DMSC Update for Instrument STAPS April 2020

1. Update from Head of DMSC
2. Data Reduction Analysis and Modelling update
3. Experiment Control and Data Curation update.

Update

Head of DMSC

- DMSC funded from initial operations budget since 2020.
- Initial operations (2020-2025) planning ongoing. Planned staff effort is reduced by 62 PY
- In-kind development from STFC, PSI & FZJ continues until 2021
- Some additional PSI development effort funded via contract
- ESS Reorganisation - Experiment Control and Data curation group (Tobias) now part of technical directorate in Project Division (PD).

- Prototype data pipeline development complete and tested at V20
- SANS science case used to show integration between controls - reduction and analysis.
- Ongoing planning with PD to develop plan for instrument development according to the updated instrument plan. This will include all scope from DMSC.
- Software development in all areas makes excellent progress.
- FZJ in-kind has recovered from staff shortage that impacted deliverable.
- Data andlysis group will now run a Python training course at each IKON. First couse in Q1 2020 – 25 particpants.

Update

Data reduction, analysis, and modelling

- Continues to develop core frameworks, most noticeably the scipp library for data reduction
- Focusing on delivering integrated software solutions for data treatment for DREAM and ODIN in 2020, similarly to what has been demonstrated for LoKI at full flux.
- Consolidate instrument simulations with and without sample environments for testing purposes

Imaging:

-PSI in kind extended with post doc focusing on Bragg edge analysis

- first advert out for instrument data scientist. In this case for imaging and engineering diffraction

- Mantid continues to be used for V20 Bragg edge analysis treatment (incl. WFM). Latest developments resolve and visualise anisotropy in strain across different lattice directions by analysing different Bragg edges.

- Good progress with using scipp on V20 Bragg edge analysis (incl. WFM). Comparison against Mantid shows scipp to be faster and much better suited to image processing.

- Paper published on energy-resolved (Bragg edge) computed tomography

- MuhRec 4.2 and 4.2.1 released improving user experience and speed-up.

- started on defining data format and organization for ToF data

- Python interface added to MuhRec & KipTool

- Batch processing prototyped

Update

Data reduction, analysis, and modelling

Diffraction

- Work started on integrated workflow for live (and post experiment) data reduction and analysis based on scipp

- Basic powder data reduction demonstrated in scipp.

- Early scipp performance measurements made against Mantid.

- Started working on describing relevant LLB instruments in Mantid with the goal to further extend this description on the MAGIC instrument.

- first version of GUI and Python API for analysis software interfacing to existing diffraction libraries ready for testing (www.easydiffraction.org)

- Collaborates with LLB on interfacing CrysPy (MAGIC, DREAM, BEER, HEIMDAL) and with ILL on interfacing CrysFML (DREAM, BEER, HEIMDAL)

Update

Data reduction, analysis, and modelling

Large-scale structures

- FZJ in kind contribution staffed with new developers (one senior and one junior). Promising work on seperate GUI for reflectometry.

- SasView 5.0.1 released and 5.0.2 release candidate available

- Initial steps for LoKI towards using scipp for making defining masks easier than with Mantid based on easier working with logical coordinate systems

- Started work on defining proper ToF resolution functions for LoKI

Spectroscopy

- Continues to collaborate with ISIS PACE project on analysis software for spectroscopy where ESS' major deliverable will be a Python SpinW integrated with PACE

- Started work on Python interface for spectroscopy in conjunction with work on Python interface for diffraction

- ISIS received funding from Ada Lovelace Centre for converting SpinW core to efficient C++ library.

Update

Experiment Control and Data Curation

- Group formed to hold responsibility for all controls and DAQ scope for instruments

- started collecting deliverables and milestone on first 3 instruments from the TG3 process, to develop plan for instruments, ICS integration, custom user interfaces etc

- NICOS UI reviewed and made improvements to better suit the standard workflow after user experience workshop

- Prototype data pipeline development tested at V20: SANS science case used to show integration between controls, reduction, analysis and data curation (including electronic logbook)

- Working through lessons learned input from this to improve user experience and robustness of the software

- Established “Ymir” instrument as new development and test platform in Utgard to be available after the shutdown of BER/V20

- Performed successful scalability tests with parallel storage loan system (IBM spectrum scale) in Utgard to confirm we meet the data rate challenge for data streaming and file writing

- Made progress with the detector readout integration, now with more realistic DG prototypes

- Plans and interface definitions for event formation under discussion for many detector types

- We are interested in potential early procurements that instruments or sample environment could do, so we can front load some development work and have more time for testing