applied sciences

MDPI

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.); debeerschmlm@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

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.

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/).

Figure S1. Check Q Setups tab in the Panel Scans interface. The yellow outline highlights buttons that are required to be clicked to ensure the output parameters to be calculated.

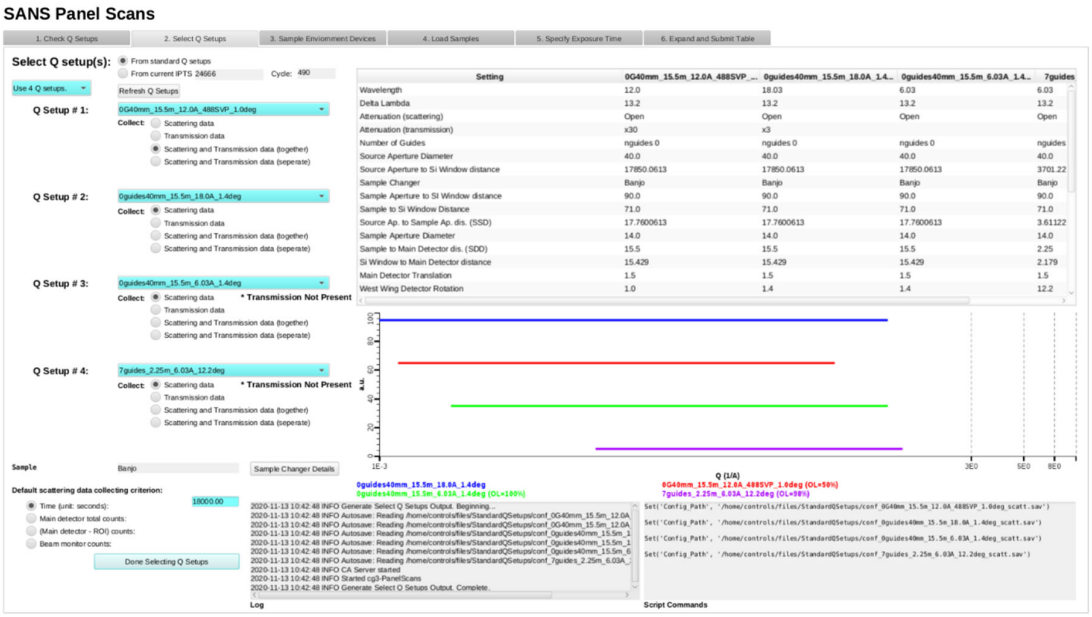

Figure S2. Select Q Setups tab in the Panel Scans interface.

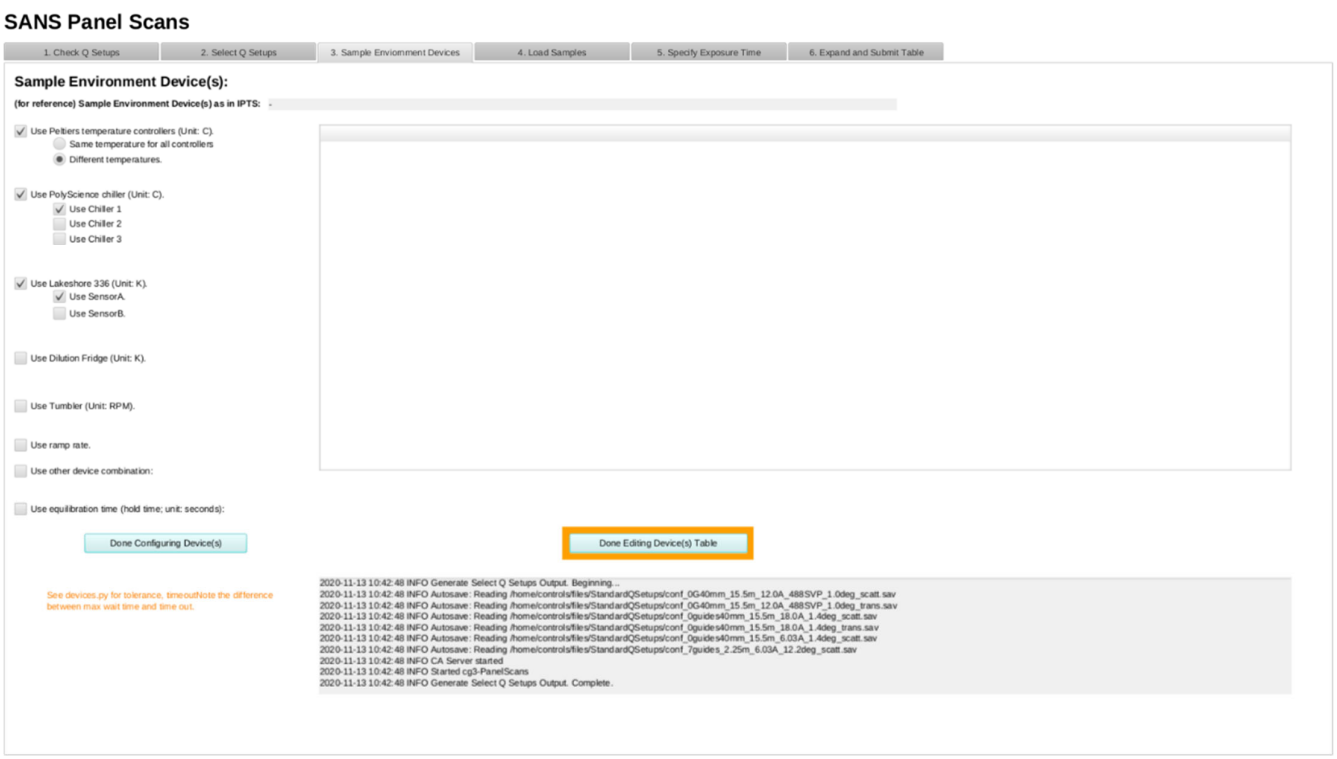

Figure S3. Sample Environment Devices tab in the Panel Scans interface, for selecting specific sample environment for the current experiment. "Use other device combination:" will reveal the text input box to type a comma separated parameter names or aliases.

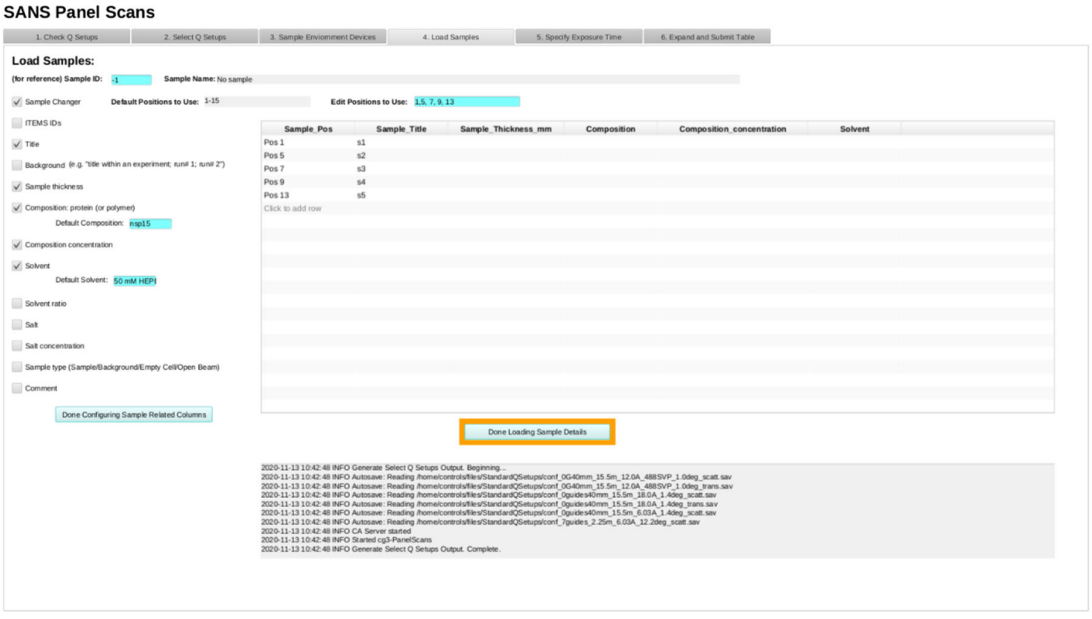

Figure S4. Load Samples tab in the Panel Scans interface, for more specific sample information.

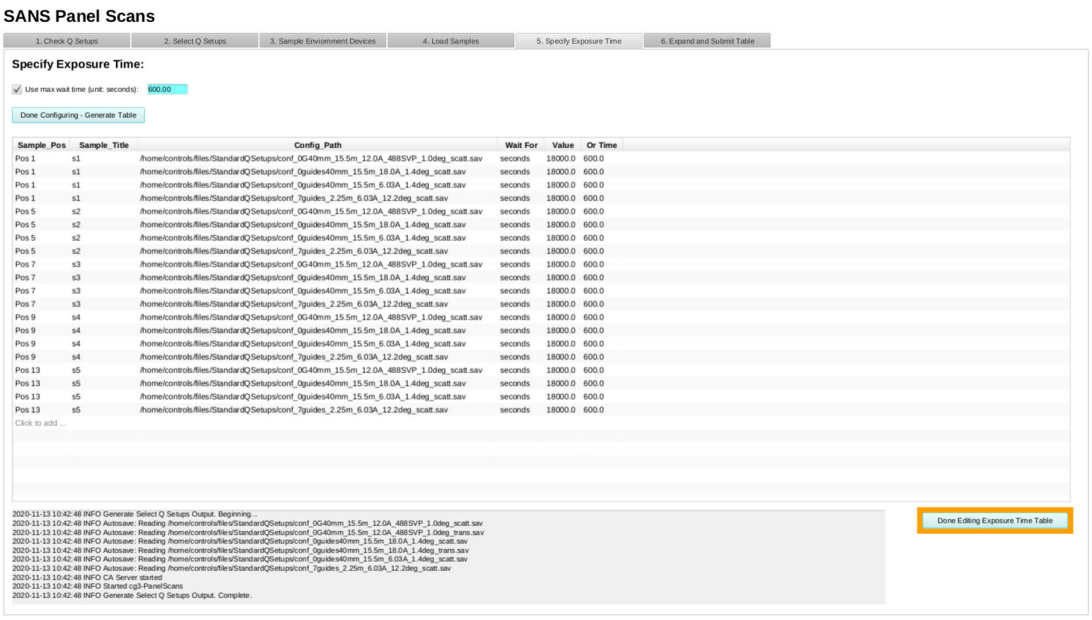

Figure S5. Specify Exposure Time tab in the Panel Scans interface to setup measurement time or detector count at different configurations and samples

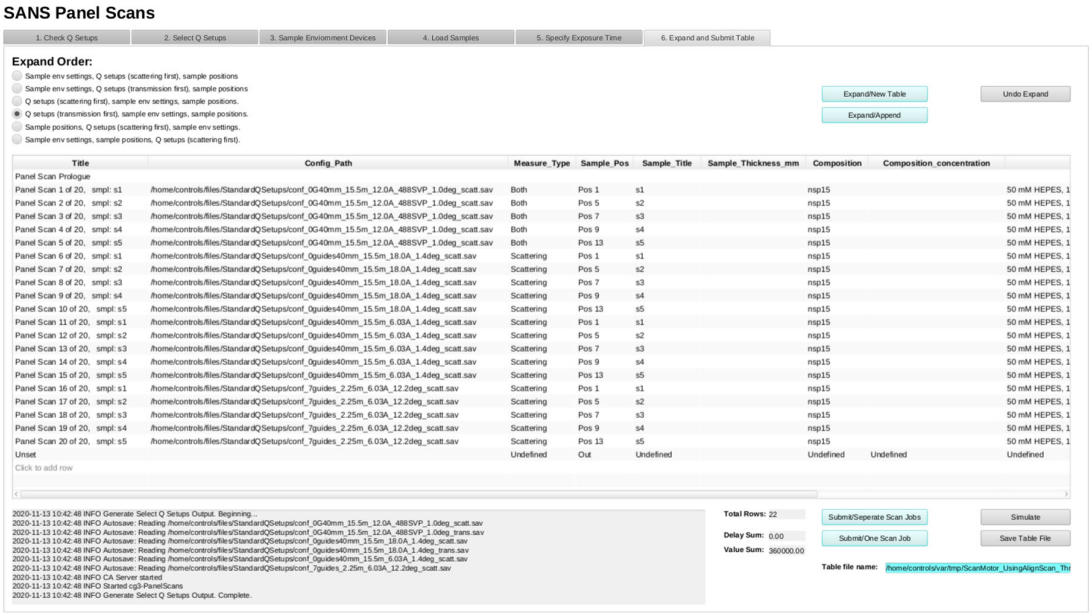

Fig. S6 Expand and Submit tab in the Panel Scans interface. It expands the scans in different ways with all conditions from previous setups (such as samples, sample environment, configurations, measurement type (transmission, scattering or both)), only part of the columns are shown in the screenshot

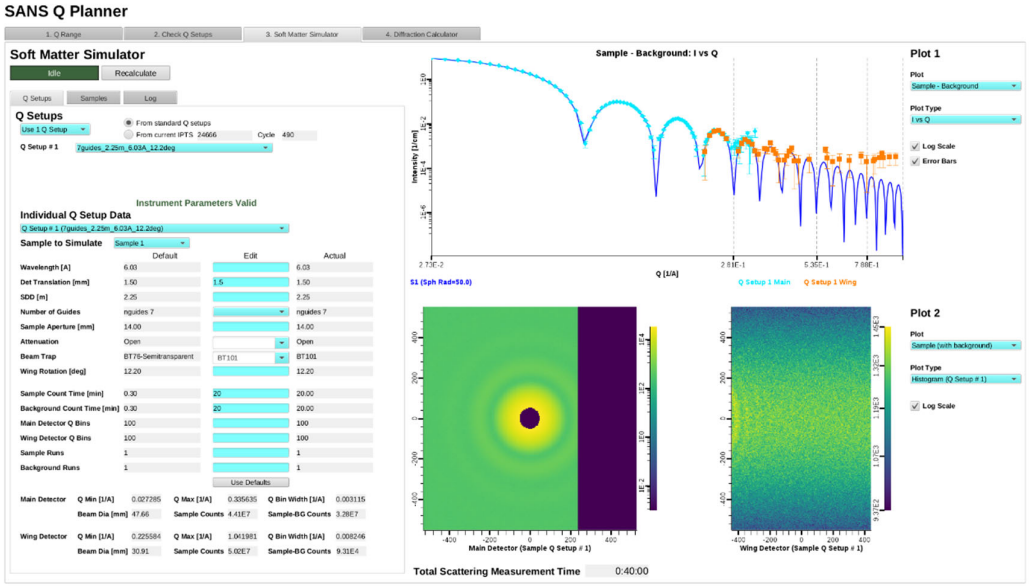

Figure S7. The soft matter simulator with instrument specific parameters.