

## Article

# A Unified User-Friendly Instrument Control and Data Acquisition System for the ORNL SANS Instrument Suite

Xingxing Yao, Blake Avery, Miljko Bobrek, Lisa Debeer-Schmitt, Xiaosong Geng, Ray Gregory, Greg Guyotte, Mike Harrington, Steven Hartman, Lilin He, Luke Heroux, Kay Kasemir, Rob Knudson, James Kohl, Carl Lionberger, Kenneth Littrell, Matthew Pearson, Sai Venkatesh Pingali, Cody Pratt, Shuo Qian \*, Mariano Ruiz-Rodriguez, Vladislav Sedov, Gary Taufer, Volker Urban and Klemen Vodopivec

Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA; xingxingyao@gmail.com (X.Y.); averybe@ornl.gov (B.A.); bobrekm@ornl.gov (M.B.); debeerschlm@ornl.gov (L.D.-S.); geng@ornl.gov (X.G.); gregoryrd@ornl.gov (R.G.); guyottegs@ornl.gov (G.G.); harringtonml@ornl.gov (M.H.); hartmansm@ornl.gov (S.H.); hel3@ornl.gov (L.H.); herouxla@ornl.gov (L.H.); kasemirk@ornl.gov (K.K.); knudsoniroiv@ornl.gov (R.K.); kohlja@ornl.gov (J.K.); calionberger@lbl.gov (C.L.); littrellkc@ornl.gov (K.L.); pearsonmr@ornl.gov (M.P.); pingalis@ornl.gov (S.V.P.); prattcl@ornl.gov (C.P.); ruizmm@ornl.gov (M.R.-R.); sedovvn@ornl.gov (V.S.); tauferga@ornl.gov (G.T.); urbanvs@ornl.gov (V.U.); vodopiveck@ornl.gov (K.V.)

\* Correspondence: qians@ornl.gov; Tel.: +1-865-241-1934

**Citation:** Yao, X.; Avery, B.; Bobrek, M.; Debeer-Schmitt, L.; Geng, X.; Gregory, R.; Guyotte, G.; Harrington, M.; Hartman, S.; He, L.; et al. A Unified User-Friendly Instrument Control and Data Acquisition System for the ORNL SANS Instrument Suite. *Appl. Sci.* **2021**, *11*, 1216. <https://doi.org/10.3390/app11031216>

Academic editor:

Received: date

Accepted: date

Published: 28 January 2021

**Publisher's Note:** MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



**Copyright:** © 2021 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).

**Abstract:** In an effort to upgrade and provide a unified and improved instrument control and data acquisition system for the Oak Ridge National Laboratory (ORNL) small-angle neutron scattering (SANS) instrument suite—biological small-angle neutron scattering instrument (Bio-SANS), the extended q-range small-angle neutron scattering diffractometer (EQ-SANS), the general-purpose small-angle neutron scattering diffractometer (GP-SANS)—beamline scientists and developers teamed up and worked closely together to design and develop a new system. We began with an in-depth analysis of user needs and requirements, covering all perspectives of control and data acquisition based on previous usage data and user feedback. Our design and implementation were guided by the principles from the latest user experience and design research and based on effective practices from our previous projects. In this article, we share details of our design process as well as prominent features of the new instrument control and data acquisition system. The new system provides a sophisticated Q-Range Planner to help scientists and users plan and execute instrument configurations easily and efficiently. The system also provides different user operation interfaces, such as wizard-type tool Panel Scan, a Scripting Tool based on Python Language, and Table Scan, all of which are tailored to different user needs. The new system further captures all the metadata to enable post-experiment data reduction and possibly automatic reduction and provides users with enhanced live displays and additional feedback at the run time. We hope our results will serve as a good example for developing a user-friendly instrument control and data acquisition system at large user facilities.

**Keywords:** SANS; neutron scattering; instrument control; data acquisition; user facility; GUI

This supplemental information presents screenshots for various tabs in the new system.



## SANS Panel Scans

1. Check Q Setups
2. Select Q Setups
3. Sample Environment Devices
4. Load Samples
5. Specify Exposure Time
6. Expand and Submit Table

### Sample Environment Device(s):

(for reference) Sample Environment Device(s) as in IPTS:

☒ Use Peltiers temperature controllers (Unit: C).  
☐ Same temperature for all controllers  
☒ Different temperatures.

☒ Use PolyScience chiller (Unit: C).  
☒ Use Chiller 1  
☐ Use Chiller 2  
☐ Use Chiller 3

☒ Use Lakeshore 336 (Unit: K).  
☒ Use SensorA.  
☐ Use SensorB.

☐ Use Dilution Fridge (Unit: K).

☐ Use Tumbler (Unit: RPM).

☐ Use ramp rate.

☐ Use other device combination:

☐ Use equilibration time (hold time; unit: seconds):

Done Configuring Device(s)
Done Editing Device(s) Table

See devices.py for tolerance, time out to the difference between max wait time and time out.

```

2020-11-13 10:42:48 INFO Generate Select Q Setups Output. Beginning...
2020-11-13 10:42:48 INFO Autosave: Reading home/control/ffilers/StandardQSetups/conf_0G40mm_15.5m_12.0A_4885VP_1.0deg_scatt.sav
2020-11-13 10:42:48 INFO Autosave: Reading home/control/ffilers/StandardQSetups/conf_0G40mm_15.5m_12.0A_4885VP_1.0deg_trans.sav
2020-11-13 10:42:48 INFO Autosave: Reading home/control/ffilers/StandardQSetups/conf_0guides40mm_15.5m_18.0A_1.4deg_scatt.sav
2020-11-13 10:42:48 INFO Autosave: Reading home/control/ffilers/StandardQSetups/conf_0guides40mm_15.5m_18.0A_1.4deg_trans.sav
2020-11-13 10:42:48 INFO Autosave: Reading home/control/ffilers/StandardQSetups/conf_7guides_2.25m_6.03A_12.2deg_scatt.sav
2020-11-13 10:42:48 INFO CA Server started
2020-11-13 10:42:48 INFO Started cg3-PanelScans
2020-11-13 10:42:48 INFO Generate Select Q Setups Output. Complete.

```

**Figure S3.** Sample Environment Devices tab in the Panel Scans interface, for selecting specific sample environment for the current experiment. “Use other device combination:” will reveal the text input box to type a comma separated parameter names or aliases.

## SANS Panel Scans

1. Check Q Setups
2. Select Q Setups
3. Sample Environment Devices
4. Load Samples
5. Specify Exposure Time
6. Expand and Submit Table

### Load Samples:

(for reference) Sample ID: 3 Sample Name: No sample

☒ Sample Changer Default Positions to Use: 1-15 Edit Positions to Use: 1,5,7,9,13

☐ ITEMS IDs

☒ Title

☐ Background (p.g. Title within an experiment, run1 1, run1 2)

☒ Sample thickness

☒ Composition: protein (or polymer) Default Composition: **14p15**

☒ Composition concentration

☒ Solvent Default Solvent: **50 mM HEPES**

☐ Solvent ratio

☐ Salt

☐ Salt concentration

☐ Sample type (Sample/Background/Empty Cell/Open Beam)

☐ Comment

Done Configuring Sample Related Columns
Done Loading Sample Details

Sample_Pos	Sample_Title	Sample_Thickness_mm	Composition	Composition_concentration	Solvent
Pos 1	s1				
Pos 5	s2				
Pos 7	s3				
Pos 9	s4				
Pos 13	s5				

Click to add row

```

2020-11-13 10:42:48 INFO Generate Select Q Setups Output. Beginning...
2020-11-13 10:42:48 INFO Autosave: Reading home/control/ffilers/StandardQSetups/conf_0G40mm_15.5m_12.0A_4885VP_1.0deg_scatt.sav
2020-11-13 10:42:48 INFO Autosave: Reading home/control/ffilers/StandardQSetups/conf_0G40mm_15.5m_12.0A_4885VP_1.0deg_trans.sav
2020-11-13 10:42:48 INFO Autosave: Reading home/control/ffilers/StandardQSetups/conf_0guides40mm_15.5m_18.0A_1.4deg_scatt.sav
2020-11-13 10:42:48 INFO Autosave: Reading home/control/ffilers/StandardQSetups/conf_0guides40mm_15.5m_18.0A_1.4deg_trans.sav
2020-11-13 10:42:48 INFO Autosave: Reading home/control/ffilers/StandardQSetups/conf_7guides_2.25m_6.03A_12.2deg_scatt.sav
2020-11-13 10:42:48 INFO CA Server started
2020-11-13 10:42:48 INFO Started cg3-PanelScans
2020-11-13 10:42:48 INFO Generate Select Q Setups Output. Complete.

```

**Figure S4.** Load Samples tab in the Panel Scans interface, for more specific sample information.

## SANS Panel Scans

1. Check Q Setups
2. Select Q Setups
3. Sample Environment Devices
4. Load Samples
5. Specify Exposure Time
6. Expand and Submit Table

### Specify Exposure Time:

☒ Use max wait time (unit: seconds): 600.00

Done Configuring - Generate Table

Sample_Pos	Sample_Title	Config_Path	Wait_For	Value	Or Time
Pos 1	s1	homecontrols/files/StandardQSetups/conf_OG40mm_15.5m_12.0A_4885VP_1.0deg_scat.sav	seconds	18000.0	600.0
Pos 1	s1	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_18.0A_1.4deg_scat.sav	seconds	18000.0	600.0
Pos 1	s1	homecontrols/files/StandardQSetups/conf_7guides_2.25m_6.03A_12.2deg_scat.sav	seconds	18000.0	600.0
Pos 5	s2	homecontrols/files/StandardQSetups/conf_OG40mm_15.5m_12.0A_4885VP_1.0deg_scat.sav	seconds	18000.0	600.0
Pos 5	s2	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_18.0A_1.4deg_scat.sav	seconds	18000.0	600.0
Pos 5	s2	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_6.03A_1.4deg_scat.sav	seconds	18000.0	600.0
Pos 5	s2	homecontrols/files/StandardQSetups/conf_7guides_2.25m_6.03A_12.2deg_scat.sav	seconds	18000.0	600.0
Pos 7	s3	homecontrols/files/StandardQSetups/conf_OG40mm_15.5m_12.0A_4885VP_1.0deg_scat.sav	seconds	18000.0	600.0
Pos 7	s3	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_18.0A_1.4deg_scat.sav	seconds	18000.0	600.0
Pos 7	s3	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_6.03A_1.4deg_scat.sav	seconds	18000.0	600.0
Pos 7	s3	homecontrols/files/StandardQSetups/conf_7guides_2.25m_6.03A_12.2deg_scat.sav	seconds	18000.0	600.0
Pos 9	s4	homecontrols/files/StandardQSetups/conf_OG40mm_15.5m_12.0A_4885VP_1.0deg_scat.sav	seconds	18000.0	600.0
Pos 9	s4	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_18.0A_1.4deg_scat.sav	seconds	18000.0	600.0
Pos 9	s4	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_6.03A_1.4deg_scat.sav	seconds	18000.0	600.0
Pos 9	s4	homecontrols/files/StandardQSetups/conf_7guides_2.25m_6.03A_12.2deg_scat.sav	seconds	18000.0	600.0
Pos 13	s5	homecontrols/files/StandardQSetups/conf_OG40mm_15.5m_12.0A_4885VP_1.0deg_scat.sav	seconds	18000.0	600.0
Pos 13	s5	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_18.0A_1.4deg_scat.sav	seconds	18000.0	600.0
Pos 13	s5	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_6.03A_1.4deg_scat.sav	seconds	18000.0	600.0
Pos 13	s5	homecontrols/files/StandardQSetups/conf_7guides_2.25m_6.03A_12.2deg_scat.sav	seconds	18000.0	600.0

Click to add ...

2020-11-13 10:42:48 INFO Generate Select Q Setups Output. Beginning...  
2020-11-13 10:42:48 INFO Autotask: Reading homecontrols/files/StandardQSetups/conf\_OG40mm\_15.5m\_12.0A\_4885VP\_1.0deg\_scat.sav  
2020-11-13 10:42:48 INFO Autotask: Reading homecontrols/files/StandardQSetups/conf\_OG40mm\_15.5m\_12.0A\_4885VP\_1.0deg\_scat.sav  
2020-11-13 10:42:48 INFO Autotask: Reading homecontrols/files/StandardQSetups/conf\_Oguides40mm\_15.5m\_18.0A\_1.4deg\_scat.sav  
2020-11-13 10:42:48 INFO Autotask: Reading homecontrols/files/StandardQSetups/conf\_Oguides40mm\_15.5m\_18.0A\_1.4deg\_scat.sav  
2020-11-13 10:42:48 INFO Autotask: Reading homecontrols/files/StandardQSetups/conf\_Oguides40mm\_15.5m\_6.03A\_1.4deg\_scat.sav  
2020-11-13 10:42:48 INFO Autotask: Reading homecontrols/files/StandardQSetups/conf\_7guides\_2.25m\_6.03A\_12.2deg\_scat.sav  
2020-11-13 10:42:48 INFO CA Server started  
2020-11-13 10:42:48 INFO Started up PanelScans  
2020-11-13 10:42:48 INFO Generate Select Q Setups Output. Complete.

Done Editing Exposure Time Table

**Figure S5.** Specify Exposure Time tab in the Panel Scans interface to setup measurement time or detector count at different configurations and samples

## SANS Panel Scans

1. Check Q Setups
2. Select Q Setups
3. Sample Environment Devices
4. Load Samples
5. Specify Exposure Time
6. Expand and Submit Table

### Expand Order:

☐ Sample env settings, Q setups (scattering first), sample positions  
☐ Sample env settings, Q setups (transmission first), sample positions  
☐ Q setups (scattering first), sample env settings, sample positions.  
☒ Q setups (transmission first), sample env settings, sample positions.  
☐ Sample positions, Q setups (scattering first), sample env settings.  
☐ Sample env settings, sample positions, Q setups (scattering first).

Expand/New Table    Undo Expand

Expand/Append

Title	Config_Path	Measure_Type	Sample_Pos	Sample_Title	Sample_Thickness mm	Composition	Composition_concentration
Panel Scan Prologue							
Panel Scan 1 of 20, smpl: s1	homecontrols/files/StandardQSetups/conf_OG40mm_15.5m_12.0A_4885VP_1.0deg_scat.sav	Both	Pos 1	s1		nsip15	50 mM HEPES, 1
Panel Scan 2 of 20, smpl: s2	homecontrols/files/StandardQSetups/conf_OG40mm_15.5m_12.0A_4885VP_1.0deg_scat.sav	Both	Pos 5	s2		nsip15	50 mM HEPES, 1
Panel Scan 3 of 20, smpl: s3	homecontrols/files/StandardQSetups/conf_OG40mm_15.5m_12.0A_4885VP_1.0deg_scat.sav	Both	Pos 7	s3		nsip15	50 mM HEPES, 1
Panel Scan 4 of 20, smpl: s4	homecontrols/files/StandardQSetups/conf_OG40mm_15.5m_12.0A_4885VP_1.0deg_scat.sav	Both	Pos 9	s4		nsip15	50 mM HEPES, 1
Panel Scan 5 of 20, smpl: s5	homecontrols/files/StandardQSetups/conf_OG40mm_15.5m_12.0A_4885VP_1.0deg_scat.sav	Both	Pos 13	s5		nsip15	50 mM HEPES, 1
Panel Scan 6 of 20, smpl: s1	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_18.0A_1.4deg_scat.sav	Scattering	Pos 1	s1		nsip15	50 mM HEPES, 1
Panel Scan 7 of 20, smpl: s2	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_18.0A_1.4deg_scat.sav	Scattering	Pos 5	s2		nsip15	50 mM HEPES, 1
Panel Scan 8 of 20, smpl: s3	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_18.0A_1.4deg_scat.sav	Scattering	Pos 7	s3		nsip15	50 mM HEPES, 1
Panel Scan 9 of 20, smpl: s4	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_18.0A_1.4deg_scat.sav	Scattering	Pos 9	s4		nsip15	50 mM HEPES, 1
Panel Scan 10 of 20, smpl: s5	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_18.0A_1.4deg_scat.sav	Scattering	Pos 13	s5		nsip15	50 mM HEPES, 1
Panel Scan 11 of 20, smpl: s1	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_6.03A_1.4deg_scat.sav	Scattering	Pos 1	s1		nsip15	50 mM HEPES, 1
Panel Scan 12 of 20, smpl: s2	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_6.03A_1.4deg_scat.sav	Scattering	Pos 5	s2		nsip15	50 mM HEPES, 1
Panel Scan 13 of 20, smpl: s3	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_6.03A_1.4deg_scat.sav	Scattering	Pos 7	s3		nsip15	50 mM HEPES, 1
Panel Scan 14 of 20, smpl: s4	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_6.03A_1.4deg_scat.sav	Scattering	Pos 9	s4		nsip15	50 mM HEPES, 1
Panel Scan 15 of 20, smpl: s5	homecontrols/files/StandardQSetups/conf_Oguides40mm_15.5m_6.03A_1.4deg_scat.sav	Scattering	Pos 13	s5		nsip15	50 mM HEPES, 1
Panel Scan 16 of 20, smpl: s1	homecontrols/files/StandardQSetups/conf_7guides_2.25m_6.03A_12.2deg_scat.sav	Scattering	Pos 1	s1		nsip15	50 mM HEPES, 1
Panel Scan 17 of 20, smpl: s2	homecontrols/files/StandardQSetups/conf_7guides_2.25m_6.03A_12.2deg_scat.sav	Scattering	Pos 5	s2		nsip15	50 mM HEPES, 1
Panel Scan 18 of 20, smpl: s3	homecontrols/files/StandardQSetups/conf_7guides_2.25m_6.03A_12.2deg_scat.sav	Scattering	Pos 7	s3		nsip15	50 mM HEPES, 1
Panel Scan 19 of 20, smpl: s4	homecontrols/files/StandardQSetups/conf_7guides_2.25m_6.03A_12.2deg_scat.sav	Scattering	Pos 9	s4		nsip15	50 mM HEPES, 1
Panel Scan 20 of 20, smpl: s5	homecontrols/files/StandardQSetups/conf_7guides_2.25m_6.03A_12.2deg_scat.sav	Scattering	Pos 13	s5		nsip15	50 mM HEPES, 1
Unset		Undefined	Out	Undefined		Undefined	Undefined

Click to add row

2020-11-13 10:42:48 INFO Generate Select Q Setups Output. Beginning...  
2020-11-13 10:42:48 INFO Autotask: Reading homecontrols/files/StandardQSetups/conf\_OG40mm\_15.5m\_12.0A\_4885VP\_1.0deg\_scat.sav  
2020-11-13 10:42:48 INFO Autotask: Reading homecontrols/files/StandardQSetups/conf\_OG40mm\_15.5m\_12.0A\_4885VP\_1.0deg\_scat.sav  
2020-11-13 10:42:48 INFO Autotask: Reading homecontrols/files/StandardQSetups/conf\_Oguides40mm\_15.5m\_18.0A\_1.4deg\_scat.sav  
2020-11-13 10:42:48 INFO Autotask: Reading homecontrols/files/StandardQSetups/conf\_Oguides40mm\_15.5m\_18.0A\_1.4deg\_scat.sav  
2020-11-13 10:42:48 INFO Autotask: Reading homecontrols/files/StandardQSetups/conf\_Oguides40mm\_15.5m\_6.03A\_1.4deg\_scat.sav  
2020-11-13 10:42:48 INFO Autotask: Reading homecontrols/files/StandardQSetups/conf\_7guides\_2.25m\_6.03A\_12.2deg\_scat.sav  
2020-11-13 10:42:48 INFO CA Server started  
2020-11-13 10:42:48 INFO Started up PanelScans  
2020-11-13 10:42:48 INFO Generate Select Q Setups Output. Complete.

Total Rows: 22  
Delay Sum: 0.00  
Value Sum: 360000.00

Submit/Seperate Scan Jobs    Simulate  
Submit/One Scan Job    Save Table File

Table file name: homecontrols/vertemp/scanMotor\_UsingAlgoScan\_Th

**Fig. S6** Expand and Submit tab in the Panel Scans interface. It expands the scans in different ways with all conditions from previous setups (such as samples, sample environment, configurations, measurement type (transmission, scattering or both)), only part of the columns are shown in the screenshot

# SANS Q Planner

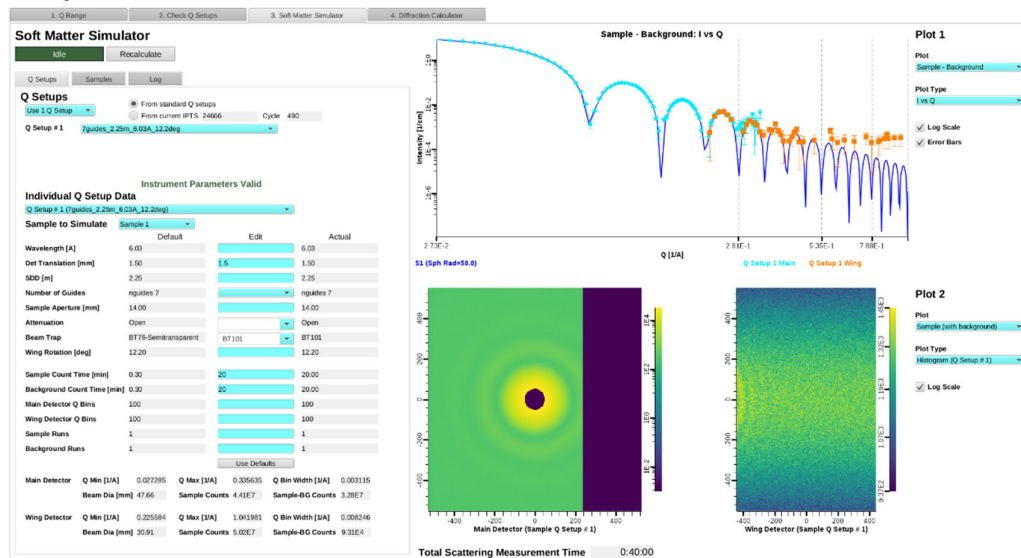


Figure S7. The soft matter simulator with instrument specific parameters.