EUROPEAN SPALLATION SOURCE

Data management and scientific computing at scattering facilities, what it is and why it is important

Jon Taylor

Raciri summer school

August 2019

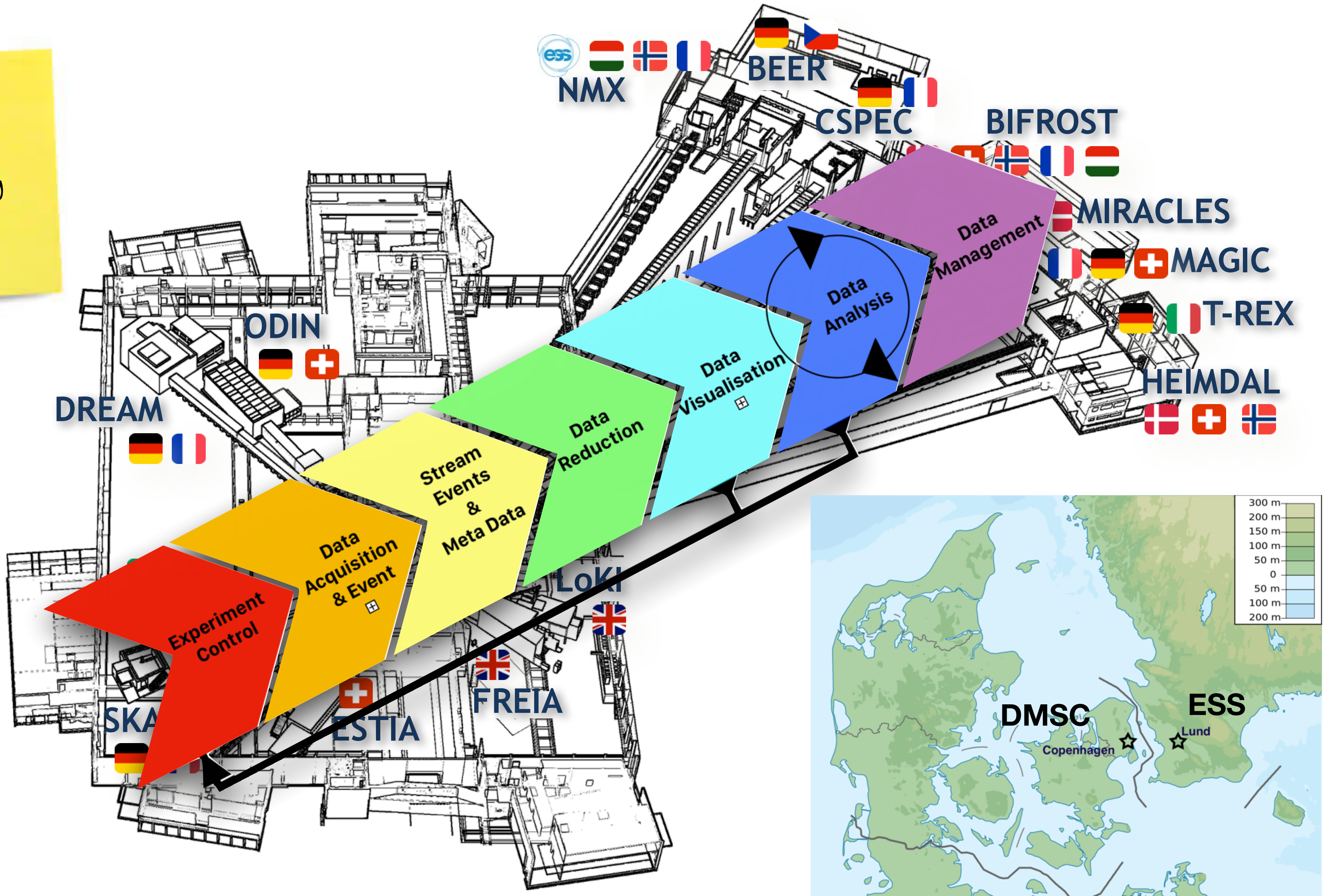
Introduction

EUROPEAN SPALLATION SOURCE

- FAIR data for European Photon and Neutron sources.
- Data Acquisition to Data analysis.
- Jupyter Notebooks for FAIR science.
- Some examples for the tutorial sessions.

DMSC - Data Management and Software Centre

TO DO:
Scientific
computing
for this



The Team: ESS and InKind Partners

JÜLICH FORSCHUNGSZENTRUM

PAUL SCHERRER INSTITUT PSI

Science & Technology Facilities Council ISIS

Our Agenda

Collaborative Open Source Software

Developed with modern practices

Minimise Single point failures

Community Engagement

Promote User Experience

FAIR Data

Open Science

European Photon and Neutron Landscape

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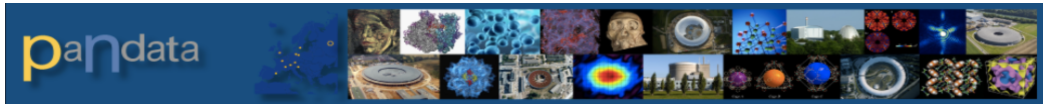
	alba	anka	als	ansto	aps	australian	cls	desy	dls	elettra	esrf	frm2	ber2	bessy2	ill	isis	lcls	lnls	maxIV	nsls	nsrrc	ornl	sinq	sls	sacla	soleil	spring8	ssls	ssrl
alba	1745	31	201	74	171	74	82	189	394	233	982	78	36	229	262	167	41	40	47	65	83	86	81	315	7	213	97	8	79
anka	31	1525	202	56	127	73	67	233	223	115	643	64	31	212	120	95	60	15	40	46	48	42	47	184	6	114	67	14	54
als	201	202	19761	682	3463	780	1675	1125	2234	968	3390	430	206	1403	937	985	1185	178	400	1042	992	1009	310	2110	107	755	1364	130	3479
ansto	74	56	682	3699	665	864	313	326	730	222	1123	479	340	339	1192	1065	134	47	111	222	398	610	386	472	40	178	561	63	381
aps	171	127	3463	665	7699	663	1392	805	1535	514	2837	371	177	612	921	930	805	113	231	779	560	1317	294	1388	93	421	792	93	2092
australian	74	73	780	864	663	6075	336	292	841	312	1147	166	83	271	412	472	174	59	119	198	398	300	123	517	22	187	430	85	531
cls	82	67	1675	313	1392	336	5593	386	776	315	1206	175	78	450	367	361	228	113	173	408	470	407	129	720	34	287	504	99	1003
desy	189	233	1125	326	805	292	386	8508	1171	780	3228	486	194	1450	749	559	834	130	472	299	292	322	276	1401	96	619	605	88	488
dls	394	223	2234	730	1535	841	776	1171	17843	979	6881	501	222	1217	1473	2337	653	223	467	574	639	649	374	2335	71	939	887	94	1163
elettra	233	115	968	222	514	312	315	780	979	7621	2519	210	93	1007	592	467	458	175	316	248	243	264	177	929	62	894	472	57	390
esrf	982	643	3390	1123	2837	1147	1206	3228	6881	2519	40207	1225	624	2939	3510	2454	977	643	1101	1146	868	1105	932	5225	176	3124	1632	125	1823
frm2	78	64	430	479	371	166	175	486	501	210	1225	3769	504	472	1558	838	111	63	96	146	209	559	615	474	27	207	257	26	208
hzb-ber	36	31	206	340	177	83	78	194	222	93	624	504	1817	364	755	532	52	45	43	60	92	305	425	231	13	68	155	10	74
hzb-bessy	229	212	1403	339	612	271	450	1450	1217	1007	2939	472	364	9272	752	585	512	141	582	323	361	369	300	1602	54	669	571	60	571
ill	262	120	937	1192	921	412	367	749	1473	592	3510	1558	755	752	10610	2630	227	183	264	333	423	1188	1049	982	54	641	763	55	441
isis	167	95	985	1065	930	472	361	559	2337	467	2454	838	532	585	2630	8442	239	120	230	358	406	1056	762	816	49	385	800	45	480
lcls	41	60	1185	134	805	174	228	834	653	458	977	111	52	512	227	239	3295	23	112	231	192	213	81	707	141	351	453	36	818
lnls	40	15	178	47	113	59	113	130	223	175	643	63	45	141	183	120	23	5802	45	40	61	59	40	162	5	165	82	9	102
max	47	40	400	111	231	119	173	472	467	316	1101	96	43	582	264	230	112	45	3220	126	123	108	72	471	25	260	160	30	201
nsls	65	46	1042	222	779	198	408	299	574	248	1146	146	60	323	333	358	231	40	126	2296	301	392	100	480	42	239	342	62	620
nsrrc	83	48	992	398	560	398	470	292	639	243	868	209	92	361	423	406	192	61	123	301	3560	478	147	523	37	184	843	101	568
ornl	86	42	1009	610	1317	300	407	322	649	264	1105	559	305	369	1188	1056	213	59	108	392	478	4766	437	551	34	186	662	63	582
psi-sinq	81	47	310	386	294	123	129	276	374	177	932	615	425	300	1049	762	81	40	72	100	147	437	2590	570	15	115	259	19	147
psi-sls	315	184	2110	472	1388	517	720	1401	2335	929	5225	474	231	1602	982	816	707	162	471	480	523	551	570	14510	106	1011	851	82	1072
sacla	7	6	107	40	93	22	34	96	71	62	176	27	13	54	54	49	141	5	25	42	37	34	15	106	454	97	416	4	62
soleil	213	114	755	178	421	187	287	619	939	894	3124	207	68	669	641	385	351	165	260	239	184	186	115	1011	97	6398	424	39	325
spring8	97	67	1364	561	792	430	504	605	887	472	1632	257	155	571	763	800	453	82	160	342	843	662	259	851	416	424	9066	79	732
ssls	8	14	130	63	93	85	99	88	94	57	125	26	10	60	55	45	36	9	30	62	101	63	19	82	4	39	79	404	90
ssrl	79	54	3479	381	2092	531	1003	488	1163	390	1823	208	74	571	441	480	818	102	201	620	568	582	147	1072	62	325	732	90	9665

40k users per year

10's PB of data

- Multi disciplinary programmes
- Individual researchers —> Large collaborations
- Industrial and commercial use



Data & Meta Data

data

/ˈdeɪtə/

noun

noun: **data**

facts and statistics collected together for reference or analysis.
"there is very little data available"
synonyms: facts, figures, statistics, details, particulars, specifics, features; More

- the quantities, characters, or symbols on which operations are performed by a computer, which may be stored and transmitted in the form of electrical signals and recorded on magnetic, optical, or mechanical recording media.
- PHILOSOPHY
  things known or assumed as facts, making the basis of reasoning or calculation.

Origin

LATIN

datum → data

mid 17th century

metadata

/ˈmɛtədeɪtə/

noun

noun: **meta-data**

a set of data that describes and gives information about other data.

Where is my Data?

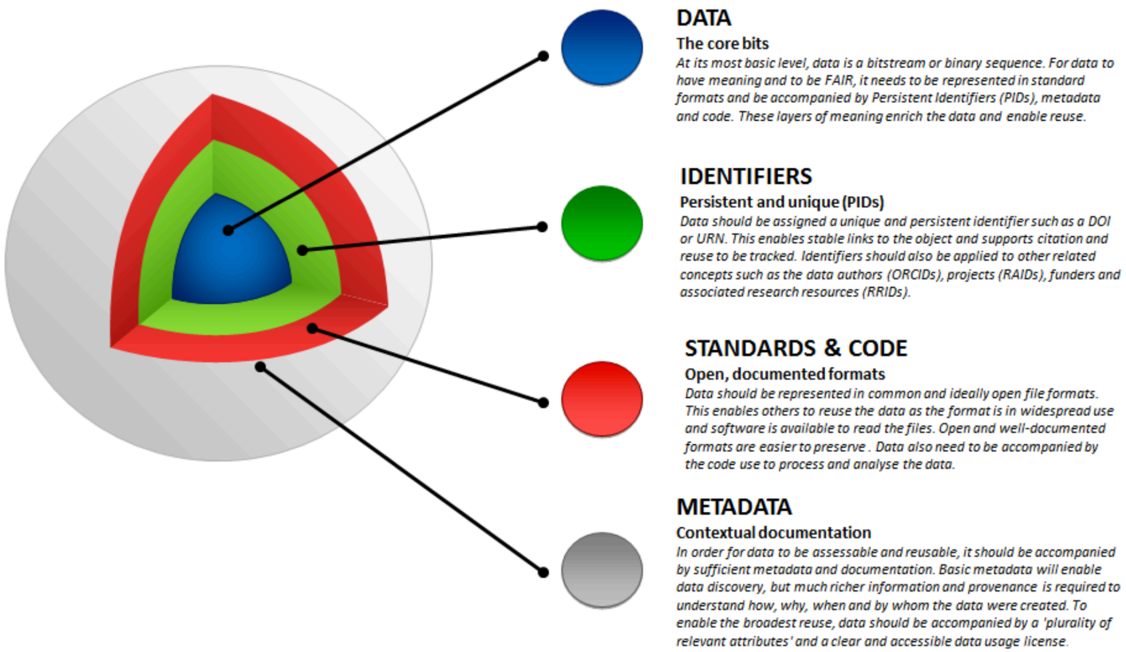
How do I get it?

How do I look at it?

What does it mean?

Is it right?

Data Is Our ‘Core Product’



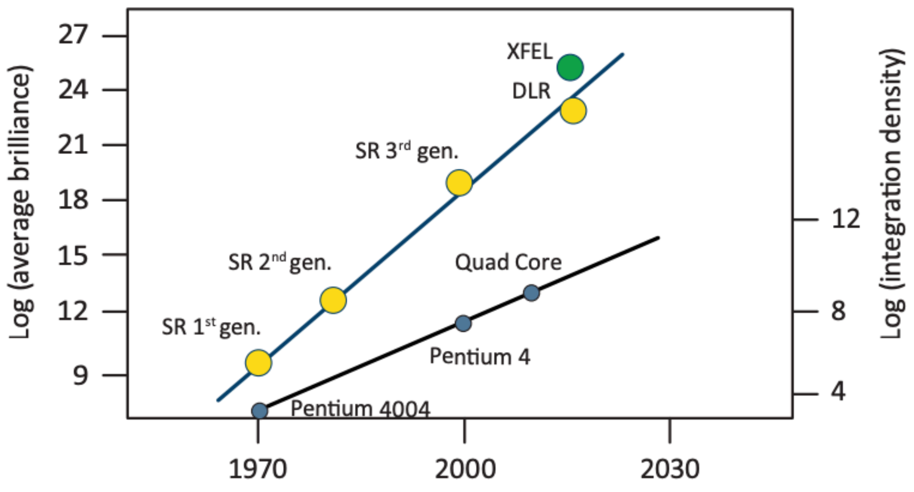


Fig. 1. Comparison of the brilliance of X-rays delivered by photon facilities over the years (LEAPS’ law) with the gain in transistor density in integrated circuits (Moore´s law). (DLR = Diffraction Limited Rings with ultimate performance; XFEL = X-ray free-electron laser)

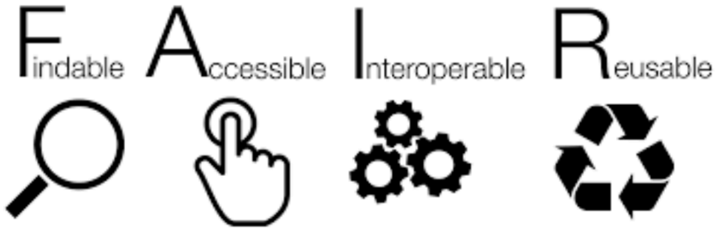
- EuXFEL ~500TB - 2PB data per experiment.
- ESS ~ 250TB per day.
- Data volume is too much for user portable drives.
- Central access is needed.
- Data management is essential.

FAIR Principles.

Wilkinson, M. D. et al. (2016). The FAIR Guiding Principles for scientific data management and stewardship. Scientific Data, 3, 160018. doi:10.1038/sdata.2016.18

To be **Findable**:

F1. (meta)data are assigned a globally unique and eternally persiste
F2. data are described with rich metadata.
F3. (meta)data are registered or indexed in a searchable resource.
F4. metadata specify the data identifier.



To be **Accessible**:

A1 (meta)data are retrievable by their identifier using a standardized communications protocol.
A1.1 the protocol is open, free, and universally implementable.
A1.2 the protocol allows for an authentication and authorization procedure, where necessary.
A2 metadata are accessible, even when the data are no longer available.

To be **Interoperable**:

I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
I2. (meta)data use vocabularies that follow FAIR principles.
I3. (meta)data include qualified references to other (meta)data.

To be **Re-usable**:

R1. meta(data) have a plurality of accurate and relevant attributes.
R1.1. (meta)data are released with a clear and accessible data usage license.
R1.2. (meta)data are associated with their provenance.
R1.3. (meta)data meet domain-relevant community standards.

Core Product is Data

- FAIR is a real challenge for facilities and for **users**

- 1500 + individual experiments (data sets) per year
  - Each experiment may have 200+ individual files

- Data rate has increased considerably

- Photon sources generate increasingly large volumes
  - Up to PBs per experiment on some beam lines

- Neutron sources produce much more data than ever
  - ESS at full specification 250TB per day (10GB/Minute/Instrument)
    - ~10^9 Events / s each event is 32bit position + 64bit Time stamp

The FAIR Data & Meta Data Challenge

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What role does the Fermi Surface play in frustrated metallic magnets?

3 Facility Experiments - 3TB of data
Inelastic X-Ray Scattering
Neutron Diffraction
Inelastic Neutron Scattering

Evernote

Data reduction and processing
Visualisation Scripts
Raw Data files
Correction and normalisation data
Sample details and characterisation
Experiment set-up and experimental log

ELK band-structure calculations

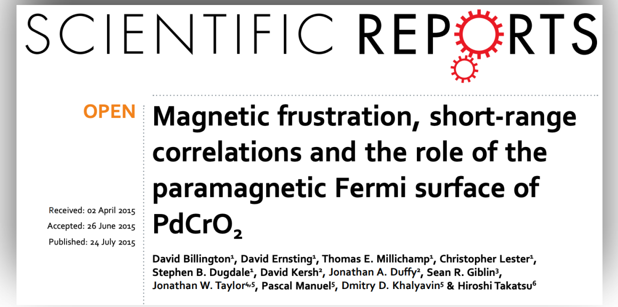
Fermi Surface reconstruction

Dynamic susceptibility calculations

Parameter and set-up files

Processing and visualisation scripts

Convolution procedure


SCIENTIFIC REPORTS

OPEN

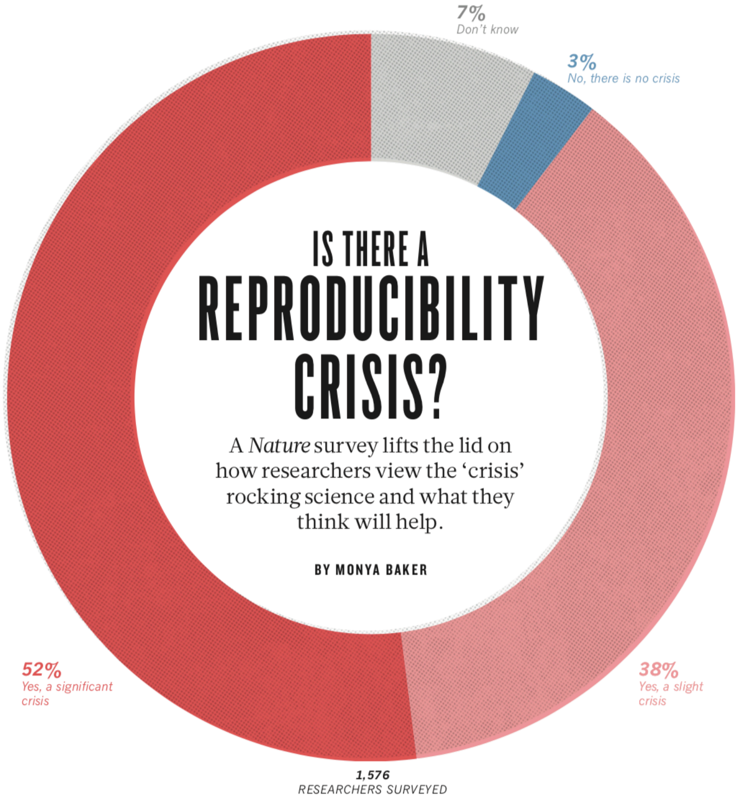
Received: 02 April 2015
Accepted: 26 June 2015
Published: 24 July 2015

Magnetic frustration, short-range correlations and the role of the paramagnetic Fermi surface of $PdCrO_2$

David Billington[1], David Ernsting[1], Thomas E. Millichamp[1], Christopher Lester[1], Stephen B. Dugdale[1], David Kersh[2], Jonathan A. Duffy[2], Sean R. Giblin[3], Jonathan W. Taylor[4,5], Pascal Manuel[5], Dmitry D. Khalyavin[5] & Hiroshi Takatsu[6]

What makes good science

- One metric is reproducibility
  - How to reproduce a measurement.
  - How to reproduce an analysis.
  - How to reproduce a calculation.
- FAIR applies to software as much as to Data



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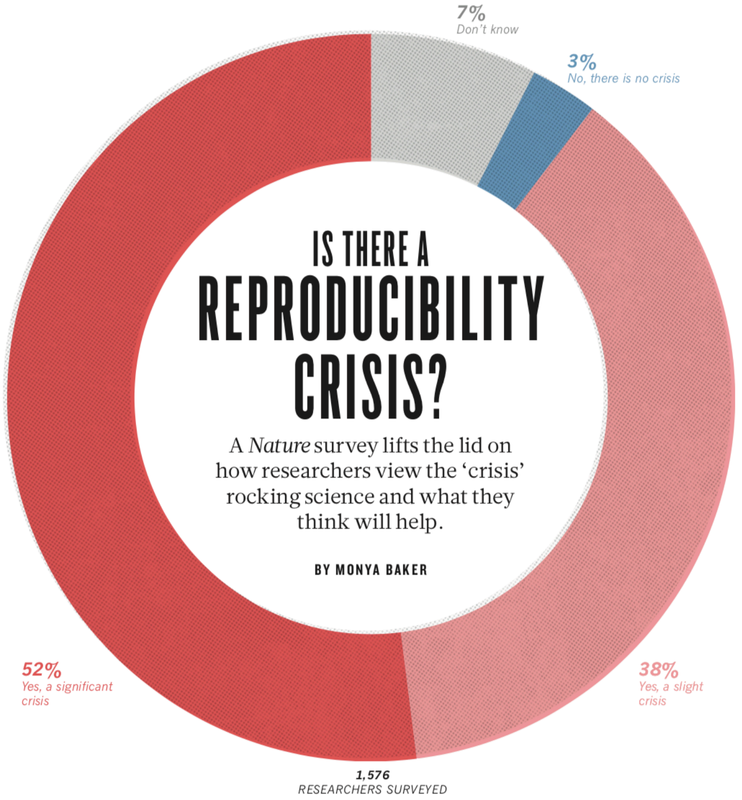
FAIR Enables Reproducibility

- Current tooling is not sufficient for FAIR*

- Beneficial for original research team

- The push for Open Science drives investment that benefits all

- * For ~75% of facility research programmes



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FAIR Data. FAIR Software.

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- Common data types that are complete descriptors
- Capture Rich Meta Data
- Catalogue and Curate with a data policy
- Persistently identify Data and Software

SciCat Project

SciCat is a metadata catalogue for scientists

MANTID

NeXus

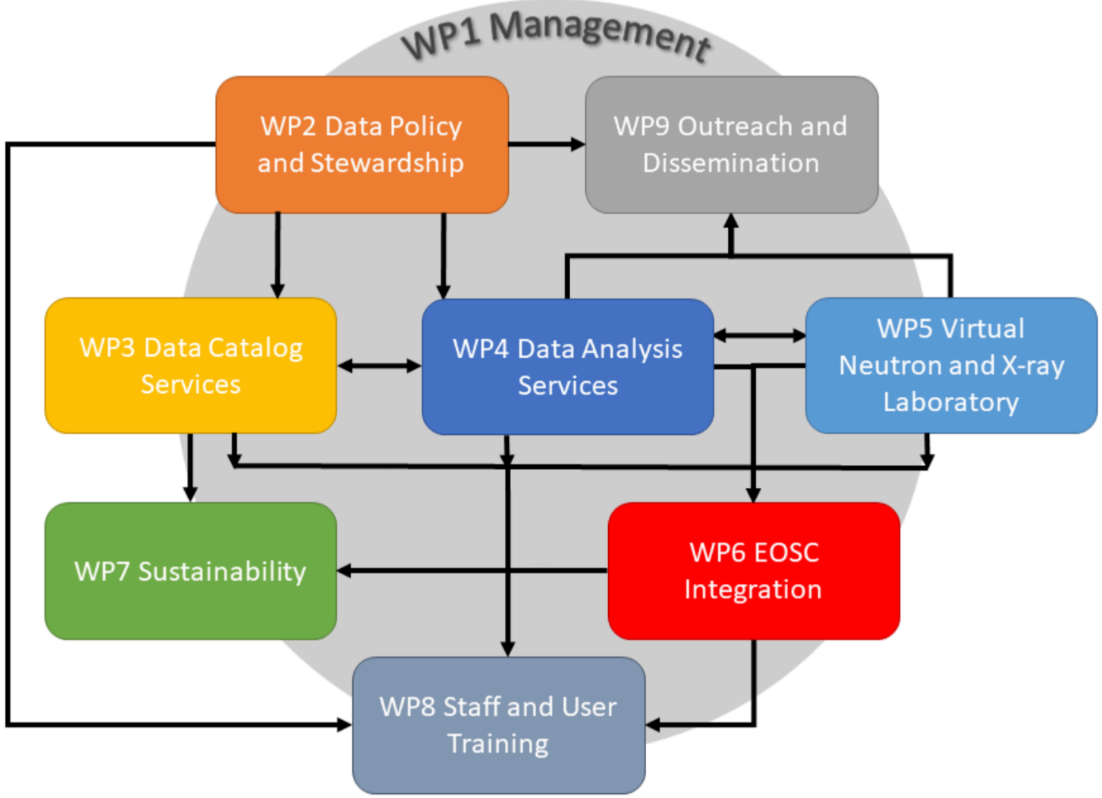
NeXus is developed as an international standard by scientists and programmers representing major scientific facilities in Europe, Asia, Australia, and North America in order to facilitate greater cooperation in the analysis and visualization of neutron, x-ray, and muon data.

Make Fair data a reality for Photon and Neutron **ESRFI** facilities.

FAIR - PaNOSC will comply with the FAIR principles in the following ways:

Findable	- all data will have a doi, rich metadata, common api for federated search
Accessible	- api will support open protocol, metadata accessible even without data
Inter-operable	- metadata to follow community standards (NeXus), register metadata
Reusable	- follow community standardise metadata, clear licence (CC-BY)

Vision- PaNOSC will help fastrack new Photon and Neutron facilities, improve data services for existing users, create a new class of virtual users of open data, help build and integrate the PaN RIs to the **EOSC**.

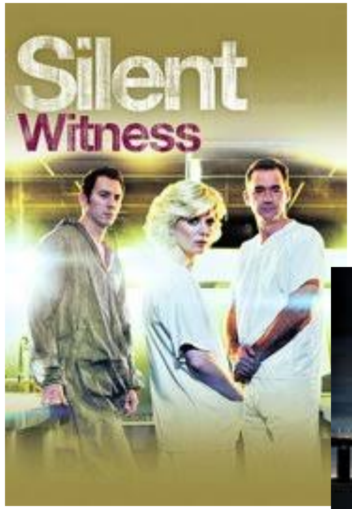


This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 823852

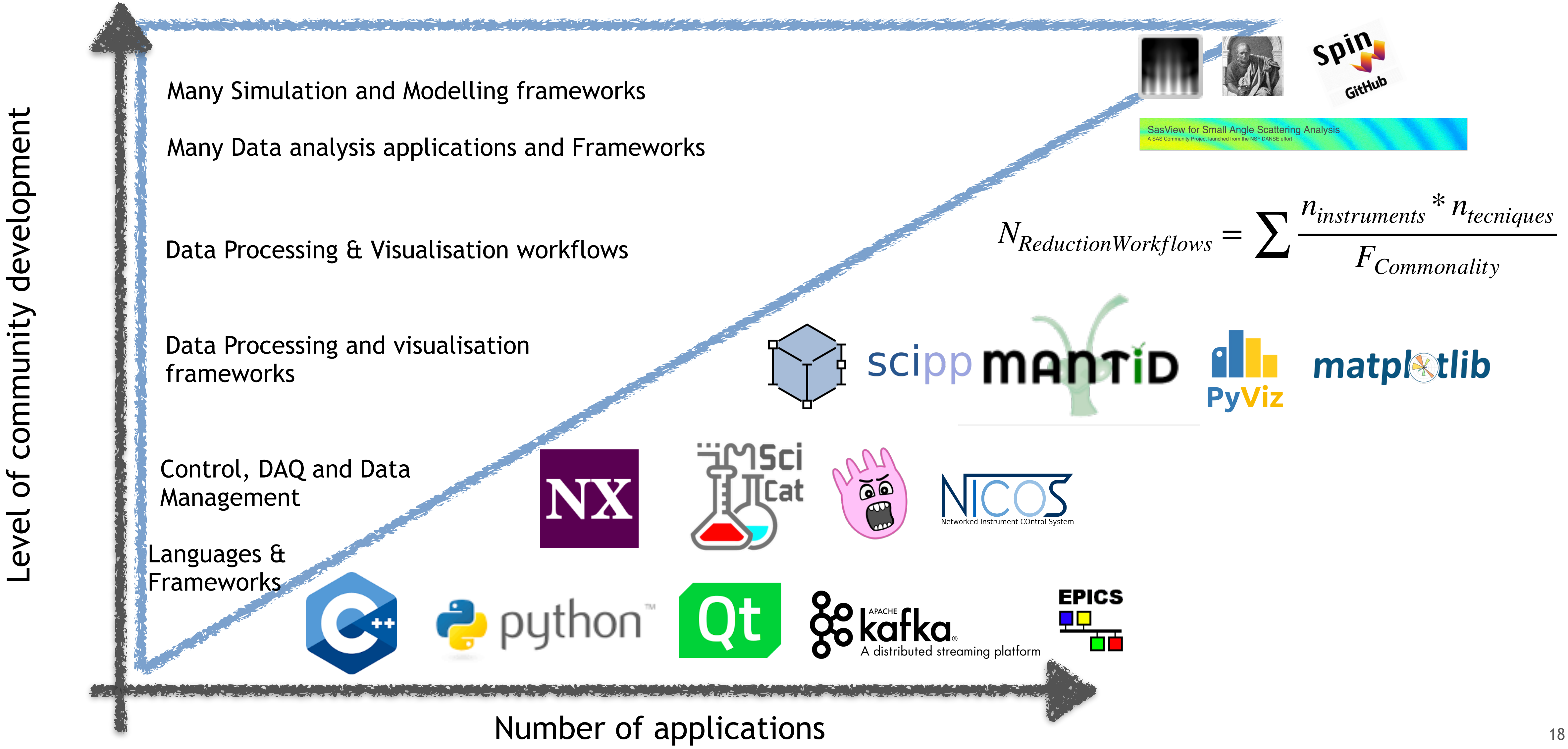
How To Improve Scientific Efficiency (A TV series analogy)

Move from Post Mortem Analysis

To Live Analysis



Scientific Application Stack



Real Time Pipelines.

- Stream data through processing to analysis.

Real-time analysis diffraction SANS

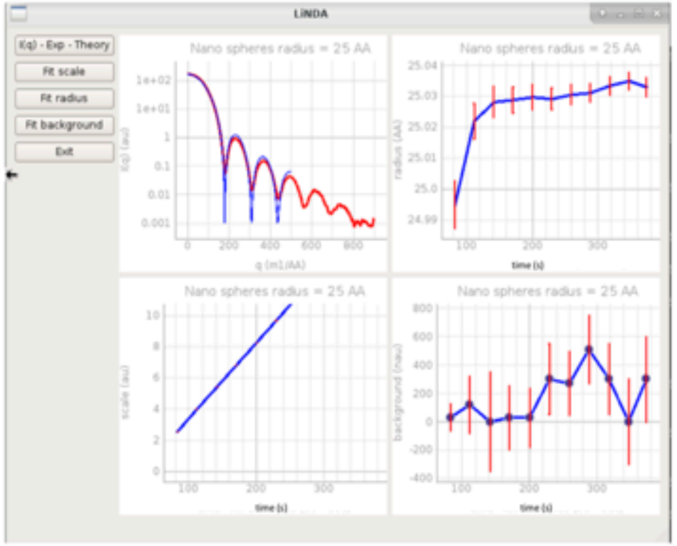
- >10^7 Events per second
- Data reduction using Mantid
- prototype for two techniques

→ diffraction & SANS

- Pipeline incudes analysis

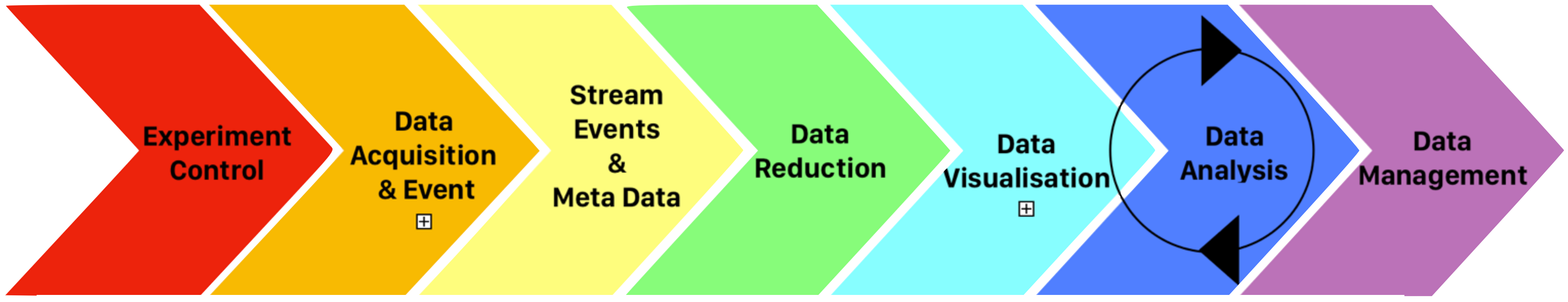
diffraction → FullProf

SANS → SasView



Whats in a pipeline

- A few million lines of code
- C++, Python
- Continuous integration automated testing, build and deploy
- 100Gb High performance networking
- Enterprise servers
- High performance storage systems
- Team of scientists, computer scientists, data scientists and developers

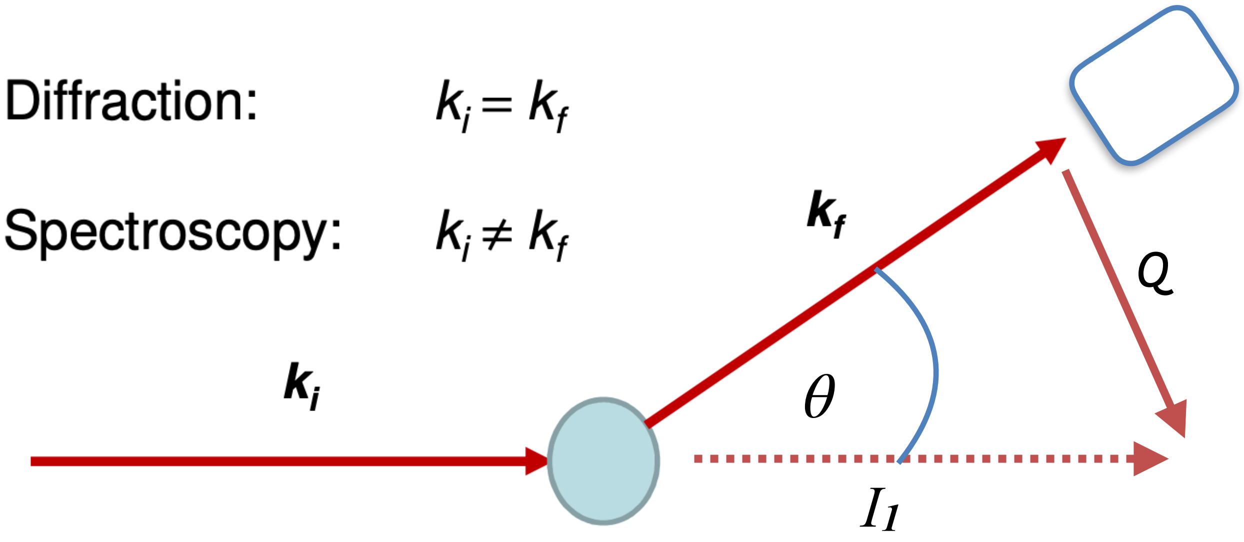


TOF Neutron scattering instrumentation

- The neutron energy is encoded in its *Time of Flight*

Diffraction: $k_i = k_f$

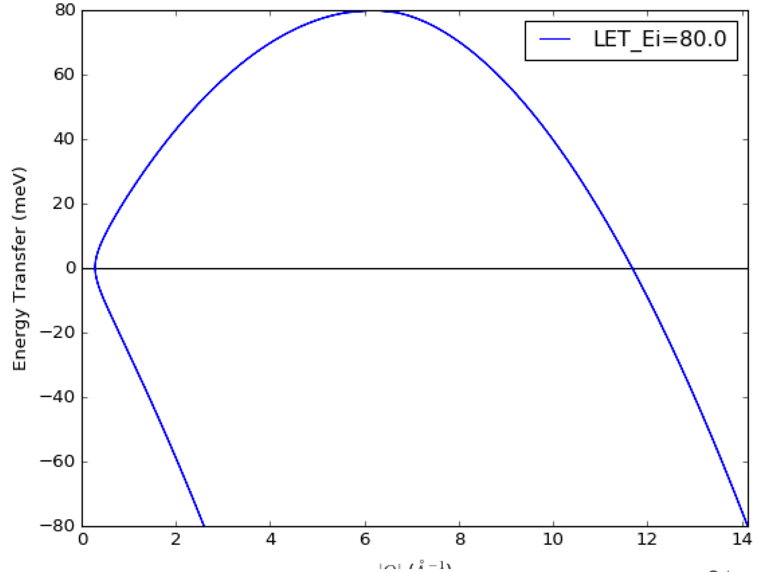
Spectroscopy: $k_i \neq k_f$



Detector Solid angle $\delta\Omega$
Detector efficiency
Detector Counts (n)

I_0 *with* $\dfrac{\delta\lambda}{\lambda}$

$$T = \frac{I_1}{I_0} = \exp(-n_s \sigma t)$$



- Volume sampled in Q is limited by kinematics of scattering.
- Most experiments scatter ~10% of incident neutrons
- Detectors have a finite performance. Dead time is an issue.
- Most (not all) detectors work as single particle counters.
    - Assume Poisson statistics.

Time of Flight Neutron Scattering

Pulsed sources rely on an accurate time system better than 1ns

Many instruments count in event mode or list mode.

Every neutron detected as good is given a timestamp.

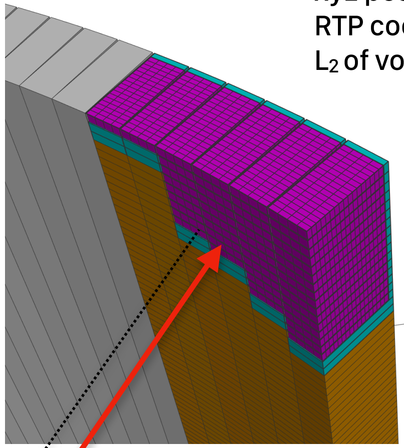
All the meta data can be timestamped

Save data lists to a hdf5 file along with the geometry of the experiment

List data can then be evaluated in software.

Detector List mode DAQ
offsets from Wall clock
:05
:06
...
+Pixel ID

xyz position
RTP coordinates
L_2 of voxel



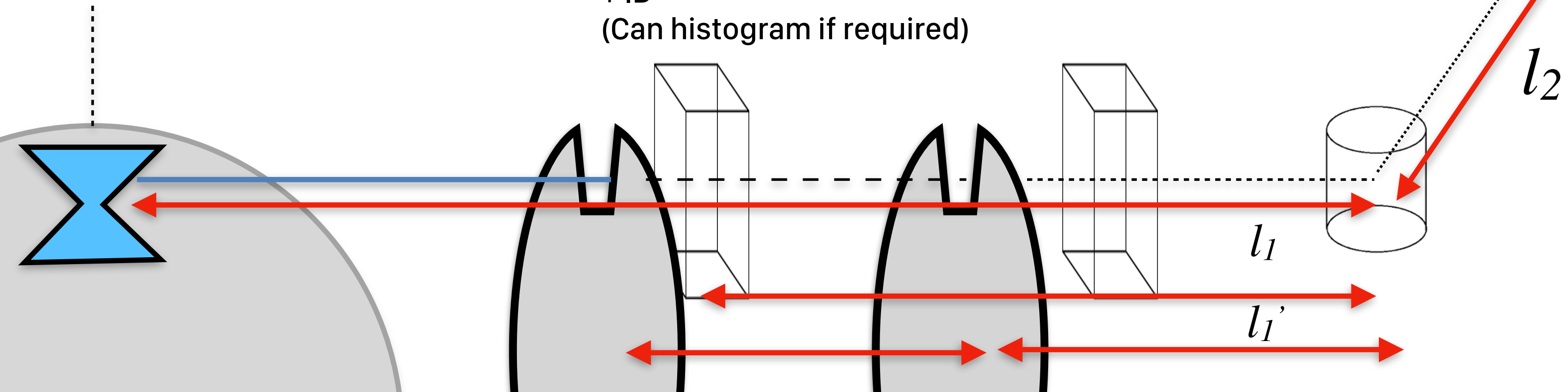
$$\lambda = \frac{h}{p} = \frac{h\,.\,tof}{m_N\,.\,L_{tot}} = 2dsin\theta$$

$$tof = t - t_0$$

$$L_{tot} = L_1 + L_2$$

Wall clock time proton pulse
11:10
Proton Pulse ID

Monitor List mode DAQ
offsets from Wall clock
:01
:02
...
+ ID
(Can histogram if required)



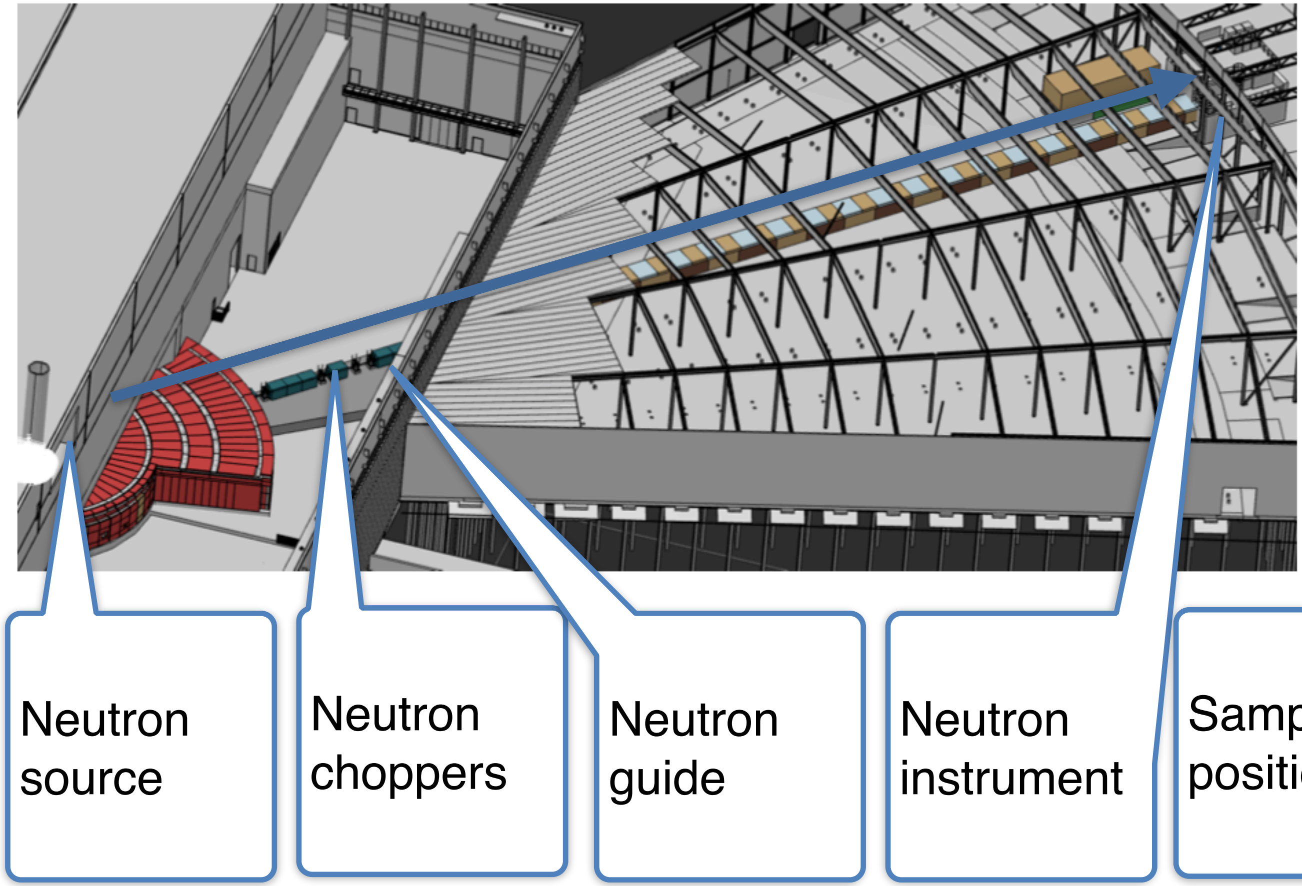
Calibration required for:
Motion axis
chopper offsets and transmission
Flight paths
Detector voxel / pixel positions

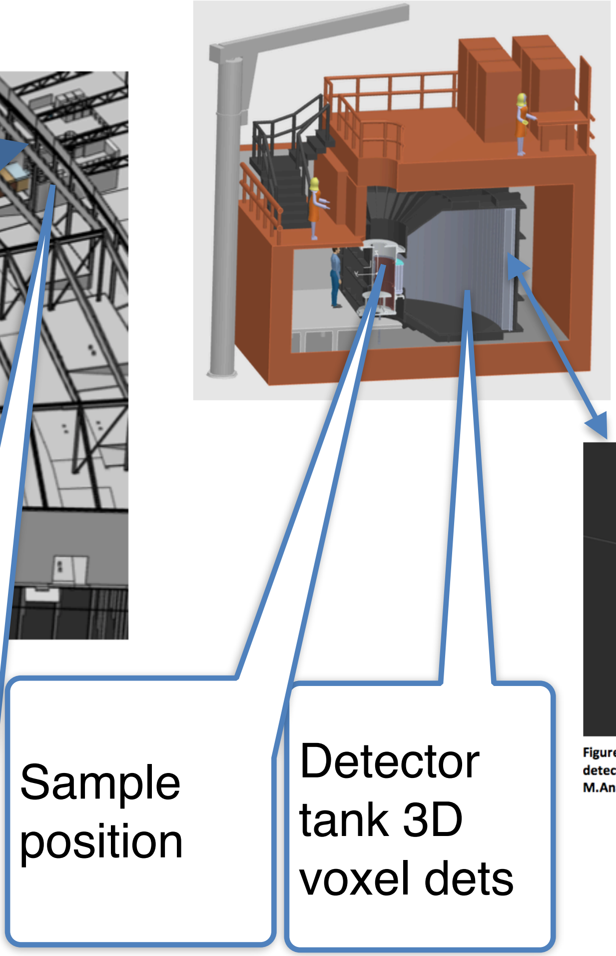
TOF Neutron scattering instrumentation

- The neutron energy is encoded in its *Time of Flight*

10^6 Detector elements
>10^7 n/s

~5TB of data per day





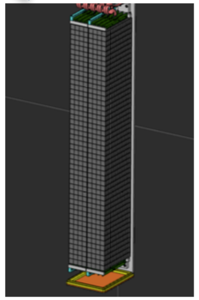


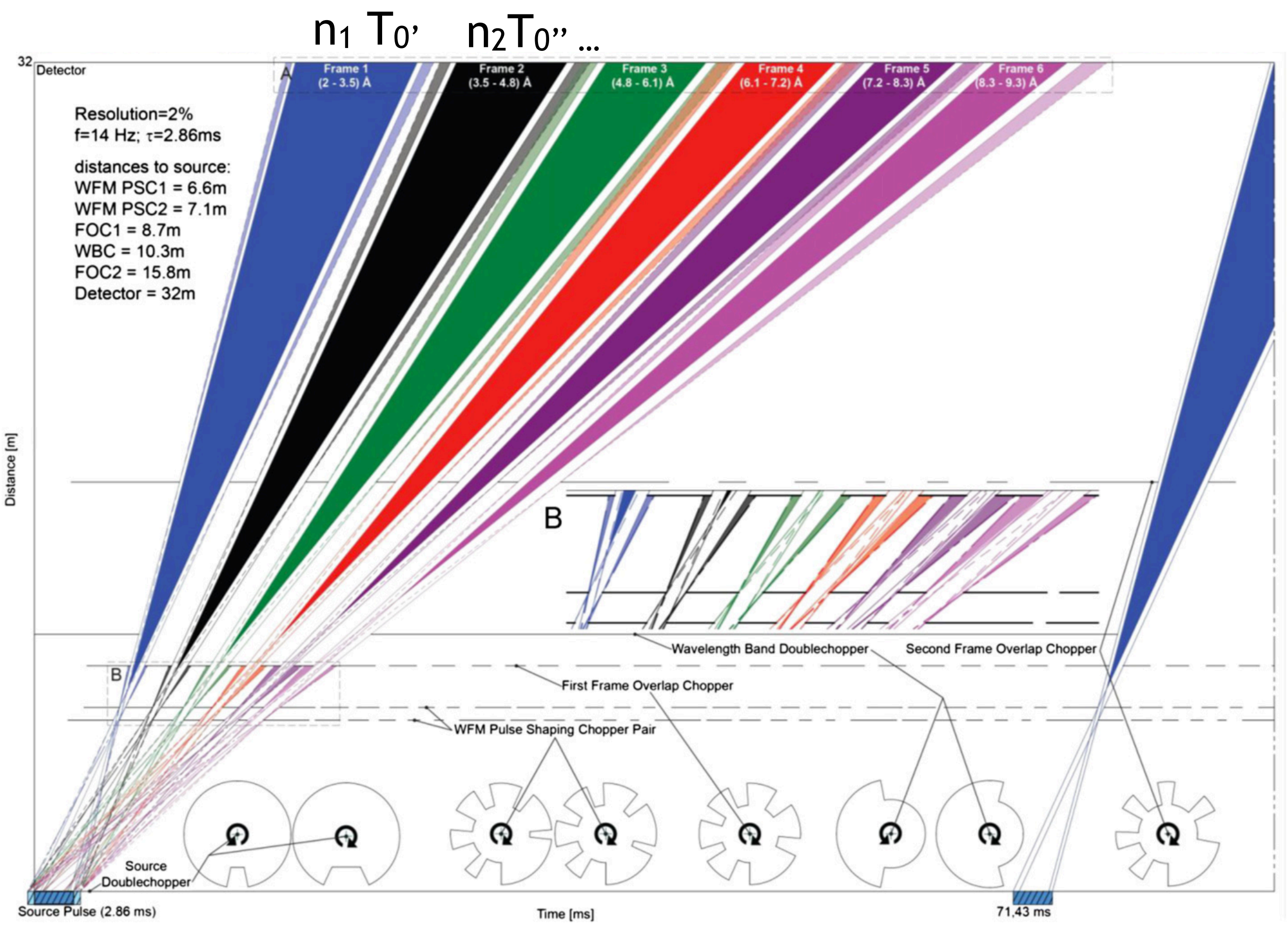
Figure 18: CAD image of a B10 detector module. M.Anastasopoulos

Data reduction / processing at TOF Neutron facilities

- Loading experimental data.
- Loading calibration data.
- Normalisation.
  - Intensity normalisation, $I / I_{Monitor}$
  - Solid Angle correction, $I / I_{Vanadium}$

- Convert Units
  - Spectrum to Theta, Q…
  - ToF to D, meV…

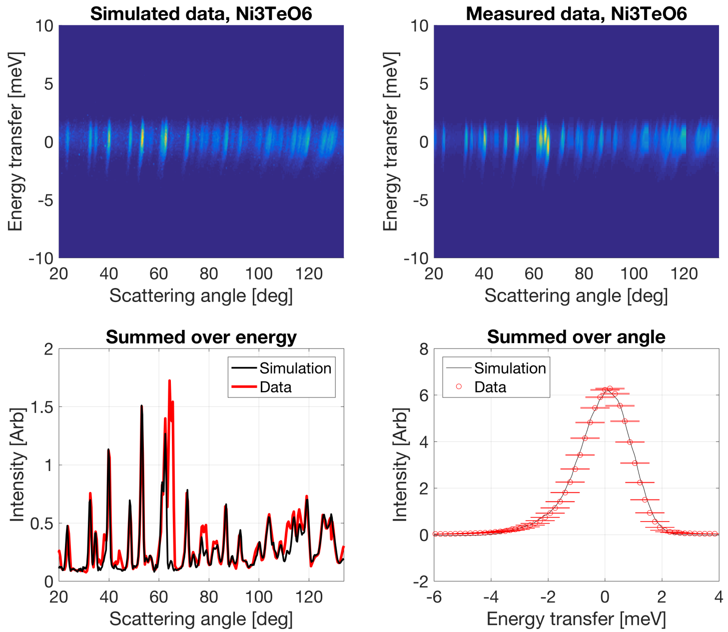
- Correct for experimental effects …

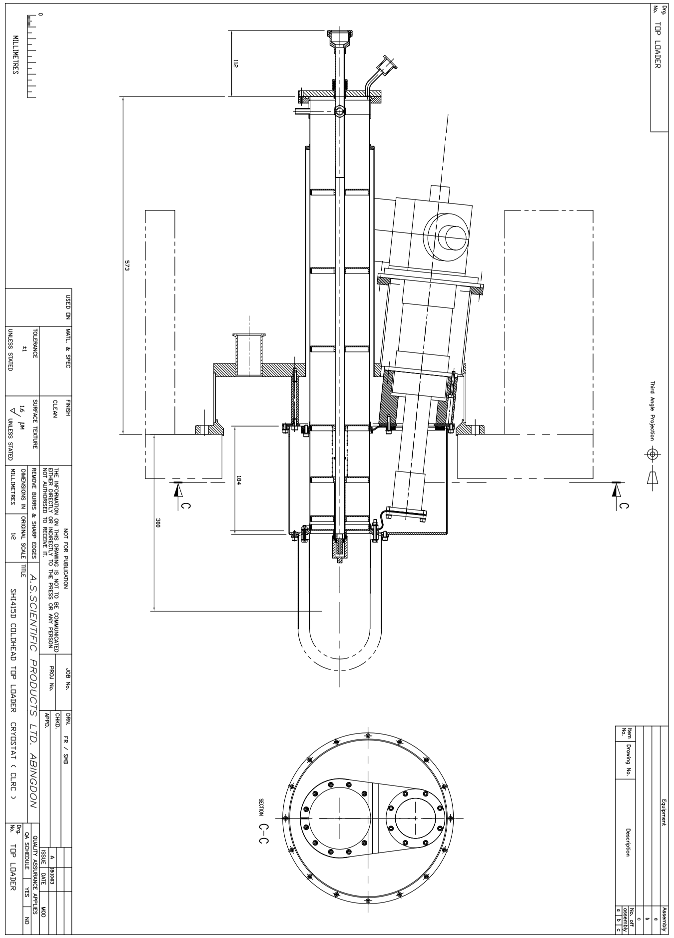


Experimental / Instrument effects

- Detector efficiency.
- Sample absorption.
- Background scattering.
  - Elastic or inelastic
- Multiple scattering.
- Inelasticity effects.

- Solve analytically or with MC
  - McStas Union component - model complex geometries
  - Source + instrument + SE +sample
  - Sample environment multiple scattering simulation
  - Get the resolution and flux for free





Event Mode Data Acquisition

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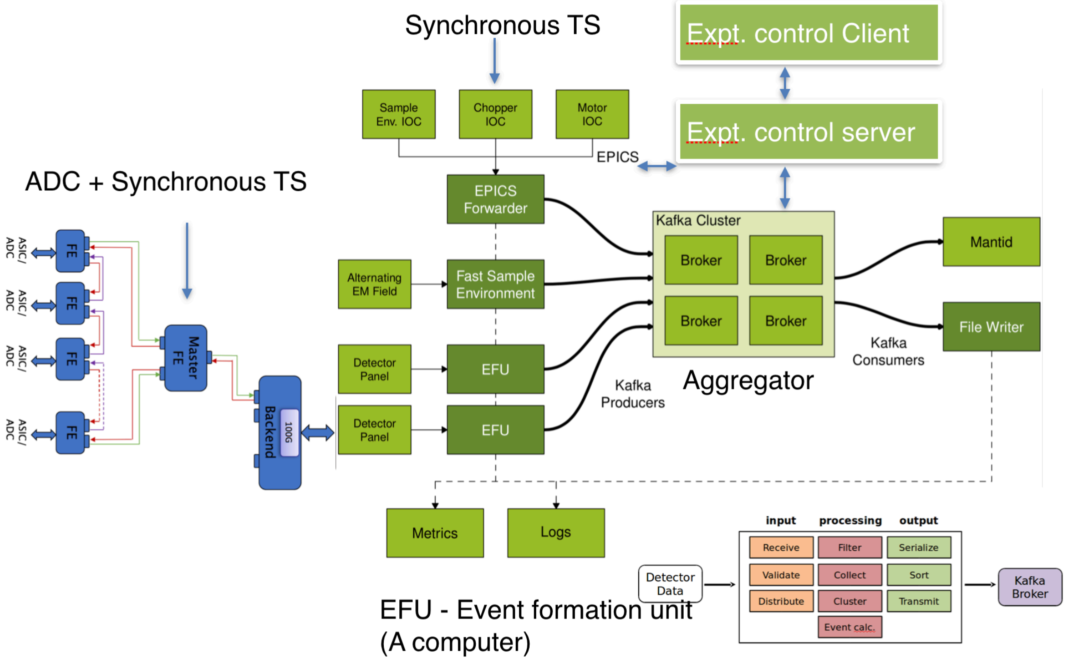
- TimeStamp everything. (Neutrons, Choppers, Motion control)
- Filter Neutron events in software.
  - The Good from the Bad and Ugly.
- Go Fast.



Event Mode Data Acquisition examples from SNS

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research papers

JOURNAL OF APPLIED CRYSTALLOGRAPHY

ISSN 1600-5767

Event-based processing of neutron scattering data at the Spallation Neutron Source[1]

Garrett E. Granroth,[a*] Ke An,[a] Hillary L. Smith,[b] Pamela Whitfield,[a,c] Joerg C. Neuefeind,[a] Jooseop Lee,[a,d] Wenduo Zhou,[a] Vladislav N. Sedov,[e] Peter F. Peterson,[a] Andre Parizzi,[a] Harley Skorpenske,[a] Steven M. Hartman,[e] Ashfia Huq[a] and Douglas L. Abernathy[a]

[a]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, [b]California Institute of Technology, Department of Applied Physics and Materials Science, Pasadena, California, USA, [c]Paul Scherrer Institute, 5232 Villigen PSI, Switzerland, [d]CHESS, Cornell University, Ithaca, New York, USA, and [e]Neutron Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA. *Correspondence e-mail: granrothge@ornl.gov

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Edited by M. Arai, European Spallation Source, Lund, Sweden

- Ramp control parameter - T, H/E Field.
- Collect data continuously.
- Filter events in software.

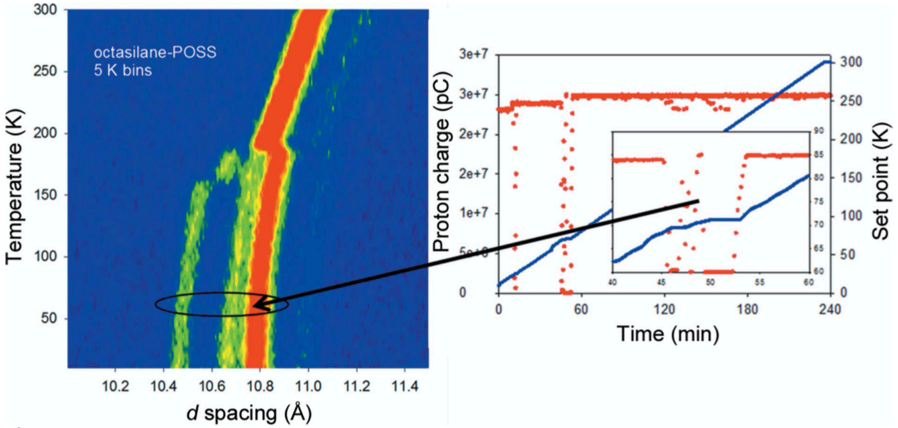

Figure 4
A contour plot of both transitions in octasilane-POSS during heating from 10 to 300 K at 2 K min^{-1} and the corresponding plot of temperature/proton charge *versus* time. The graph shows that the temperature holds when the beam has tripped. Had the temperature ramp not paused during this time there would be a gap in the data in the region indicated on the contour plot.

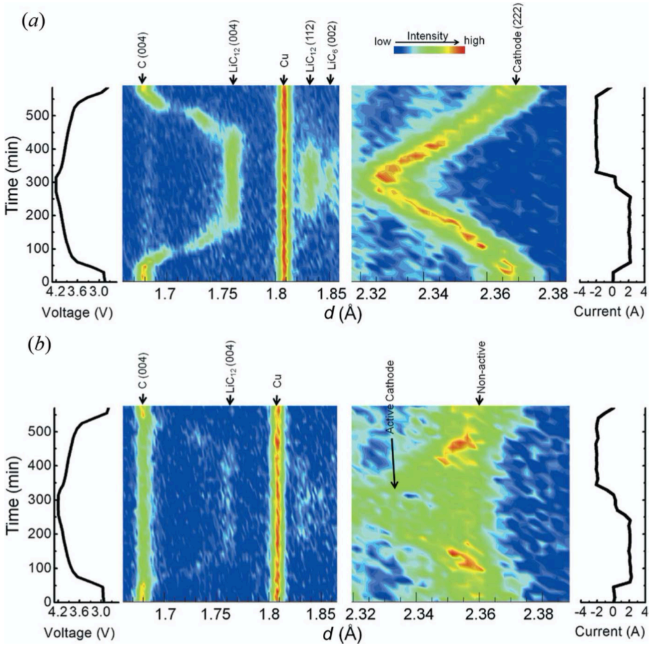

Figure 7
Contour plots during charge–discharge cycles, showing signs of degradation of a large-format battery (*a*) before and (*b*) after long-term cycling, with limited Li^+ insertion/removal processes in an active material (Cai, An *et al.*, 2013).

Data Streaming & Event Data

- How to process events without creating a histogram.
- In some cases it allows fast execution
- Realtime Processing of neutron data
- Modern photon detectors can count in event mode (TimePixIII)

Nuclear Instruments and Methods in Physics Research A 803 (2015) 24–28

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Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

Event-based processing of neutron scattering data

Peter F. Peterson*, Stuart I. Campbell, Michael A. Reuter, Russell J. Taylor, Janik Zikovsky

Neutron Data Analysis and Visualization, Oak Ridge National Laboratory, Oak Ridge, TN, USA

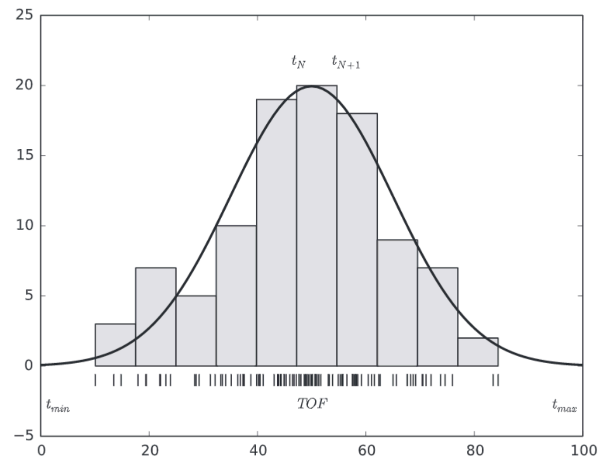
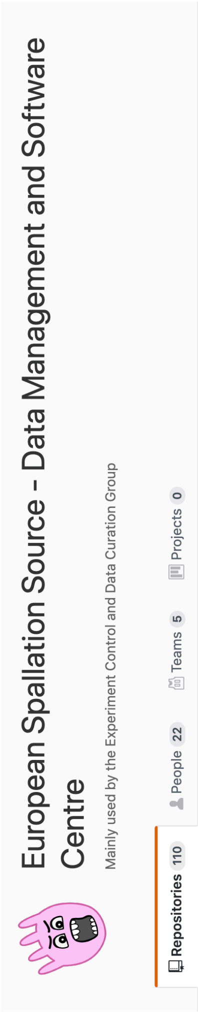
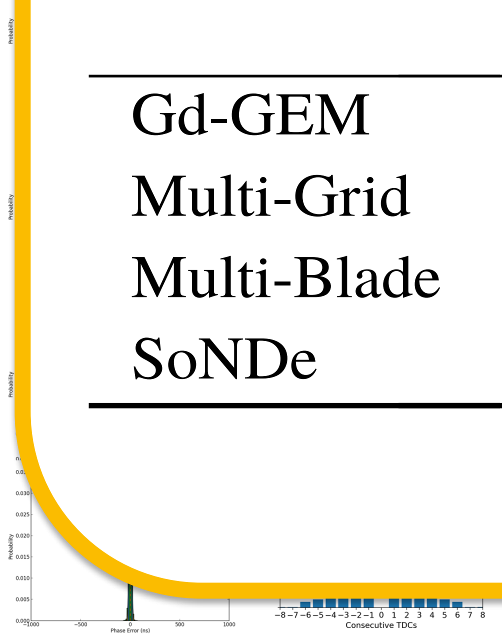


Fig. 1. Schematic diagram of histogramming. Dashes below are individual events. Boxes are the histogram representation. Curved line is the normal distribution for reference.

Testing ESS DAQ Architecture.

EUROPEAN SPALLATION SOURCE





Event formation throughput on 1 or 2 cores

Detector	Packet Rate [pkt/s]	Trigger Rate [readouts/s]	Event Rate [events/s]	cores
Gd-GEM	n/a	18.6 M	500 k – 1 M	1
Multi-Grid	86.000	3.0 M	2.46 M	1
Multi-Blade	82.000	5.6 M	2.31 M	2
SoNDe	94.000	23.5 M	23.5 M	2

EUROPEAN SPALLATION SOURCE

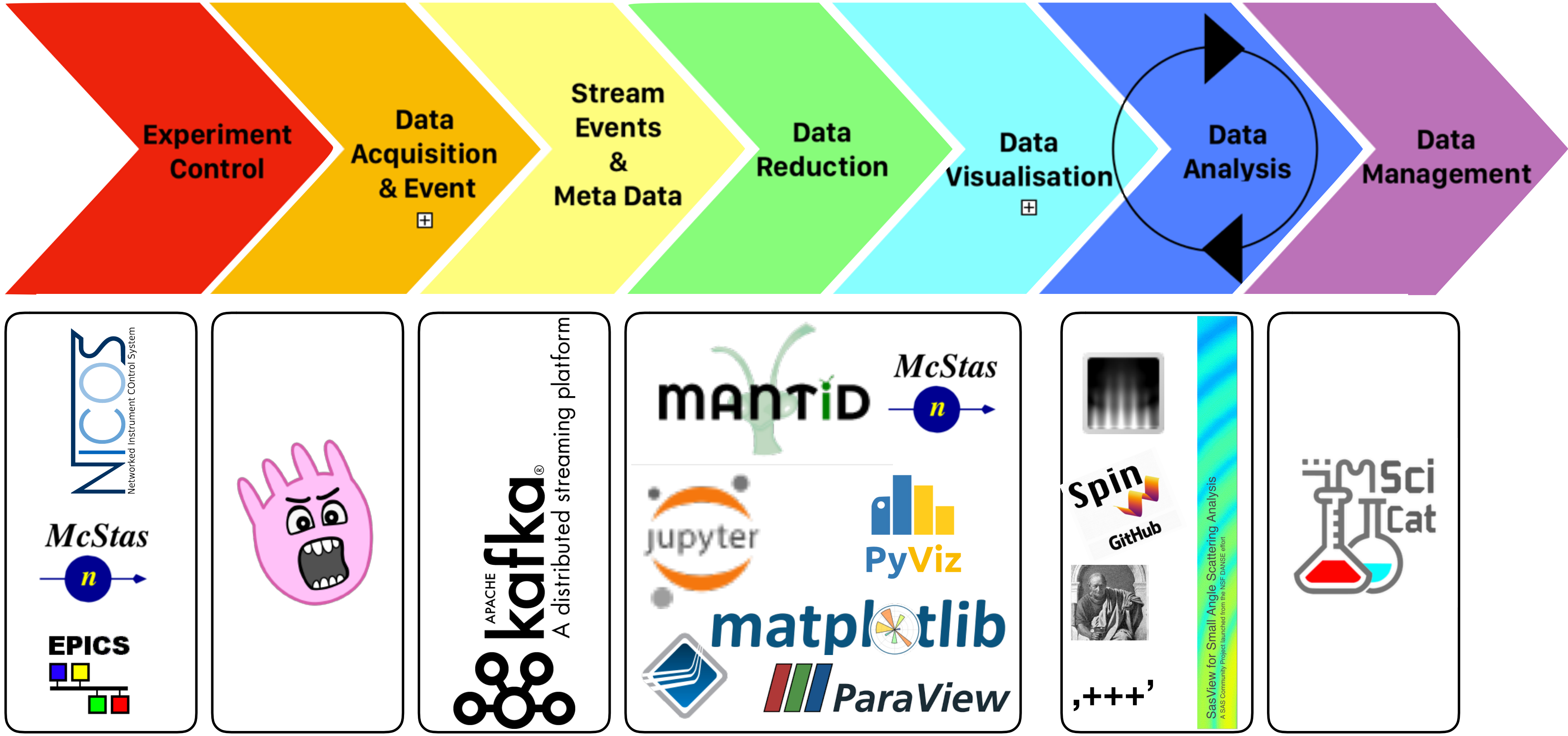
Stitched in Mantid

ESS Scientific Computing Pipeline

Core acquisition, controls and reduction stack tested on V20 test beam line.

- Detectors
- Monitors
- Motion
- Choppers
- Sample environment

- Highlights successful implementation
- Areas for further development



Data files & Data Containers for FAIR

CrossMark

computer programs

Journal of
Applied Crystallography
ISSN 1600-5767

Received 17 November 2014
Accepted 17 December 2014

The NeXus data format

Mark Könnecke,[a]* Frederick A. Akeroyd,[b] Herbert J. Bernstein,[c] Aaron S. Brewster,[d] Stuart I. Campbell,[e] Björn Clausen,[f] Stephen Cottrell,[b] Jens Uwe Hoffmann,[g] Pete R. Jemian,[h] David Männicke,[i] Raymond Osborn,[j] Peter F. Peterson,[e] Tobias Richter,[k] Jiro Suzuki,[l] Benjamin Watts,[m] Eugen Wintersberger[n] and Joachim Wuttke[o]

[a]Laboratory for Development and Methods, Paul Scherrer Institute, 5232 Villigen-PSI, Switzerland, [b]ISIS Facility, STFC, Rutherford Appleton Laboratory, Didcot, Oxfordshire OX11 0QX, England, [c]imgCIF, Dowling College, Shirley, NY 11769, USA, [d]Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, [e]Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, [f]Los Alamos National Laboratory, Los Alamos, NM 87545, USA, [g]Helmholtz-Zentrum Berlin für Materialien und Energie Gmb, 14109 Berlin, Germany, [h]Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA, [i]ANSTO, New South Wales 2234, Australia, [j]Argonne National Laboratory, Argonne, IL 60439, USA, [k]Diamond Light Source, Didcot, Oxfordshire OX11 0DE, England, [l]KEK, Ibaraki 305-0801, Japan, [m]Swiss Light Source, Paul Scherrer Institute, 5232 Villigen-PSI, Switzerland, [n]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany, and [o]Forschungszentrum Jülich, JCNS at MLZ, 85747 Garching, Germany. Correspondence e-mail: mark.koennecke@psi.ch

NeXus is an effort by an international group of scientists to define a common data exchange and archival format for neutron, X-ray and muon experiments. NeXus is built on top of the scientific data format HDF5 and adds domain-specific rules for organizing data within HDF5 files, in addition to a dictionary of well defined domain-specific field names. The NeXus data format has two purposes. First, it defines a format that can serve as a container for all relevant data associated with a beamline. This is a very important use case. Second, it defines standards in the form of application definitions for the exchange of data between applications. NeXus provides structures for raw experimental data as well as for processed data.

- Custom Photon and Neutron classes
- Based on HDF5 (h5Py)
- Used at ISIS, DLS, SLS, ESRF, ILL, SNS …
- The most common data type at facilities?
- Paper is cited 41 times?
- Structured Container for data and meta data.
- Classes for Raw and processed data
- Special classes for domain types SANS —> NXSAS
- Definition for Instrument Geometry and setup

Processing Data.

MANTID

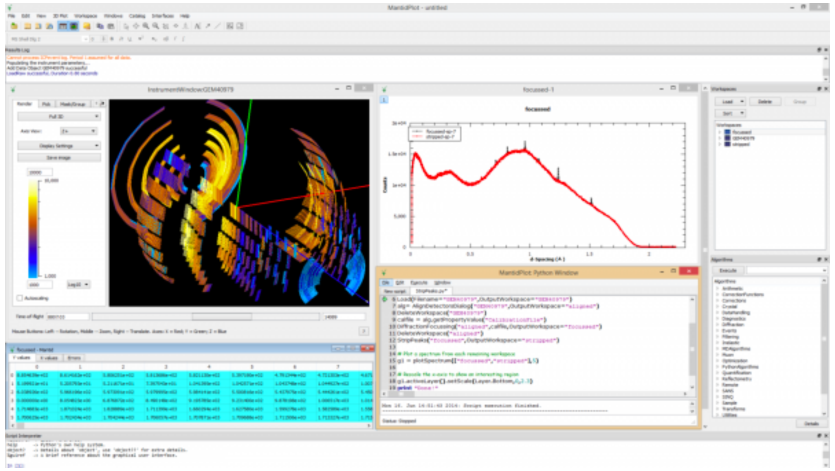
- Use a framework
- Define the processing steps
- Make Processed data documented and FAIR

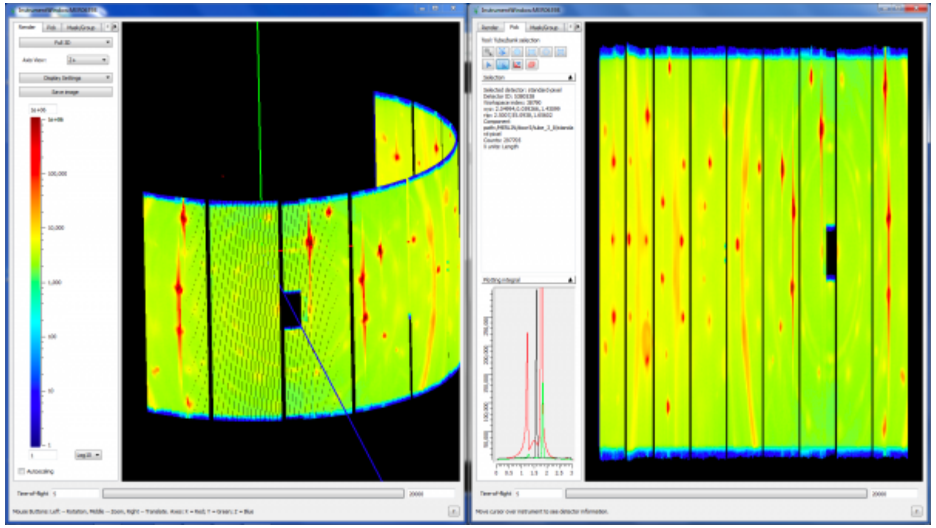
xarray

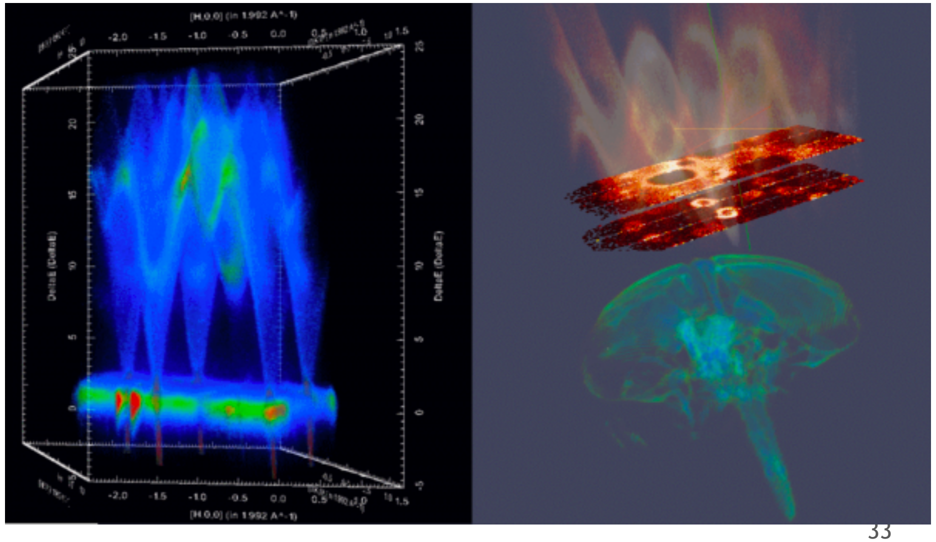
scipp

Mantid

- Data Processing & Analysis
- Neutron TOF and reactor data
- Used at ISIS, ILL, SNS, ESS
- Python & C++

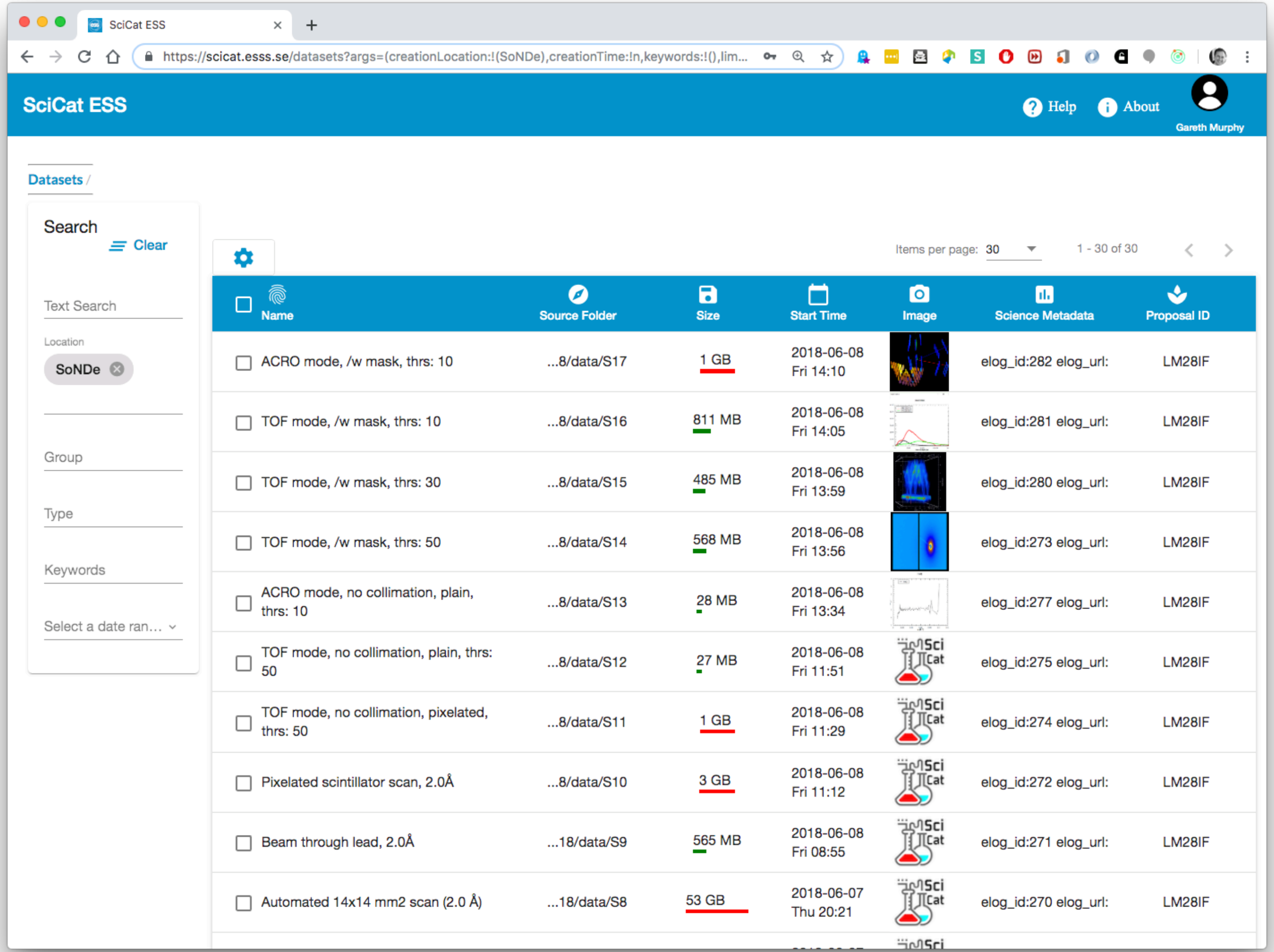






SciCat – the ESS metadata catalogue

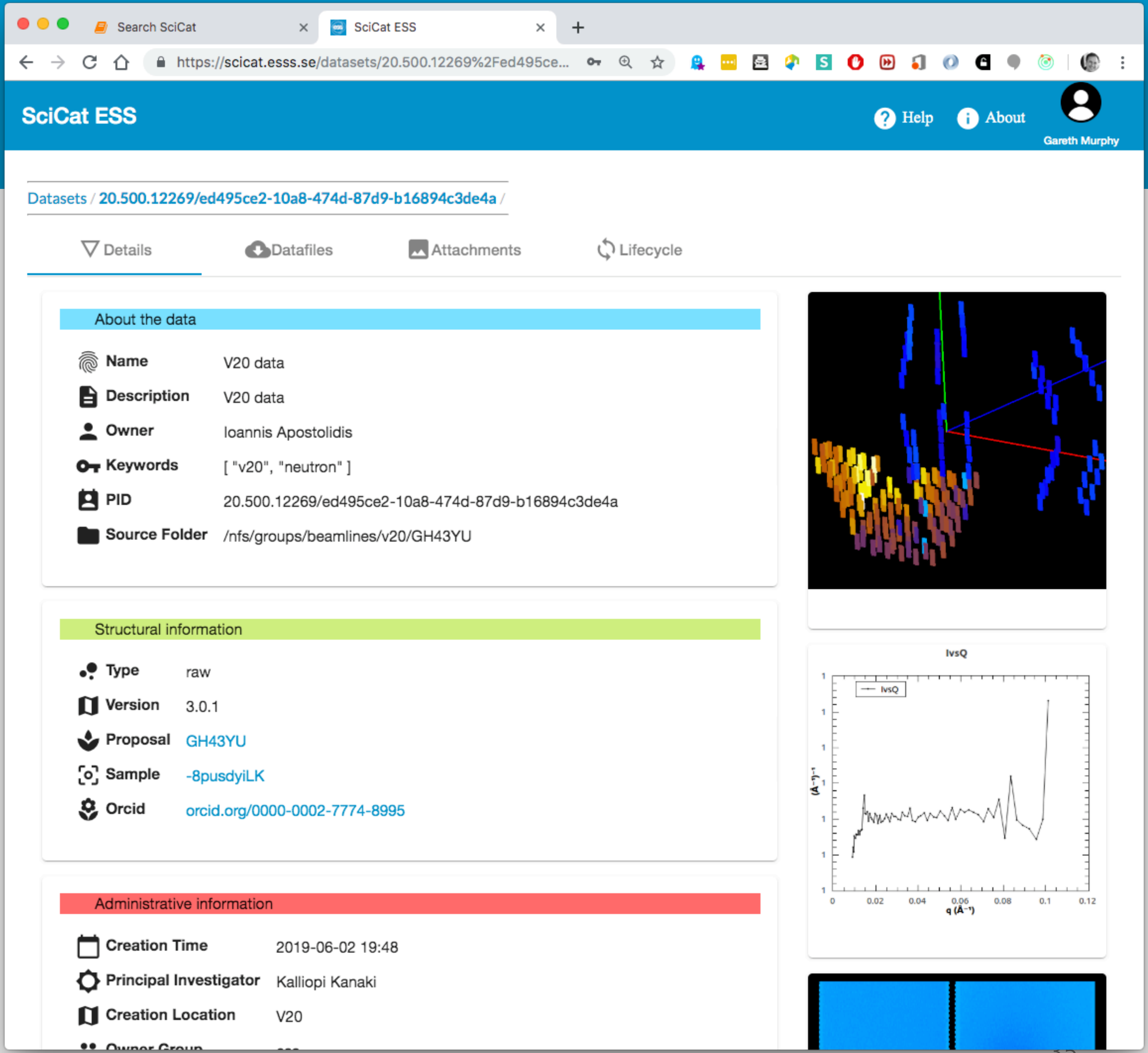
- SciCat stores metadata from experiments at ESS
- Users can search, sort and filter by types of experiment and preview images



SciCat features

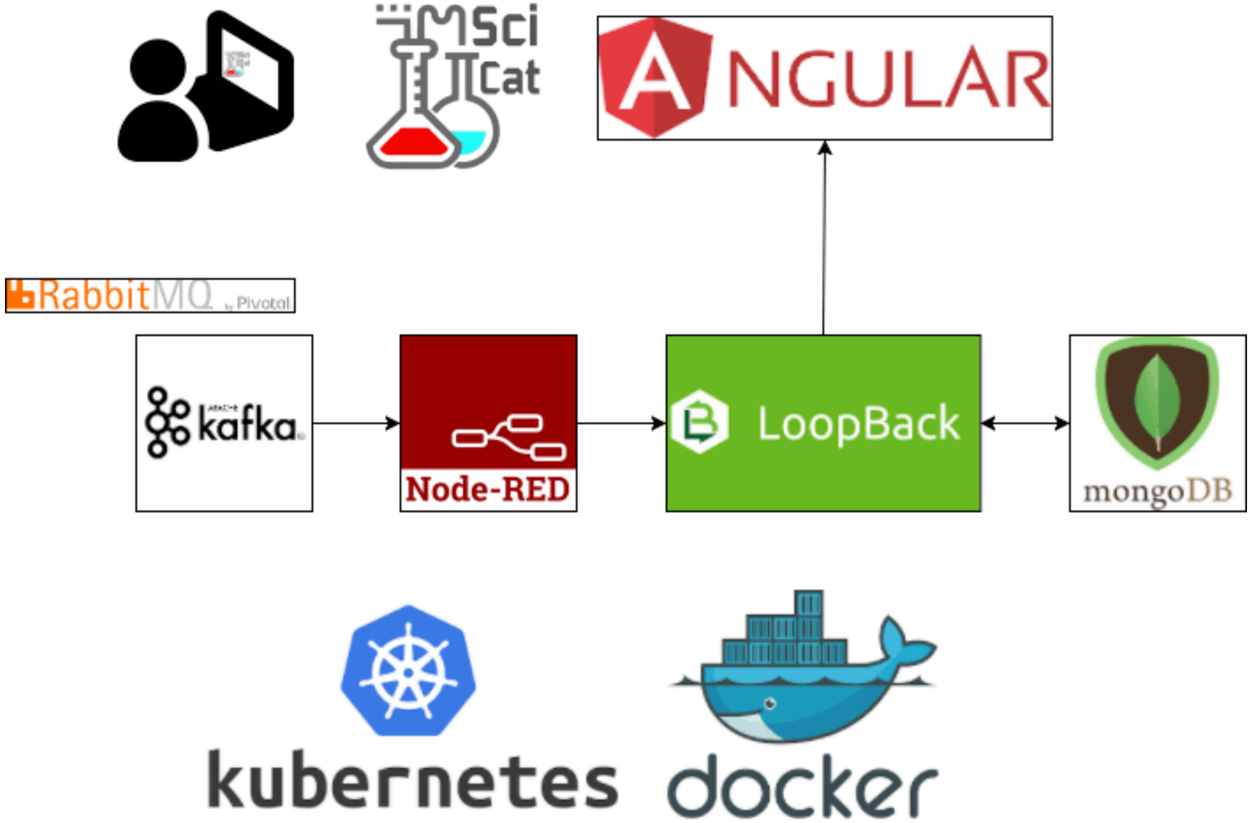
- Search for your own and public data
- Publish a DOI
- Link to proposal and sample

- Coming soon …
  - Data reduction!
  - Logbook integration!



How it works

- Data is fed in from Kafka and stored in a MongoDB database by the scicat metadata server
- Users access a web application written in Google's Angular framework
- The SciCat server runs on Docker image in a Kubernetes cluster



python™ Is A Preferred Language.

EUROPEAN SPALLATION SOURCE

- Easy to learn.
- Fast enough for most problems.
- Object oriented.
- Scientific packages.
- Learn Python
- Write code
- Share your work on Github

In [8]: Slide Type Sub-Slide

```
from mantid.simpleapi import *
def workspace2dToDataSet(workspace):
    signal = mtd[workspace].extractY()
    error  = mtd[workspace].extractE()
    TOF    = mtd[workspace].extractX()[0]
    wkspDim=signal.shape

    TOFAxis=(TOF[0:wkspDim[1]])
    d = sc.Dataset(
        {'data': sc.Variable(dims=[Dim.X, Dim.Y], values=signal),
        },
        coords={
        Dim.X: sc.Variable([Dim.X], values=np.arange(signal.shape[0]), unit=sc.units.m),
        Dim.Y: sc.Variable([Dim.Y], values=TOFAxis, unit=sc.units.us)},
        )
    print(d)
    return d
```

In [ ]: Slide Type

In [9]: Slide Type Sub-Slide

```
d = workspace2dToDataSet('data')
```

```
<scipp.Dataset>
Dimensions: {{Dim.Y, 1900}, {Dim.X, 922}}
Coordinates:
    Dim.X                     int64     [m]              (Dim.X)
    Dim.Y                     double    [µs]             (Dim.Y)
Labels:
Data:
    data                      double    [dimensionless]  (Dim.X, Dim.Y)
Attributes:
```

Managing Environments

EUROPEAN SPALLATION SOURCE

CONDA

- Conda manages environments and installation
- Conda install …

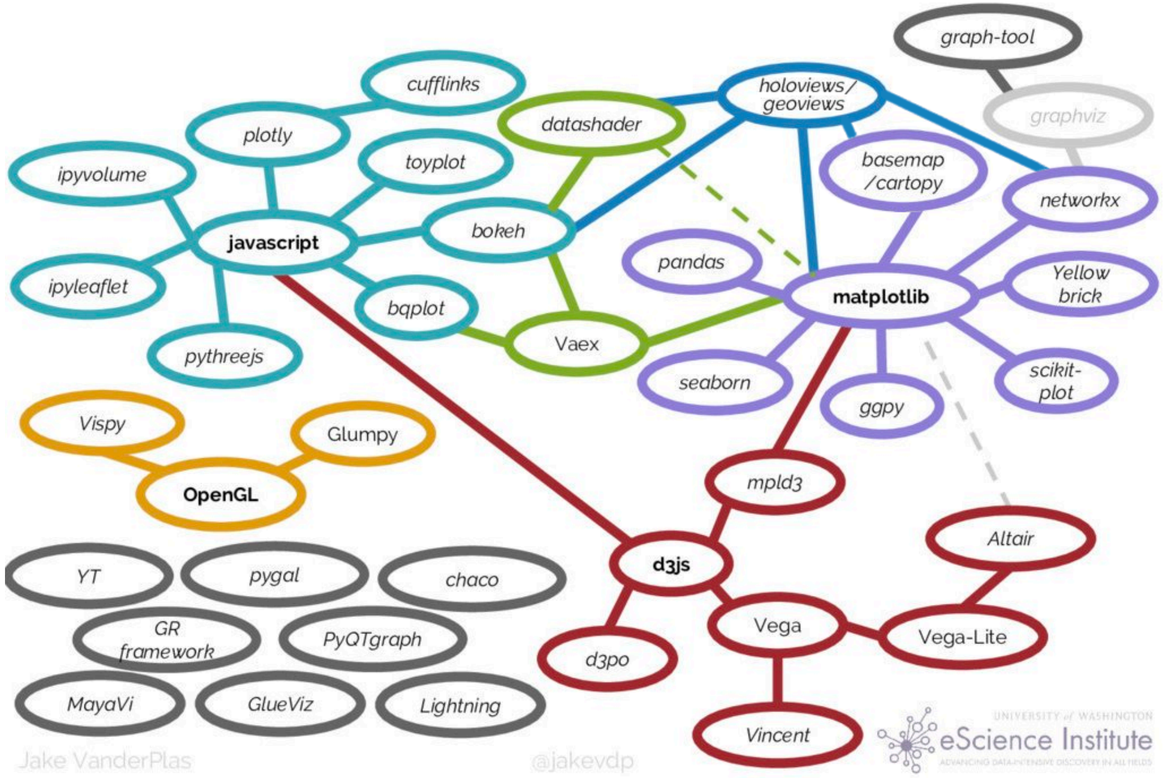
python jupyter scipp MANTID matplotlib

pandas NumPy xarray INTAKE DASK Numba SciPy HoloViews GeoViews Bokeh Datashader Param

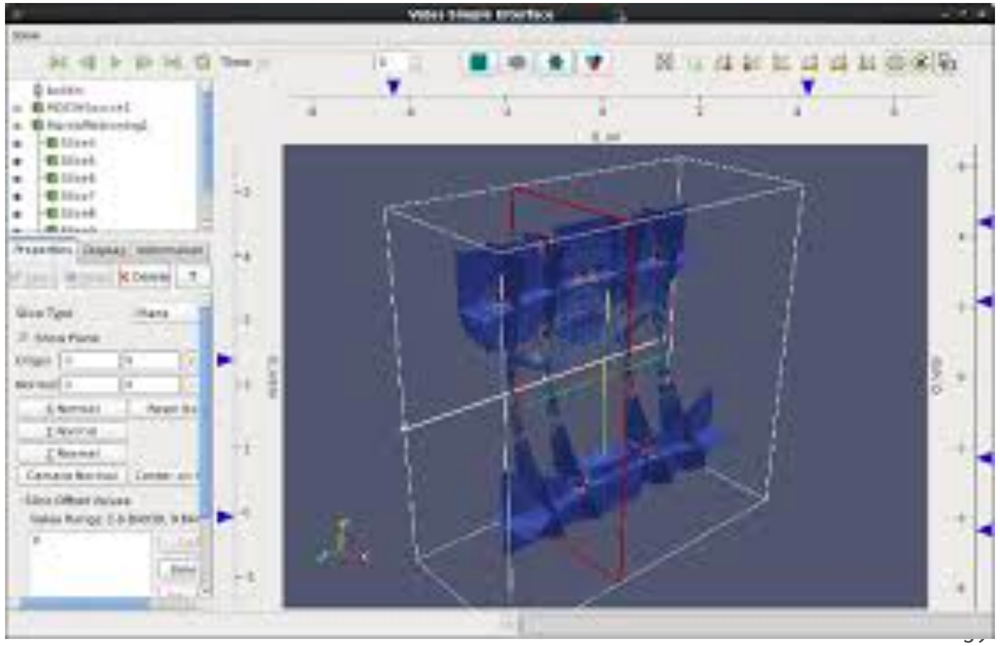
NetworkX GeoPandas Cartopy Iris yt SymPy Panel hvPlot

Visualising Data in Python

1D and 2D



3D



The jupyter EcoSystem

EUROPEAN SPALLATION SOURCE

MENU **nature** International journal of science

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TOOLBOX · 30 OCTOBER 2018

Why Jupyter is data scientists' computational notebook of choice

An improved architecture and enthusiastic user base are driving uptake of the open-source web tool.

- Notebooks capture process, data, and visualisation.
- Great for documenting complex data processing.
- Can be Central or Local
- Easy to use …

jupyter

Project Jupyter exists to develop open-source software, open-standards, and services for interactive computing across dozens of programming languages.

Language of choice

Jupyter supports over 40 programming languages, including Python, R, Julia, and Scala.

Share notebooks

Notebooks can be shared with others using email, Dropbox, GitHub and the Jupyter Notebook Viewer.

Interactive output

Your code can produce rich, interactive output: HTML, images, videos, LaTeX, and custom MIME types.

Jupyter examples for Neutron data.

- Some example jupyter & Python 3 notebooks at
  - https://github.com/Jon-Taylor/raciri-2019.git

- Data Processing with mantid, data visualisation, ipywidgets for UI Holoviews and data shader.
- Atomic simulation environment for calculation of PDoS

In [26]: Slide Type Sub-Slide

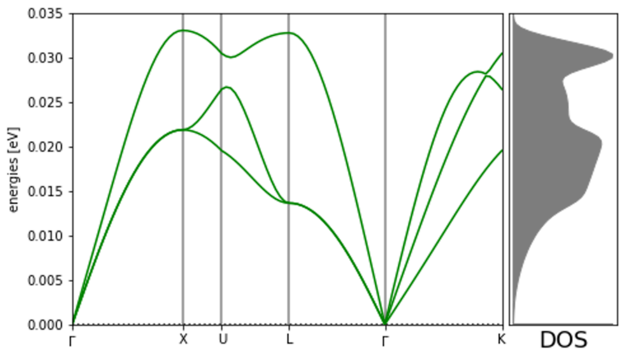
```python
# Plot the band structure and DOS:
%matplotlib inline
import matplotlib.pyplot as plt


fig = plt.figure(1, figsize=(7, 4))
ax = fig.add_axes([.12, .07, .67, .85])

emax = 0.035
bs.plot(ax=ax, show=False, emin=0.0, emax=emax)
aa=bs.todict()
aa.keys
dosax = fig.add_axes([.8, .07, .17, .85])
dosax.fill_between(dos.weights[0], dos.energy, y2=0, color='grey',edgecolor='k', lw=1)

dosax.set_ylim(0, emax)
dosax.set_yticks([])
dosax.set_xticks([])
dosax.set_xlabel("DOS", fontsize=18)
```

Out[26]: Text(0.5, 0, 'DOS')



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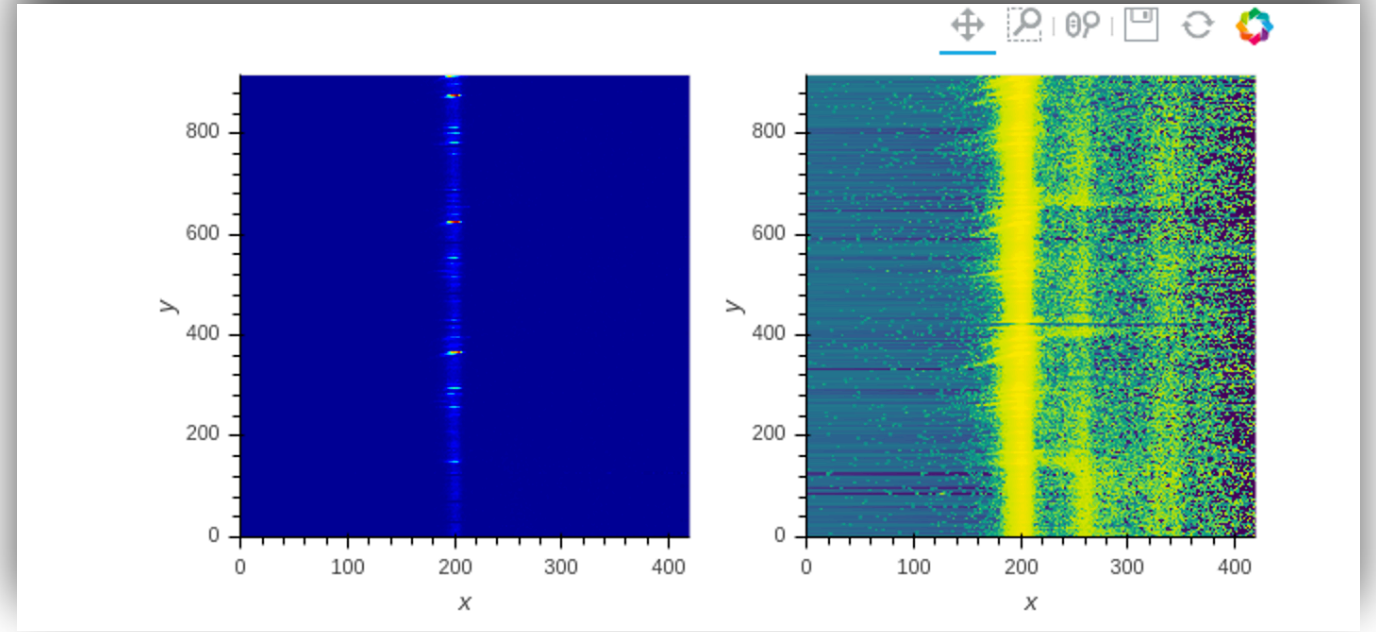

Jupyter examples for Neutron data.

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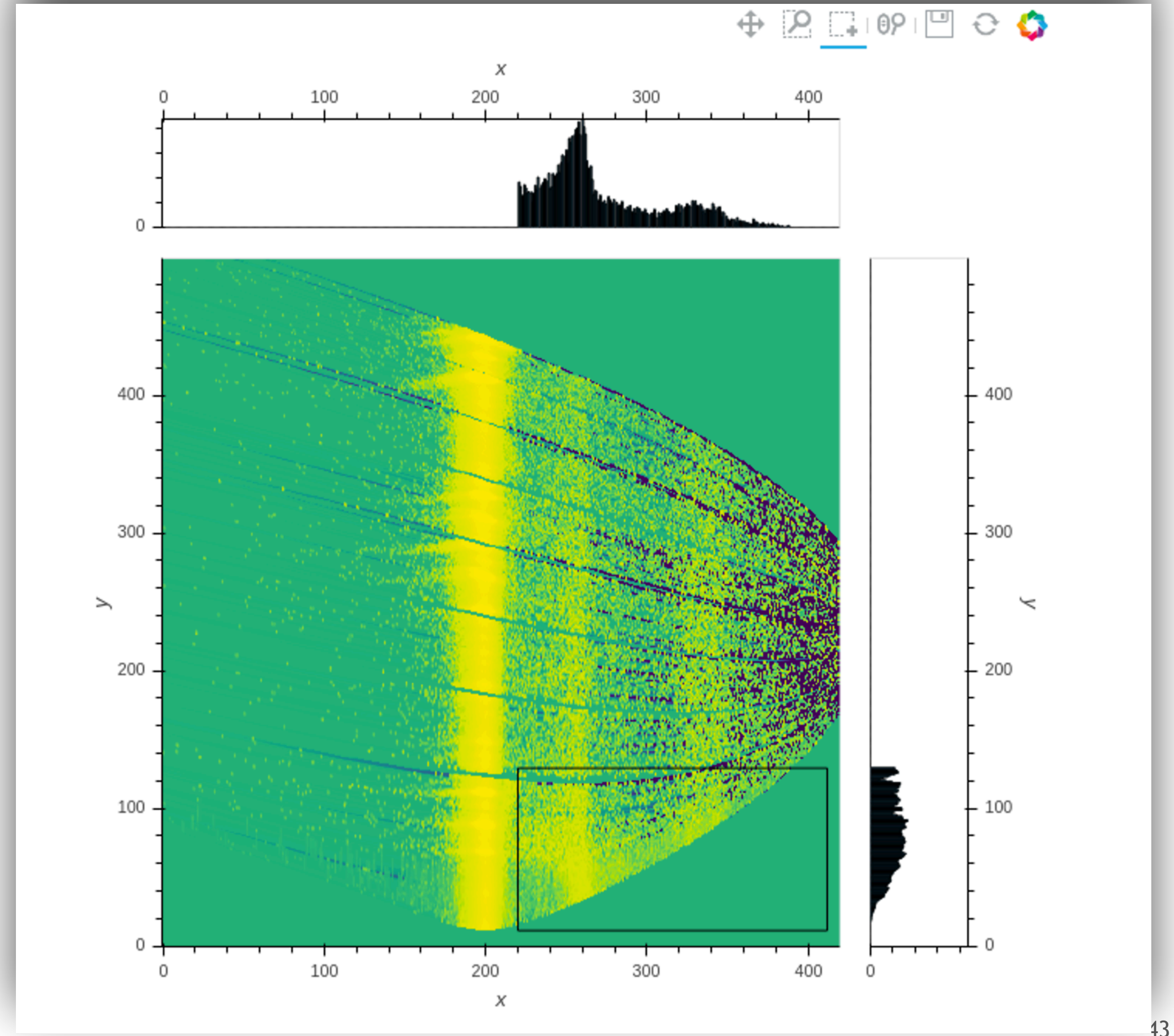
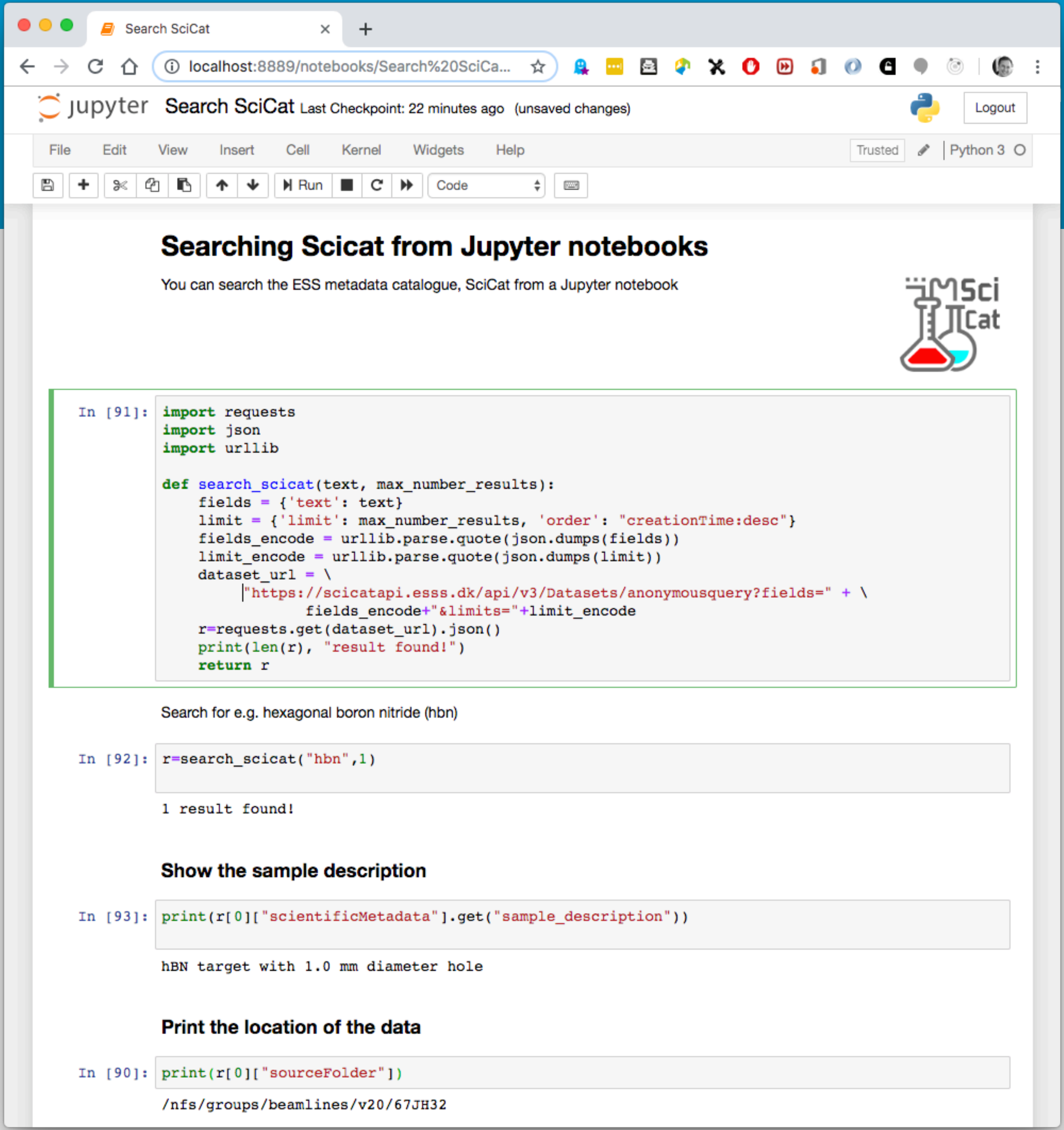


Jupyter & SciCat

- SciCat can be accessed directly from your jupyter notebook!
- You can search for metadata about different experiments at ESS

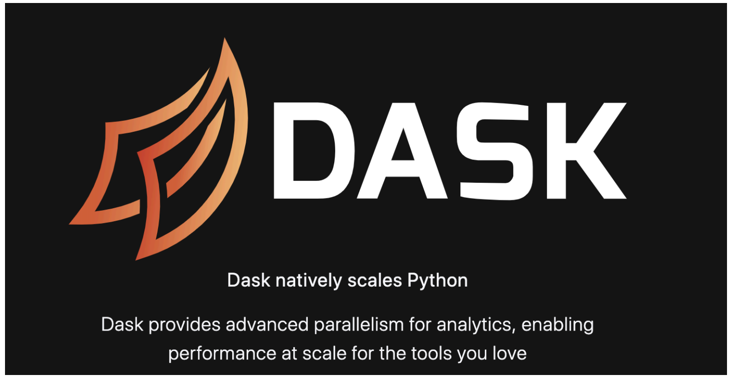


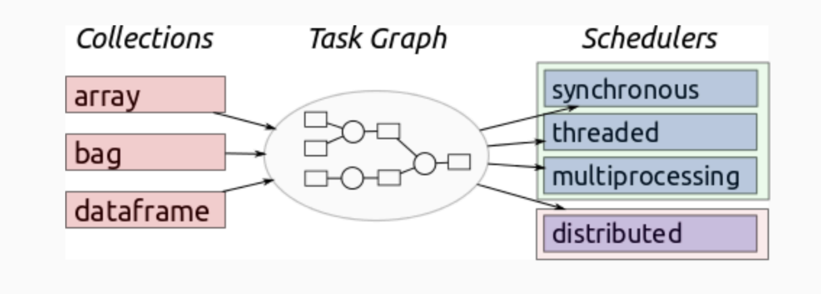
https://git.io/fjSFG

Scaling Python and Machine Learning

EUROPEAN SPALLATION SOURCE

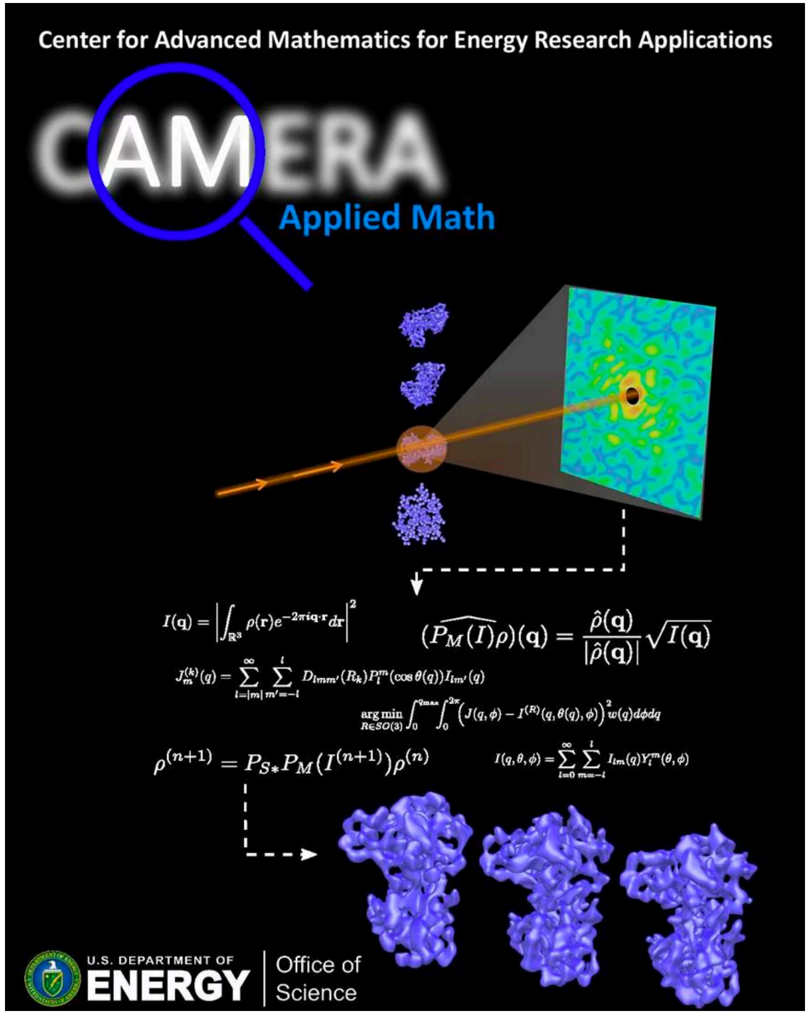
- Some Problems are too large to fit on a single machine.





- Some Problems can be automated with Machine learning.
- https://www.camera.lbl.gov/

TensorFlow

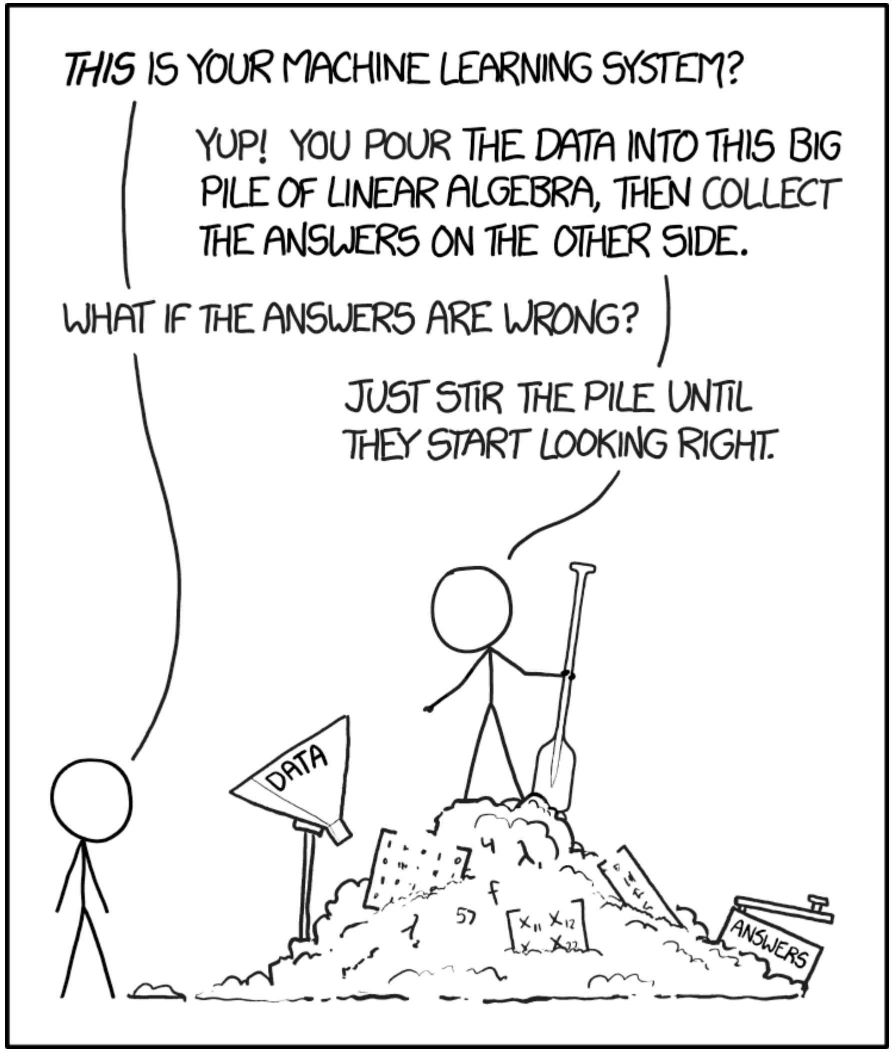


How could Deep Learning and AI be used for scattering experiments.

- A trained neural network can define a likelihood that a requested parameter is true or exists, in an automated workflow.

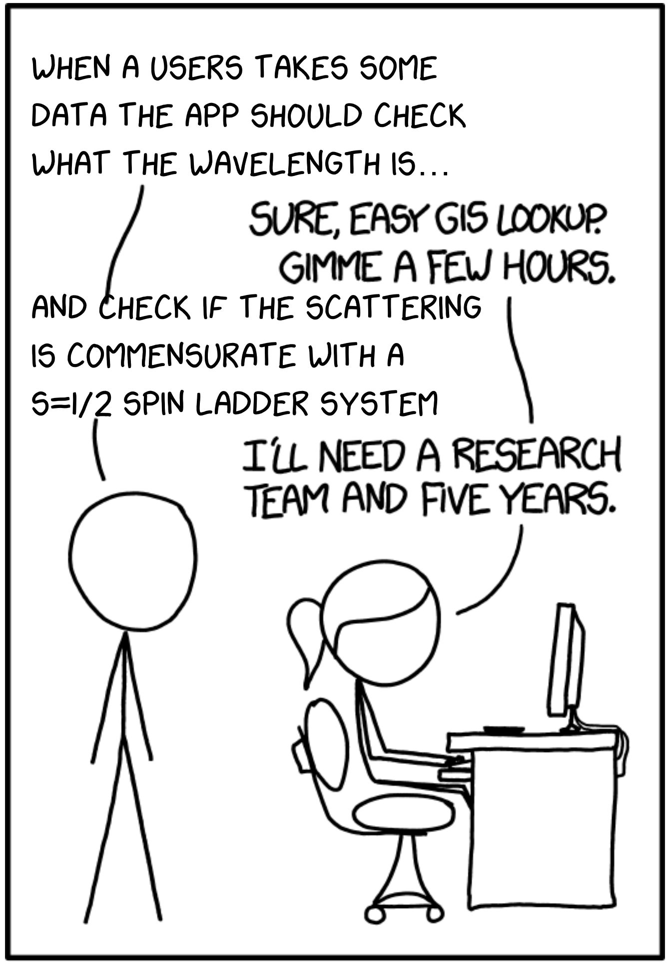
- There could be real benefits for automation and high throughput processing of data.

  - Is the sample well aligned
  - Is the instrument configured for best resolution at …
  - What is the space group point symmetry
  - Is the sample poly disperse
  - What is the value of the exchange interaction
  - and so forth



Machine / Deep learning and AI for Neutron Science

- Deep learning is a fast moving research field.
- There are both technical and ethical challenges for science.
  - Zero Bias is not guaranteed by default



IN CS, IT CAN BE HARD TO EXPLAIN THE DIFFERENCE BETWEEN THE EASY AND THE VIRTUALLY IMPOSSIBLE.

Any questions?

- AI & Deep leaning workshops for neutron & photon scattering
  - Copenhagen September 24 https://indico.nbi.ku.dk/event/1256
  - Grenoble November 12 https://workshops.ill.fr/e/ai2019

Data Reduction, Data Analysis and Modelling.

EUROPEAN SPALLATION SOURCE

Mantid @ ESS

- volumetric slicing (see figure)
- support for novel detector geometries (Band-Gem).
- support for NeXus Geometry

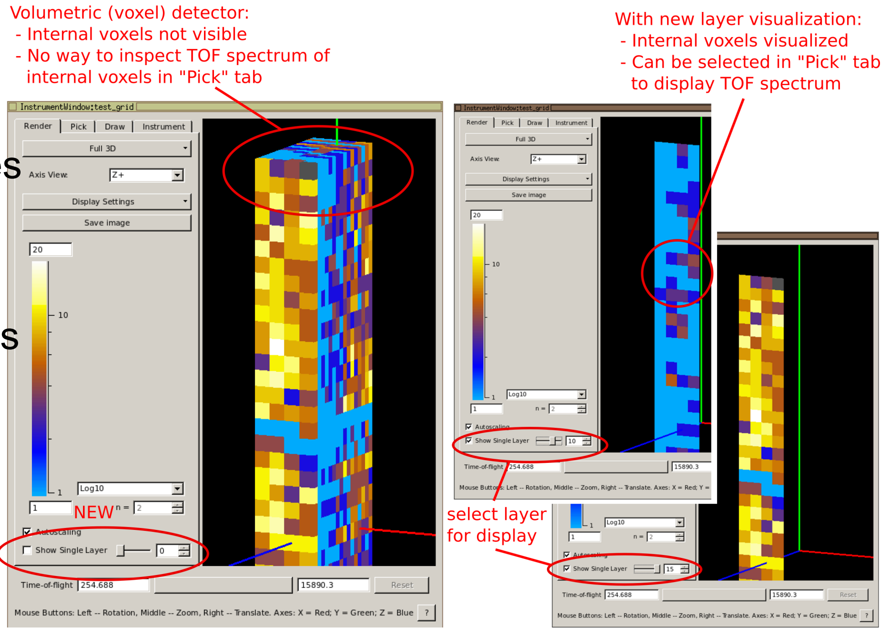
→ significant speed-up for instruments with many pixels

- speed-ups from Instrument-2.0

Facilities involved

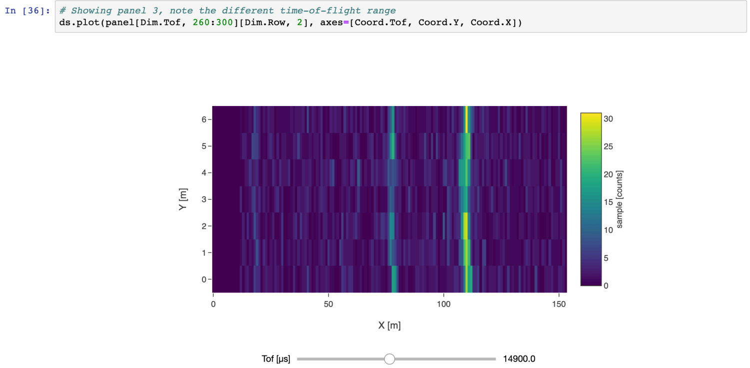
EUROPEAN SPALLATION SOURCE

Science & Technology Facilities Council ISIS



http://www.mantidproject.org

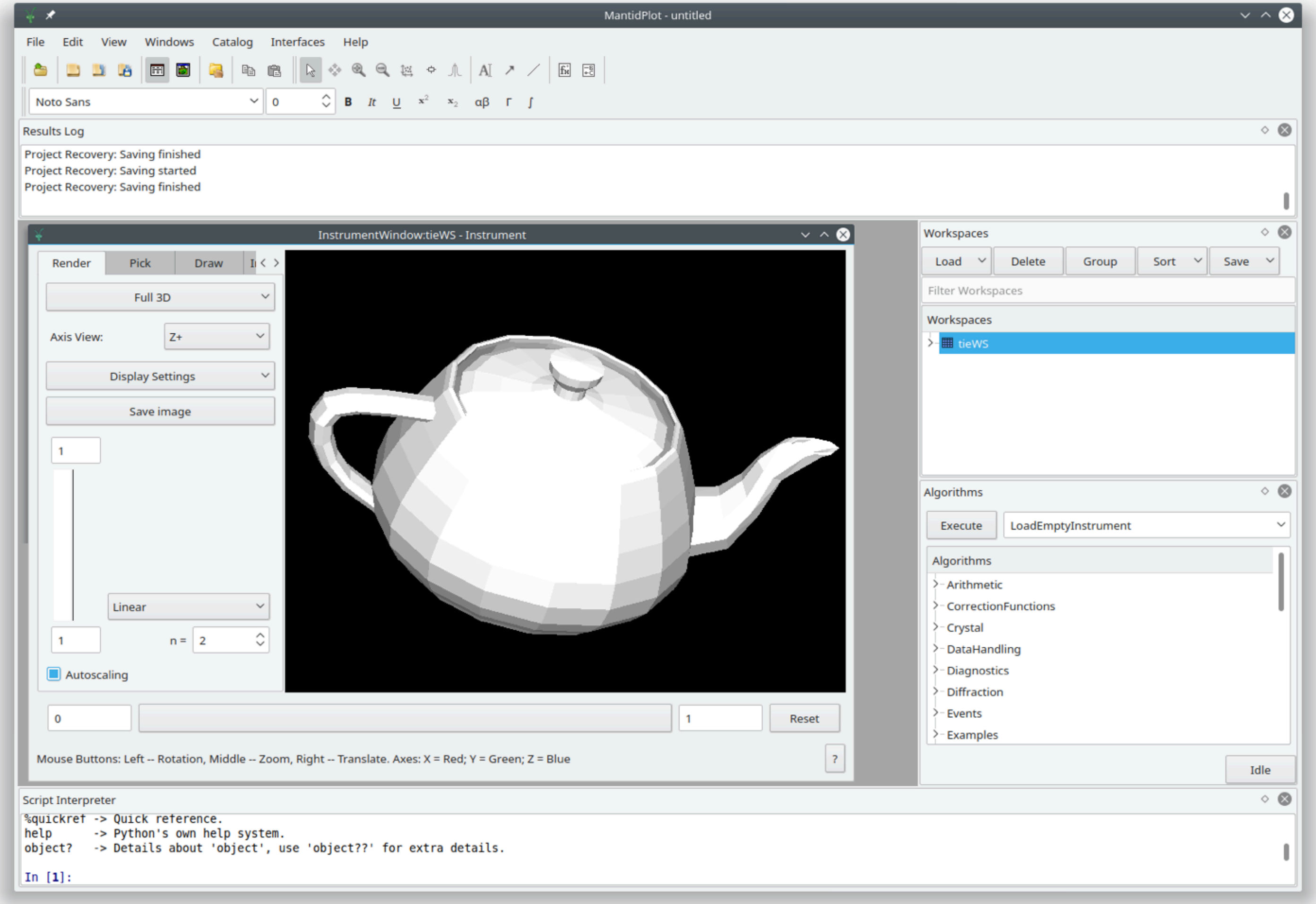
- X Array for Neutron Scattering data
- Jupiter & Python (PaNOSC)
- Multi Dimensional Data structure.
- Units
- Errors
- Geometry



Flexible Instrument Geometry

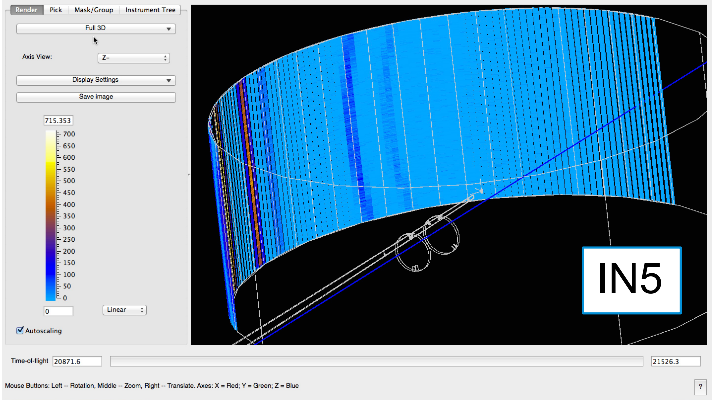
NeXus

NeXus is developed as an international standard by scientists and programmers representing major scientific facilities in Europe, Asia, Australia, and North America in order to facilitate greater cooperation in the analysis and visualization of neutron, x-ray, and muon data.

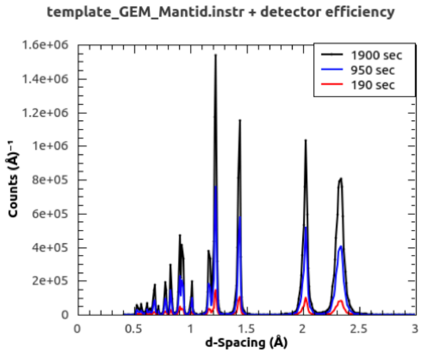


Data Reduction, Data Analysis and Modelling.

McStas



IN5

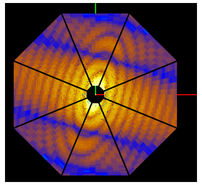


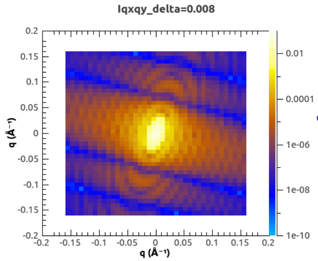
McStas → MANTID

- virtual experiment of ESS instruments
  moderator → detector
- models of samples
- instrument model repository

→ preparation for reduction & analysis

LoKI

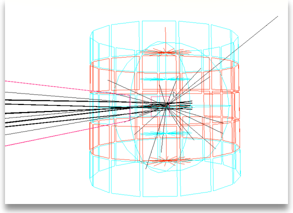




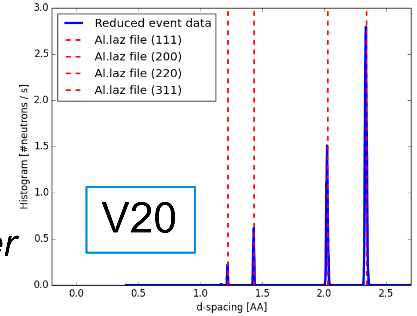
← SasView 2D scattering kernel

← MANTID instrument view

- MANTID reduced McStas event data



Single crystal diffractometer with cylindrical detector geometry



V20

http://www.mcstas.org/

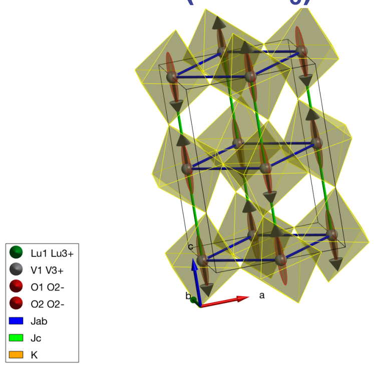
EUROPEAN SPALLATION SOURCE NEUTRONS FOR SOCIETY DTU

Data Reduction, Data Analysis and Modelling.

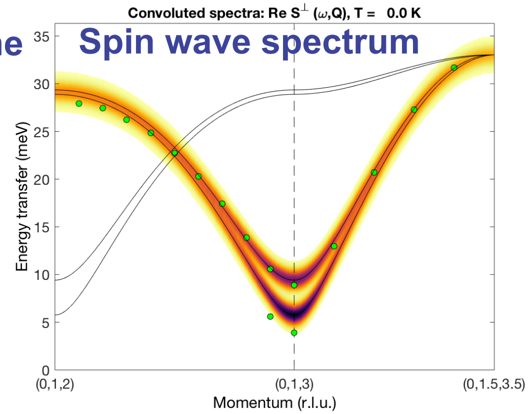
SpinW

modularizing with C++ core and Python interface.

Magnetic and crystalline structures ($LuVO_3$)



Spin wave spectrum



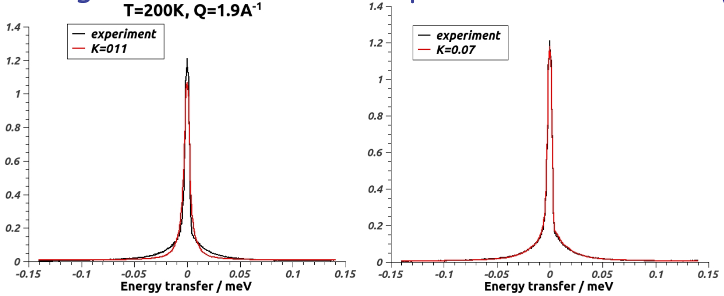
https://www.psi.ch/spinw

Fitting QENS data

fitting potential to QENS data ➜ dynamical version of EPSR method

Original force-field

Optimized force-field



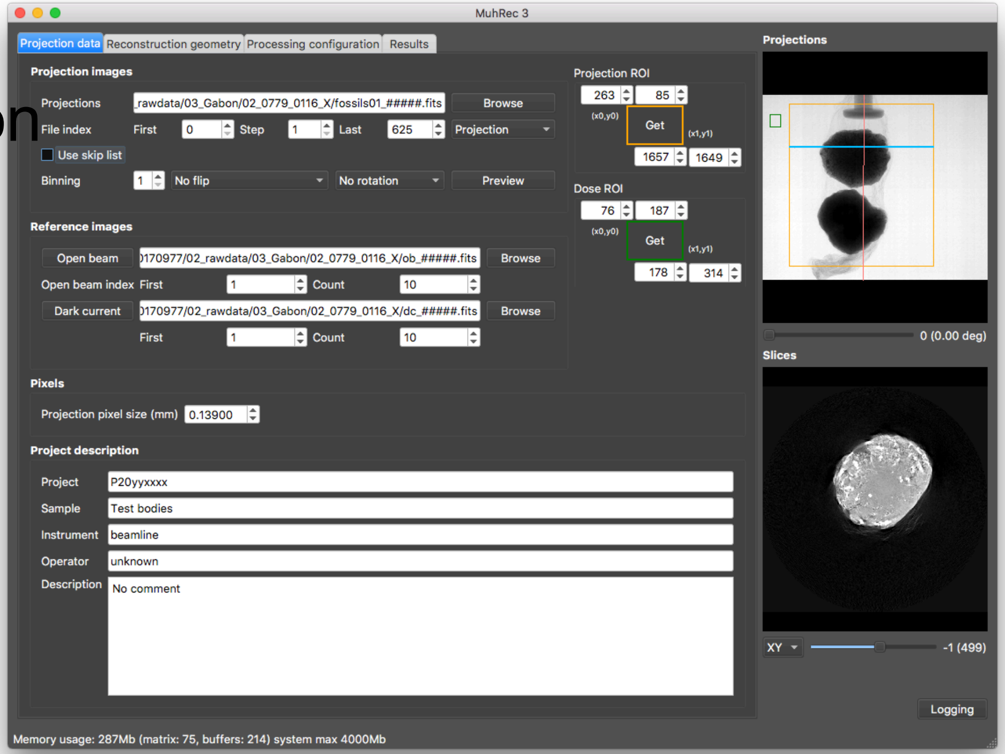
methyl rotations in methyl-Polyhedral oligomeric silsesquioxanes

M. Hagen, J. Borreguero (SNS/NDAV), M. Crawford (Dupont), N. Jalarvo (Jülich)

Data Reduction, Data Analysis and Modelling.

MuhRec imaging

- support for cone beam reconstruction
  - algorithm to correct biases due to background scattering
    - more pre-processing opti
      - revised user interface
      - stability improvements
    - support for NeXus file formats



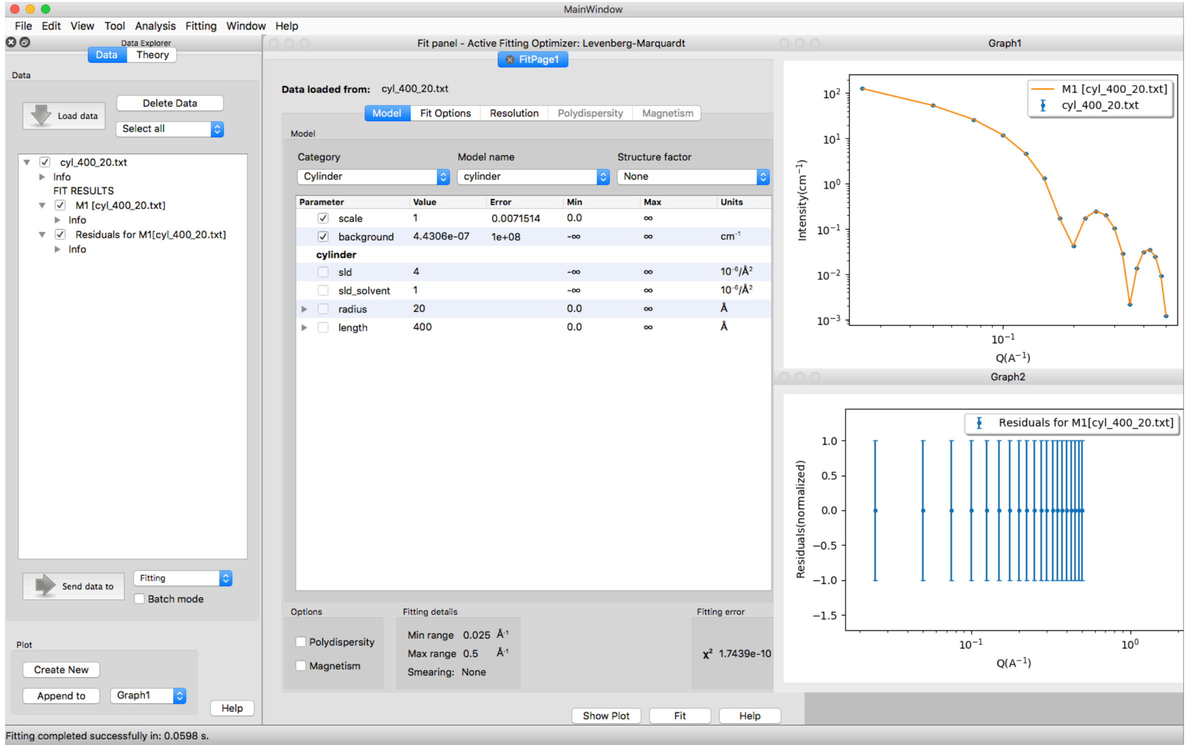
https://github.com/neutronimaging/imagingsuite/wiki/User-manual-MuhRec

Data Reduction, Data Analysis and Modelling.

EUROPEAN SPALLATION SOURCE

SasView SANS

- code modularization
- GUI re-design (Qt5)
- code optimization for faster analysis methods using GPUs
- incorporation of model functions from SasFit*
- Sasmodels marketplace



* https://kur.web.psi.ch/sans1/SANSSoft/sasfit.html

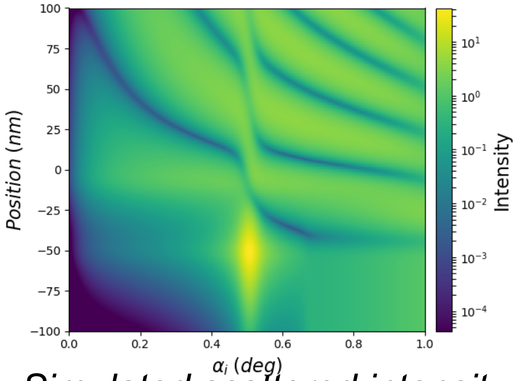
http://www.sasview.org

Data Reduction, Data Analysis and Modelling.

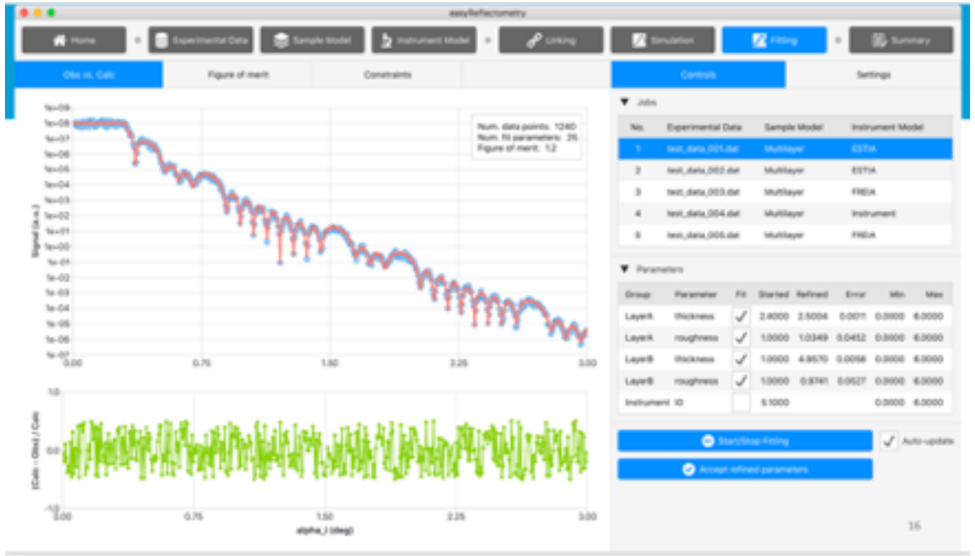
EUROPEAN SPALLATION SOURCE

BornAgain reflectometry

- basic functionality for reflectometry simulations
- simulation functionality → GUI
- usability check on experimental data
- depth probe simulation for experimental setup (see figure)



Simulated scattered intensity from Ti/Pt resonator with beam divergence



SINE 2020

JÜLICH FORSCHUNGSZENTRUM

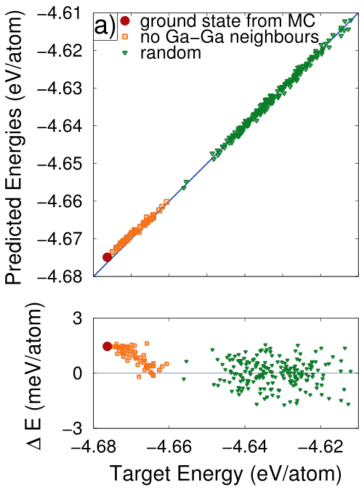
Data Reduction, Data Analysis and Modelling.

EUROPEAN SPALLATION SOURCE

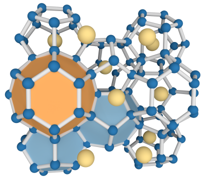
Icet

diffraction

- simulating ordering and segregation in multi-component systems
- DFT calculation
- construction and sampling of cluster expansions



Ångqvist & Erhart, Chem. Mat.



$Ba_8Ga_{16}Ge_{30}$

CHALMERS

Interreg Öresund-Kattegat-Skagerrak European Regional Development Fund

EUROPEAN UNION

EUROPEAN SPALLATION SOURCE

ESS & MAX IV: Cross Border Science and Society

https://www.materialsmodeling.org/

- Collaborative development of the FullProf Suite with ILL

User experience.

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- Sustainable software development for Neutron Scattering data analysis.
- Enable the community with easy to use feature rich software