Data Reduction Software Overview

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Data reduction software for ESS is developed at DMSC in Copenhagen, as European Spallation Source(ESS) is built in Lund.
Here is an overview of various software packages that our Data reduction team(scipp) has built to support various instruments at ESS and other neutron source experiments data reduction.

Quick Links

Open Source — All our software is under BSD-3 license.. Scan the QR code to see all codebase at scipp github organization. github.com/scipp

scipp — Scan the QR code to see scipp documentation scipp.github.io

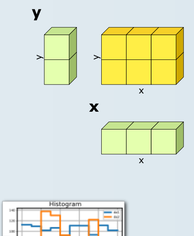
Scan the QR code to see scipp tutorial on Youtube at EuroPython2023

Scientific Software Cores

Data Structure
Computation
Visualization

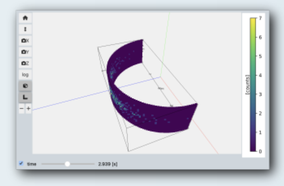
scipp - The core project of all our data reduction software.

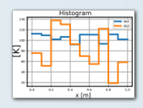
- Numpy like multi dimensional arrays data structure and computational functionalities
- Physical units and coordinates
- Physical properties propagation along computation (units, errors, masks, etc…)
- Flexible binning of data without losing original information
- String formatting and HTML data representation



plopp - Scientific visualization tool (using scipp).

- Various automatic plotting (1,2,3d histogram, line plots etc…)
- Ipywidgets (data slicer, 3d instrument view)

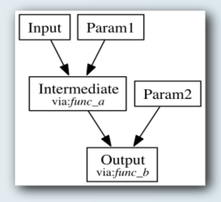




sciline - Workflow framework for data reduction routine development.

- Type-hint-based dependency injection
- Visualization of components and workflow as a graph
- Map-reduce interface of a workflow
- Reproducibility support (provenence)

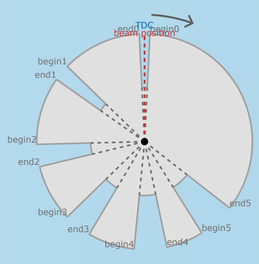
Name	Value	Source
Input	1	
Intermediate		▸ func_a
Output		▸ func_b
Param1	2	
Param2	3	



Generic Neutron Experiment Libraries

scipp neutron - (scippneutron) Neutron related data structure and computation functionalities.

- Neutron related coordinate transformation graphs,
i.e. time-of-flight transformation to wavelength, Q, (h,k,l), etc…
- Chopper data structure, visualization and computation tools for long pulse

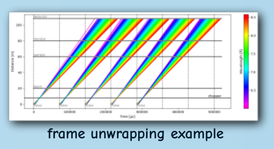


scipp NeXus - (scippnexus) Python IO interface for NeXus(hdf5) files

- Loading dataset with physical attributes using scipp data structure
- Loading neutron event data (NXevent) along with corresponding static information
- Resolving transformation chains (NXtransformation)
- Coordinate based data slicing

essreduce - (essreduce) Generic data reduction workflows for ESS

- Frame unwrapping workflow
- Wavelength frame multiplication stitching workflow
- Mutli files/Run type mapping workflow

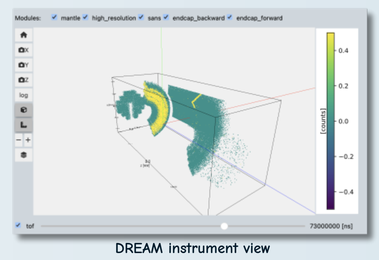

frame unwrapping example

Technique and Instrument Specific Data Reduction Libraries

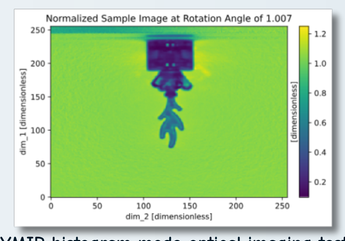
The ess* packages provide instrument/technique specific functionalities and workflows.
Some instruments are supported by a sub package of a higher level technique specific packge.
i.e. loki is under esssans. Heret is the list of early ESS instruments/techniques
that each package supports. Many of packages can save reduced data into relevant format.

*Some of packages also has example workflows for external instruments out of ESS in the documentation
Some instruments uses multiple ess packages if they use multiple techniques. i.e. esspolarization will be used by all instruments that provide polarization experiments.

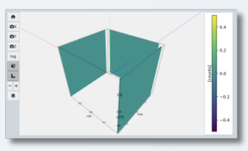
essdiffraction	DREAM
essimaging	ODIN, Test Beam Line, YMIR
essnmx	NMX
essreflectometry	ESTIA, FREIA
esssans	LoKI
essspectroscopy	BIFROST

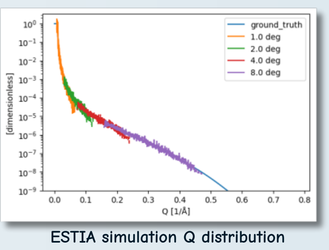


DREAM instrument view

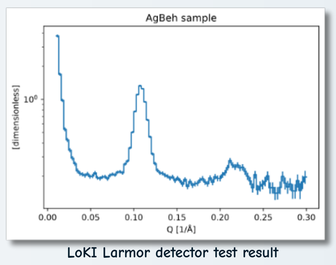


YMIR histogram mode optical imaging test

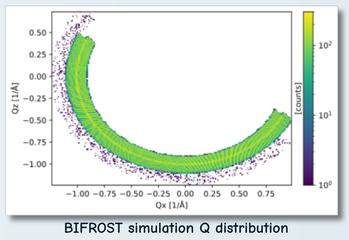

NMX instrument view



ESTIA simulation Q distribution



LoKI Larmor detector test result



BIFROST simulation Q distribution

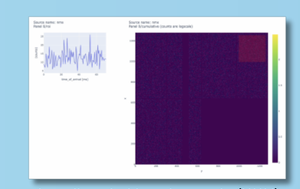
Live Data Reduction Application

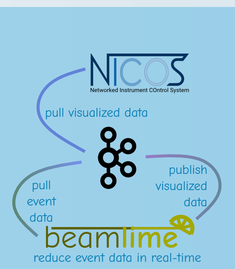
beamlime

Live data reduction framework/application.

- Live visualization of event counts along physical coordinates
- Visualization integrated in NICOS
- Selection of region of interest

*More features are under development


beamlime dashboard example (NMX)



Interface with Other Services

SciCat SCITACEAN

SCITACEAN - High level Python package for down/uploading datasets from/to SciCat

scitiff - (Scitiff) Neutron imaging tiff format and metadata schema

CI/CD tools

*that we did not make but heavily dependent on

copier - Create/update projects from template. (copier.readthedocs.io)

Gitlab/Github - Automated CI/CD using gitlab/github

The project template for python packages is also public on our organization.
Scan the QR code to check our python package copier template
github.com/scipp/copier_template