SCTB review:
Computing and data analysis

Nicolas Soler - 09/11/2021
Computing Division

The Computing division

Computing & Controls

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Computing Division Head

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New
Feb 2021

Controls and DAQ

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Electronics

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IT Systems

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IT Systems Section Head

MIS

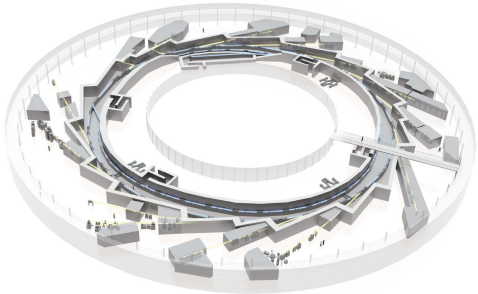
MIS Section Head

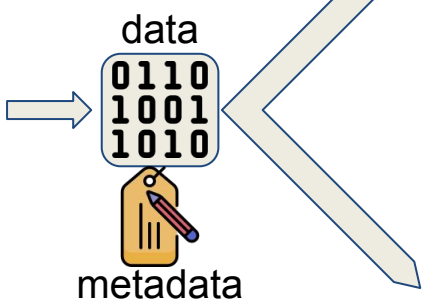
SDM

Nicolas Soler
SDM Section Head

2021: Scientific Data Management

A new section inside the Computing & Controls division

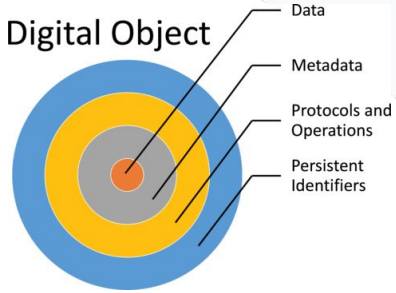




Data processing

Data reusability

- Metadata ingestion
- Provenance
- Persistent identifiers
- Catalogue
- DAaaS



4 people hired with hybrid science / computing profiles (+1 more in the beginning of 2022)

- Beamlines support
- Occasional accelerators support

https://www.nist.gov/programs-projects/facilitating-adoption-fair-digital-object-framework-material-science

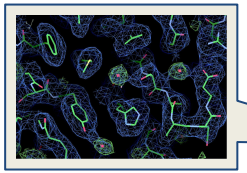
Data availability

The data supporting this study can be made available from the corresponding author upon request.

Towards FAIR synchrotron data

panosc

ExPaNDS



User: connection from local workstation or home laboratory

re-process

Data analysis as a service (WP4)

- EOSC Service portal
- PaN portal
- Containers
  Virtual machines
  Remote desktops
  Jupyter notebooks
- HPC
- Reference datasets

Use
re-use

Process
raw data

Annotate &
store processed data + provenance

FAIR-ready data (WP2)

- **Certified** (meta)data repository
- Standard metadata framework
- FAIR Data Management Plan (**DMP**) for each technique
- Persistent Identifier (**PID**) for data, instrument, software, sample)
- Common **data policy** framework

Data catalogues (WP3)

- **API / UI**
- **EOSC hub**
- **Metadata ontologies** (shared vocabulary)
- PaNOSC **federated catalogue**
- **Metadata formats** (NeXus)
- **Catalogues** (eg iCAT, SciCat)

Data reduction / compression

- Metrics
- New algorithms
- Software vs hardware
- Technique-specific
- Lossy vs non lossy
- Meta-compressors (ML)

LEAPS INNOVATION (WP7)

Implementation of a data catalogue at ALBA

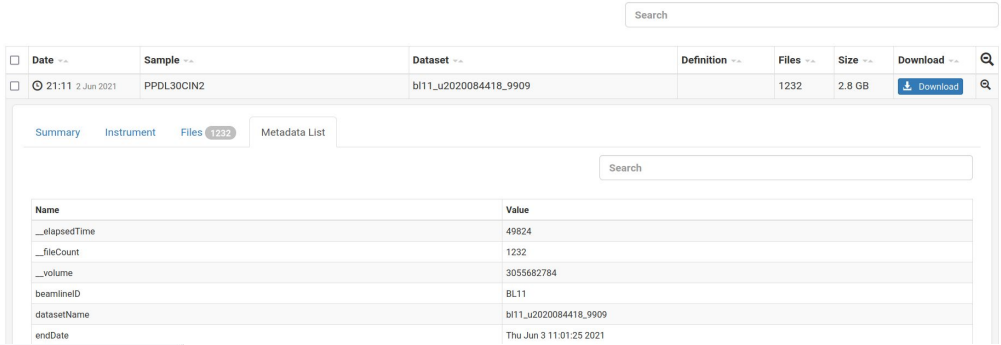
EOSC portal

PaNOSC Federated Metadata catalogue

- iCAT
- iCAT
- SciCAT
- …..

Experimental data, metadata, derived data and related info (i.e PIDs)

European facilities data catalogues



B2FIND

doi .org

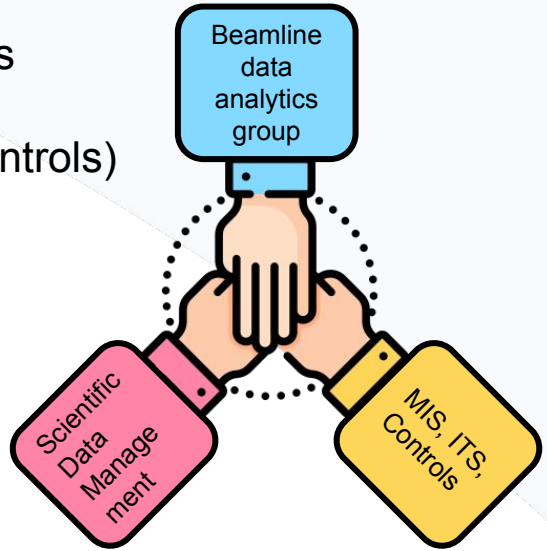
OpenAIRE

- Data have an embargo period of 3 years
- iCAT already in use for NCD-SWEET
- Next: Implementation in MIRAS and MSPD
- Open externally by the end of the year

2021: Scientific Data Management

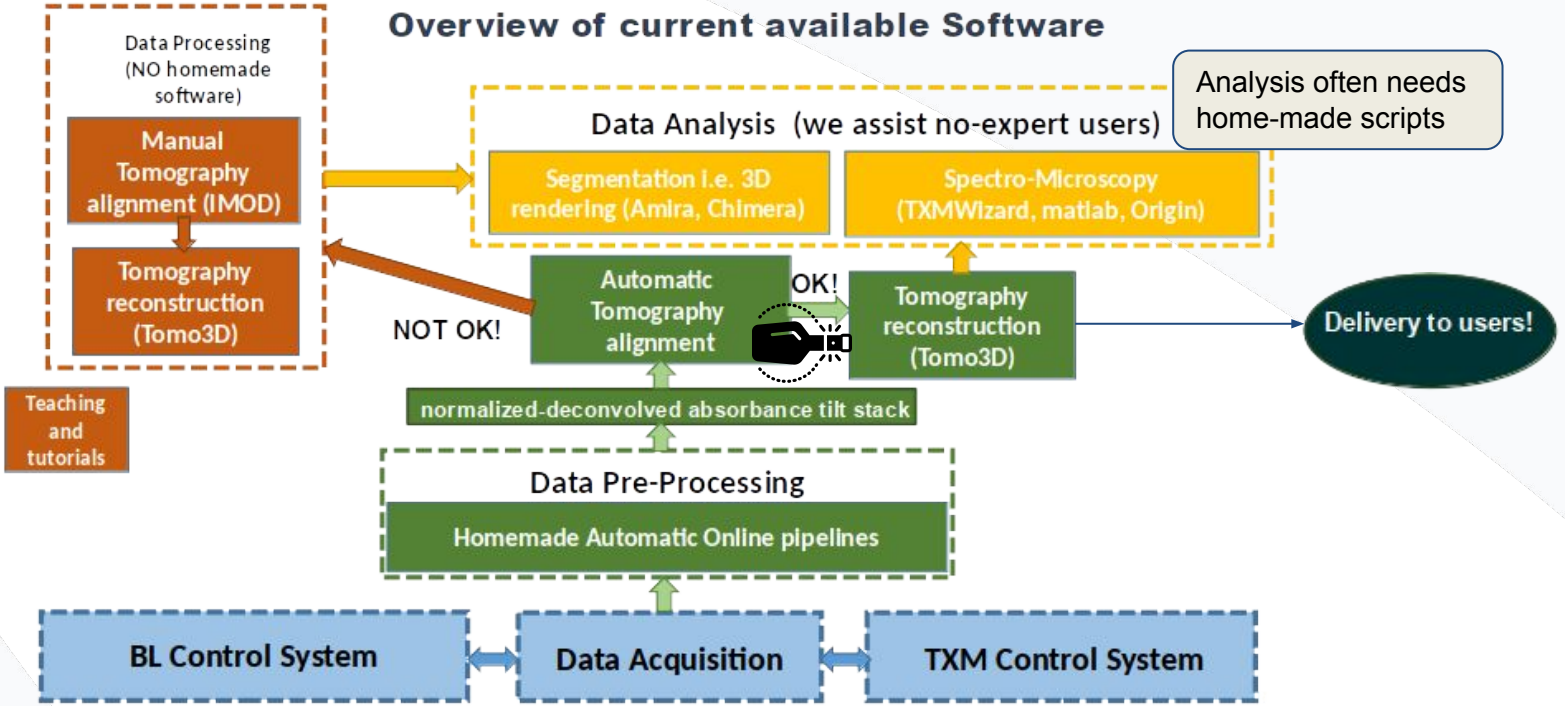
BUILDING A SYNERGIC SOFTWARE DEVELOPMENT PROCESS BETWEEN COMPUTING ENGINEERS AND METHOD DEVELOPMENT SCIENTISTS AT THE BEAMLINE

- Building downstream data processing and analysis pipelines
- Real-time data processing triggering and feedback (with Controls)
- Data visualization tools and GUI
- Databases and APIs
- Data reusability (ExPaNDS, with MIS and Controls)
- **Collaborating in data analysis methods development**



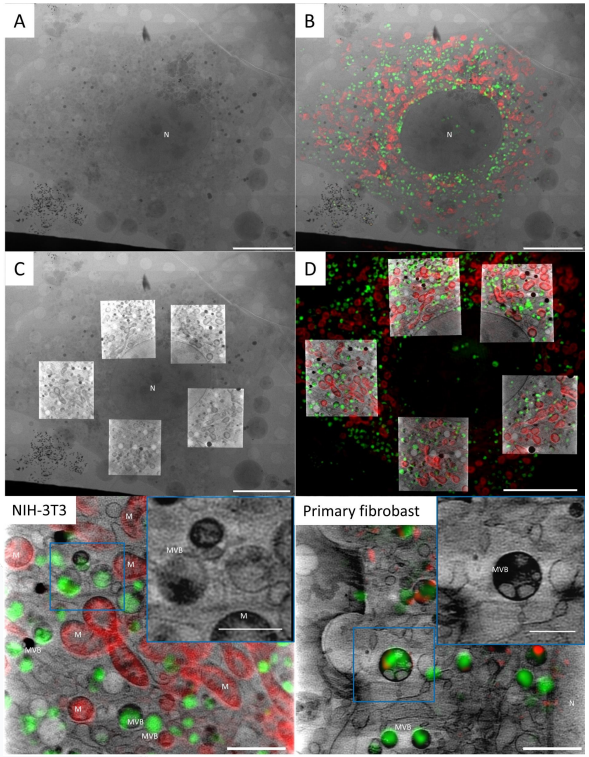
MISTRAL data flow (cryo-SXT)

(from A.Sorrentino' slide



Example of data analysis

Effect of an antifibrotic novel therapeutic agent at the cellular level



Chemical Science

ROYAL SOCIETY OF CHEMISTRY

EDGE ARTICLE

Cite this: DOI: 10.1039/d1sc04183e

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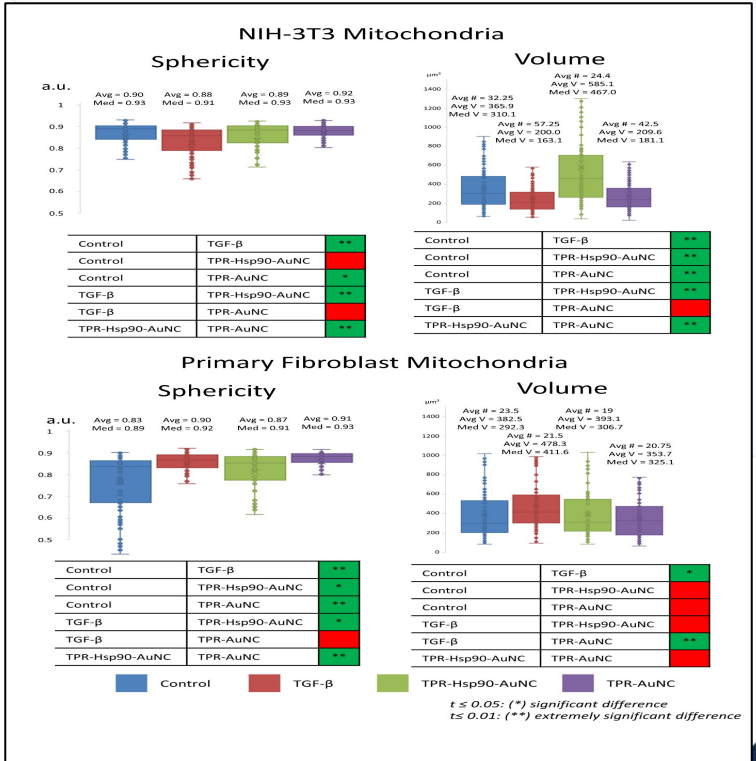
Correlative 3D cryo X-ray imaging reveals intracellular location and effect of designed antifibrotic protein–nanomaterial hybrids†

J. Groen, [a] A. Palanca, [bc] A. Aires, [d] J. J. Conesa, [ae] D. Maestro, [b] S. Rehbein, [f] M. Harkiolaki, [g] A. Villar, [bh] A. L. Cortajarena [*di] and E. Pereiro [*a]



MISTRAL DP/DA: GAP analysis

DP feature	Current setup	Problem / disadvantage	Mitigation / future setup
User interface	user interface	Scripts-based	GUI / workflow manager
Preprocessing	Custom pipelines (single/multiple images per angle for tomos, spectroscopy 2D & 3D)	has to be launched manually after data acquisition	Automatic triggering to be installed
Alignment (tomo & spectra)	IMOD, EFTEM-TOMOJ & 2D correlation Image J or python (2D spectroscopy)	presence of fiducials required but hardly controllable	Optical flow, TomoPy
Reconstruction	SIRT (Tomo3D), ART of TOMOJ	ok but could be GUI-monitored	followed on workflow manager
Segmentation & analysis	AMIRA, Chimera, SuRVoS	Not enough automation?	ML approaches
Correlative microscopy 3d	in progress	to test	*Icy- eC-CLEM?*
Data access, reprocessing	via sFTP, HDD	preservation, provenance	Data catalogue, DAaaS

MISTRAL data processing & analysis

- Bring more **automation** in the current data processing pipeline. Bring graphical interfaces and data workflows where needed. Improve current pipelines.

- Install a robust, parallelized xy **fiducialess alignement** correction program (e.g Tomopy) that could be use by default (whether or not fiducials are present).

- Provide software support for **correlative microscopy** (cryoET and cryo3DSIM volume superposition) and **segmentation methods**

- Together with on-site experts, assist in the development of **analysis** software.

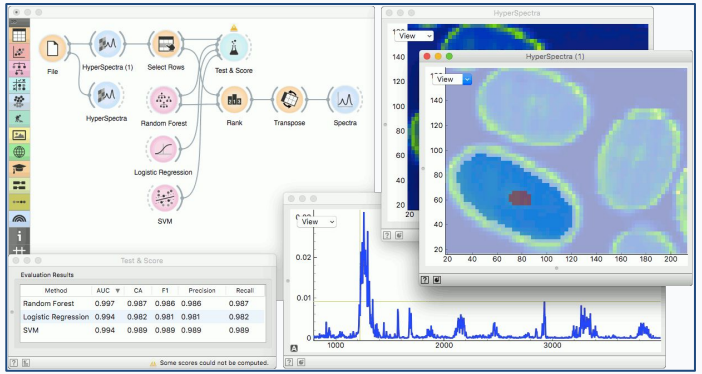
FAXTOR hard X-ray µCT: *Future issues to consider*

- Workflow manager and previews (GUI)
- preprocessing: from raw data to phase retrieval, (normalisation etc).
- computer reconstruction (aiming at real-time, parallelized on the cluster)
- image registration (re-aligning / shifting)
  - on angular projection
  - on reconstructed volume
- Machine learning for low dose, segmentation, denoising, missing angles etc
  - on angular projection
  - on reconstructed volume
- Managing and visualizing big data volumes (size: few GB to several TB)
  - distributed memory visualization (NVIDIA index, paraview plugin)
  - Data selection (automated?), Database of scans (iCAT)
  - Data compression (probably lossy)

Cell and tissue biology beamlines:

How can SDM help?

MIRAS IR spectroscopy & microscopy



- Move from proprietary to **open source solutions** (e.g Orange, Quasar). Join the IR quasar network (SOLEIL, Elettra, Sirius, Canadian light source etc), especially bringing **data workflows**, **machine learning** capabilities and nice feature to explore **imaging**/hyperspectral data.
- Improve the data analysis as a service by switching to these solution.
- Provide advice for **statistical methods** (eg t-SNE instead of PCA)
- **Multimodal** experiments: correlation with other types of spectroscopies

quasar

biolab

SOLEIL SYNCHROTRON

Elettra Sincrotrone Trieste

Canadian Light Source | Centre canadien de rayonnement synchrotron

BioSpec Norway

LNLS Brazilian Synchrotron Light Laboratory

PHOTOTHERMAL SPECTROSCOPY CORP

orange

Summary

- SDM has been created 9 months ago to support Experiments with data processing, analysis and visualization needs as well as with future data reusability (FAIRness)
- The first 2 engineers started in September, 1 in November, 1 more to come until in Jan. 2022, 1 to be hired next year.
- SDM will coordinates the metadata ingestion scheme and catalogue, as well as the transition towards data analysis as a service for remote users.
- Computing engineers with scientific background will work hand in hand with data analytics beamline method developers to:
    - produce and maintain data processing & analysis pipelines, bringing expertise in software development and other relevant technologies (i.e machine learning.
    - Provide support for integration of heterogeneous data.