



**EUROPEAN  
SPALLATION  
SOURCE**



# Proposals, DMPs and FAIR

@ESS

PRESENTED BY CARINA LOBLEY & FREDRIK BOLMSTEN

2023-08-31

# Agenda



- 1 Proposals
- 2 Proposal do's and don'ts
- 3 Data Policy
- 4 Data Management Plans

# Proposals



Sign in

Email

carina.lobley@ess.eu

Password

\*\*\*\*\*

SIGN IN

[Forgot password?](#)

[Don't have an account? Sign Up](#)

or

iD | SIGN IN WITH ORCID



# Obtaining Access to ESS

## Who might be an ESS user?

Five access routes are specified:

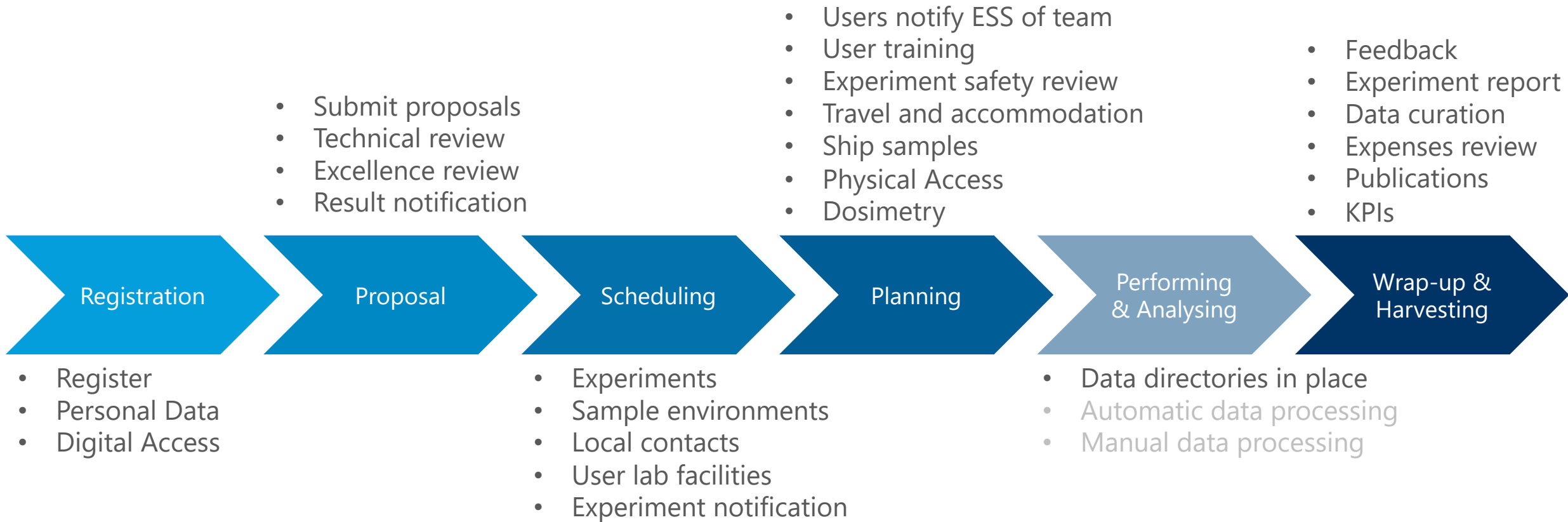
- 1) Peer Reviewed Access
- 2) Quick Access
- 3) Discretionary Access
- 4) Proprietary Access
- 5) Alternative Access Routes

Access routes 1, 2, 3 & 5 are free at the point of use and represent the majority of users. Proposals are selected on the basis of excellence.

Proprietary access will be via a negotiated contract for each user

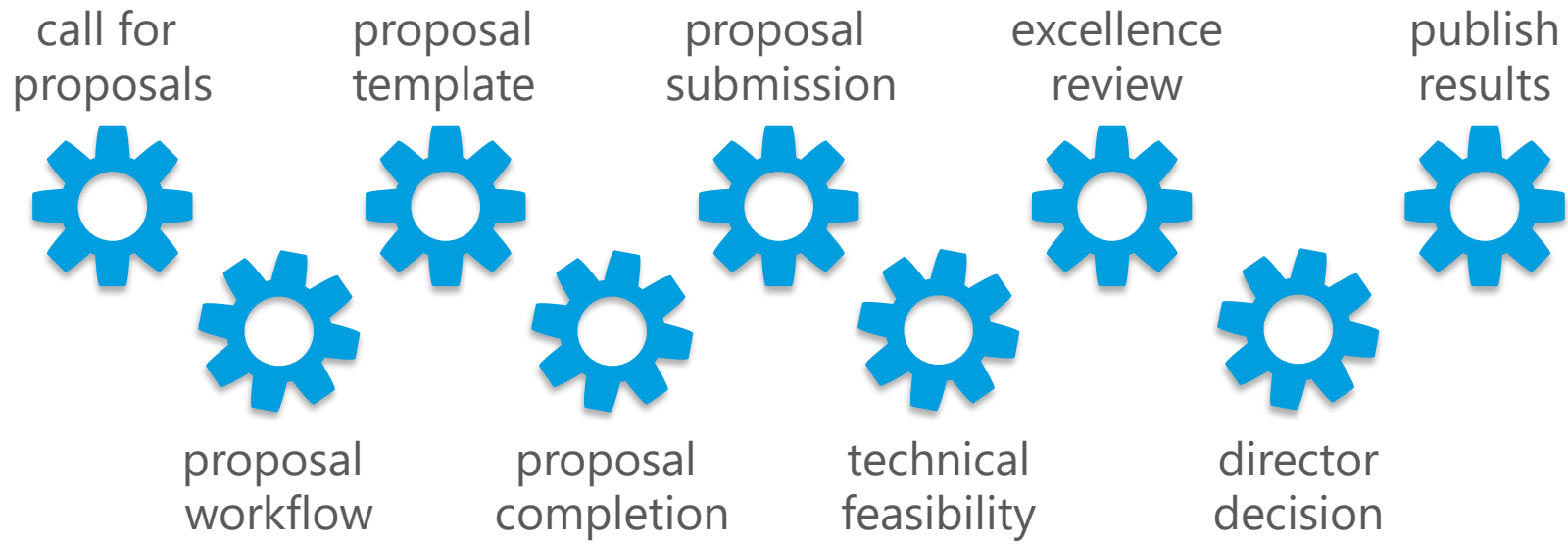


# The User Journey





# Proposal Submission and Review



The software for this process are fully developed and are in operation on a small scale at ESS. We have a collaboration and this software is in use at ISIS and CLF in the UK.



# Draft/Submission

## Proposal Topics

- General
- Support
- Instruments
- Sample & Sample Environment
- Other Facilities
- Proposal Text

### New Proposal

1 General — 2 Support — 3 Instruments — 4 Sample & SE Equipment — 5 Other facilities — 6 Proposal text — 7 Review


Title \*

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Abstract \*


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Principal Investigator \*

Fredrik Bolmsten; European Spallation Source ERIC (ESS) 

Co-Proposers

Actions	Firstname	Lastname	Preferred name	Organisation
No Users				

 ADD



# Technical Review

Is it possible and safe to carry out the experiment

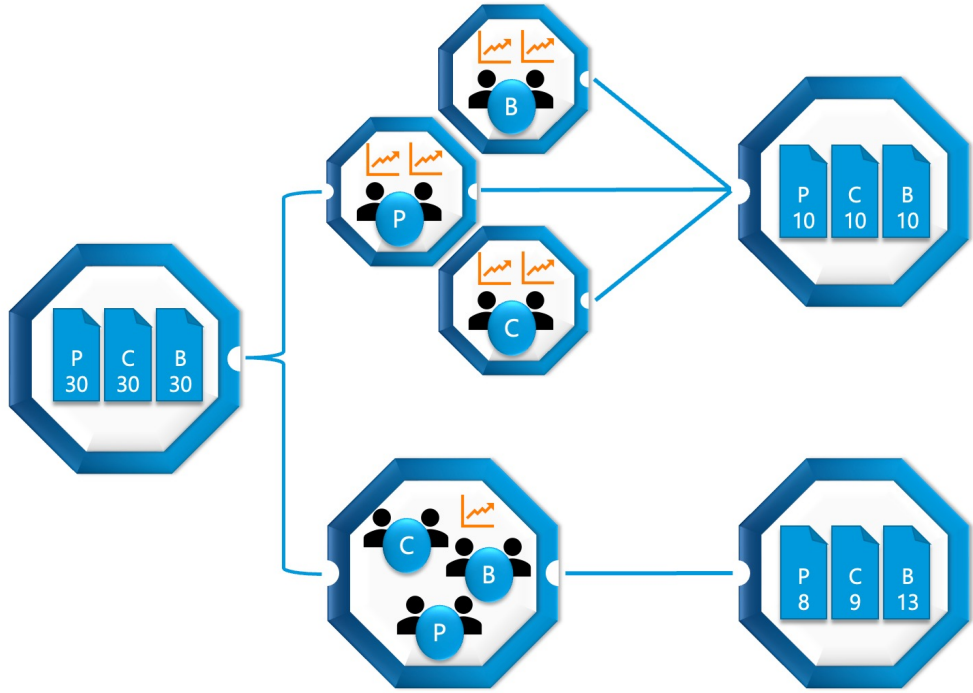
- Investigate the feasibility of the proposed experiment
- An unfeasible technical review does not necessarily mean no scientific merit
- Give an estimate for days required
- Check with safety regarding concerns
- Give general comment to reviewers



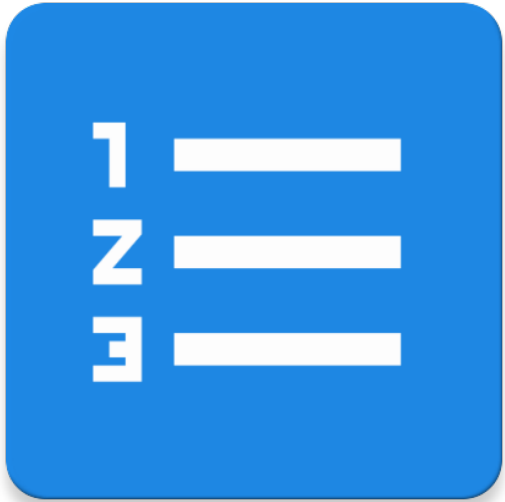
# Excellence Review

## Scientific Evaluation and Access Policy

- Judge scientific excellence
  - Grade
  - Comment
  - Control feasibility
  - Check previous work



- Meeting:
  - Rank proposals
  - Time allocate



# Proposal do's and don'ts



# Preparing a Winning Proposal

## Scientific Evaluation and Access Policy

### Practical tips:

- 1) start early
- 2) always talk to the instrument scientist(s) for the latest updates and advice
- 3) check all the questions you need to answer and carefully review that they are suitably addressed
- 4) ask the user office for help if using the software is presenting challenges – as far ahead of time as you can
- 5) do not miss the deadline for submission

### Writing tips:

- 1) write for a well educated, scientifically interested audience
- 2) use grammatical, uncomplicated language (usually English) to be easily read and understood
- 3) comply with length guidelines and number of figures
- 4) be precise about the sample(s) and experiment(s) you plan
- 5) explain why the science requires the tools you are asking for and why it needs to be done now very clearly



# Adding value to a proposal

## Scientific Evaluation and Access Policy

Always remember:

1. Make the impact of the research clear – you can't afford wasted words
2. Clearly state the need for the instrument you request
3. Indicate what other research will complement this experiment
4. Demonstrate the prior art that your team has which will make this successful
5. Explain why now is the time for this work
6. Let the reviewer know if the sample is ready to go – if it isn't clearly explain how it will be ready in time and any mitigation for problems
7. The peer reviewers have a collective memory – they will know if they rejected this proposal before so be clear what has changed in the new approach
8. Express your motivation – why does this work give you joy? In a bundle of proposals in the same format, it's amazing how enthusiasm stands out

# Data Policy





# ESS Data Policy

## Main elements

- ESS is the custodian of raw data and metadata from all instruments
- ESS will automatically collect metadata for all experiments
- ESS will store metadata in a metadata catalogue
- High level metadata will be published as soon as possible, i.e. Title, Authors, Beamline, Abstract
- Experimental team has sole access to the data during the so-called embargo period of 3 years; request to extend embargo period can be made
- After embargo ESS will make the data "Open Access"
- Proprietary i.e. commercial data belong by default to the PI and are not archived unless explicitly agreed



# ESS Data Policy

## Questions

- Analysis
  - Access to the results of analysis performed on raw data and metadata is restricted to the person or persons performing the analysis, unless otherwise requested by those persons. If the raw data being analysed is still restricted, access to the analysis results must be granted by the PT.
- Long term storage
  - If ESS decides to stop acting as a custodian of some scientific research data after 10 years, ESS will inform the PIs concerned in a timely manner allowing them to make a copy of the scientific research data that was generated by their proposal(s), provided ESS is aware of the e-mail address of the PI.



# Data Management Plans

## 3 Who is allowed to access the dataset?

Horizon 2020 DMP

e.g. project members, partners of the project, only in-house, external partners

Desirable: *Before Submitting the DMP*

Experiment team for 3 years and then open access

Answered in less than 5 seconds by Albert Einstein.

## 4 Is this dataset interoperable, i.e. allowing data exchange with other institutions, organisations, countries etc.?

Horizon 2020 DMP

Datasets is following the NeXus standard for NMX

Answered in less than 5 seconds by Albert Einstein.

## 5 Will this dataset be published or shared?

Horizon 2020 DMP

a. Yes, internally with everyone, as long as they don't pass on the d



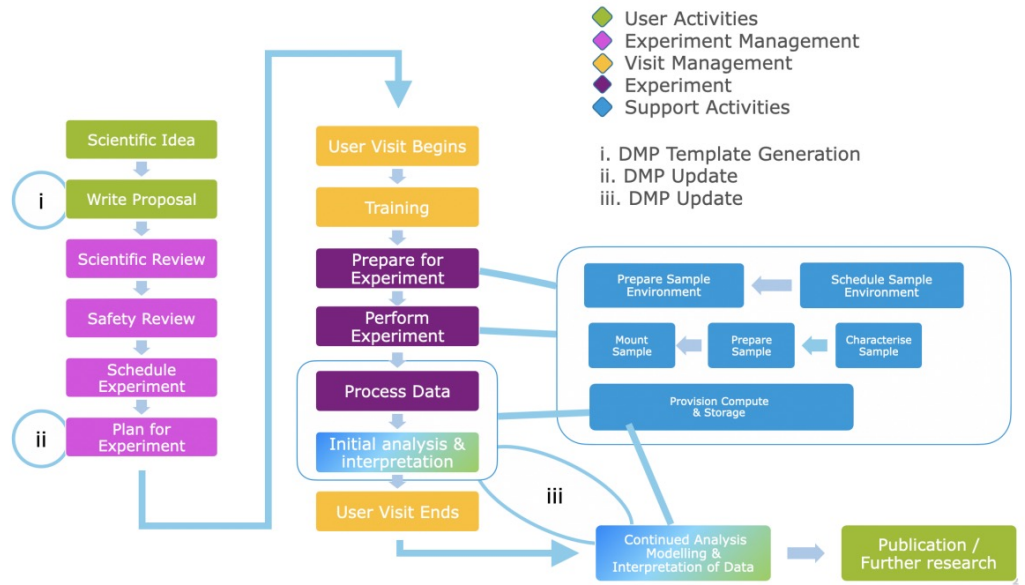
# Overview

## Theory

A data management plan, or DMP, is **a document where information about the data management in a research project is collected**. The plan covers all phases of the project, from planning and collection, production or generation of data, to analysis, publication, and archiving.

## Purpose

A communication channel between the facility and the user to understand the needs that will arise from the data collected at experiment time and analysis.



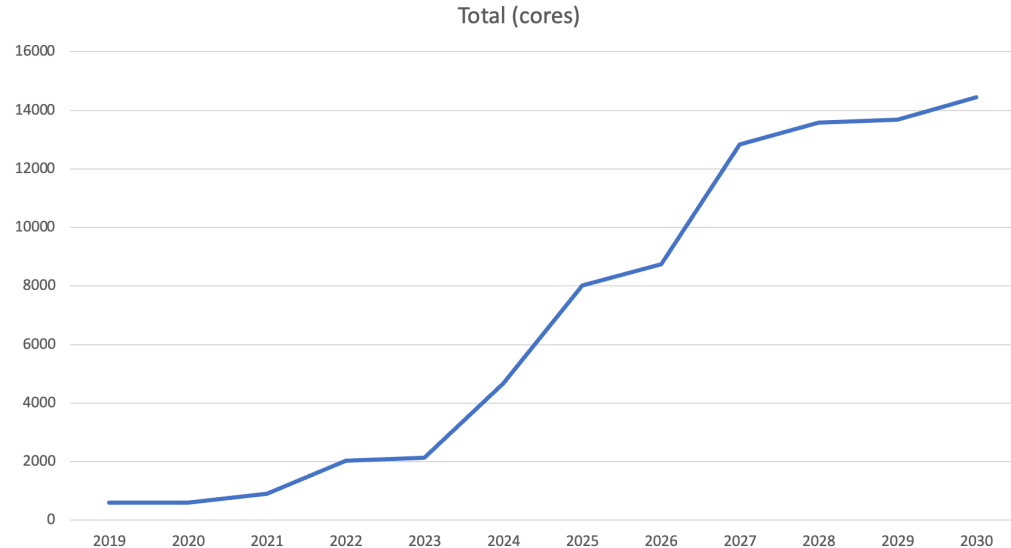
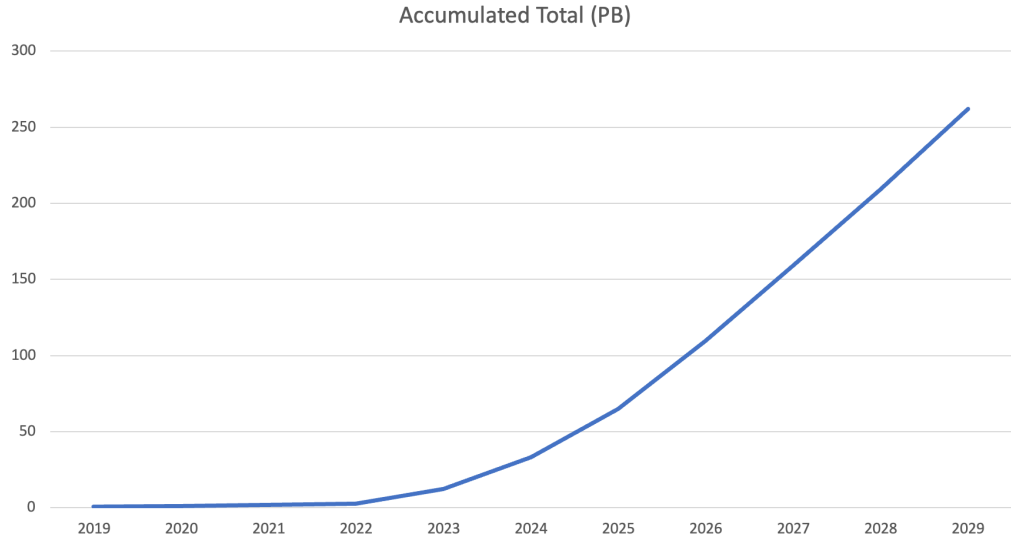


# Storage & Processing

## Handling the data

The increasing data rates caused by next generation detectors is making data handling a key issue for facilities as users are less capable of handling storage and processing themselves.

These storage and processing requirements has made data management plans a requisite for users and the facility to understand the needs that will arise from the experiment.





# Questions

## PaNOSC & Horizon 2020

- Which file formats are used?
- Which tools, software, technologies or processes are used to generate or collect the data?
- Which software, processes or technologies are necessary to use the data?
- Are different versions of the dataset created?
- Which versioning strategy is applied for this dataset?
- Which technology or tool is used for versioning?
- To what extent will infrastructure resources be required (e.g. CPU hours, bandwidth, storage space... etc.).
- Where is the dataset stored during the project?
- Under which URL can the dataset be accessed during the project?
- Are there internal project guidelines for a consistent organisation of the data? If so, where they are documented?
- ...

# Data Curation



## General Information

<b>Name</b>	Last Neutrons Ever at HZB.
<b>Description</b>	V20 data
<b>PID</b>	20.500.12269/2511nicos_00002511.hdf
<b>Type</b>	raw
<b>Creation Time</b>	2019-12-11 13:48
<b>Keywords</b>	<span>v20</span> <span>neutron</span>



## Creator Information

<b>Owner</b>	Peter Kadletz
<b>Principal Investigator</b>	Tobias Richter
<b>Orcid</b>	default
<b>Contact Email</b>	<a href="mailto:Tobias.Richter@esss.se">Tobias.Richter@esss.se</a>
<b>Owner Group</b>	ess
<b>Access Groups</b>	ess,brightness



## File Information

<b>Source Folder</b>	/nfs/groups/beamlines/v20/YC7SZ5
<b>Size</b>	203 MB
<b>Data Format</b>	NeXus HDF5

# What is data curation?

Data curation - organizing, integrating data and metadata, presenting and publishing, preserving and archiving



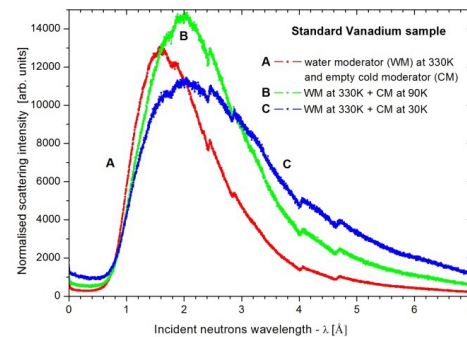
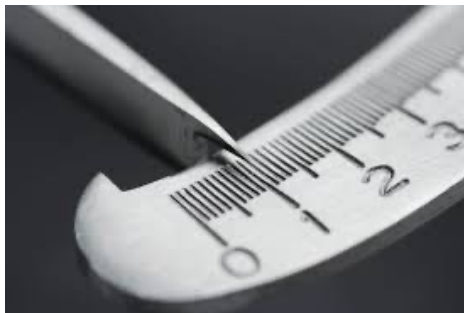
# Raw, reduced and derived data

Raw data - unprocessed data at full resolution, with communications artifacts removed (e.g. frame headers)

Reduced - transformed and corrected from instrument units to physical units,

Derived data - images, plots, statistics

How to manage all this data?

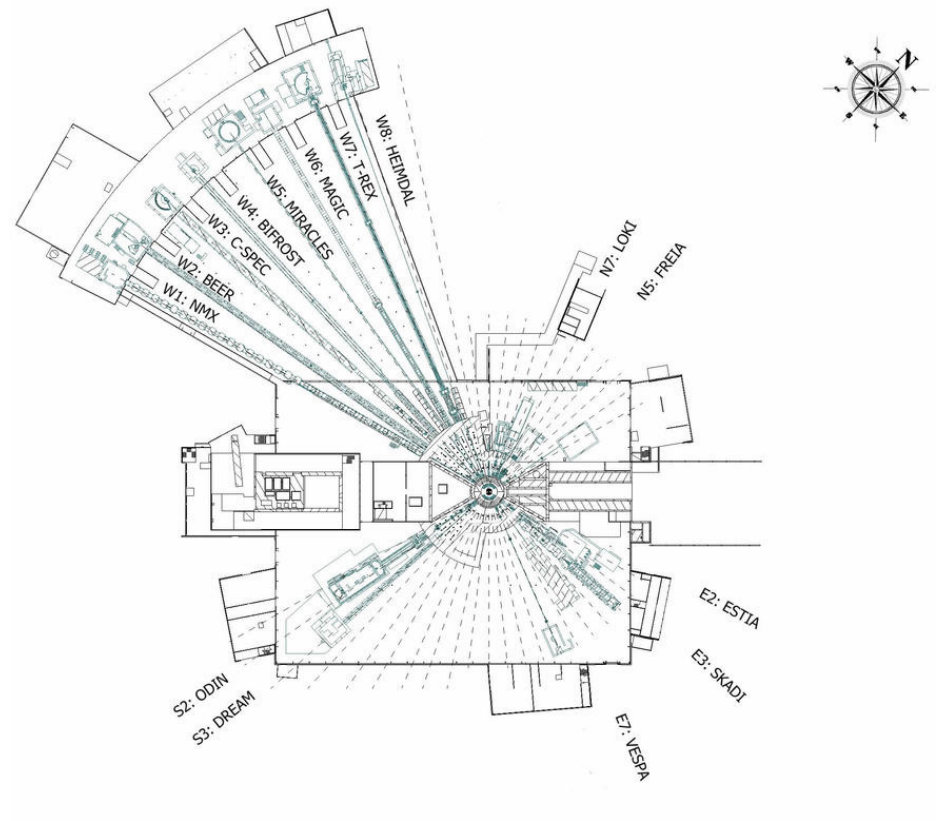


# Data @ ESS

Imaging, spectroscopy, diffraction  
Each instrument has different data requirements

Traditionally, communities have had different data types, formats, analysis and reduction methods, standards - problem for data management

By standardizing across instruments, we can make this process simpler and quicker



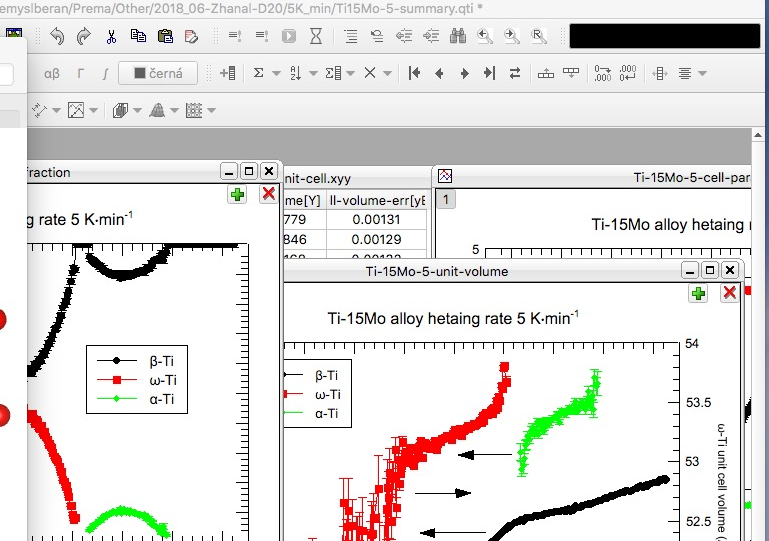
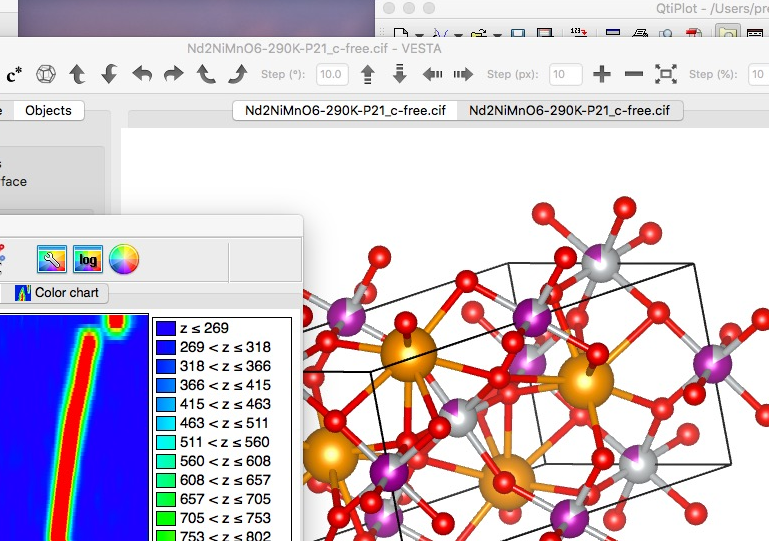
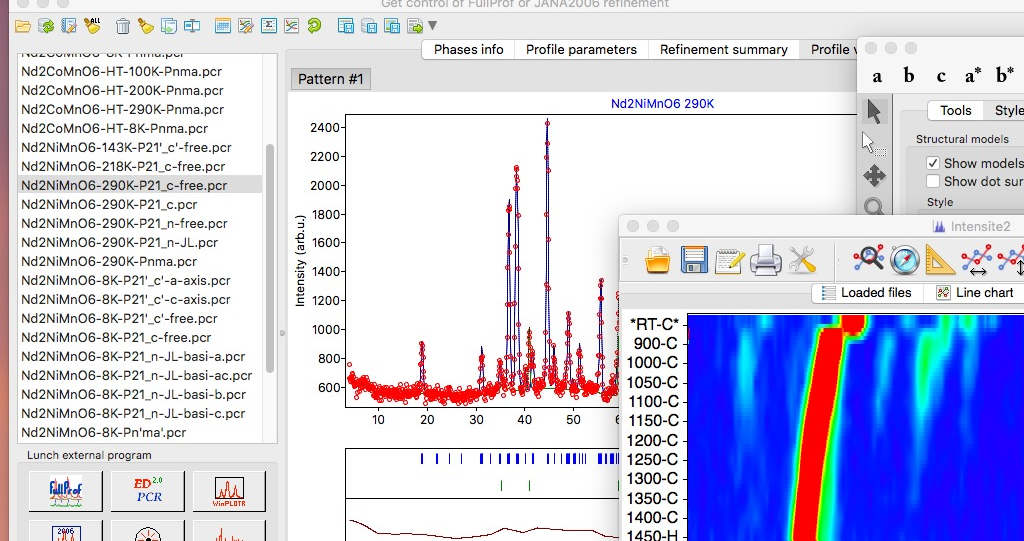


# Scientific metadata

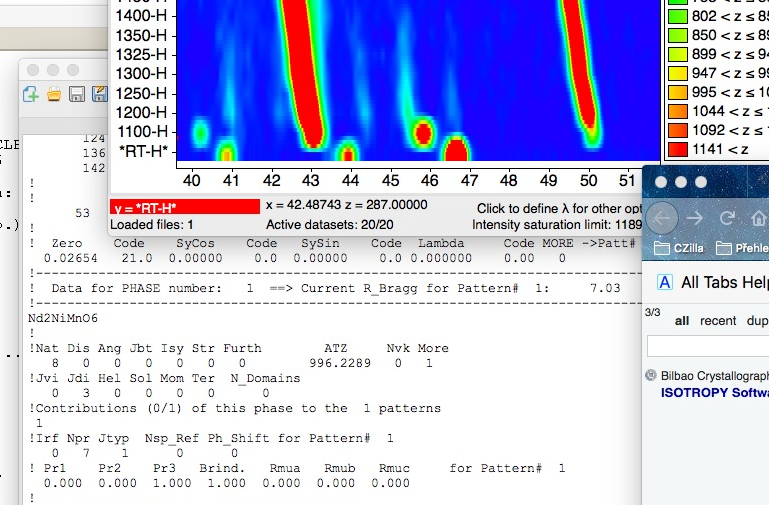
"... is often notoriously incomplete. Additional quantities and assumptions necessary to interpret the data may initially only be recorded on scraps of paper, hard-coded into analysis software or only exist in the experimenter's head"

Clive Davenhall - Digital Curation Centre





```
FullProf Program
Load Edit PCR Mode Run Exit
=> RP-factor : 5.458
=> Phase: 2
=> Bragg R-factor: 7.004
=> RP-factor : 3.442
=> Convergence reached at this CYCLE !!!!: CYCLE 124
=> R-Factors: 3.49 Chi2: 1.36
=> Expected : 3.76
=> Conventional Rietveld R-factors for Pattern:
=> Rp: 23.5 Rwp: 19.6 Rexp: 16.80
=> Global user-weighted Chi2 (Bragg contrib.)
=> -----> Pattern# 1
=> Phase: 1
=> Bragg R-factor: 7.028
=> RP-factor : 5.458
=> Phase: 2
=> Bragg R-factor: 7.004
=> RP-factor : 3.442
=> Normal end, final calculations and writing...
=> Contribution to Yi for phase: 1
=> Contribution to Yi for phase: 2
=> CPU Time: 0.906 seconds
=> 0.015 minutes
=> END Date:05/11/2018 Time => 15:47:39.297
```



Bilbao Crystallographic Server

ISOTROPY Software Suite

iso.byu.edu/iso/isotrop

### ISOTROPY Software Suite

Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA, stokes@byu.edu

**Description:** The ISOTROPY software suite is a collection of software which applies group theoretical methods to the analysis of phase transitions in crystalline solids.

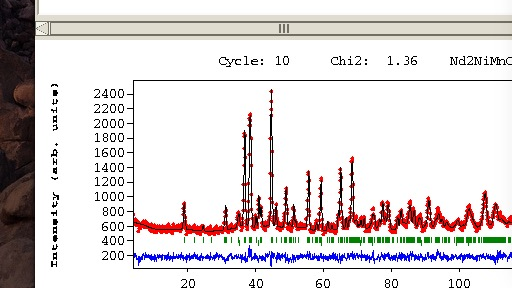
**How to cite:** ISOTROPY Software Suite, iso.byu.edu.

#### References and Resources

- ISODISTORT:** Explore and visualize distortions of crystalline structures. Possible distortions include atomic displacements, atomic ordering, strain, and magnetic moments.
- ISOSUBGROUP:** Interactive program using user-friendly interface to list isotropy subgroups.
- ISOTROPY:** Interactive program using command lines to explore isotropy subgroups and their associated distortions.
- SMODES:** Find the displacement modes in a crystal which brings the dynamical matrix to block-diagonal form, with the smallest possible blocks.
- FROZSL:** Calculate phonon frequencies and displacement modes using the method of frozen phonons.

#### Space groups and irreducible representations

- ISOCIF:** Create or modify CIF files.
- FINDSYM:** Identify the space group of a crystal, given the positions of the atoms in a unit cell.
- ISO-IR:** Tables of Irreducible Representations. The 2011 version of IR matrices.



```
!Nat Dis Ang Jbt Isy Str Furth ATZ Nvk More
8 0 0 0 0 0 0 0 996.2289 0 1
!Jvi Jdi Hel Sol Mom Ter N_Domains
0 3 0 0 0 0 0 0
!Contributions (0/1) of this phase to the 1 patterns
1
!Irf Npr Jtj Nsp_Ref Ph_Shift for Pattern# 1
0 7 1 0 0 0
!Pr1 Pr2 Pr3 Brind. Rmua Rmub Rmuc for Pattern# 1
0.000 0.000 1.000 1.000 0.000 0.000 0.000
!Max dst(dist) (angles) Bond-Valence Calc.
3.3000 2.2000 BVS
!N_cations N_anions Tolerance(%) / Name or cations/ and Anions
5 1 1.000 0.00
ND+3 NI+3 NI+2 MN+3 MN+4
O-2
!
P 21/c <--Space group symbol
!Atom Typ X Y Z Biso Occ In Fin N_t Spc /C
Nd_1 ND 0.24357 0.04759 0.25300 0.77093 1.00000 0 0 0 1
Ni_1 NI 120.20 110.20 520.20 470.20 0.00 0 0 0 3
Mn_1 MN 0.50000 0.00000 0.00000 1.28838 0.40857 0 0 0 4
Ln_2 LT 0.00000 0.00000 0.50000 1.28838 -160.20 0.09143 0 0 0 2
```

Ext	Size	Date	
<DIR>		09/03/201	
ST-1000-C	75.6 K	08/03/201	
ST-1000-C	34.4 K	19/03/201	
ST-1000-C	15.3 K	19/03/201	
ST-1000-C	194.3 K	08/03/201	
ST-1000-C	15.4 K	08/03/201	
ST-1000-C	104.4 K	08/03/201	
ST-1000-C	24.6 K	08/03/201	
ST-1000-C	373	16/03/201	
ST-1000-C	373	08/03/201	
ST-1000-C1	609	08/03/201	
ST-1000-C1	mic	7.5 K	08/03/201
ST-1000-C1	sub	46.0 K	08/03/201
ST-1000-C2	fst	609	08/03/201
ST-1000-C2	mic	5.7 K	08/03/201
ST-1000-C2	sub	46.0 K	08/03/201
ST-1000-C3	fst	609	08/03/201
ST-1000-C3	mic	5.7 K	08/03/201
ST-1000-C3	sub	46.0 K	08/03/201
ST-1000-C4	fst	909	08/03/201

files: 0 of 553, folders: 0 of 0

# How to capture metadata?

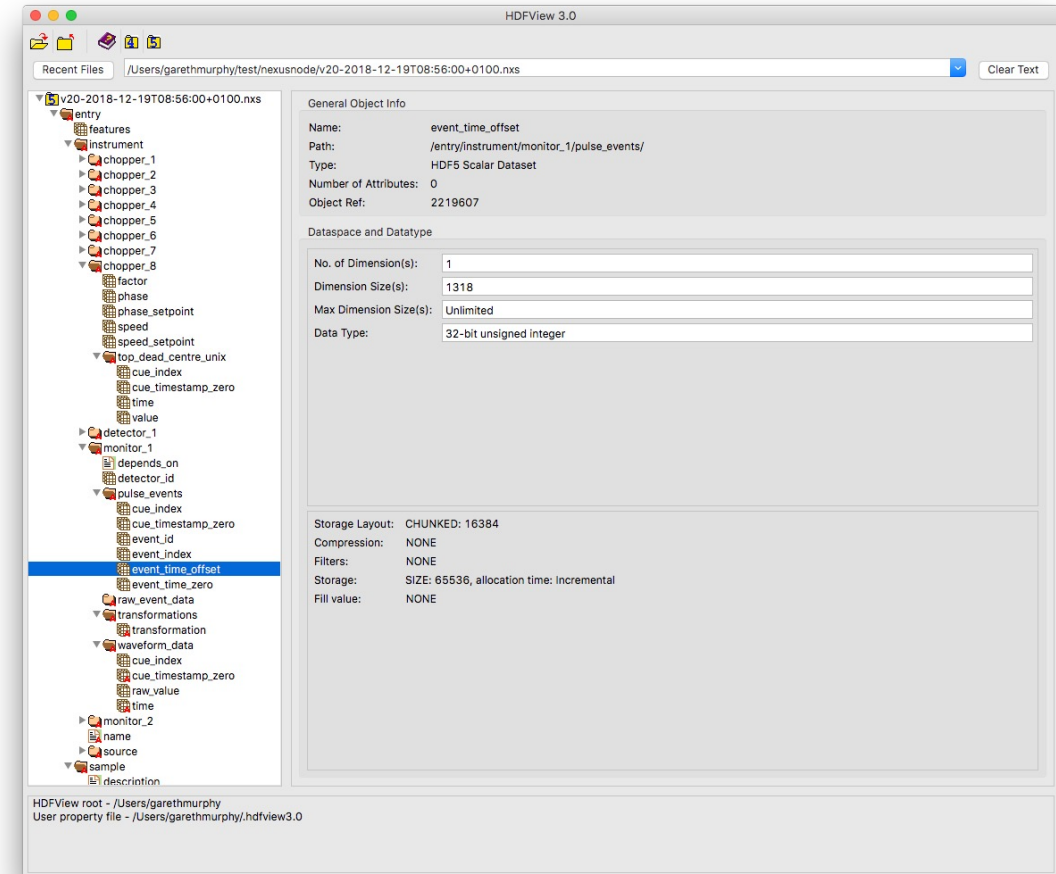


Each instrument has its own type of data

Own methods of data reduction/analysis

We use the same format across instruments  
HDF5 file format with NeXus format

Metadata is generated automatically and added  
to our data catalogue





# SciCat: Data Catalogue

Manages the metadata of raw and derived data which is taken at experiment facilities

administrative metadata : data steward, data management lifecycle, file details, size etc

scientific metadata: describing the sample, beamline and experiment parameters relevant for the users data analysis



Published Datasets / 10.17199/BRIGHTESS/V200115 /

**Publication Status**

Status	registered
Registered Time	2020-09-01, 16:22

**General Information**

Title	Sample Data from V20
Abstract	This data was collected as part of BrightNESS, funded by the European Union Framework Programme for Research and Innovation Horizon 2020, under grant agreement 676548. It consists of test data for the detector.
DOI	10.17199/BRIGHTESS/V200115
URL	<a href="https://doi.org/10.17199/BRIGHTESS/V200115">doi.ess.eu/detail/10.17199/BRIGHTESS/V200115</a>
Publication Year	2018

**Creator Information**

Creator	Tobias Richter
Authors	Tobias Richter
Affiliation	ESS
Publisher	ESS

**File Information**

Size	90 MB
Number of Files	1
Resource Type	hdfs files
Data Description	<a href="#">HDFS</a>

**Organization**

**ESS**  
The European Spallation Source ESS is a European Research Infrastructure Consortium (ERIC), a multi-disciplinary research facility based on the world's most powerful neutron...

**read more**

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**Dataset**

**Sample Data from V20**

This data was collected as part of BrightNESS, funded by the European Union Framework Programme for Research and Innovation Horizon 2020, under grant agreement 676548. It consists of test data for the detector.

PaN Photon and neutron ...

**Identifier**

DOI	<a href="https://doi.org/10.17199/BRIGHTESS/V200117">https://doi.org/10.17199/BRIGHTESS/V200117</a>
Metadata Access	<a href="https://scicat.ess.eu/openaire/oa?verb=GetRecords&amp;metadataPrefix=oa1_datacite&amp;identifier=10.17199/BRIGHTESS/V200117">https://scicat.ess.eu/openaire/oa?verb=GetRecords&amp;metadataPrefix=oa1_datacite&amp;identifier=10.17199/BRIGHTESS/V200117</a>

**Provenance**

Creator	Richter, Tobias (ESS)
Publisher	ESS
Publication Year	2018
Rights	OpenAccess: info:eu-repo/semantics/openAccess
OpenAccess	true

**Representation**

Resource Type	Dataset
Size	155 MB
Version	1
Discipline	Particles, Nuclei and Fields