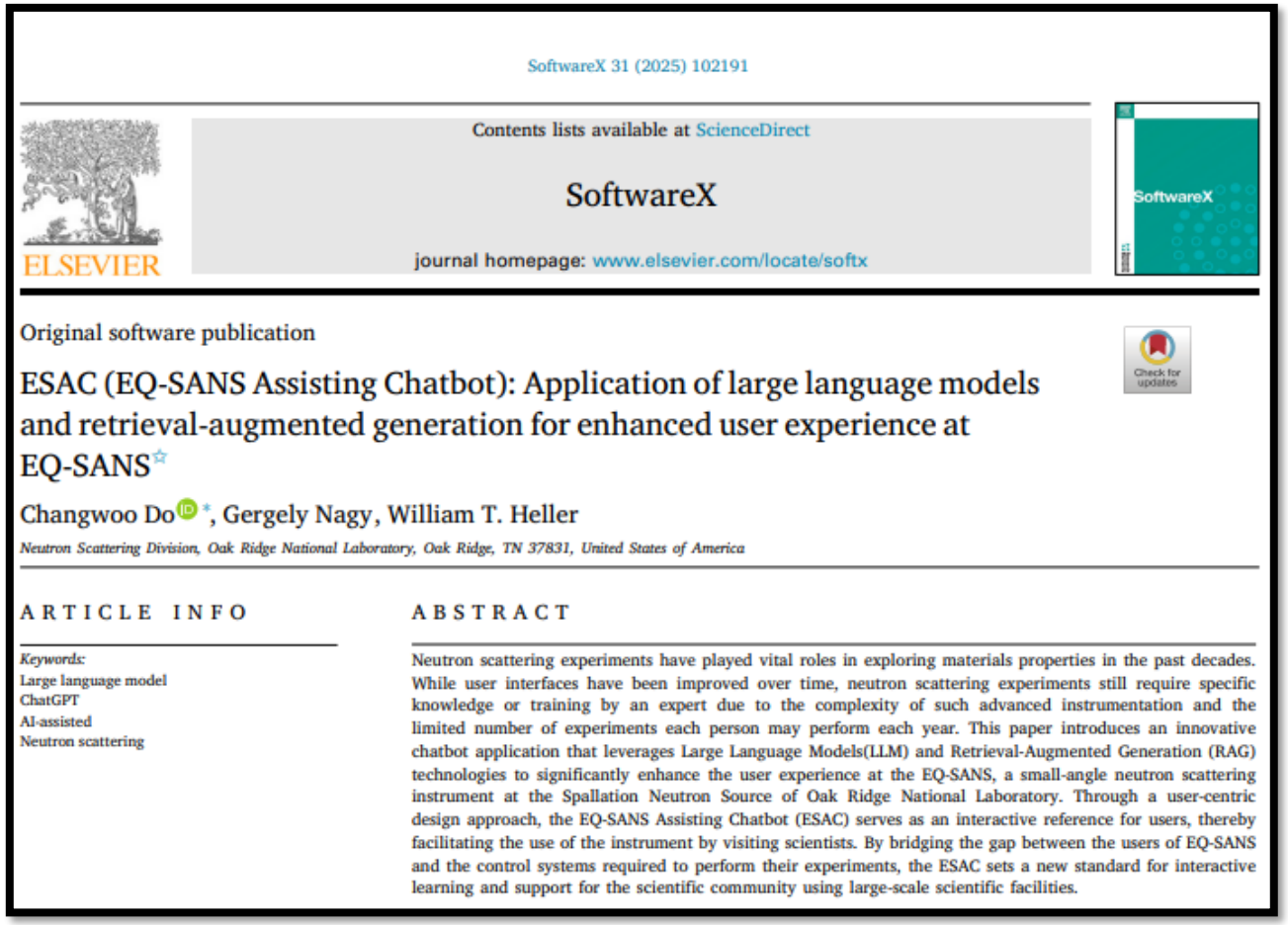
- New chopper installation (Jan 2026)
  - Enables monochromatic wavelength experiments



- Continued SE and automation expansion
- Software aligned with suite strategy

Integration/Application of ML & AI Approaches (Q7)

- ESAC: AI-Assisted Chatbot for EQ-SANS Users
  - Domain-specific AI chatbot
  - Help users:
    - Write experiment scripts
    - Understand instrument functions
  - Produces transparent, editable scripts
  - User Workflow
    - User describes experiment intent
    - ESAC proposes script
    - User reviews/ modifies
    - Script executed normally
    - Data collected as usual



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journal homepage: www.elsevier.com/locate/softx

Original software publication

ESAC (EQ-SANS Assisting Chatbot): Application of large language models and retrieval-augmented generation for enhanced user experience at EQ-SANS☆

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ARTICLE INFO

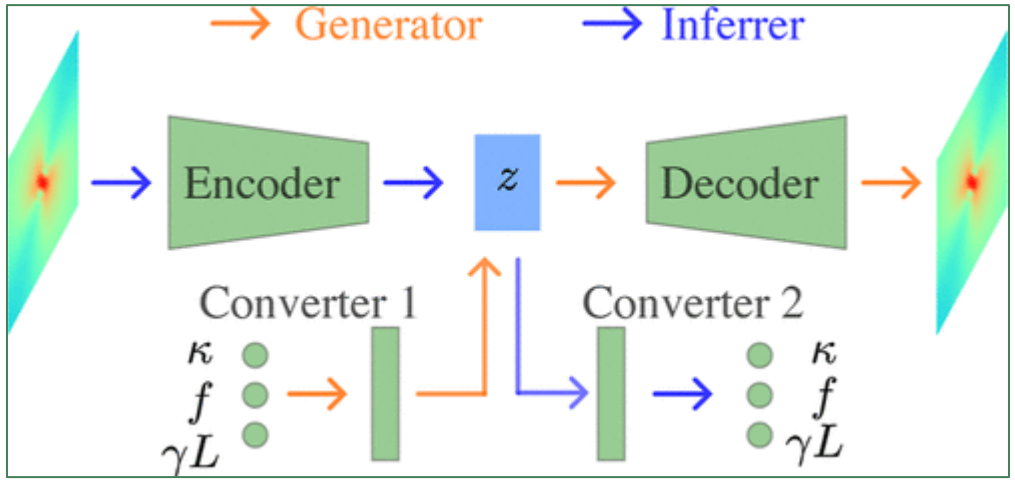
Keywords:
Large language model
ChatGPT
AI-assisted
Neutron scattering

ABSTRACT

Neutron scattering experiments have played vital roles in exploring materials properties in the past decades. While user interfaces have been improved over time, neutron scattering experiments still require specific knowledge or training by an expert due to the complexity of such advanced instrumentation and the limited number of experiments each person may perform each year. This paper introduces an innovative chatbot application that leverages Large Language Models(LLM) and Retrieval-Augmented Generation (RAG) technologies to significantly enhance the user experience at the EQ-SANS, a small-angle neutron scattering instrument at the Spallation Neutron Source of Oak Ridge National Laboratory. Through a user-centric design approach, the EQ-SANS Assisting Chatbot (ESAC) serves as an interactive reference for users, thereby facilitating the use of the instrument by visiting scientists. By bridging the gap between the users of EQ-SANS and the control systems required to perform their experiments, the ESAC sets a new standard for interactive learning and support for the scientific community using large-scale scientific facilities.

Integration/Application of ML & AI Approaches (Q7)

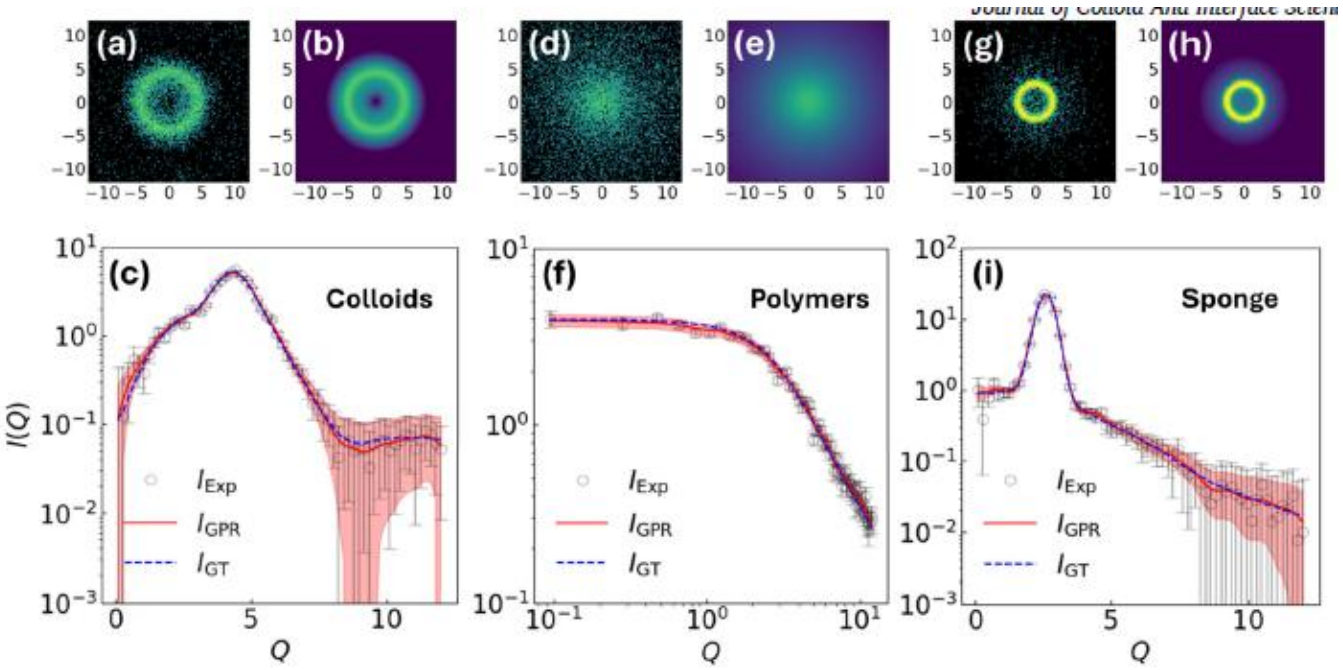
- Machine Learning-Assisted SANS Analysis
  - Result of a completed LDRD project "ML-Assisted SANS Data Analysis"
  - ML models developed for:
    - Interacting polydisperse hard spheres
    - Charged polymers
    - Interacting charged spheres
    - Lamellar phases
    - Ladder polymers
    - Mechanically driven polymers
    - Interacting hard rods (in progress)



[1] Tung, C. H. *et al.* **Inferring effective electrostatic interaction of charge-stabilized colloids from scattering using deep learning**. *Journal of Applied Crystallography* **57**, 1047–1058 (2024).
[2] Tung, C.-H. *et al.* **Insights into distorted lamellar phases with small-angle scattering and machine learning**. *J Appl Crystallogr* **58**, 523–534 (2025).
[3] Ding, L., Tung, C.-H., Sumpter, B. G., Chen, W.-R. & Do, C. **Machine learning inversion from scattering for mechanically driven polymers**. *J Appl Crystallogr* **58**, 1526–1532 (2025).
[4] Ding, L., Tung, C.-H., Sumpter, B. G., Chen, W.-R. & Do, C. **Deciphering the Scattering of Mechanically Driven Polymers Using Deep Learning**. *J. Chem. Theory Comput.* **21**, 4176–4182 (2025).
[5] Ding, L., Tung, C.-H., Carrillo, J.-M. Y., Chen, W.-R. & Do, C. **Machine learning inversion from small-angle scattering for charged polymers**. *Digital Discovery* 10.1039.D5DD00038F (2025) doi:10.1039/D5DD00038F.
[6] Ding, L. *et al.* **Machine learning-assisted profiling of a kinked ladder polymer structure using scattering**. *Digital Discovery* **4**, 1570–1577 (2025).
[7] Ding, L. & Do, C. **Deciphering the small-angle scattering of polydisperse hard spheres using deep learning**. *APL Machine Learning* **3**, 036112 (2025).

Integration/Application of ML & AI Approaches (Q7)

- Augmenting Sparse SANS Measurements with Bayesian Inference
  - Result of a completed LDRD project "ML-Assisted SANS Data Analysis"
  - **1D High-Fidelity Reconstruction**: A "one-shot" GPR approach that reconstructs smooth 1D profiles from sparse data
  - **2D anisotropic Recovery**: Extends Bayesian inference to 2D patterns using symmetry-aware basis functions to recover complex features from noisy or occluded detector data
  - **Real-Time Convergence Metric**: A dimensionless forecasting tool that predicts optimal measurement duration from early-time data by identifying universal power-law scaling in profile evolution.



(1) Tung, C. H.; Yip, S.; Huang, G. R.; Porcar, L.; Shinohara, Y.; Sumpter, B. G.; Ding, L.; Do, C.; Chen, W. R. **Unlocking Hidden Information in Sparse Small-Angle Neutron Scattering Measurements**. *Journal of Colloid and Interface Science* **2025**, *692*, 137554–137554. https://doi.org/10.1016/J.JCIS.2025.137554.
(2) Tung, C.-H.; Ding, L.; Shinohara, Y.; Huang, G.-R.; Carrillo, J.-M.; Chen, W.-R.; Do, C. **A Convergence Metric for Counting Statistics in Time-Resolved Small Angle Neutron Scattering**. *The Journal of Chemical Physics* **2025**, *163* (7), 074107. https://doi.org/10.1063/5.0281134.
(3) Tung, C.-H.; Wang, Y.; Carrillo, J.-M.; Shinohara, Y.; Chen, C.-Y.; Lin, J.-M.; Porcar, L.; Murphy, R. P.; Huang, G.-R.; Ding, L.; Do, C.; Chen, W.-R. **Bayesian Inference of Anisotropic 2D Small-Angle Scattering from Sparse Measurement**. *The Journal of Chemical Physics* **2025**, *163* (15), 154103. https://doi.org/10.1063/5.0291081.

User-Driven Development Since 2020 (Q6)

- Time-resolved Rheometer & Tensile stage
- Robotic sample changer deployed (Q7, automation)
- Light sample environment
- New high-throughput furnace (under development)
  - 12 samples vs 6
  - Compatibility with Nb top-loading cells (NSE & BASIS)
- GI-SANS (under development)

Recent SEs at EQ-SANS

Peltier block

- Improved speed and precision for temperature control

Rheometer

- Stroboscopic Rheology Capability since 2024B

Robotic sample changer

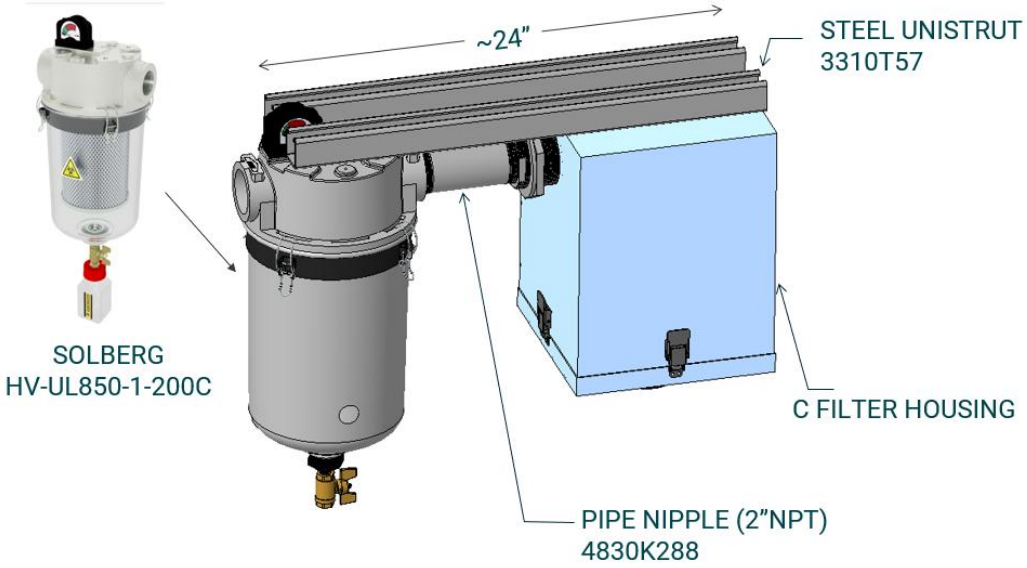
SE contacts:

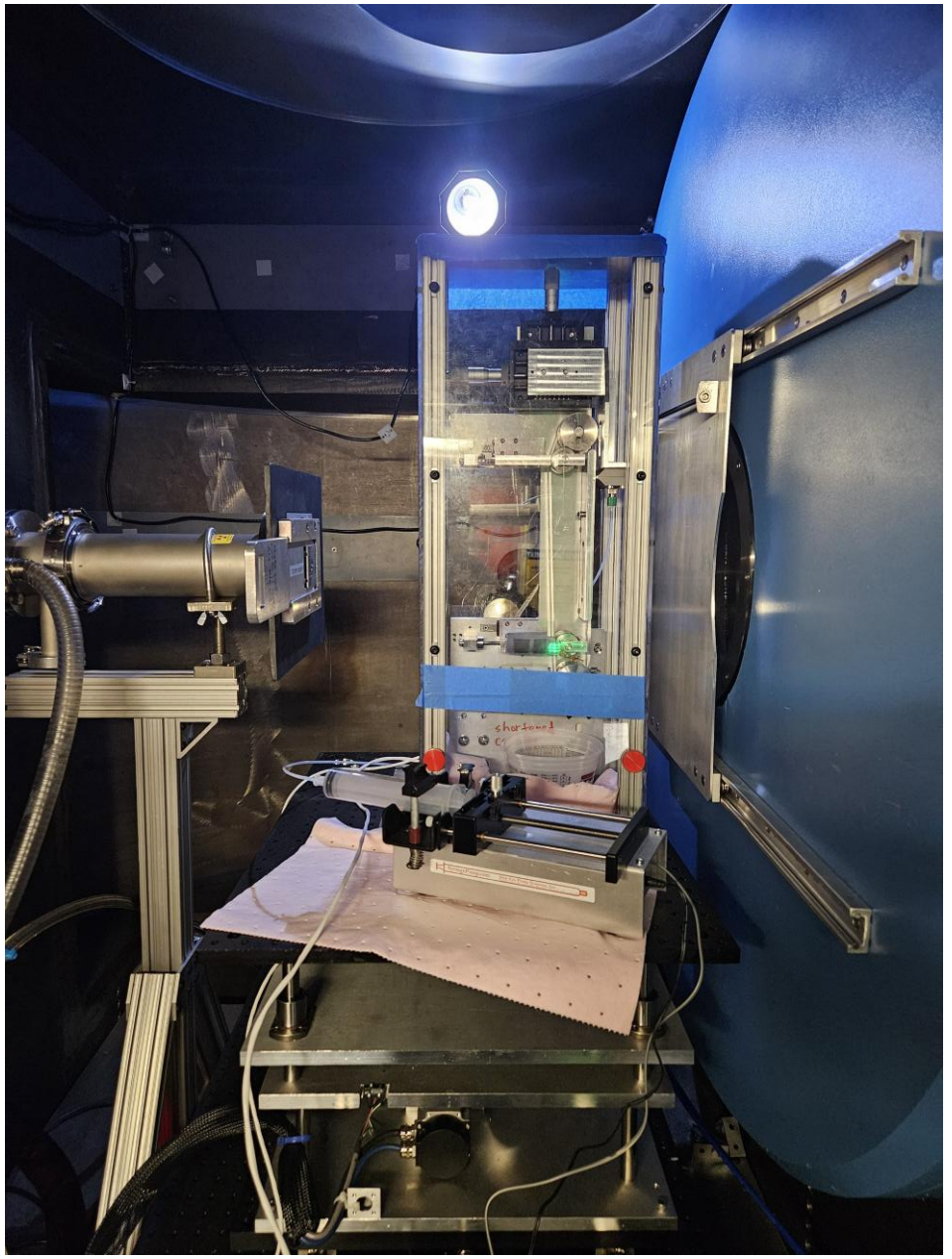
- Sunho Lee
- Mark Loguillo

User Inspired SEs

In-situ battery electrode casting

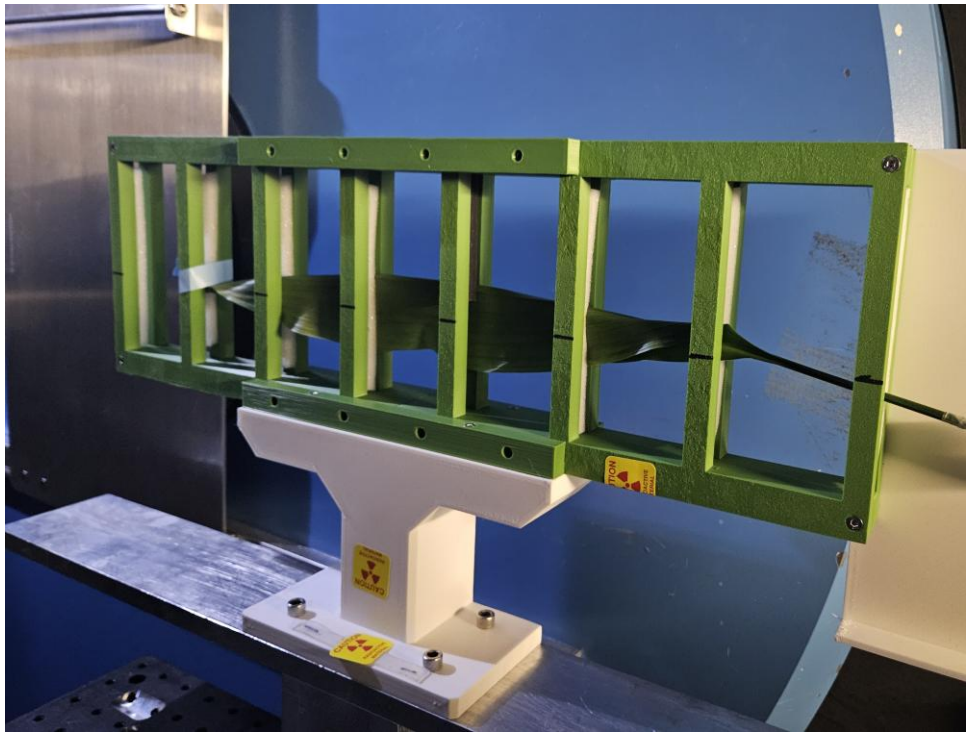
- Collaborative development proposal
- Safety developments allowing:
  - Unbound nanomaterial
  - Flammable solvent



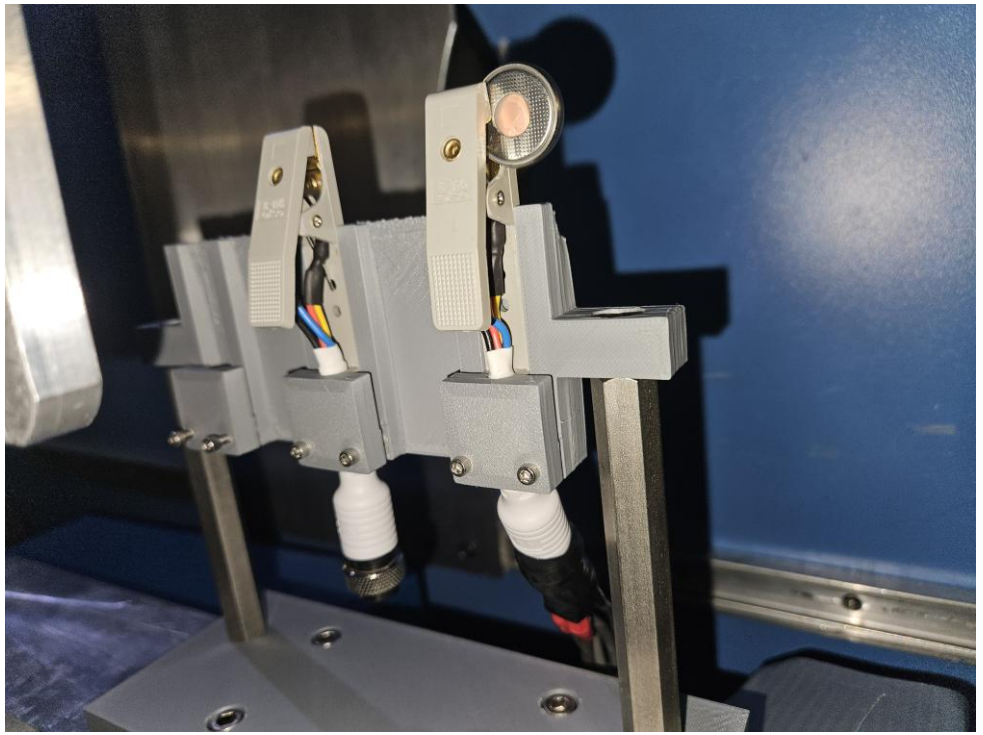


User Inspired SEs – 3D printing

Multi-position leaf sampling



In operando battery testing

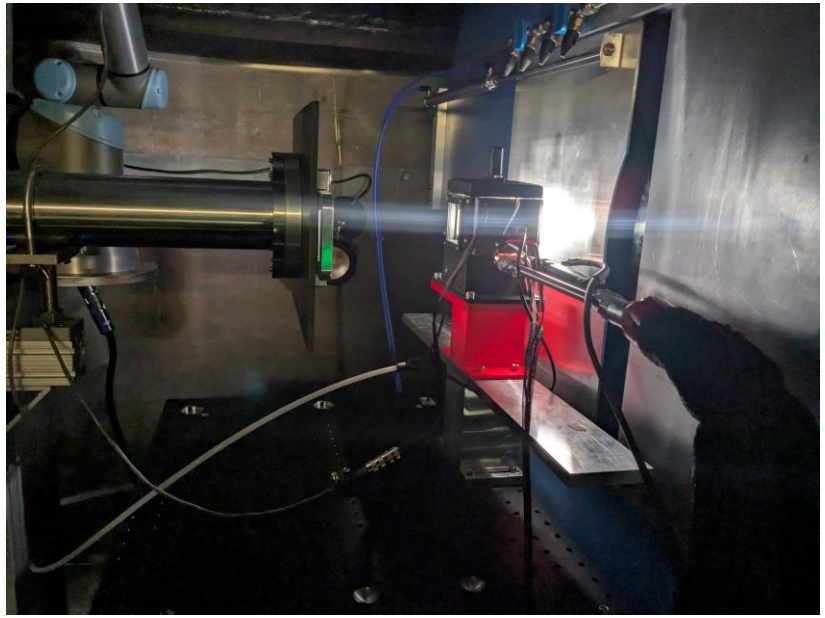


SE contact: Christopher Neal

User Inspired SEs

In-situ illumination, precise T-control

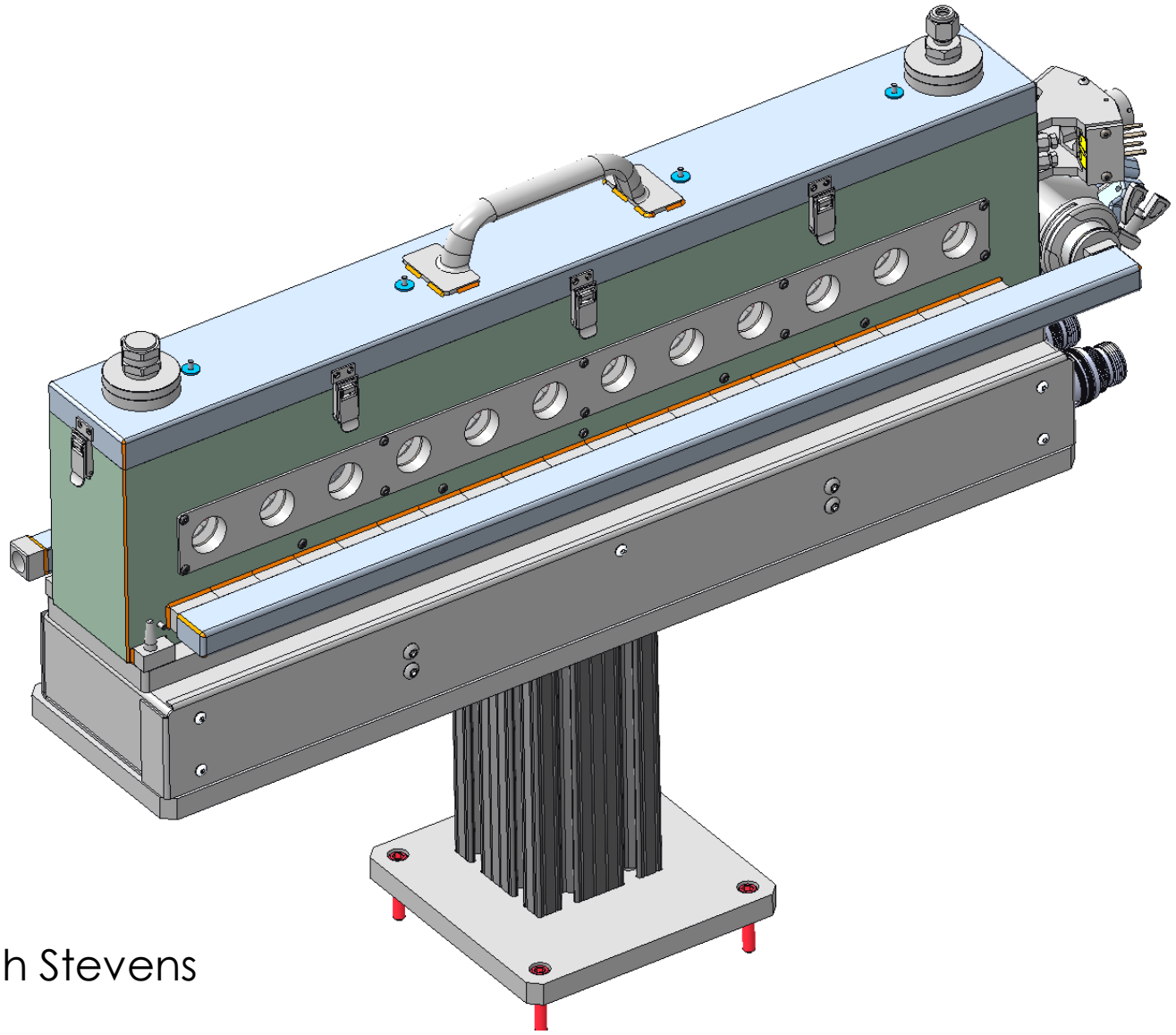
- Interchangeable LED spectral choices, UV, Vis, solar spectra
- Photosynthetic membranes
- Photoresponsive polymers



SE contact: Christopher Neal

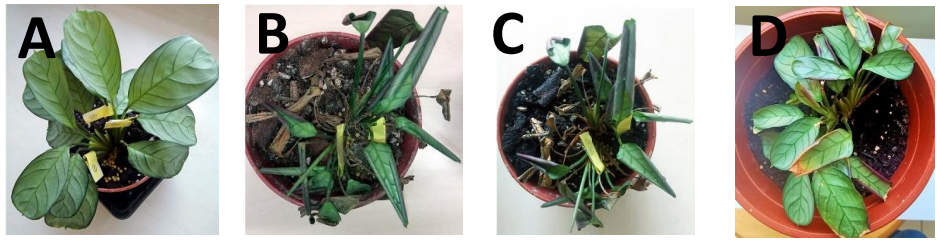
High-throughput furnace – under development

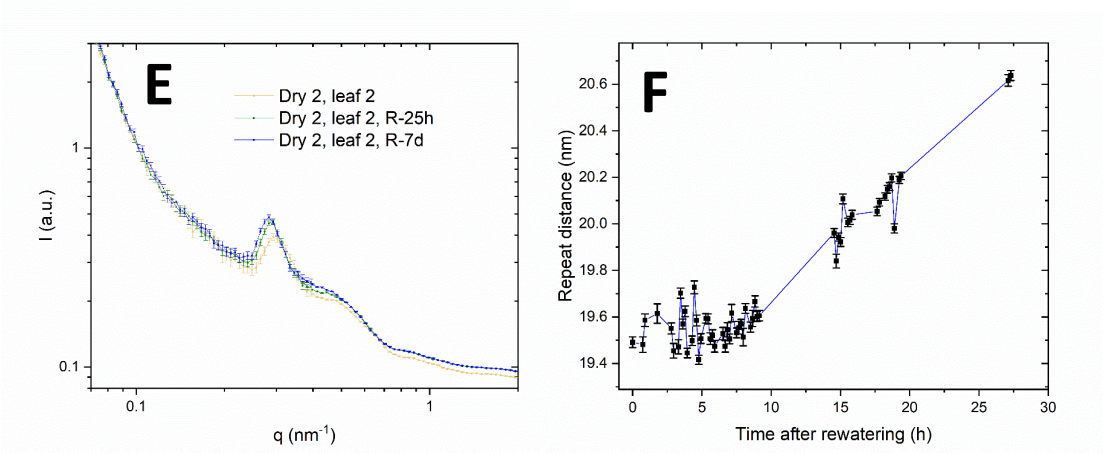
- 12 positions (instead of 5)
- Versatile (SANS, NSE/QENS cells)
- 20 – 300 °C
- Easier/safer installation (lighter)
- Offers gas environment
- Faster cooling times – active air cooling



SE contact: Elijah Stevens

Drought induced changes in plant photosynthesis and subsequent recovery





- Combined SANS, optical spectroscopy, proteomics, light and transmission electron microscopy study
- SANS – unique insight in vivo into the fast structural recovery of the grana structure of drought-stressed leaves

OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

R. Hembrom, R. Ünnep, É. Sárvári, G. Nagy and K. Solymosi, *Physiologia Plantarum* **177** (1), e14621S. doi:10.1111/ppl.14621 Work was performed at SNS: EQ-SANS BL-6

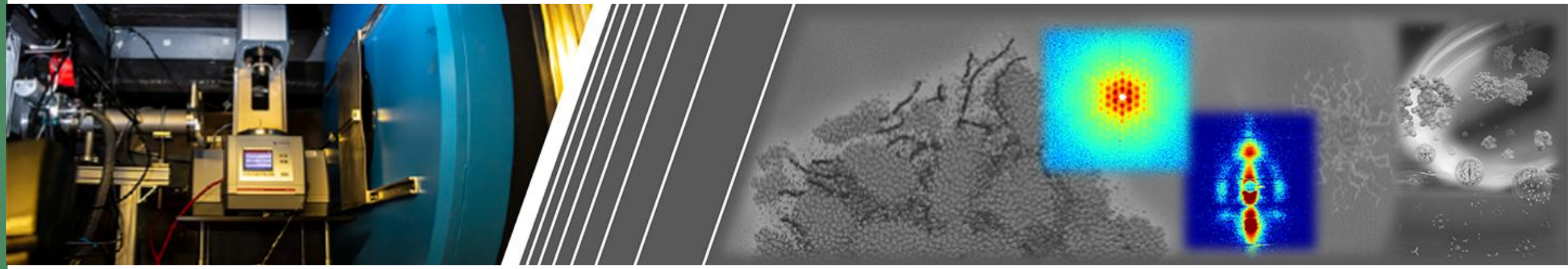
Instrument Team Summary

- Competitive, differentiated capabilities (Q1)
- Day-to-day user needs met (Q3)
- Development plans justified and user-driven (Q6)
- Automation and AI/ML credible and integrated (Q7)

EQ-SANS is a mature, evolving instrument with a clear scientific niche and a disciplined, forward-looking development strategy.

Capitalizing on being a good Q-resolution SANS with high performance at mid and high-Q making EQ-SANS ideal for in-situ and kinetic studies.

THANK YOU



Charges

- **(Q1)** Do the technical capabilities and performance of the individual instruments and instrument suites compare favorably with peer instruments at leading national and international neutron facilities?
- **(Q3)** Do the beamlines meet users' day-to-day needs for data collection, reduction, and analysis? Are planned software developments sufficient to meet anticipated future user needs?
- **(Q6)** Are the plans for development appropriate and well justified to meet current and future user requirements? Please consider aspects of instrument techniques, sample environments, sample preparation and characterization infrastructure, data analysis and modeling capabilities.
- **(Q7)** Are there well-defined and credible plans for future automation and integration of artificial intelligence or machine-learning approaches?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- User describes experiment intent
- ESAC proposes script
- User reviews/ modifies
- Answer questions about instrument
- Search past script