SNAPRed: A Novel Approach to Data Reduction for the Highly Re-configurable SNAP Diffractometer

Malcolm Guthrie, Michael Walsh, Reece Boston, Kort Travis, Daniel Caballero and Darsh Dinger

Streamlining Data Processes from Collection to Analysis for the SNAP Instrument

Overview of SNAP

The **SNAP** diffractometer is a beacon of versatility at the SNS, meticulously designed to scrutinize materials ranging from powdered, single-crystal to amorphous forms. Augmented with state-of-the-art area detectors, beam-focusing optics, and a vast angular coverage, SNAP epitomizes precision and breadth in neutron diffraction analysis. Its distinctive arsenal includes an array of pressure devices — from conventional Paris-Edinburgh presses reaching up to 25 GPa, to the progressive integration of large-volume diamond anvil cells targeting an impressive 50 to 100 GPa pressure range. This advanced configuration positions SNAP at the forefront of studies necessitating extreme pressure and temperature conditions, facilitating groundbreaking research into domains like planetary ices and intricate hydrogen bonding dynamics.

Challenges of Data Reduction

The **SNAP** diffractometer at **SNS**, with its advanced features like movable detectors, bandwidth-shifting choppers, and wide angular coverage, introduces complexities in data reduction. Its high pixelation requires strategic pixel groupings to balance data quality, while diverse sample environments add layers of interpretation nuances. Real-time changes in sample conditions, like nuclei displacements due to high pressures, complicate the analysis. Consequently, full comprehension of diffraction patterns can be delayed post-experiment. Addressing these challenges is crucial for accurate studies, necessitating solutions like the **SNAPRed** project.

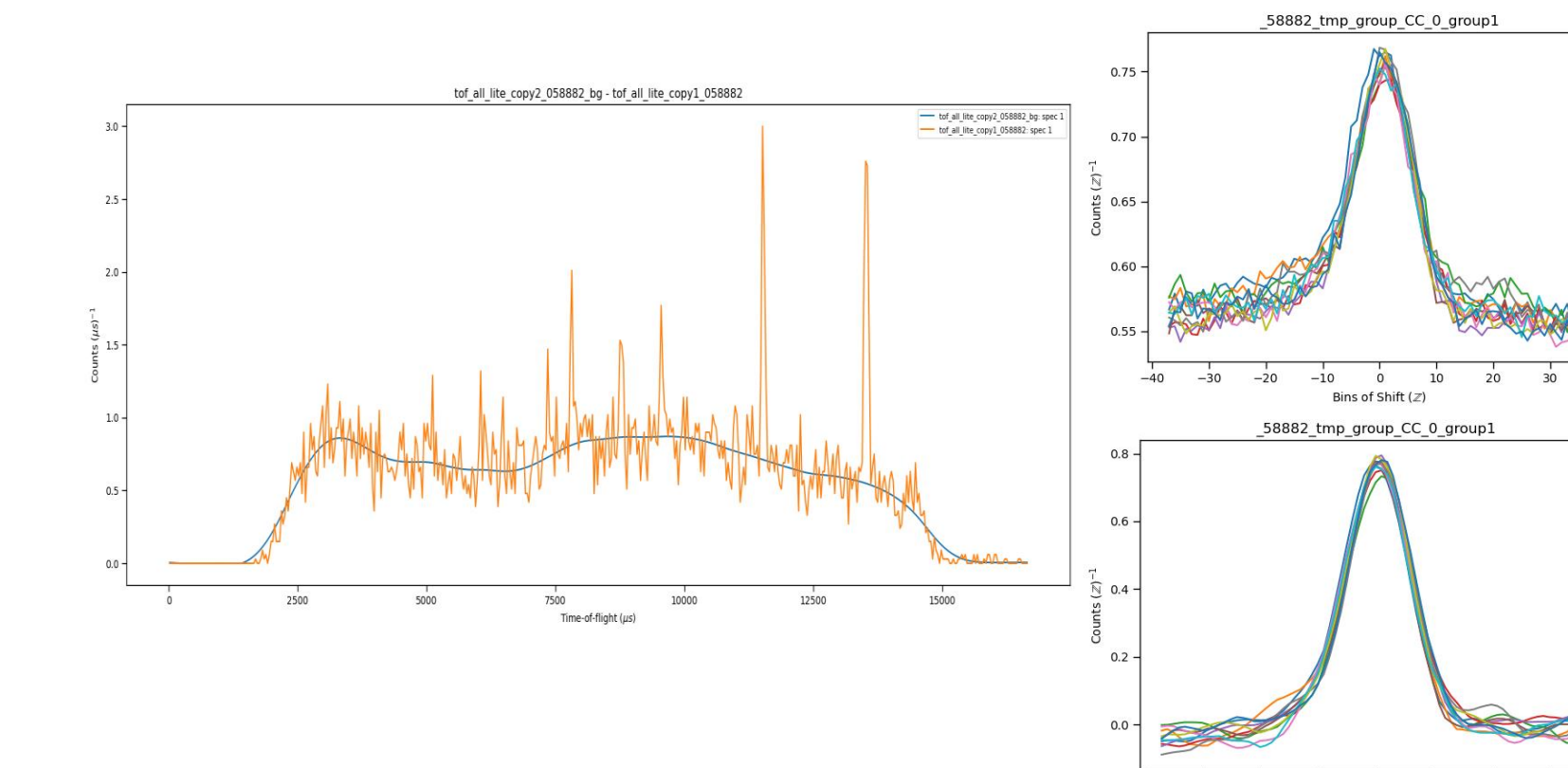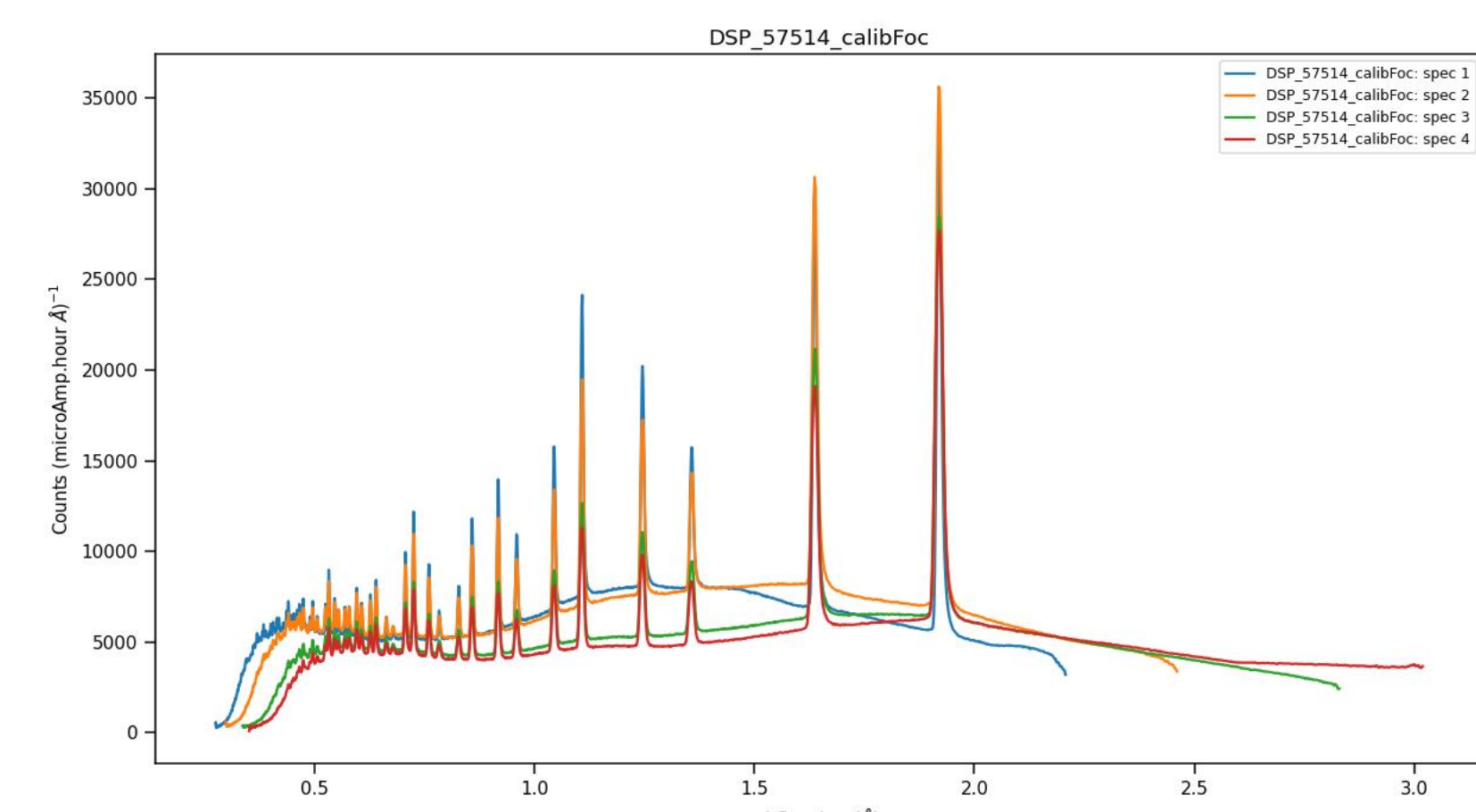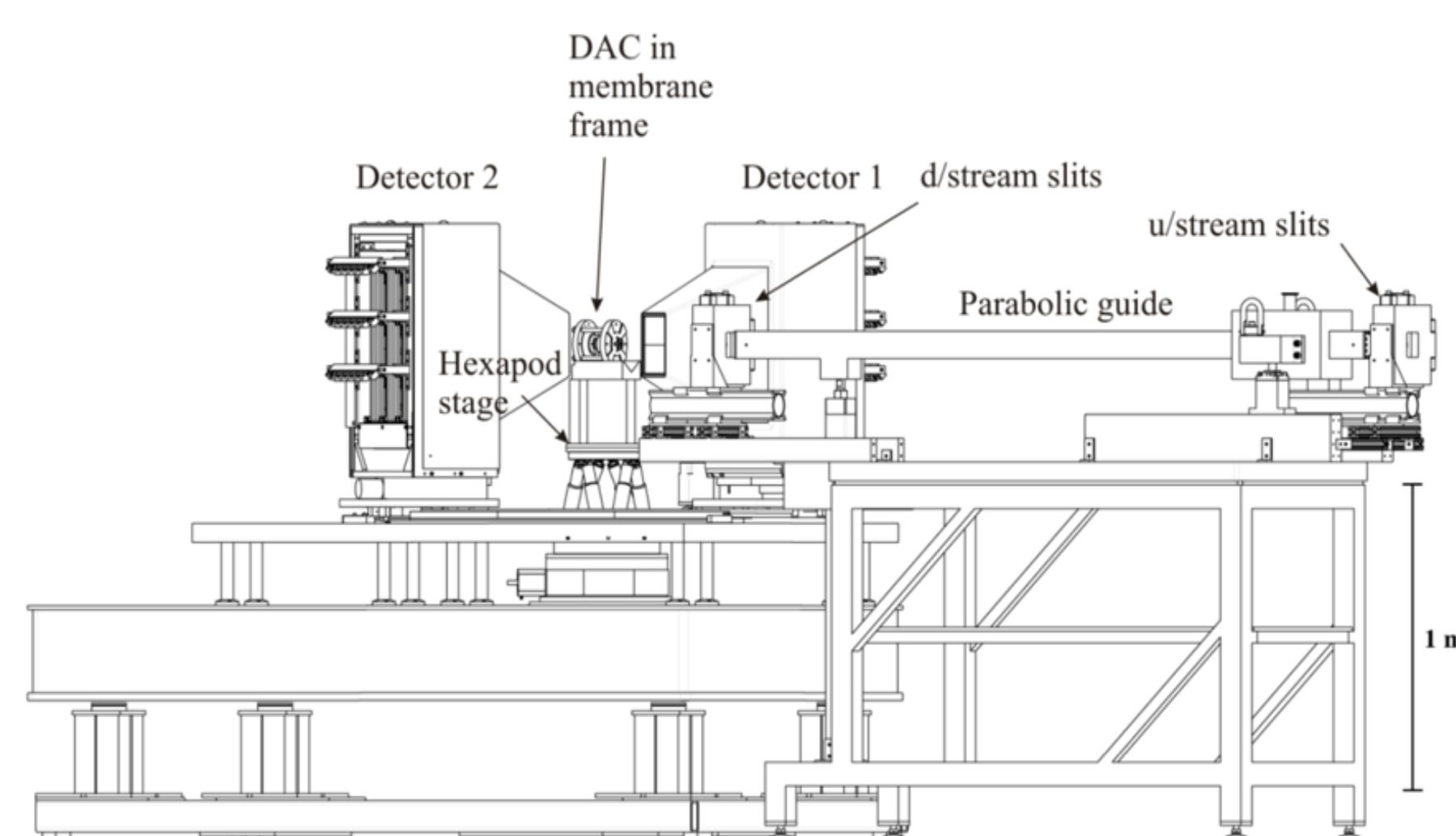## SNAPRed: Streamlining Data Reduction

SNAPRed is a desktop application for Lifecycle Management of data collected from the SNAP instrument. Here are some of the details pertinent to **SNAPRed**:

Conceptual Design:
- Minimal input with maximal extrapolation, a single run number often being enough to complete a reduction.
- Unique Instrument States index and organize finely tuned calibration configurations appropriate for the instrument's physical setup.
- Retain historical configurations to ensure repeatable results.
- Leaverage Mantid algorithms for enhanced data manipulation [1].

User Experience (UX)

SNAPRed: Streamlining Data Reduction (Cont.)

Calibration/Normalization:
- Rapid, standardized process with visual peak fitting feedback.
- Quality metrics ensure consistent and reliable results.
- Tuned for instrument state, sample, and historical relevance.

Managing a Highly Re-Configurable Instrument:
- Addresses dynamic wavelength-dependent backgrounds due to pressure changes.
- Algorithms counteract attenuation effects from nuclei from nuclei displacement, ensuring data integrity.

Application Use Cases

Currently the functional methods included within **SNAPRed**:
- Instrument Configuration and Data Lifecycle Management
- SNAP Data Reduction
- SNAP Instrument Diffraction and Normalization Calibration

In addition to these explicit functionalities, there are a lot of implied benefits for SNAP instrument data as a whole: ***Consistency.***

SNAPRed will provide the facilities and ease of use to encourage users to adopt it as their tool of choice for Reductions and Calibration, and a byproduct of this is an implied standardization of Reduction and Calibration practices. Whereas currently the standard practice is determined by a given CiS's opinionated python script, which can be error prone, subject to undocumented change and irrecoverable deletion.

Future Integration

SNAPRed currently plans to include the following:
- Reduction and Calibration Diagnostics Mode
  - Data Exploration and Visualization
- Low friction and informative User Experience
- Performance Tune-ups
- Advanced Reduction and Calibration parameter tweaking
- On-the-fly Lite Mode data file generation
- Container/Pressure Cell Profiling and Correction

References

[1] Mantid 6.6.0: Manipulation and Analysis Toolkit for Instrument Data.;
Mantid Project. doi: 10.5286/SOFTWARE/MANTID6.6, Arnold, O. et al. Mantid-
Data Analysis and Visualization Package for Neutron Scattering and mu-SR
Experiments. Nuclear Instruments and Methods in Physics Research Section
A: Accelerators, Spectrometers, Detectors and Associated Equipment 764
(2014): 156-166 doi: 10.1016/j.nima.2014.07.029