

Data, Metadata, and FAIR

Max Novelli, data curation scientist
SIMS team (Scientific Information Management Systems)
ESS

About Me





Data Curation Scientist SIMS team

Scientific Information Management Systems

Data Management and Software Center European Spallation Source





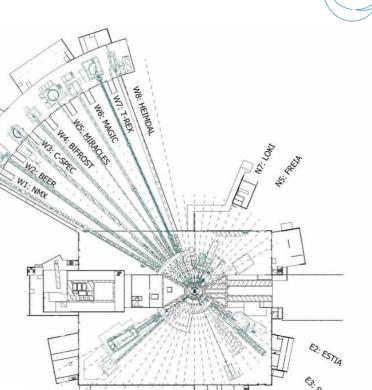




ESS Data

- 15 different instruments
- Different techniques
- Different data requirements
- Multiple scientific communities
- Multiple data types
- Multiple formats and standards
- A lot of data...





...for real!!!

Question #1 ...and #2



How do we manage all this data?



How do we deliver this data to our users?



The journey



Brett Patzke on Unsplash

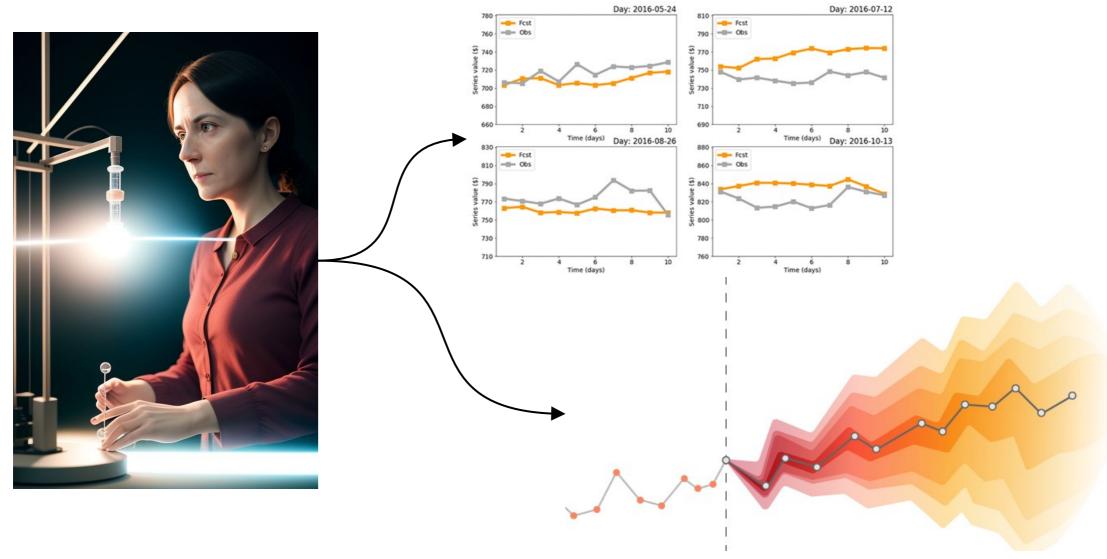
ESS User Journey



Performing Wrap-up & Registration **Proposal** Scheduling **Planning** & Analysing Harvesting Register **Experiments** Data directories in place Personal Data Sample environments Automatic data processing **Digital Access** Local contacts Manual data processing User lab facilities Permissions for files Experiment notification Submit proposals Users notify ESS of team Technical review User training Excellence review Experiment safety review Travel and accommodation Result notification Ship samples Physical Access Dosimetry

Experiment





Data: saving and transportation



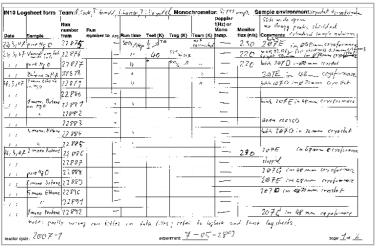


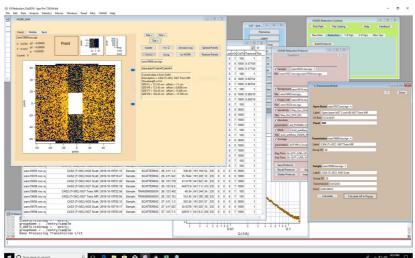


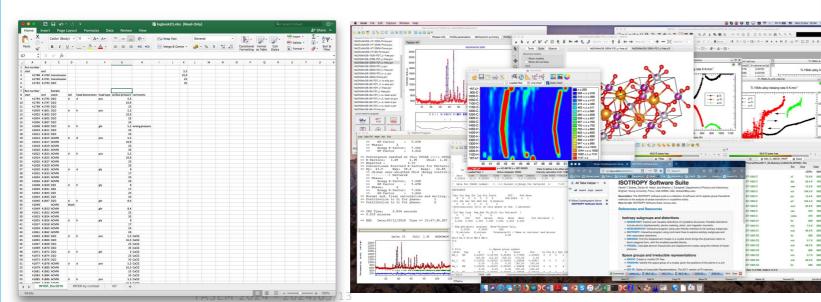


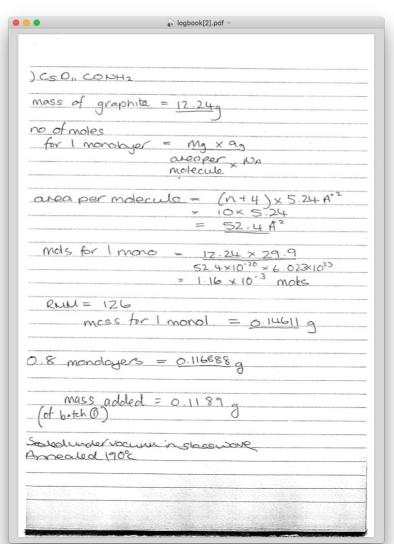
Experimental notes and log books











Evident Results

Papers

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Spectroscopic neutron imaging for resolving hydrogen dynamics changes in battery electrolytes



E. Ricardo Carreón Ruiz a, Jongmin Lee a, b, J. Ignacio Márquez Damián c, Markus Strobl b, d, Genoveva Burca e. f. Robin Woracek 8, Marc-Olivier Ebert h, Eric Winter d, Magali Cochet d, Laura Höltschi 4, Peter M. Kadletz 8, Mateusz Zlobinski 4, Anton S. Tremsin 1, Lorenz Gubler a, Pierre Boillat a, b, a

- Electrochemistry Laboratory (LEC), Paul Scherrer Institut (PSI), 5232, Villigen PSI, Switzerland
- b Laboratory for Neutron Scattering and Imaging (LNS), Paul Scherrer Institut (PSI), 5232, Villigen PSI, Switzerland Spallation Physics Group, European Spallation Source ERIC, P.O. Box 176, 22100, Lund, Sweden
- ^d Niels Bohr Institute, University of Copenhagen, Nørregade 10, 1165, Copenhagen, Denmark
- 6 STFC-Rutherford Appleton Laboratory, ISIS Facility, Harwell, OX11 OQX, UK
- Foculty of Science and Engineering, The University of Manchester, Alan Turing Building, Oxford Road, Manchester, M13 9PL, UK
- 8 European Spallation Source ERIC, P.O. Box 176, 22100, Lund, Sweden
- Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 1-5, 8093, Zurich, Switzerland
- Space Sciences Laboratory, University of California, Berkeley, CA, 94720, USA

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ABSTRACT

We present the use of spectroscopic neutron imaging (SNI), a bridge between imaging and scattering techniques, for analyzing battery electrolytes. The scattering information of CH_n-based organic solvents and electrolytes was mapped in a two-dimensional space through time-of-flight neutron imaging, which exploits the wavelength-dependent properties of hydrogen atoms. The results show partial solidification and concertation change of electrolyte as a function of temperature. Our investigation demonstrates a novel approach to tracking real-time physical and chemical changes in H-containing compounds, by which limitations of new electrolyte mixtures and additives can be evaluated. The sensitivity of SNI to hydrogen in CH_n functional groups extends the use of spectral methods to inspect electrolytes in Li-ion batteries and organic solvents for relevant applications beyond electrochemical systems.

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1. Introduction

Capabilities of neutron imaging (NI) have been significantly expanded with the advent of energy-resolved neutron imaging. which has become an essential tool for non-destructive material characterization [1-5], including studies of electrochemical energy storage and conversion devices [6,7]. The particular advantage of NI to investigate light elements of technological importance, i.e., hydrogen and lithium, even in operando processes has contributed to the improvements of green mobility technologies such as fuel cells [8,9] and lithium-ion batteries [10] (LIBs).

Electrodes in LIBs have been extensively studied by conventional (white-beam) NI [11-15], and energy-resolved NI has been effective in determining the state-of-charge via Bragg-edge analysis [16.17]. Physical or chemical changes in the electrolytes, on the other hand, are typically studied using spectroscopic techniques including Raman, nuclear magnetic resonance, and Fouriertransform infrared spectroscopies [18-22]. However, these techniques usually require specifically designed cells or involve complicated procedures to extract the electrolytes. Therefore, it is common to perform post-mortem mimicking operando conditions.

Neutron instrumentation development (detection systems [3,23-26], methods [2,27,28]) narrowed the gap [29,30] between information accessible by imaging and scattering techniques [31-33], which lead to the design of new beamlines (e.g., ODIN, ESS [31]) to exploit new opportunities, especially in the NI field. In this work, we demonstrate that a study of battery electrolytes

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^{*} Corresponding author. Electrochemistry Laboratory (LEC), Paul Scherrer Institut (PSI), 5232, Villigen PSI, Switzerland.

E-mail address: pierre.boillate@psi.ch (P. Boillat).

Less Evident Results



Data Loss



Missed Opportunity to Increase Value

FASEM 2024 - 2024/03/13

So... then...



Our Vision

...and of the funding agencies



Data Journey Ex-Bunker Bunker wall In-Bunker Acquisition Data Data Reduction Analysis System Analyzed Raw Reduced Data Data Data Data Catalog and Storage System

Paradigm Shift





MY DATA



FAIR data



Indable Accessible Interoperable Reusable

https://www.go-fair.org/fair-principles/

TRUSTed Repositories





https://www.nature.com/articles/s41597-020-0486-7

Open data





https://data.europa.eu



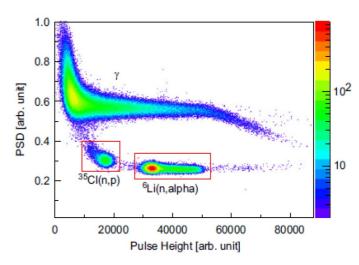
How do we get there?



Key concepts



Data





Metadata

Data

ess

METADATA

Data is a collection of discrete or continuous values that convey information, describing the quantity, quality, facts, statistics, other basic units of meaning, or simply sequences of symbols that may be further interpreted formally.

Such information is saved in one or multiple files which are generated during the experimental data acquisition or in

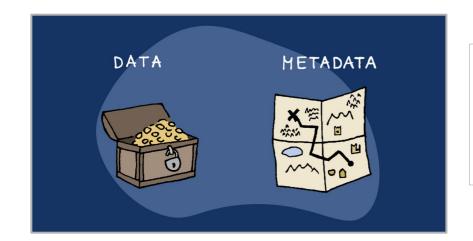
DATA

relation to that time window.

https://en.wikipedia.org/wiki/Data

Metadata





Metadata is data that provides information about other data

https://en.wikipedia.org/wiki/Metadata

Metadata are any information saved in the data catalog and available to the user to search for and retrieve the specific information she is looking for

Dataset



A **Dataset** is a collection of multi-modal items which:

- share a common purpose
- were collected for a specific purpose,
- describes an individual event or a series of events or an experiment,
- pertains to the same experimental data collection.

Metadata



Metadata can be:

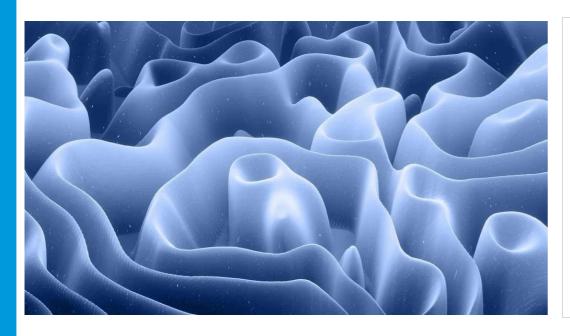
- a duplicate of any piece of data contained in the linked data files, as long it is of small size.
- any derived information that results from any type of data aggregation (like average, min, max or something more complex) performed on information contained in the linked data files
- any qualitative or quantitative information that has been collected or discovered at a later stage, which is relevant to describe and facilitate finding the dataset itself.

Metadata has to be relevant for the future utilization of the data.

Minimum Viable Metadata Set



The minimum set of key/values, descriptors that provides the best description of a dataset but is not overwhelming to use, search and maintain.



Metadata is an ever changing set of information.

They varies depending on:

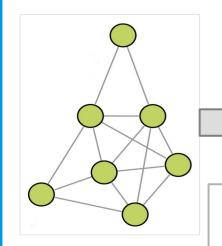
- Intended usage
- Stakeholder
- Domain knowledge

Data Curation

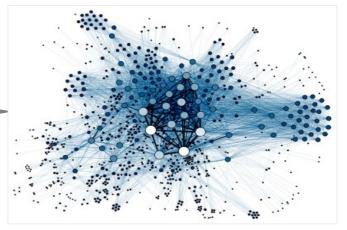


Data curation is the effort to organize and integrate data collected from various sources in a single entity, called dataset

https://en.wikipedia.org/wiki/Data_curation



Enrichment and Enhancement



Data Curation: example



Column 1

Connector 3

Channel B

Blue cable

Left light

Unknown

Resolution

Units
Which will be Metadata
Which aggregation

Other questions?

Sample Temperature

Temperature Controller 1

Sample position X axis

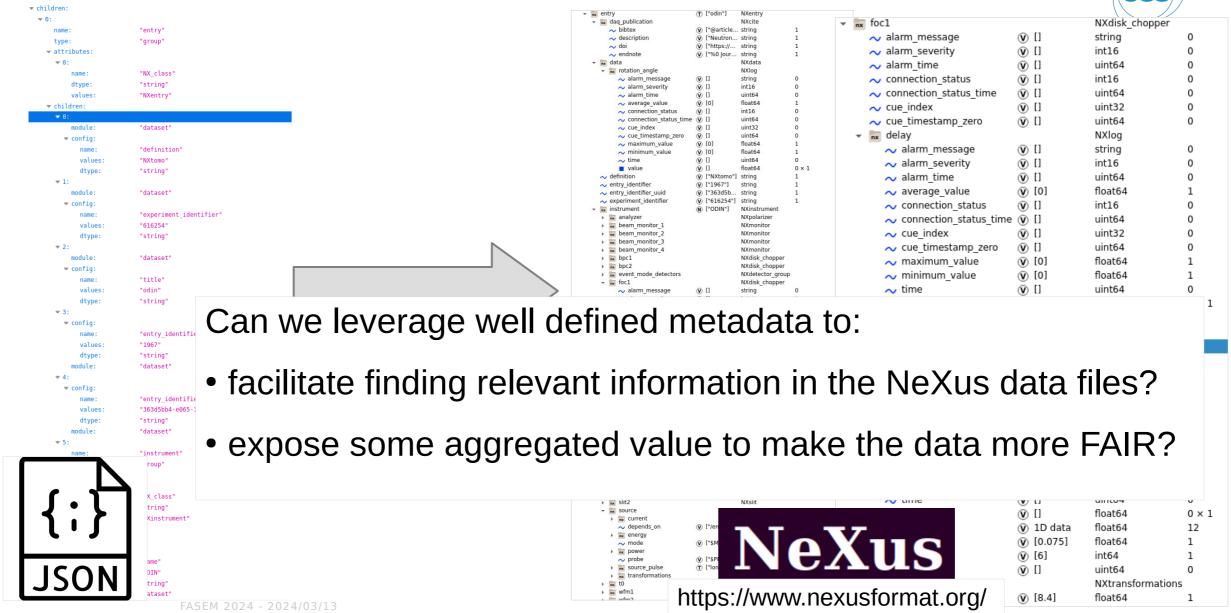
Light detector

Tomography light source

Slit position Y

Sample position resolution

Data Curation: understanding data





Which tool can help us in our data journey?



Tools: Metadata Catalog





https://scicatproject.github.io/

https://github.com/scicatproject

https://scicatproject.github.io/documentation













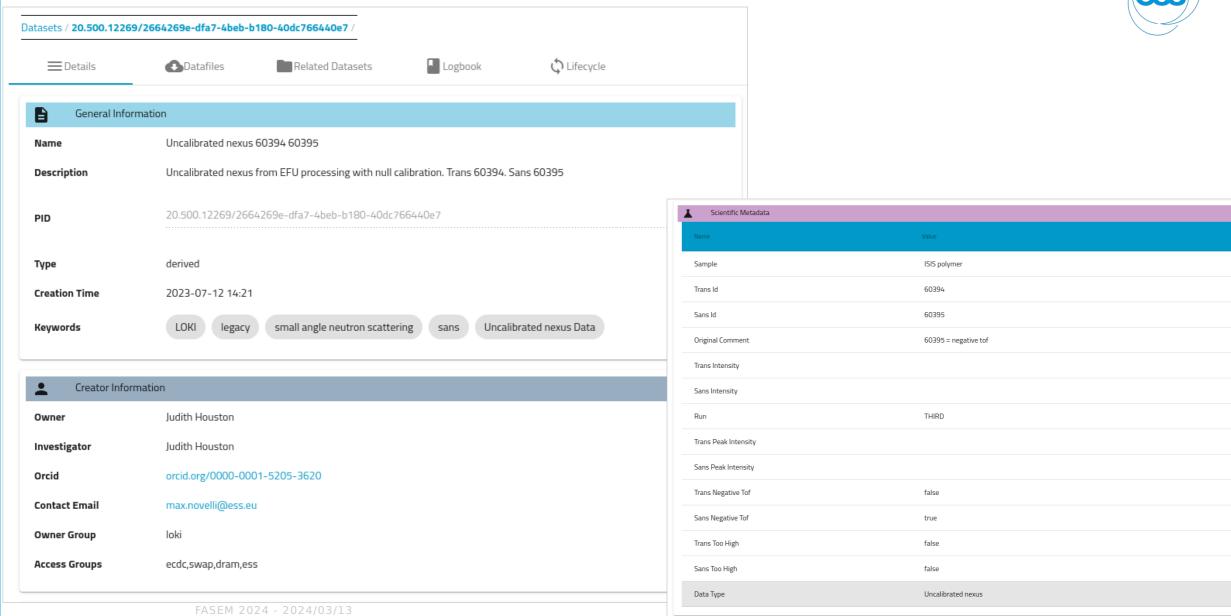






SciCat Dataset Details





Publishing Data in SciCat















Published Datasets / 10.5072/2d629944-9792-449c-ab54-3feb9bd5ccaa

Publication Status		
Status	pending_registration	
Register		

About the published data		
Title	Demo	
Creator List	clement	
Abstract	Demo	
© DOI	10.5072/2d629944-9792-449c-ab54-3feb9bd5ccaa	
○ URL	doi2.psi.ch/detail/10.5072/2d629944-9792-449c-ab54-3feb9bd5ccaa	

Administrative metadata	
O User	ldap.Henrik Johansson
Creator	clement
Data Description	None
Dataset IDs	20.500.12269/BCMFEAcceptance_297_2020-07-14-17-04- 37_3,20.500.12269/BCMFEAcceptance_297_2020-07-14-17-04- 37_2,20.500.12269/BCMFEAcceptance_297_2020-07-14-17-04-37_1
nublisher Publisher	ESS
Resource Type	raw





Digital Object Identifier



How can we foster adoption and data usage?



Tools: language libraries





SCITACEAN

Scitacean is a high level Python package for downloading and uploading datasets from and to SciCat.

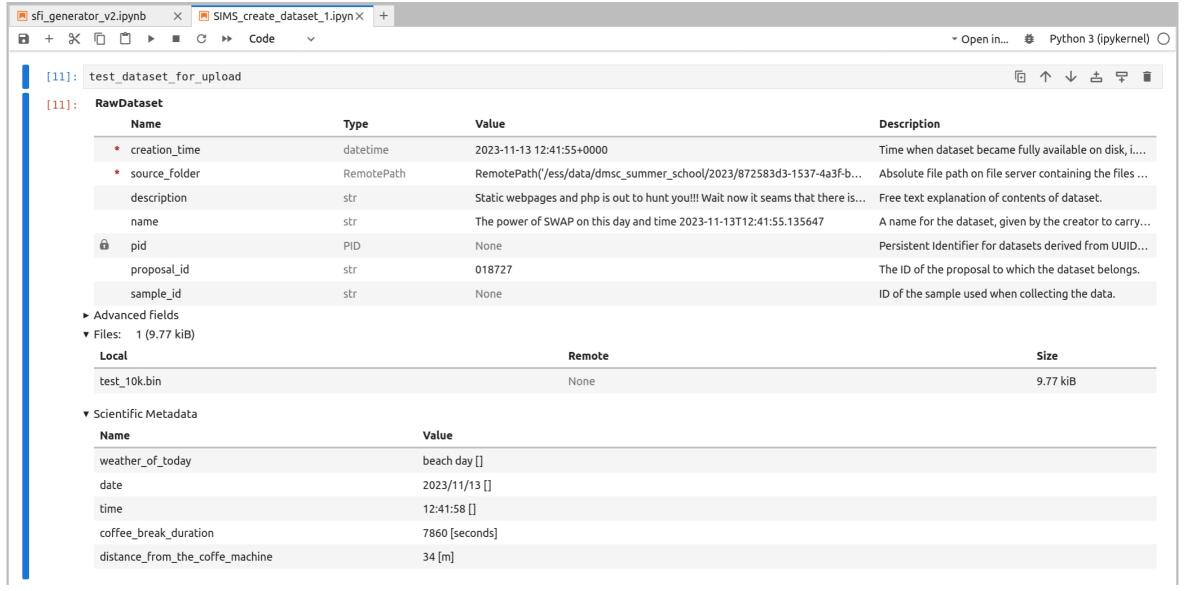
End user, data exploration, interactive

https://github.com/SciCatProject/scitacean

https://scicatproject.github.io/scitacean/

Scitacean in Jupyter Notebook







Why?





Miximizing Scientific Output Foster Innovation Methodologies and Tools





Use Cases



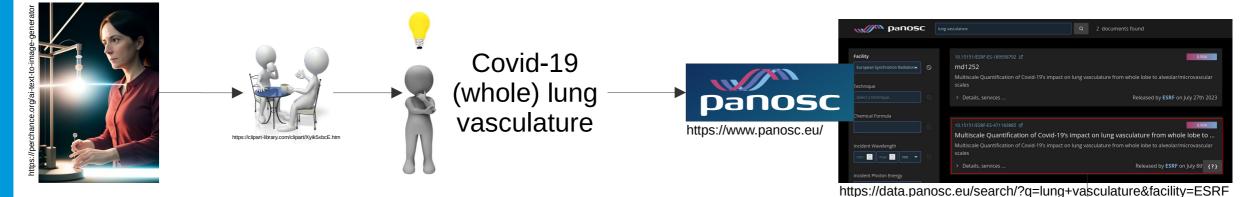
Greg Razoky on Unsplash

Use case: Story One





https://www.youtube.com/watch?v=wl kfKrfDD8

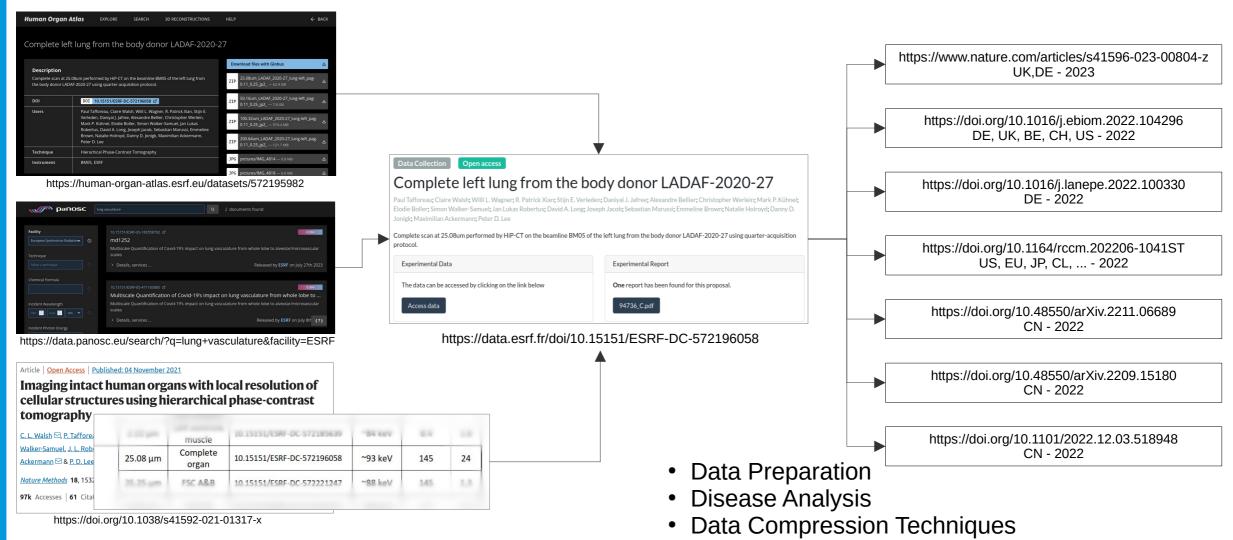




https://data.esrf.fr/doi/10.15151/ESRF-DC-572196058

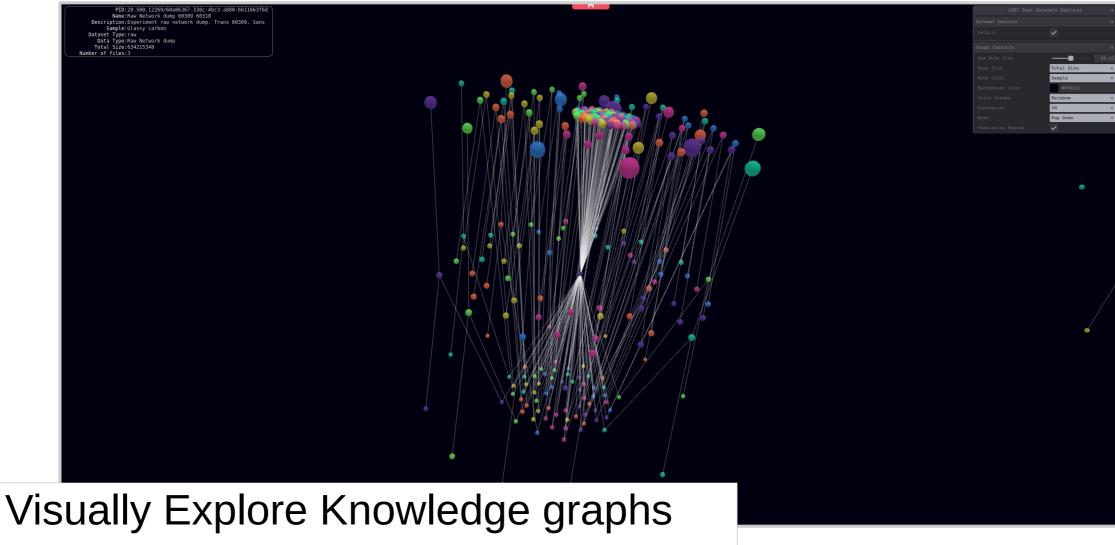
Use case: Story two





New exploratory tools





New methodologies





We are constrained by the boundaries of our domain knowledge and experience.

Only by opening our data to actors from different fields and domains, we can further push innovation beyond the borders of our knowledge and comfort zone.

Think about Machine Learning, AI and visualization.

Example: Kaggle https://www.kaggle.com/

FAIR Open Data Benefits and Challenges



Benefits

- Easy discovery of other resources
- Hidden connections
- Increase scientific output and better science quality
- Driving innovation and best practices
- Longer data life and better data quality

Challenges

- Data access and sharing
- Proper data curation
- Cross institution and cross national collaboration
- Right tools for the job





Call to Action

Talk to your data curation expert.

Include all your stakeholders in the discourse.

Prioritize FAIRness of your data.

Increase the value of your data.



Exercise 1



In small groups, discuss and list few properties of the objects shown below







http://www.pegani.dk

Exercise 2





How could you find all the balls that are intact and of the same color?

Which minimum viable metadata set would you use?

https://stock.adobe.com

Exercise 3



Which questions would you ask to capture the minimum viable metadata set for the objects shown below?



https://www.santafixie.dk



Thank you

Questions?

Max Novelli max.novelli@ess.eu