EUROPEAN
SPALLATION
SOURCE

DMSC STAP
Updates from DRAM

...

TORBEN NIELSEN

October 2022

Agenda

1 DRAM

2 Data reduction updates

3 Modelling updates

4 Data analysis updates

DRAM

Data Reduction, Analysis and Modelling


Simon Heybrock


Neil Vaytet


Jan-Lukas Wynen


Piotr Rozyczko


Simon Ward


Andrew Sazonov


Peter Willendrup


Mads Bertelsen


Justin Bergmann

Scope

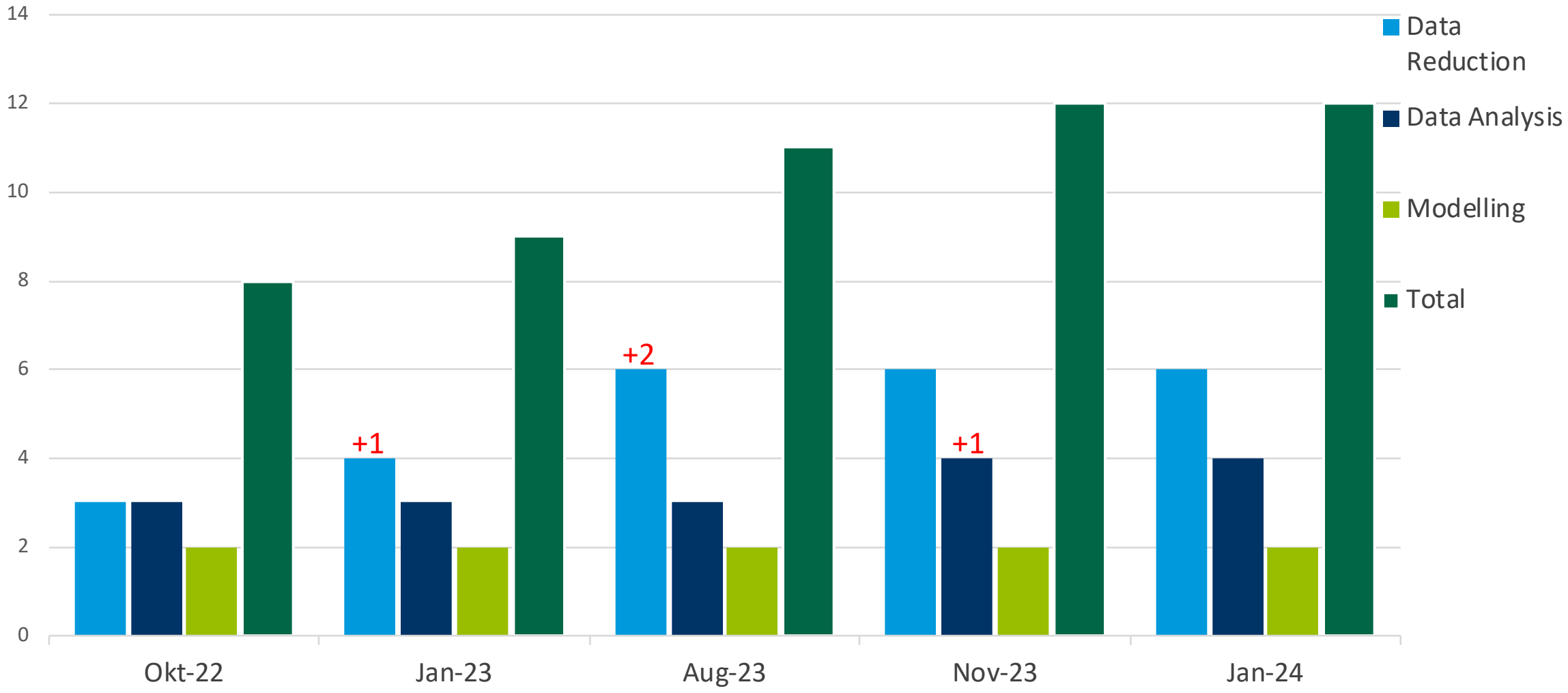
The DRAM group is responsible for providing the data reduction, analysis and modelling software for all instruments at ESS.

- 3 teams (9 persons)
  - Data Reduction (scipp)
  - Data Analysis (SasView, SpinW, EasyScience, external collaborations)
  - Modelling (McStas++, pan-learning.org, NMX)

DRAM - staff profile

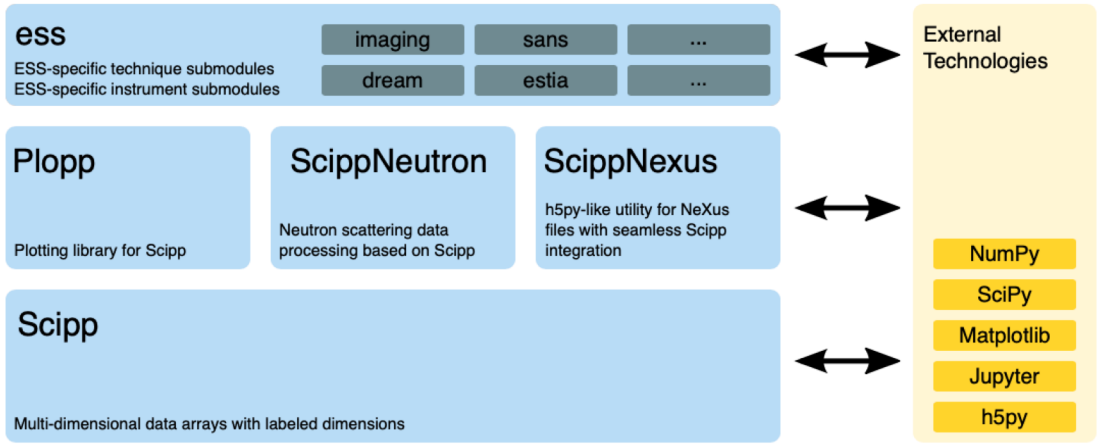
P0/P6 – spring 2022

S



scipp

scipp, scippneutron, scippnexus, plopp and ess



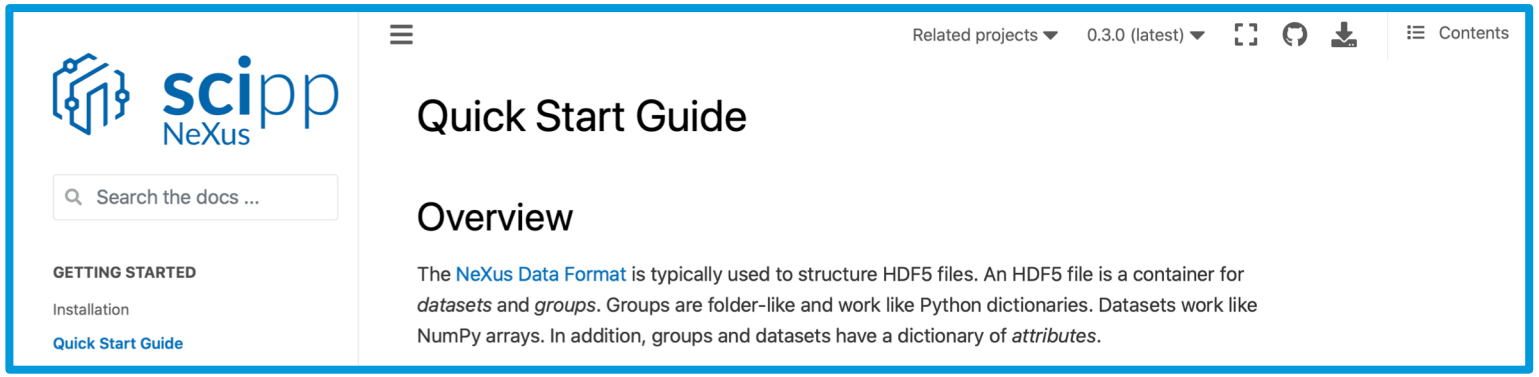
- Close collaboration between scipp and IDS team for defining data reduction workflows in scipp
- Joint meetings, pair-programming, and lively discussion on a dedicated Slack channel.

- scipp continues to be developed with input and requirements from instrument data scientists.
- Good progress
- Lots of features added & issues fixed

- From: https://scipp.github.io

scipp

Documentation on https://scipp.github.io



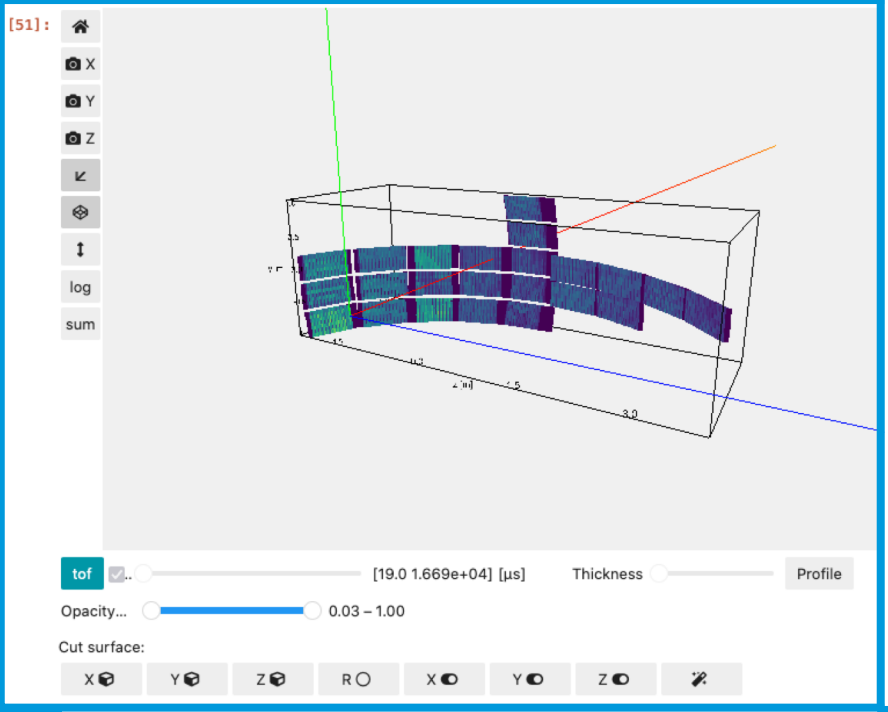
- scippnexus: An h5py-like utility for NeXus files with seamless Scipp integration

- plopp: plotting library for scipp

scippnexus

- POWGEN data
- PG3_4844_event.nxs

[51]:




```
[39]: from scippnexus import NXdetector, NXdata

      f.entry.instrument[NXdetector]
```

```
[39]: {'bank102': <NXdetector "/entry/instrument/bank102">,
       'bank103': <NXdetector "/entry/instrument/bank103">,
       'bank104': <NXdetector "/entry/instrument/bank104">,
       'bank105': <NXdetector "/entry/instrument/bank105">,
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       'bank82': <NXdetector "/entry/instrument/bank82">,
       'bank83': <NXdetector "/entry/instrument/bank83">,
       'bank84': <NXdetector "/entry/instrument/bank84">}
```

```
[40]: f.entry.instrument[NXdetector]['bank102'][()]
```

[40]: scipp.DataArray (8.75 MB)

▸ Dimensions: (**x_pixel_offset**: 154, **y_pixel_offset**: 7)

▾ Coordinates:

azimuthal_angle	(x_pixel_offset, y_pixel_offset)	float32	rad	-0.3123652, -0.2958419, ..., -0.2258334
distance	(x_pixel_offset, y_pixel_offset)	float32	m	3.2983806, 3.2987897, ..., 3.5141585, 3.5
local_name	()	string		F2
pixel_id	(x_pixel_offset, y_pixel_offset)	int32		127500, 127501, ..., 128576, 128577
polar_angle	(x_pixel_offset, y_pixel_offset)	float32	rad	1.4804635, 1.4808731, ..., 1.266226, 1.26
total_counts	()	int32		456601
x_pixel_offset	(x_pixel_offset)	float32	m	-0.3825, -0.3775, ..., 0.3775, 0.3825
y_pixel_offset	(y_pixel_offset)	float32	m	-0.1629, -0.1086, ..., 0.1086, 0.1629

▾ Data:

	(x_pixel_offset, y_pixel_offset)	DataArrayView	binned data [len=0, len=0, ..., len=0, len=(

```
[41]: f.entry.instrument[NXdetector]['bank102']['event_time_offset'][()]
```

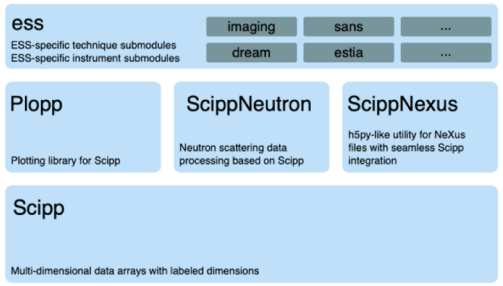
[41]: scipp.Variable (1.74 MB)

(event: 456601)	float32	µs	6027.5, 7976.1, ..., 10003.6, 3044.1

HDFView

plopp

new



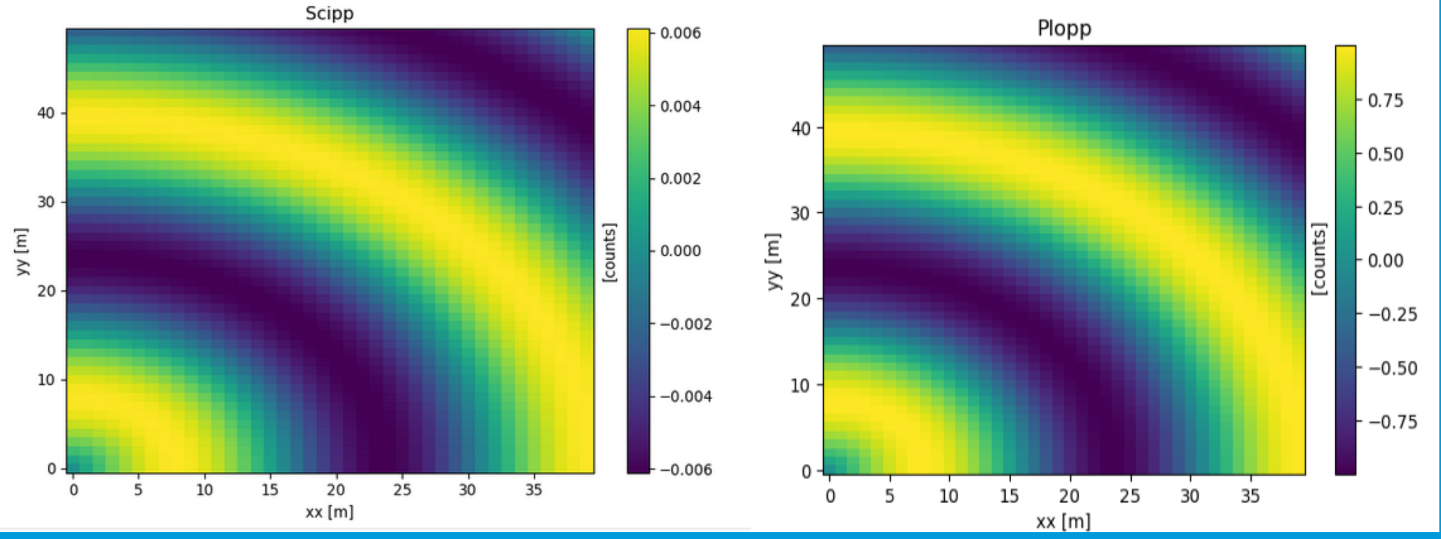
Issues with automatic resampling

[3]:
```
print(da.min().value, da.max().value)
```
```
-0.9999902065507035 0.9999886166646338
```

[4]:
```
s = sc.plot(da, title='Scipp')
p = pp.plot(da, title='Plopp')

ipw.HBox([s._to_widget(), p.to_widget()])
```

[4]:



Scipp vs Plopp

This notebook aims to illustrate the differences between the current (old) Scipp plotting, and the new Plopp package.

Background

See ADR0013 for more details.

The current plotting functionality automatically resamples 2-D (or higher) data as well as binned data of any dimension. There were three main drivers/motivations for this:

- We frequently deal with data with "long" dimensions, such as "pixel" or "spectrum" dimensions, which may exceed a million.
- We often deal with "ragged" data, i.e., data with 2-D coordinates that originate after coordinate transformations.
- We frequently plot binned data. Bins are often much larger than the target plot resolution, so histogramming must be done. This is combined with "long" dimensions and potentially high resolutions along other dimensions (exceeding 1000 or even 10000).

In the past we have therefore taken it as a given that resampling is a non-optional requirement. However, we have since then experienced a multitude of problems with this, ranging from simple bugs to complex and hard to maintain code. More importantly, the resulting plots are unpredictable and not faithful to the actual data.

One of the most compelling conclusions was:

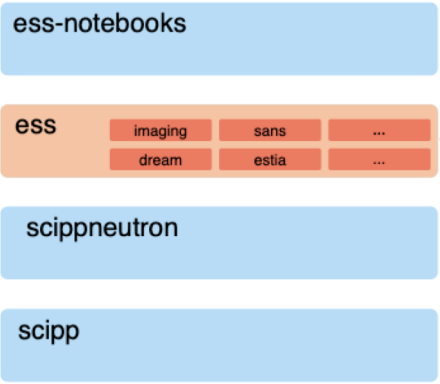
"Scientifically any plot generated with resampling is not usable, e.g., for publications."

New requirements

From scipp#2475

1. Faithful representation of data
2. Not tied to plotting/widget library
3. Updatable data
4. Both interactive and static figures
5. Customizable figures
6. Plots should still be visible in saved notebooks
7. API for adding custom tools with callback (or similar)

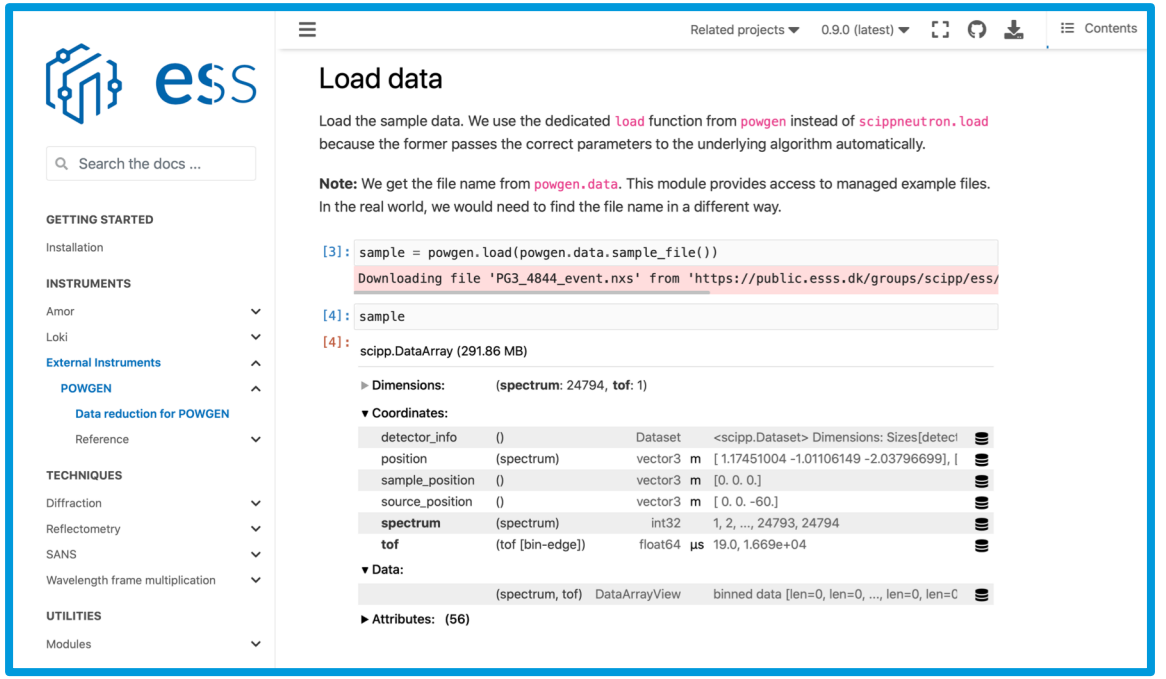
old

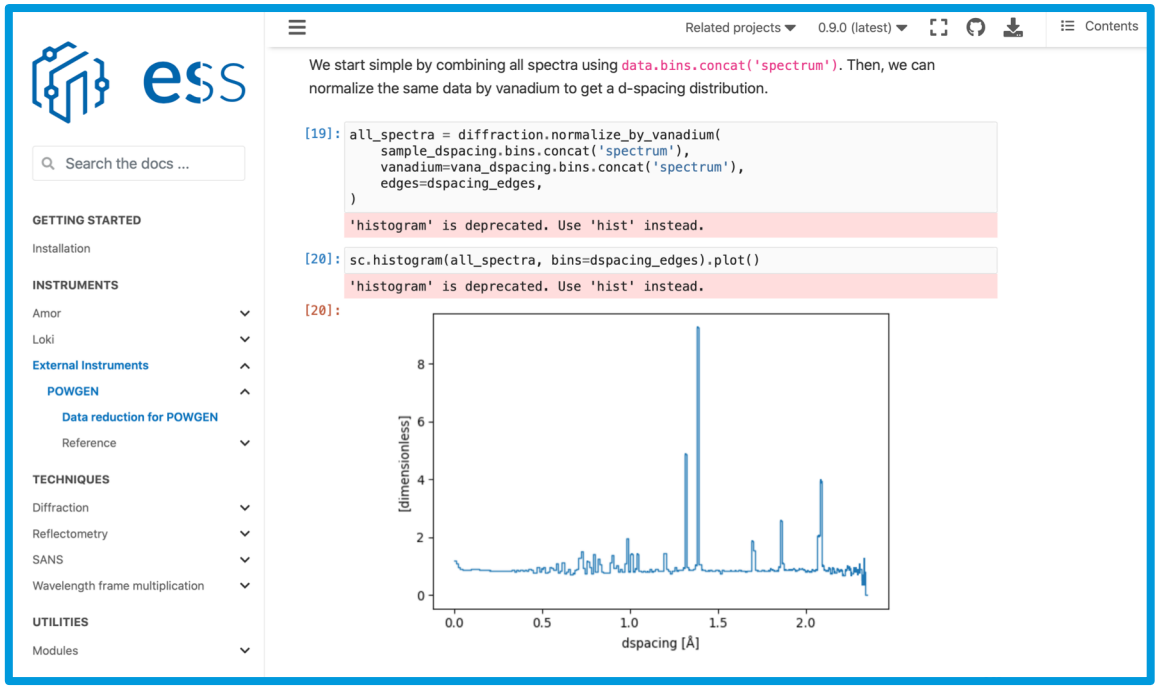


scipp / IDS

Data reduction workflow - - see ess package

- Some of the highlights include the ess package being extended for powder diffraction support such that reduction workflows are now available directly for the users on the online documentation pages.
  - Data reduction for POWGEN
  - This notebook shows a basic reduction workflow for powder diffraction for the SNS POWGEN instrument. It serves mainly to develop and present routines for powder diffraction and will eventually be removed in favor of a workflow for DREAM at ESS.
  - See ess docs on io pages





scipp

A bunch of releases

scipp: **#10**: v0.16.4 - v0.16.3 - v0.16.4 - v0.16.2 - v0.16.1 - v0.16.0 - v0.15.1 - v0.15.0 - v0.14.1 - v0.14.0 - v0.13.1 (April 01 2022)

scippneutron: **#9:** v.0.9.4 - v.0.9.3 - v.0.9.2 - v.0.9.1 - v.0.9.0 - v.0.9.4 - v.0.8.0 - v.0.7.0 - v.0.6.0 - v.0.5.3 (30 March 2022)

ess: **#7:** v0.9.0 - v0.8.0 - v0.9.0 - v0.7.1 - v0.7.0 - v0.6.0 - v0.5.0 - v0.4.0 (Feb 28 2022)

scippnexus: **#21:** v0.3.2 - v0.3.1 - v0.3.2 - v0.3.0 - v0.2.1 - v0.2.0 - v0.1.8 - v0.1.7 - v0.1.6 - v0.1.5 - v0.1.4 - v0.1.3 - v0.1.2 - v0.1.1 - v0.1.0 - v0.0.9 - v0.0.8 - v0.0.7 - v0.0.6 - v0.0.5 - v0.0.4 (31 March 2022)

plopp: **#8: :** v0.3.0 - v0.2.2 - v0.2.1 v0.2.0 – v0.1 – v0.03 – v0.0.2 – v0.0.1 (25 Aug 2022)

mpltoolbox: **#7:** v0.1 – v0.0.8 – v0.0.7 – v0.0.6 – v0.0.5 – v0.0.4 – v0.0.3 (11 Jul 2022)

62 - releases

Modelling

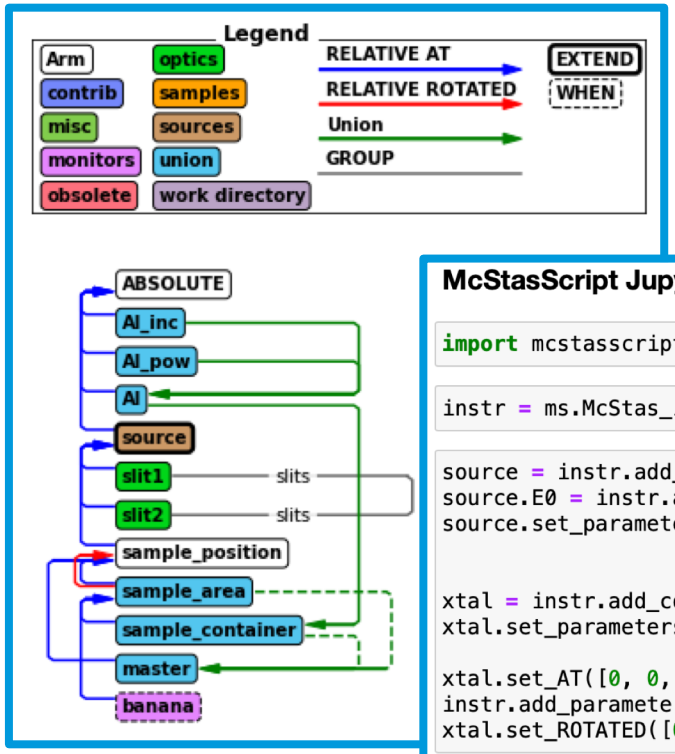
McStas Python API with tools, diagrams and widgets

New developments

- Diagrams of instrument objects
- Improved error checking
- Compatibility with McStas 3.X
- Interactive quiz system in jupyter notebooks
- Dynamic splits of instruments using MCPL

In collaboration with PaNOSC

- Instrument database with API



McStasScript Jupyter notebook

```
import mcstasscript as ms

instr = ms.McStas_instr("demo")

source = instr.add_component("source", "Source_simple")
source.E0 = instr.add_parameter("energy", comment="[meV]")
source.set_parameters(xwidth=0.12, yheight=0.03, dE="0.1*energy",
                      dist=2.0, focus_xw=0.01, focus_yh=0.01)

xtal = instr.add_component("crystal", "Single_crystal")
xtal.set_parameters(radius=0.005, reflections='"YBaCuO.lau"',
                    ax=3.8186, by=3.886, cz=11.6777, mosaic=30)
xtal.set_AT([0, 0, 2.0], RELATIVE=source)
instr.add_parameter("sample_rotation", value=0, comment="[deg]")
xtal.set_ROTATED([0, "sample_rotation", 0], RELATIVE=source)

instr.set_parameters(energy=5.0, sample_rotation=37.0)
instr.show_parameters()

 energy           = 5.0   // [meV]
 sample_rotation  = 37.0  // [deg]

data = instr.backengine()
```

Modelling: workshops and conferences

Events attended since april

Participated in following events

- DMSC McStas workshop
- McStas training days (May-July 2022)

- ICNS Argentina
  Neutron Instrumentation and Innovation award for Mads Bertelsen
- PaNOSC Summer school
- ESS-ILL User meeting
- PaNOSC WP 5 sprint (online)

McStasScript

Modelling overview

mcstasscript: #10: 0.0.51, 0.0.50, 0.0.49, 0.0.48, 0.0.46, 0.0.44, 0.0.43, 0.0.42, 0.0.41, 0.0.40 (March 22 2022)

guide_bot: #10: 0.0.27 - 0.0.26 - 0.0.25 - 0.0.24 - 0.0.23 - 0.0.22 - 0.0.21 - 0.0.20 - 0.0.19 - 0.0.18 - 0.0.16 - 0.0.15 (Feb 16 2022)

Data Analysis

Updates since last STAP

For easyScience core:

- ❑extension for multiple datasets/fit functions fitting
- ❑IO rework of easyCore for speedup in XML encoding, and hence a more responsive GUI.
- ❑Started work on asymmetric peaks fitting in easyDiffraction

For easyDiffraction:

- ❑easyDiffraction v0.8.4 was released
- ❑polarized support in the GUI
- ❑changing how experimental data are handled
- ❑starting working on file-less interface to CrysFML
- ❑Improved CrysPy interface

For easyReflectometry:

easyReflectometry v0.0.5 was released

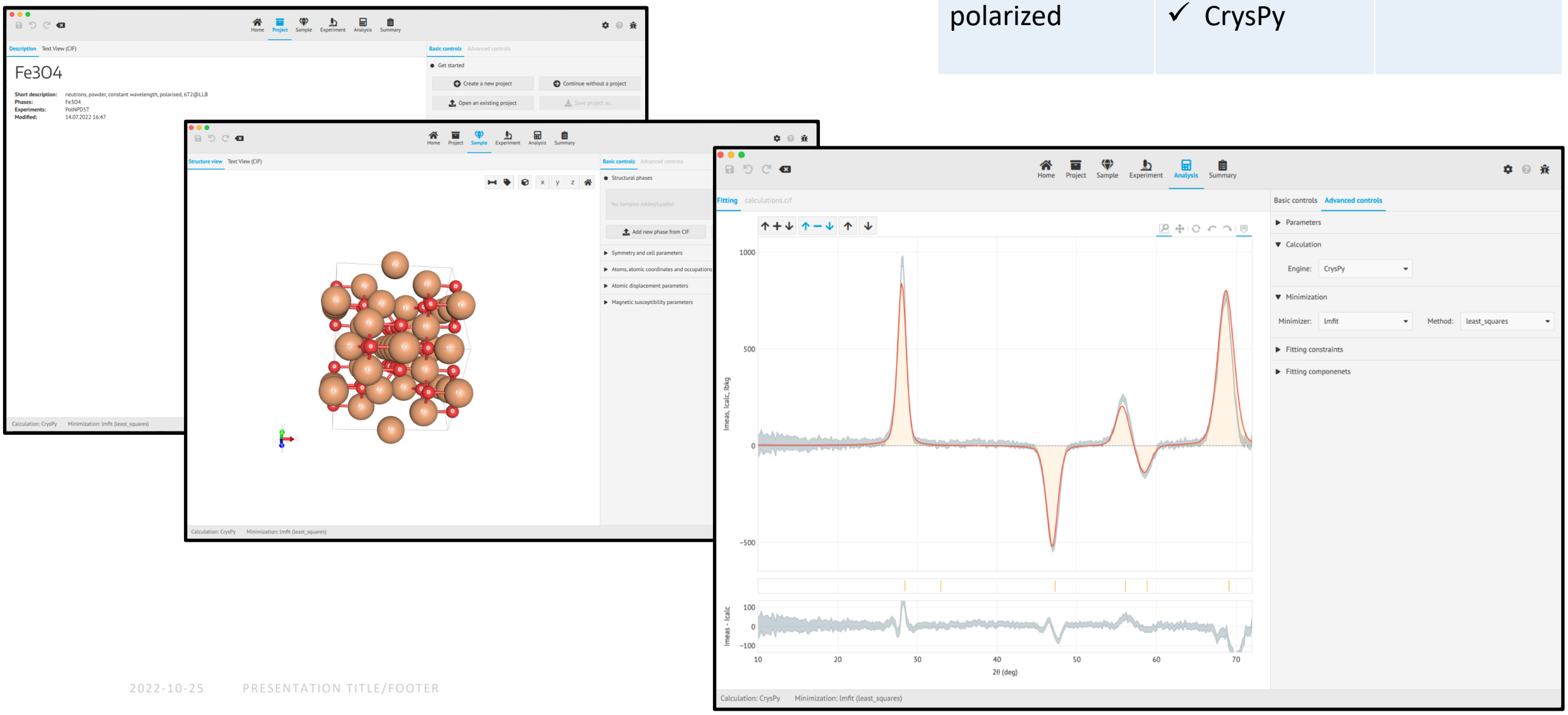
surfactant Layer in GUI was added

general bug fixes and minor improvements

easyDiffraction 0.8.4

Polarization support for CW using CrysPy

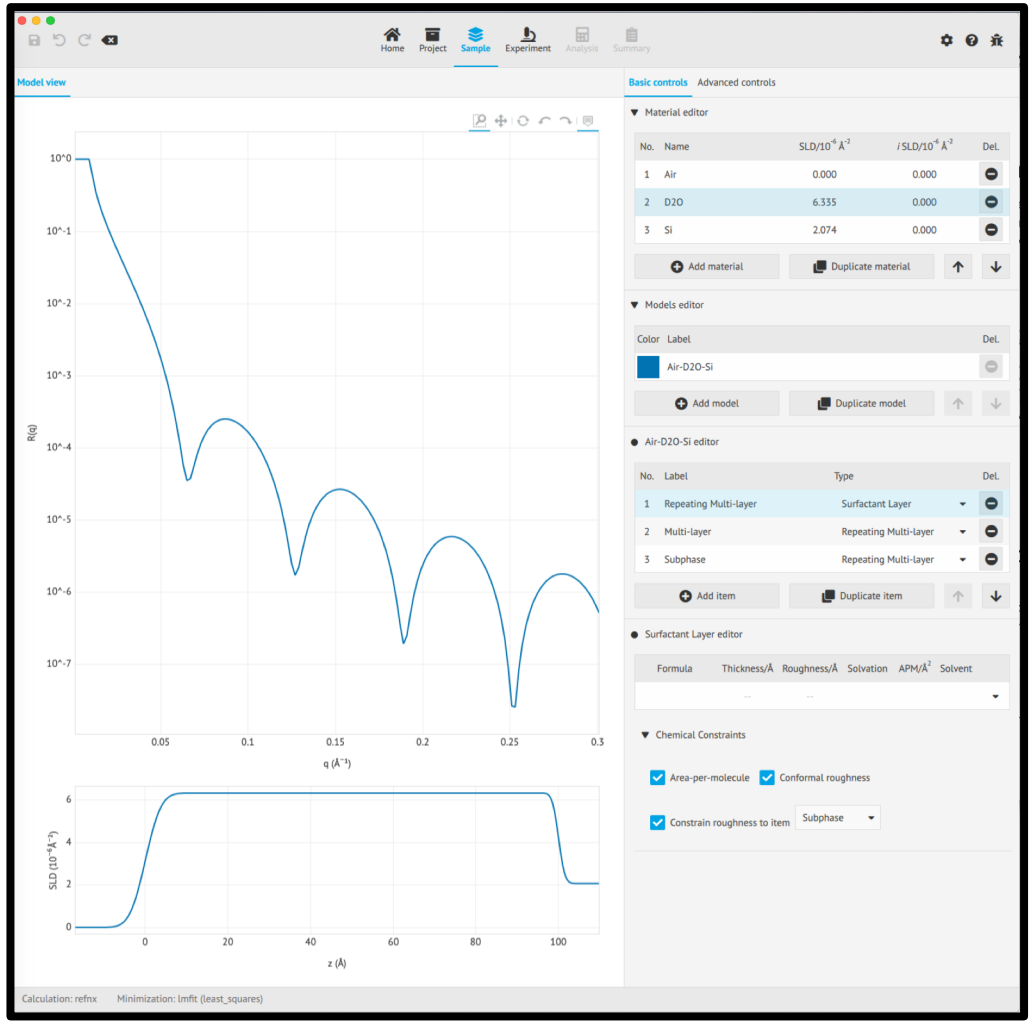
easyDiffraction	CW	TOF
un-polarized	✓ CrysFML ✓ CrysPy ✓ GSAS-II	✓ CrysPy
polarized	✓ CrysPy	



easyReflectometry

v0.0.5

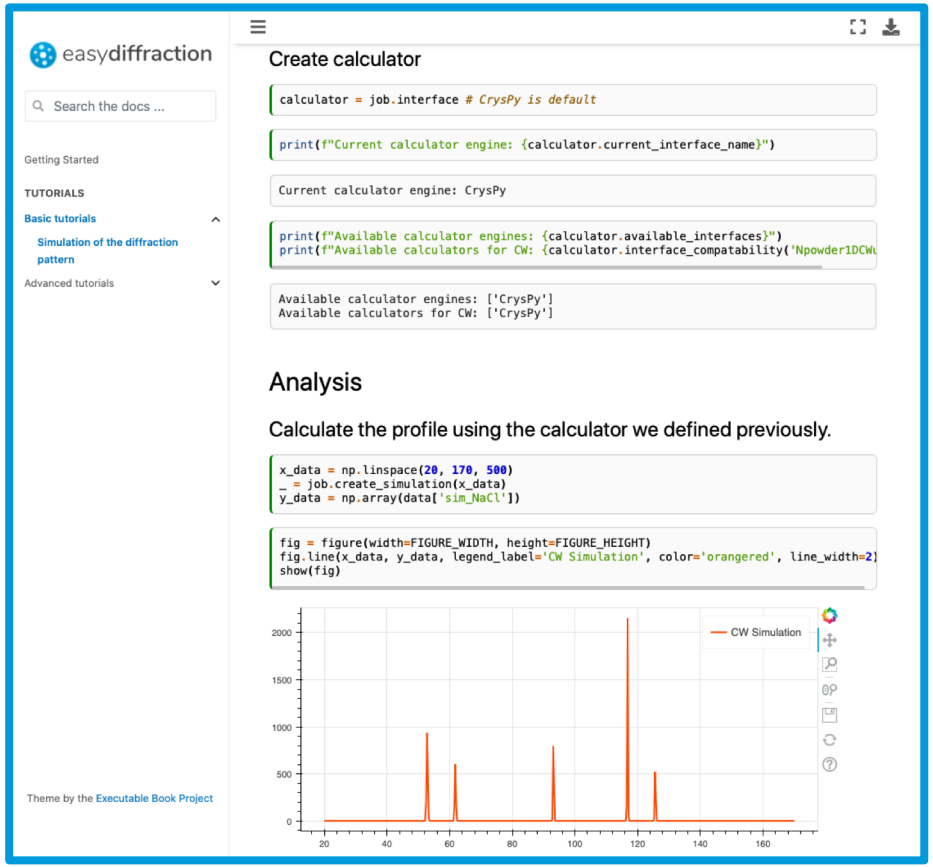
- ❑surfactant Layer in GUI was added
- ❑general bug fixes and minor improvements
- ❑Python notebooks

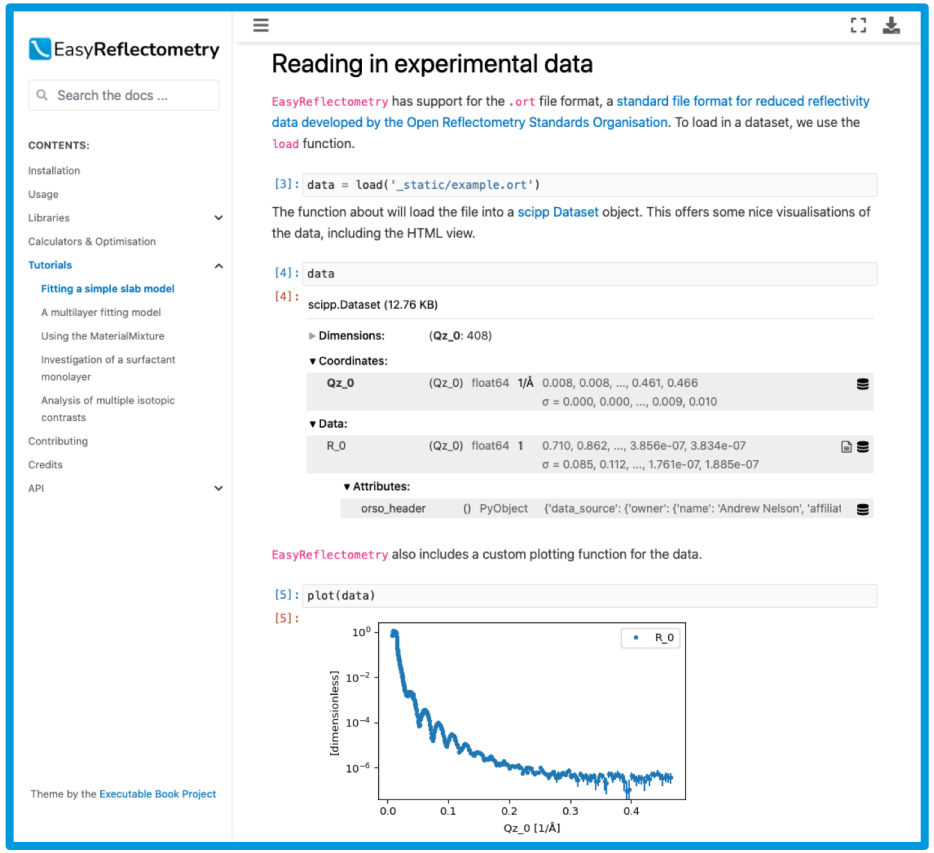


Documentation

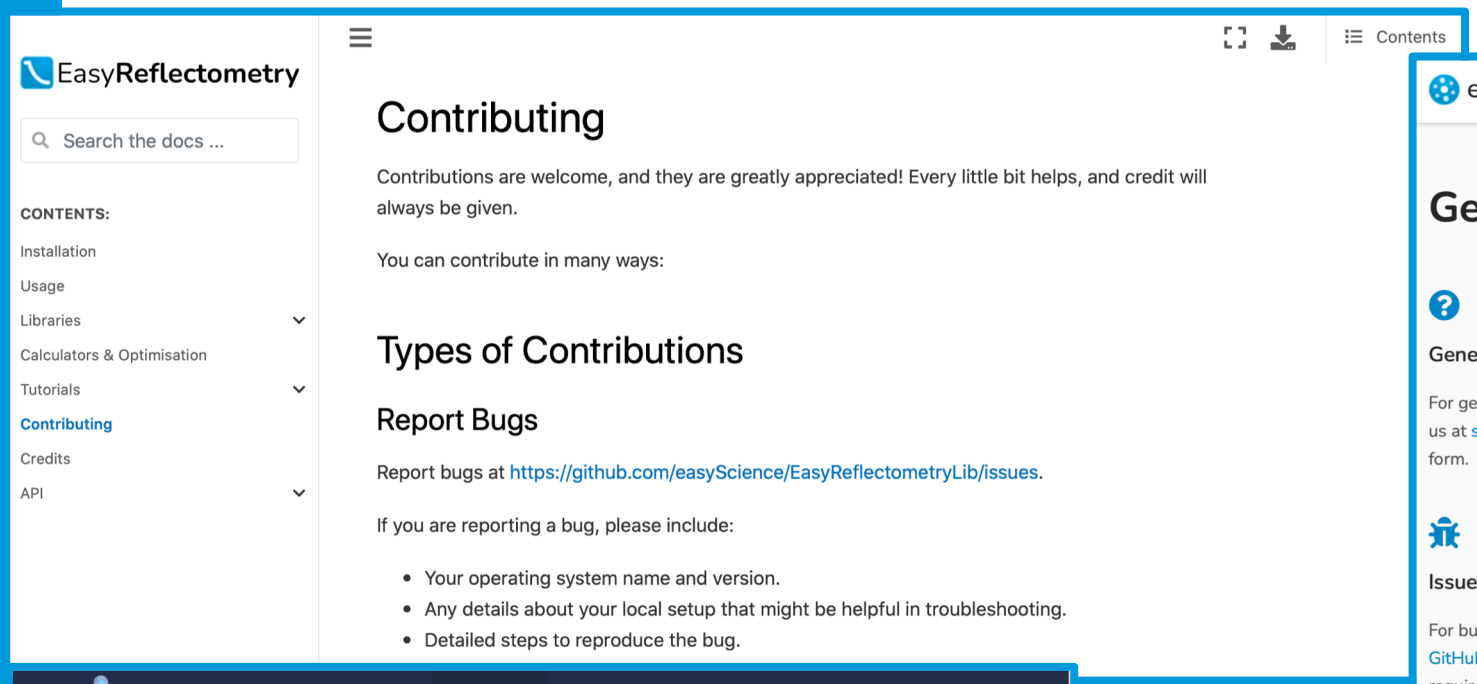
https://docs.easydiffraction.org/lib/

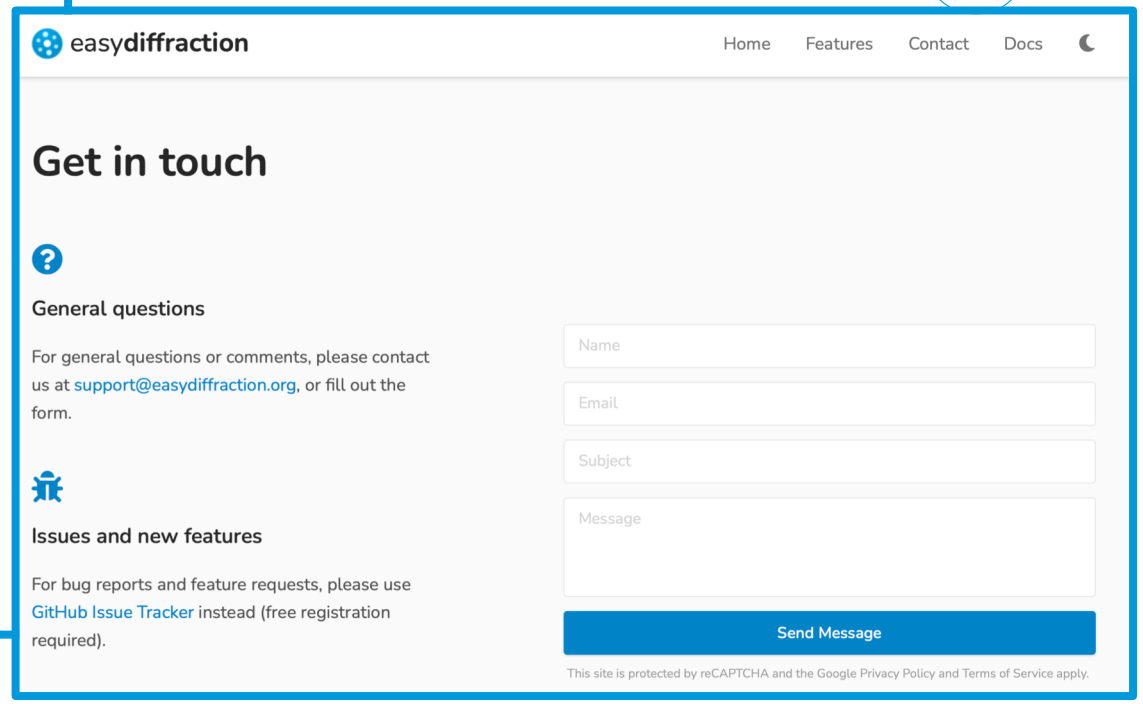
https://docs.easyreflectometry.org

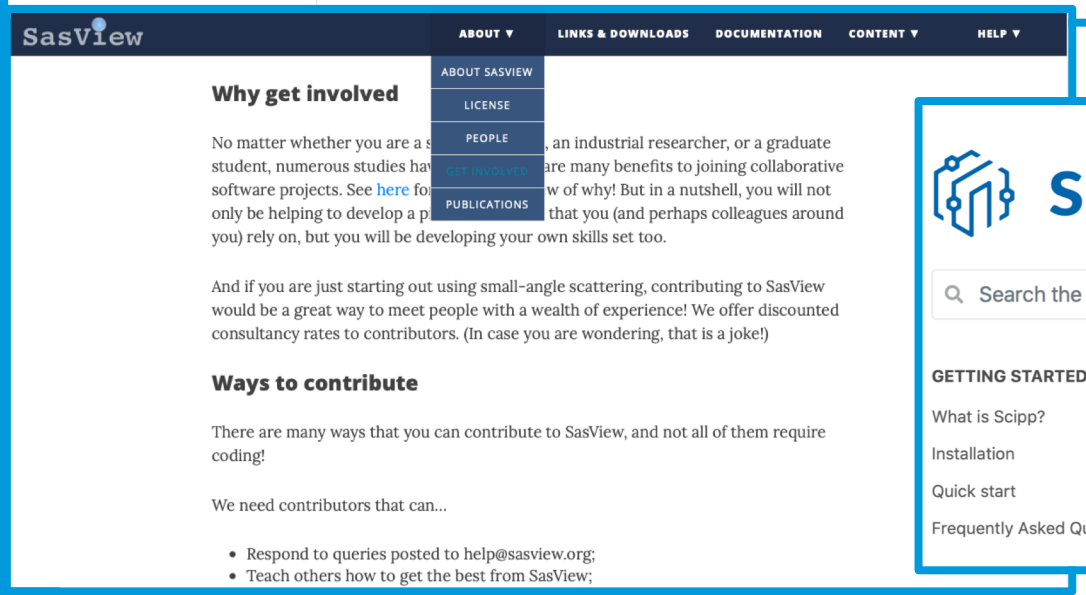


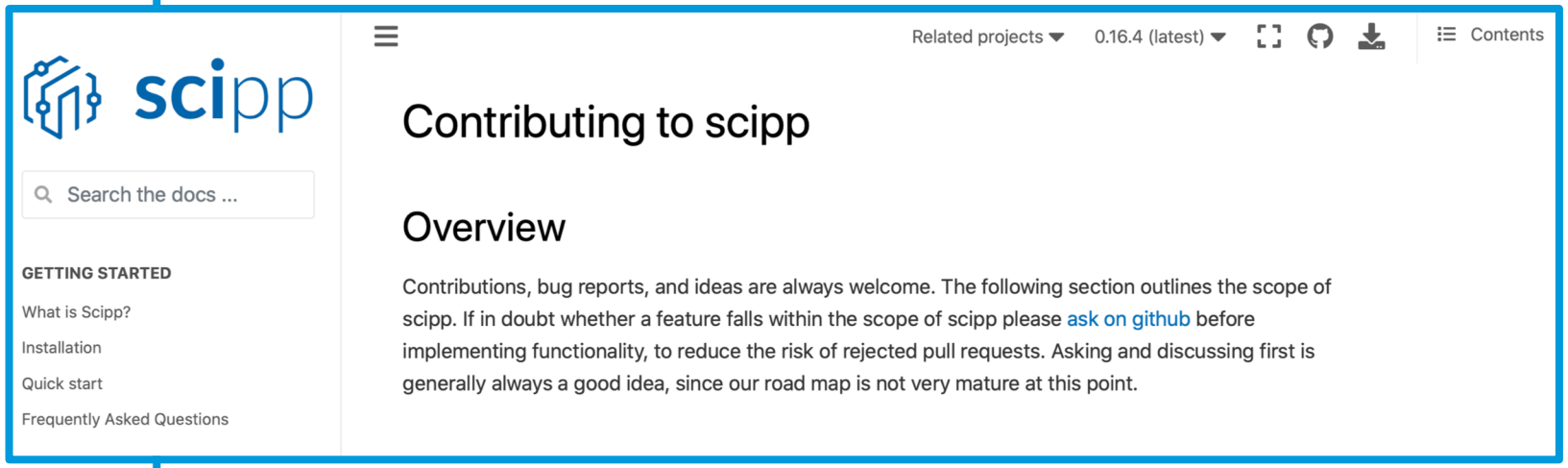


Collaborations – getting people onboard









Finish presentation