EUROPEAN
SPALLATION
SOURCE

DMSC STAP

Updates from DRAM

TORBEN NIELSEN

Agenda

1. DRAM
2. Staff
3. Updates since last STAP
4. Comments to STAP report
5. Summary

DRAM

Data Reduction, Analysis and Modelling

Data reduction

- **scipp** will be used for all instruments
- Possibly in combination with other software for NMX & Imaging
- Are looking for partners

Data analysis

- **easyScience** for powder, sxtal & reflectometry
  - possibly also QENS and TOF imaging
  - But always in combination with other libraries (backengines)
- **SasView** for SANS
- **PACE** for spectroscopy
- **MuhRec** for Tomography.

Data modelling

- **McStas** for instrument simulations
  - Now also with Python API **McStasScript**
  - and optimized for GPU
- **NCrystal**

DRAM

Data Reduction, Analysis and Modelling - Staff


Simon Heybrock


Neil Vaytet


Jan-Lukas Wynen


Sunyoung Yoo


Johannes Kasimir

MS


Piotr Rozyczko


Andrew Sazonov

Developer 3

Developer 4

Developer 4.5


Peter Willendrup


Mads Bertelsen


Thomas Kittlemann*

- 3 teams (14+ persons)
1. Data Reduction (scipp)
2. Data Analysis (SasView, SpinW, EasyScience, external collaborations)
3. Modelling (McStas++, pan-learning.org, NMX IDS, Detector Group)

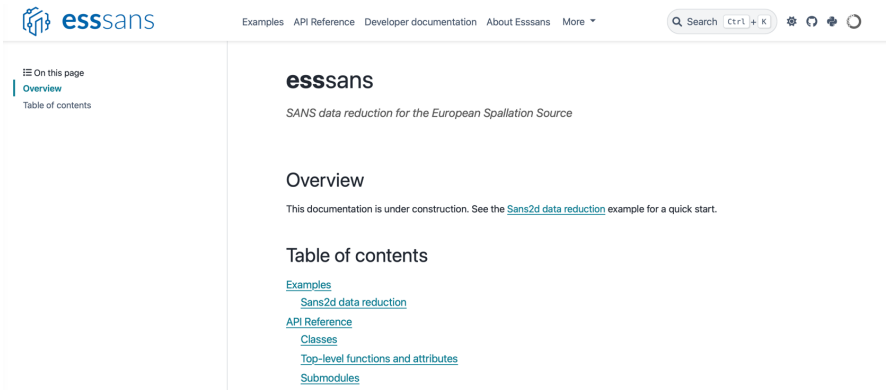
Scope

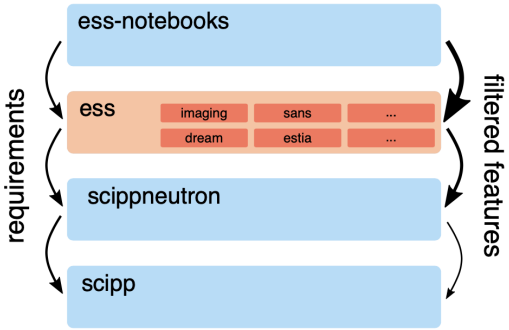
The DRAM group is responsible for providing the data reduction, analysis and modelling soft-ware for all instruments at ESS.

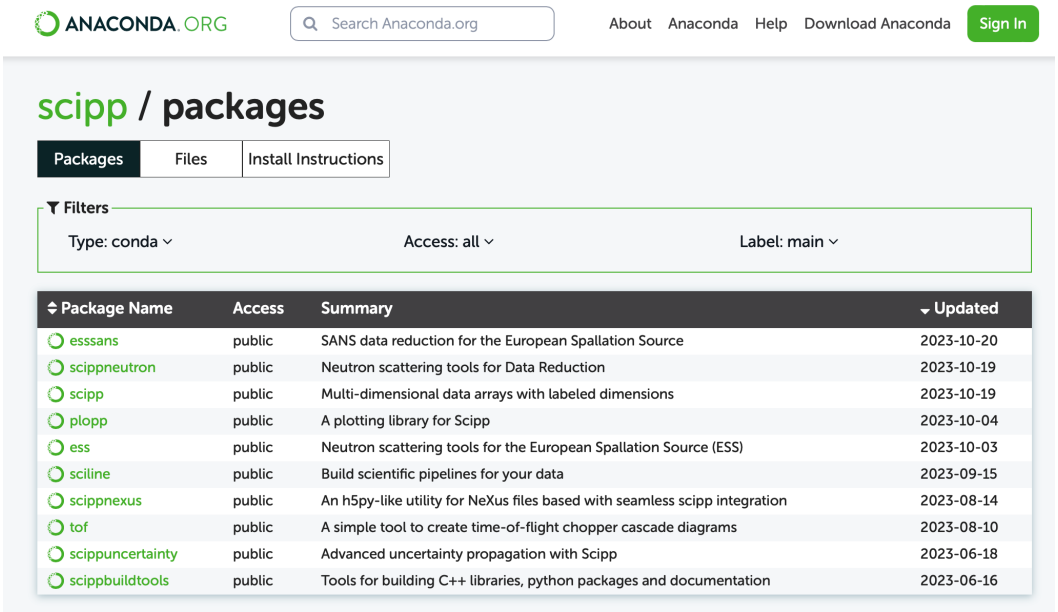
Scipp SWAT McStas

Scipp – Updates

1. **Requirements from IDS**
2. **ess**
3. **ess_sans**
4. ess_reflectormetry
5. **DMSC Summer School**
6. **Sciline**
7. Beamline
8. Scitation
9. Tof
10. New staff
11. Copier







Package Name	Access	Summary	Updated
esssans	public	SANS data reduction for the European Spallation Source	2023-10-20
scippneutron	public	Neutron scattering tools for Data Reduction	2023-10-19
scipp	public	Multi-dimensional data arrays with labeled dimensions	2023-10-19
plopp	public	A plotting library for Scipp	2023-10-04
ess	public	Neutron scattering tools for the European Spallation Source (ESS)	2023-10-03
sciline	public	Build scientific pipelines for your data	2023-09-15
scippnexus	public	An h5py-like utility for NeXus files based with seamless scipp integration	2023-08-14
tof	public	A simple tool to create time-of-flight chopper cascade diagrams	2023-08-10
scippuncertainty	public	Advanced uncertainty propagation with Scipp	2023-06-18
scippbuildtools	public	Tools for building C++ libraries, python packages and documentation	2023-06-16

Scipp – Updates 1

Requirements from the IDS

- We have previously reported efforts on gathering concrete and actionable requirements from the IDS
- While the effort has led to outcomes for some techniques, others have not been able to provide any feedback.
- We will now try to kick off workflow development in remaining techniques **by a more agile approach**: Our new idea is **that the team will take the lead in implementing a rudimentary workflow** for each technique (unless it exists already).
- **This will serve as a starting point to gather feedback from the IDS**, and to identify and prioritize missing features. Even for this first step, we will, however, require IDS involvement, in particular we need to obtain sample data.

Scipp – Updates 2

IDS Requirements - Template on Confluence

Data Analysis and Modelling

- Goal
- Context (Background Knowledge)
- References
- Environment
  - Assumptions
- Use-cases
- Preconditions
- Interfaces
- Input/Output
  - Input
  - Output
- Data Processing Procedure
- Test Cases
- Performance metric (non-functional requirements)
- Acceptance Criteria
- Potential Effects
- Followup Work

Edit View i

SANS direct beam iterations

Created by Wojciech Potrzebowski, last modified by Neil Vaytet on Jun 08, 2023

Goal

We need a notebook (or interactive script) that allows for choosing which tubes, straws or layers will be used in iterations that allow for determining direct beam function. It may be useful to provide various presets to the script e.g. have predefined list of tubes and layers to be used in analysis

Context (Background Knowledge)

D(l) is the "direct-beam function", which allows us to cross-normalise the incident spectrum to that of the empty beam (without sample) seen on the main detector. The direct-beam function also accounts for the adsorption by any windows in the beamline between the monitor and the detectors, such as Bragg dips at short wavelengths caused by the vacuum window in front of the detector. For more context see: Direct Beam notes and SANS Data reduction documents

The version of direct beam iteration in scipp was developed already in 2019: https://github.com/scipp/ess-legacy/blob/master/sans/direct-beam.ipynb. In the first approximation it may be enough to modernize the notebook so it works with latest version of scipp and ess. There is also a script in Mantid, which has been developed by Richard Heenan and Judith. The script is available from owncloud: https://project.esss.dk/owncloud/index.php/f/16903437. (This is long script but not all there is needed for achieving minimum required functionality). These two scripts should be used as reference for implementation.

Environment

Assumptions

- Flood source simulation data available from Geant 4 simulation
- The NeXus input file can be combined from multiple runs, however for the first pass is ok to use a single run

Use-cases

Instrument (Data) Scientists will use Jupyter notebook or script to input which straw, tubes or layers can be used that run the script to investigate intermediate results and then store resulting curves to the file.

Interfaces

```
Interactive Jupyter notebook
```

Input/Output

Input

LoKI detector test data, Geant4 simulations (for starting points)

I0 and Rg for different standard samples

Output

NeXus file with direct beam function defined per pixel id and the number of comparison plots.

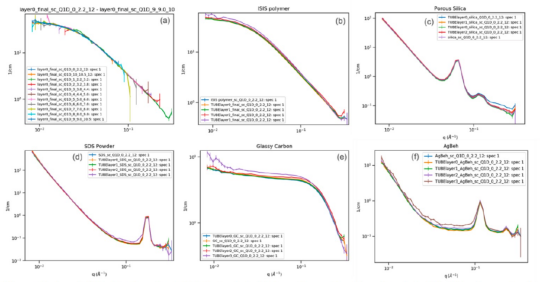


Figure 4 Reduced SANS data from the LoKI detector test. (a) Example wavelength overlap plot of the ISIS polymer standard for one layer of straws (out of 28). (b-f) Reduced data using the DB correction function. The detector data in each has been split into the four tubes layers – to illustrate (i) the current methodology works well for layer 0-2. Layer 3 is clearly out in each case, however this is not surprising, given we need to adjust rerun now the masks have been finally sorted. (b) ISIS standard polymer of partially-deuterated solid polystyrene, (c) Porous silica, (d) deuterated SDS powder, (e) glassy carbon and (f) AgBeh.

- Files:
  - Direct beam correction file (written to NeXus)
  - Text files with values from iterations e.g. I0, Rg - it maybe not necessary if it is written in notebooks

Change History

Version	Published	Char
CURRENT (v. 27)	Jun 08, 2023 12:58	
v. 26	Jun 08, 2023 10:49	
v. 25	Jun 08, 2023 09:20	
v. 24	Jun 08, 2023 09:07	
v. 23	Jun 08, 2023 08:58	
v. 22	May 12, 2023 12:48	
v. 21	May 12, 2023 12:42	
v. 20	Apr 18, 2023 09:56	
v. 19	Apr 18, 2023 09:52	
v. 18	Apr 18, 2023 09:43	

Scipp – Updates 3

Breaking apart the `ess` package

- **The `ess` package has long served as a collection of all ESS-specific data reduction code.** It contains submodules for instruments, techniques, and generic helpers. We have, however, struggled for a while with keeping it up to date with developments in Scipp and other libraries, as it proved **challenging to update all techniques "in sync"**, in particular in light of ongoing developments.

- As an example, this approach prevents releasing new features and **bugfixes for instrument A if instrument B is not yet ready for release**. While this has a relatively low impact currently, we believe it would turn into a major problem when entering hot-commissioning.

- A second issue is that dependencies for all techniques are tied together. For example, some techniques **may depend on Mantid which is not available via `pip`**. This slows down continuous-integration and releases as `conda` has to be used. Furthermore, **Mantid requires a fixed Python version**, and would thus prevent techniques that do not even depend on Mantid from using a more recent Python version.

Scipp – Updates 4

esssans

With the release of Sciline, we are now able to move existing workflows to use the new library. As SANS currently is the most developed and most actively used workflow, we have focused on this technique.

The old (pre-Sciline) workflow is available in the `ess` package, in the `ess.sans` module. We have been intending to break the `ess` package into smaller packages for more than a year (see below), and this has hereby been started: The rewrite of the `ess.sans` module can be found in the new esssans package. While the bulk of the rewrite is complete, it is not done yet, and still has to be rolled out to users.

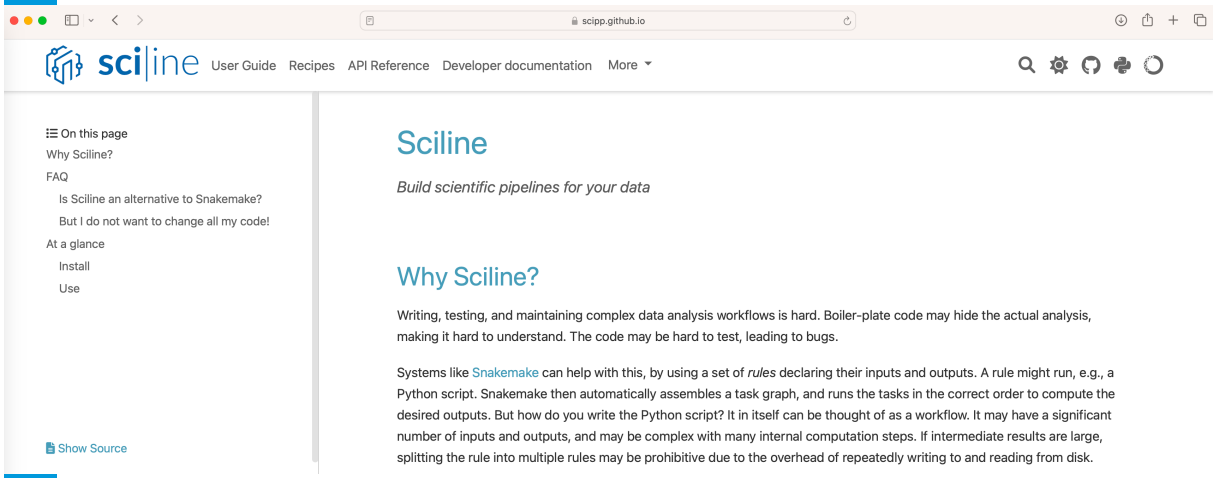
`esssans` is spearheading the move to Sciline, serving multiple purposes:

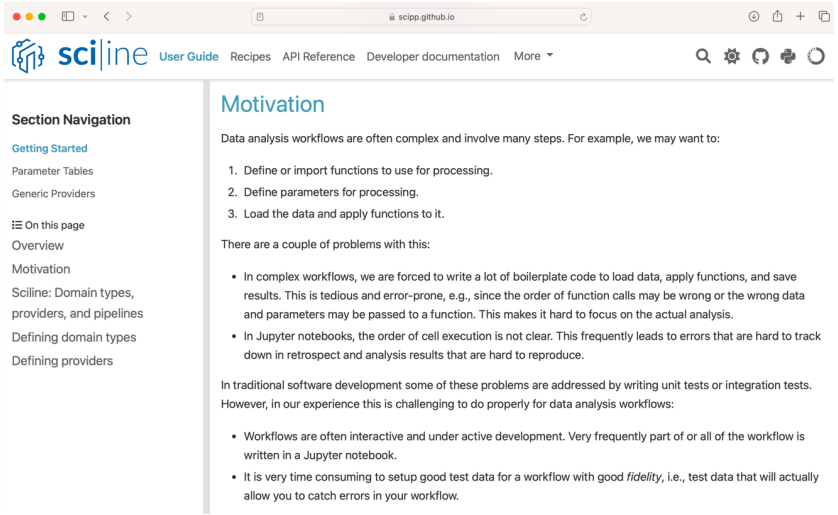
- Identify remaining problems and usability issues in Sciline.
- Serve as a full and nontrivial example for how Sciline can be used to write other data-reduction workflows.
- Enable developments that have deliberately been avoided in the old workflow due to growing complexity, e.g., combining data from multiple input files.

Scipp – Updates 5

Sciline

- After many discussions over the past year, as well as a number of small prototypes, we have converged on a solution for writing data-reduction workflows. This has resulted in our new Python library Sciline, which will be used to build such pipelines.
- Sciline builds **tasks graphs** which can be used to compute desired workflow results or intermediate results.
- It is worth noting that Sciline is independent of Scipp, i.e., it can be used with other data such as NumPy arrays of Pandas DataFrames. This might make this solution more attractive to outside users.



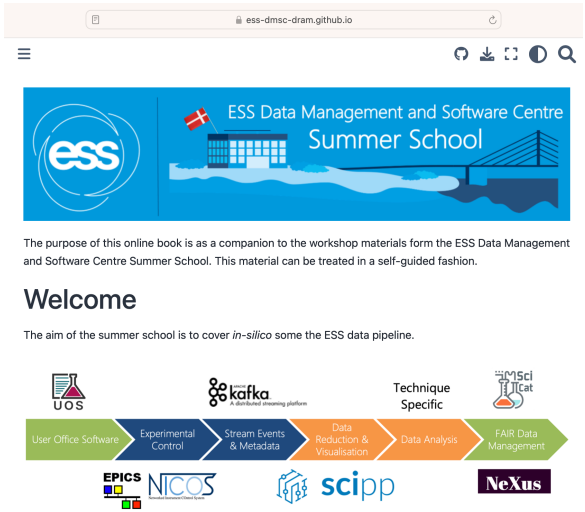


Scipp – Updates 6

DMSC Summer School 2023

The team has contributed a major session to the DMSC Summer School. As a highly valuable side effect, the work on the teaching material served as an integration test of almost the entire data pipeline. We will be looking into how we could turn this into a regular integration test, e.g., by running it as part of our continuous integration.

https://ess-dmsc-dram.github.io/dmsc-school/intro.html



Python

- Introduction to JupyterLab
- Python basics
- Using external libraries

McStas

- Simulation
- SANS exercise
- QENS exercise

Reduction with scipp

- Introduction to Scipp
- Coordinate transformations
- SANS data reduction
- QENS data reduction

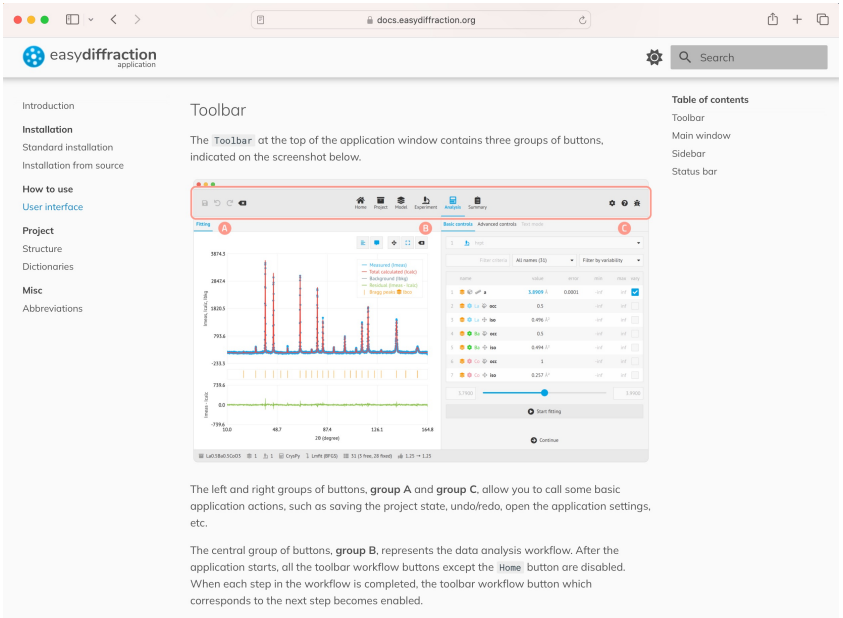
Scicat

- Dataset
- Data Curation
- FAIR Data
- Data and Metadata
- Data Catalog
- SciCat
- Python Libraries
- Example
- Data Curation Exercise

Data Analysis – Updates 1

- **Staff:** farewell to two developers: Simon W & Andrew M. In the process of hiring two new developers.

- **EasyDiffraction:** IUCr 2023 meeting and EDA demo at Software Fair (also at IUCr 2023)
- EasyDiffractionApp (EDA)
  - out to users
  - get freedback
  - Fix gui
    - fixed slow start-up
    - fixed slow gui
    - fixed slow fitting
    - fixed a few user reported issues
  - New updated user documentation



Data Analysis – Updates 2

EasyDiffractionApp

Main effort on redesigning the EasyScience based applications to provide performance comparable to most widely used software in the field

Minimization (fitting) performance has been made more robust and significantly improved (3-30 times)

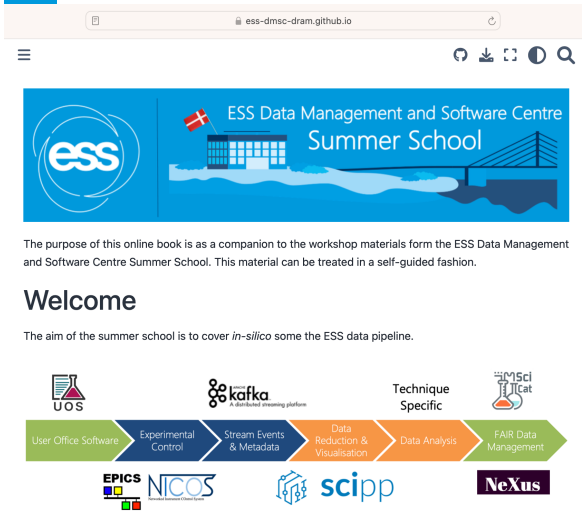
Improved **GUI design** and significantly improved visualization performance of charts and structures

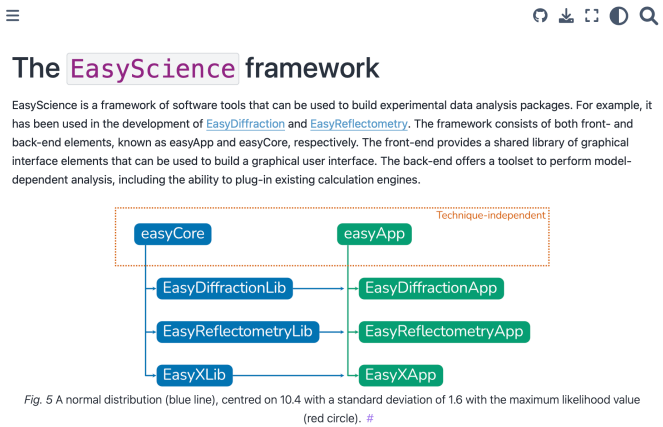
New crystal structure visualiser which will be extended to support magnetic structures
Currently on 8th alpha release (Oct 2023)

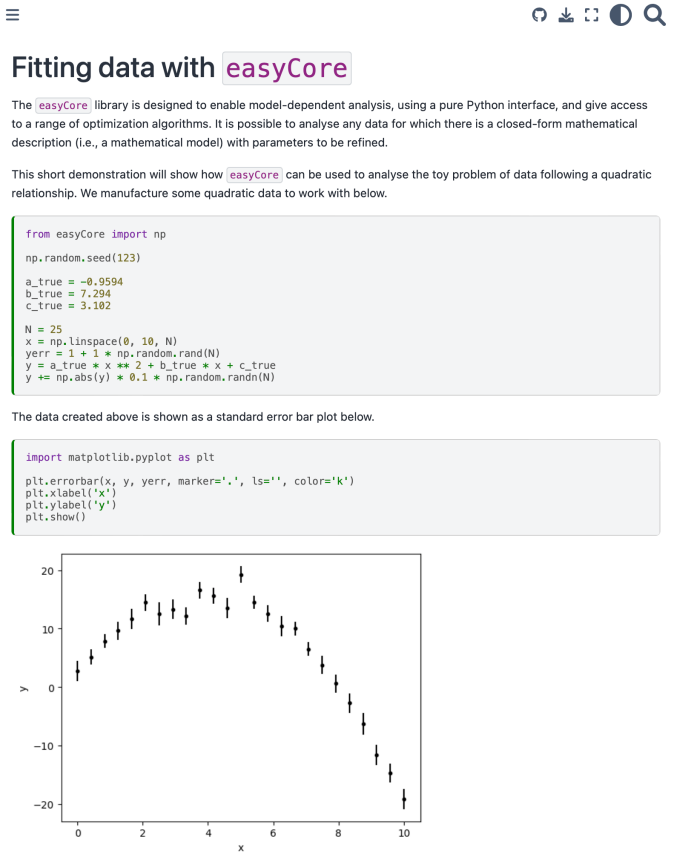
Data Analysis – Updates 3

DMSC Summer School 2023

The team has contributed a major session to the DMSC Summer School. Showing how easyCore can be used for fitting.







https://ess-dmsc-dram.github.io/dmsc-school/intro.html

Instrument modelling – Update 1

McStas etc. updates

- McStas 3.3, March 31st, 2023 (Presented at ECNS in Garching)
  - Built-in NeXus support on all platforms
  - mcgui run dialogue now allows to directly specify --format=NeXus and --format=NeXus –IDF

- McStas 3.4, September 19th, 2023
  - End of McStas 2.x releases
  - End of support for Perl tools
  - Build process for both macOS and Windows overhauled, embedded conda environment.
  - MPI support is now included with the installation on Windows

- Collaboration with SOLEIL for McXtrace school May 2023, Talk and demo at HighNESS scattering kernel school May 2023, DMSC Summer School September 2023
  - https://e-learning.pan-training.eu/course/view.php?id=135 school entry point (Federated login)
  - https://panlearningjhub.esss.dk/dmscsummerschool2023 “Fat” docker with McStas-McStasScript-NeXus-SCIPP developed and deployed

Instrument modelling – Update 2

McStas etc. updates

- McStasScript continues, the package can now load McStas generated NeXus data.
- McStas now ships with McStasScript and a JupyterLab
- The McStas package now also includes a translation tool that can write a McStasScript python file from a classic instrument file

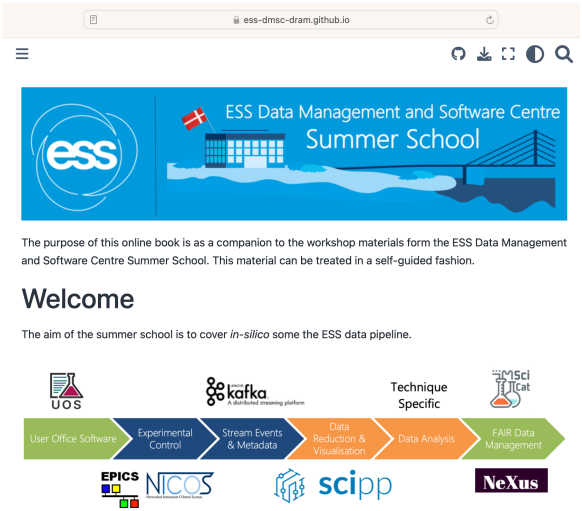
- The current development efforts on McStasScript concerns creating a widget interface to explore event data generated by McStas.
- This widget uses scipp and plopp to group the data as individual rays using the neutron id and to build interactive widgets that display the data.
- It will for example be possible to highlight a peak on the detector and see the history of the neutron rays that make up the peak.

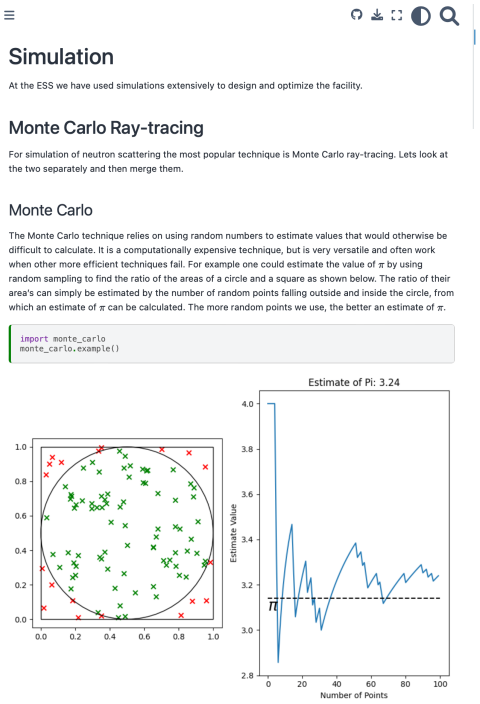
Instrument modelling – Update 3

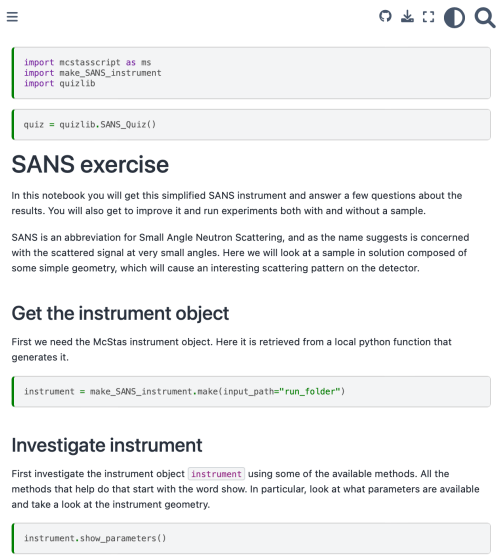
DMSC Summer School 2023

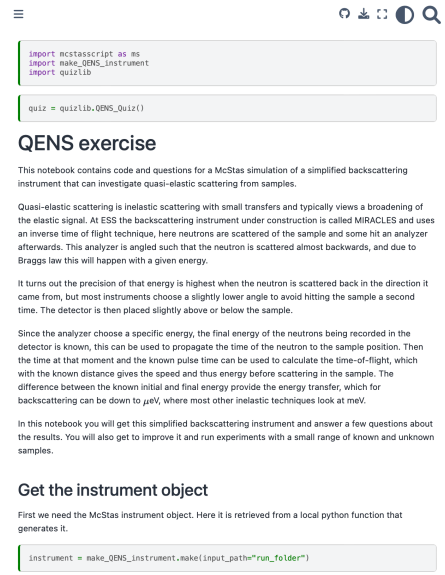
The team has contributed a major session to the DMSC Summer School. Showing how McStasScript can be used for instrument simulations.

https://ess-dmsc-dram.github.io/dmsc-school/intro.html









- https://e-learning.pan-training.eu/course/view.php?id=135
- Docker with McStas-McStasScript-NeXus-SCIPP developed and deployed

Instrument modelling – Update 4

The conclusion of the 3 year EU project HighNESS

- Simulated their performance (three conceptual instruments) on the different proposed moderators put forth in HighNESS
- The concepts were two SANS instruments, one conventional and one with focusing optics, and a simple imaging instrument.
- In the HighNESS project it was found that using a solid deuterium moderator rather than liquid deuterium could provide unprecedented intensity at wavelengths above 40 Å.
- The results were described in a thorough deliverable report and in the main HighNESS deliverable, the conceptual design report (CDR) https://arxiv.org/pdf/2309.17333.pdf

McStas timeline at a glance

When did what functionality arrive

v1.0, October 15, 1998

v1.1-1.6x, 1999-2002
mcrun, mcplot, mcgui,
Single_crystal, Source_gen,

v1.7-1.8, 2003-2004
Windows supp.
GPL license,
new tools

v1.9-1.11 2005-2007
PowderN & Isotropic_Sqw,
mcstas.org domain
Polarisation, macOS,
Debian pkg, MPI support

v1.12.x "era" 2008-2011
McXtrace project start,
ESS-oriented simulation
work, workshop efforts
take off
v1.12c is last 1.x release

v2.0-v2.1 2012-2014
/Initial Mantid support,
comp std., first
Python tools

v2.3-2.4.x 2015-2017
ESS_butterfly,
MCPL
Union subsystem, Python
tools fully default

v2.5-2.7 2018-2020
NCrystal
GPU efforts
Lots of new instruments

v3.0-3.1, 2020-2021
Official GPU support
arrives

v3.2, 2022
Official GPU support
arrives
v2.7.2 is last 2.x release

v3.3-3.4, 2023
Embedded NeXus,
mcstas-pygen,
McStasscript embedded

Steady in-flow of "smaller" developments, bugfixes, user contributions…

Addressing STAP comments & suggestions

From STAP report – and reply from DRAM

1) Workflows

- Regarding workflows, many of the IDS are having challenges in working with scientists on the instrument teams to get the calibration and reduction/analysis steps defined.
- A good starting point would be to look at the existing workflows in Mantid as an outline to at least help start a discussion.
- **A good suggestion we will keep in mind. Aligns with our new approach for handling IDS's requirements.**

2) Repository

- Having a separate repository for workflows make sense.
- ESS-Spectroscopy, ESS-Diffraction, ESS-Imaging/Engineering, ESS-SANS, ESS- Reflectometry, ESS-General?
- **We have arrived at the same conclusion. This has already been implemented a few months ago.**

3) GitHub repository tools

- Having the GitHub repository provides the ESS with a unique opportunity that other facilities did not have in the build up to operations.
- The time and process of developing specific workflow tasks can be monitored and then the process refined in response to expedite future developments.
- **A good suggestion we will keep in mind. It was mentioned durring the April STAP meeting; and point was noted.**

4) Mcstas – Geant4 coupling

- The current workflow of merging McStas and Geant for Dream is not sustainable beyond instrument design
- **This was never the design goal. The goal is to mimic all of Geant4 features in a one-stop McStas-shop for the untrained McStas user.**

Addressing STAP comments & suggestions

From STAP report – and reply from DRAM

5) Ownership

- Something that needs to be decided is who owns the simulations
- Will they be maintained long term by the instrument teams, the IDSs, centrally by the DRAM group, or by some other means
- **Already on our radar. We have more or less consensus in the team. Need to check with stakeholders.**

Finish presentation

Questions ?