



DAta for PHoton and Neutron Experiments

NFDI

Nationale Forschungsdaten Infrastruktur Initiative

Aim

Systematic exploitation of valuable research data across all scientific fields for sustainable access, use and reuse

NFDI e.V.

Foundation of NFDI e.V. in October 2020

Coordination accross all scientific areas / ‚Basisdienste‘

191 members (status 11/2021)

Implementation through **research area specific consortia** (DFG funding, 2 x 5 years foreseen)

1st call 2019: 9 consortia funded, start 01.10.2020

2nd call 2020: 10 consortia funded (a.o. DAPHNE4NFDI), start 01.10.2021

3rd call 2021: ongoing, start foreseen 01.01.2023

DAPHNE4NFDI

Data for Photon and Neutron Experiments

Consortium

Brings together 18 partners:

- University user groups
- Large scale facilities
- In addition: KFN + KFS
- > 60 participants (without funding)
- Kick-off meeting 1.12.2021

Task Area Leader:

Anton Barty (DESY, Speaker)

Bridget Murphy (CAU, KFS)

Astrid Schneidewind (FZJ)

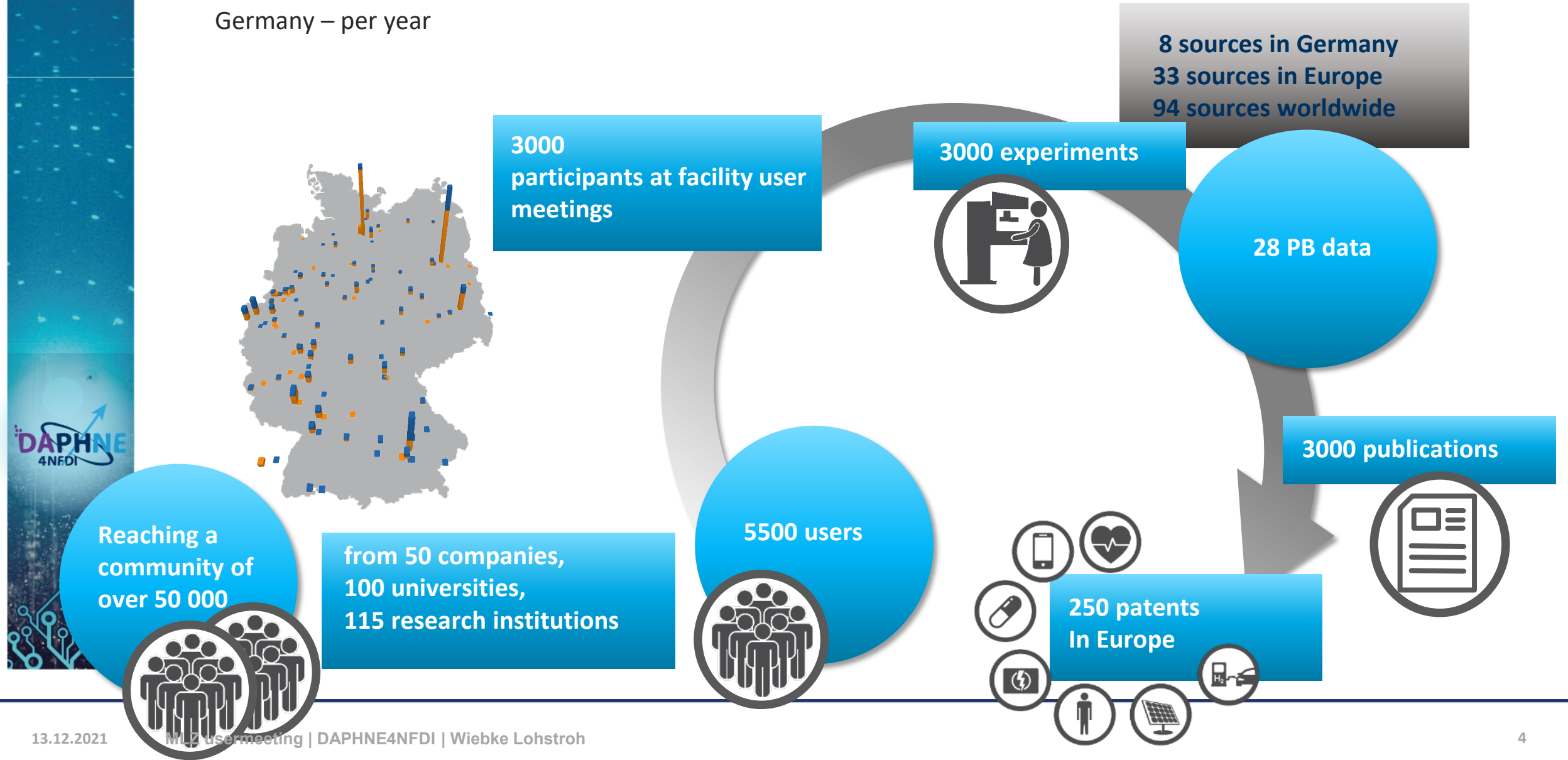
Christian Gutt (U Siegen)

Wiebke Lohstroh (TUM)



Research with photons and neutrons

Germany – per year



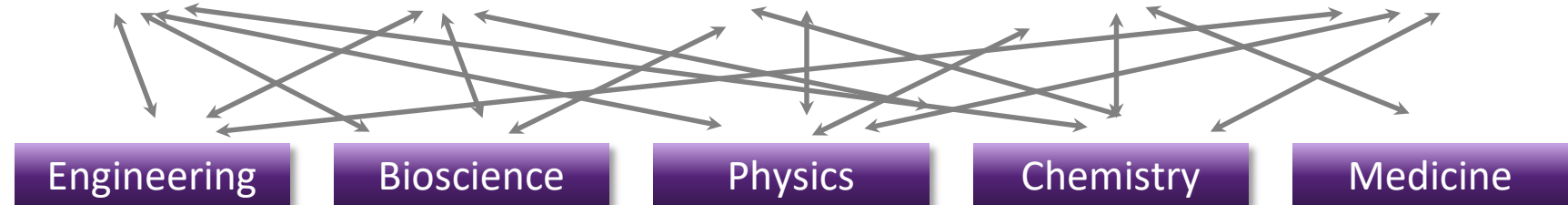
Our research community impacts on global challenges

Impact extends far beyond the physics or materials science community

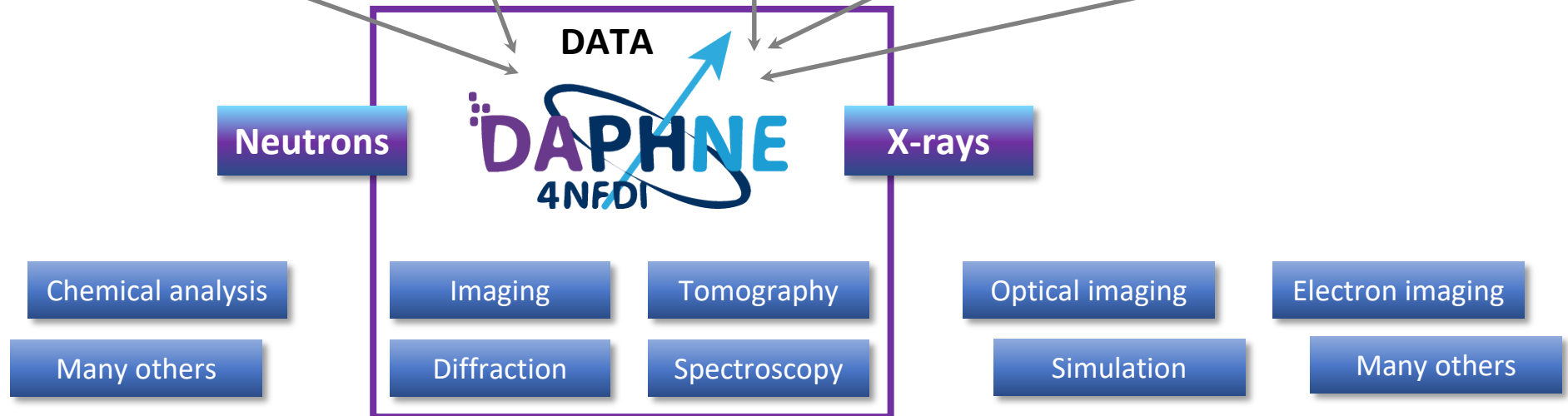
Society
challenges



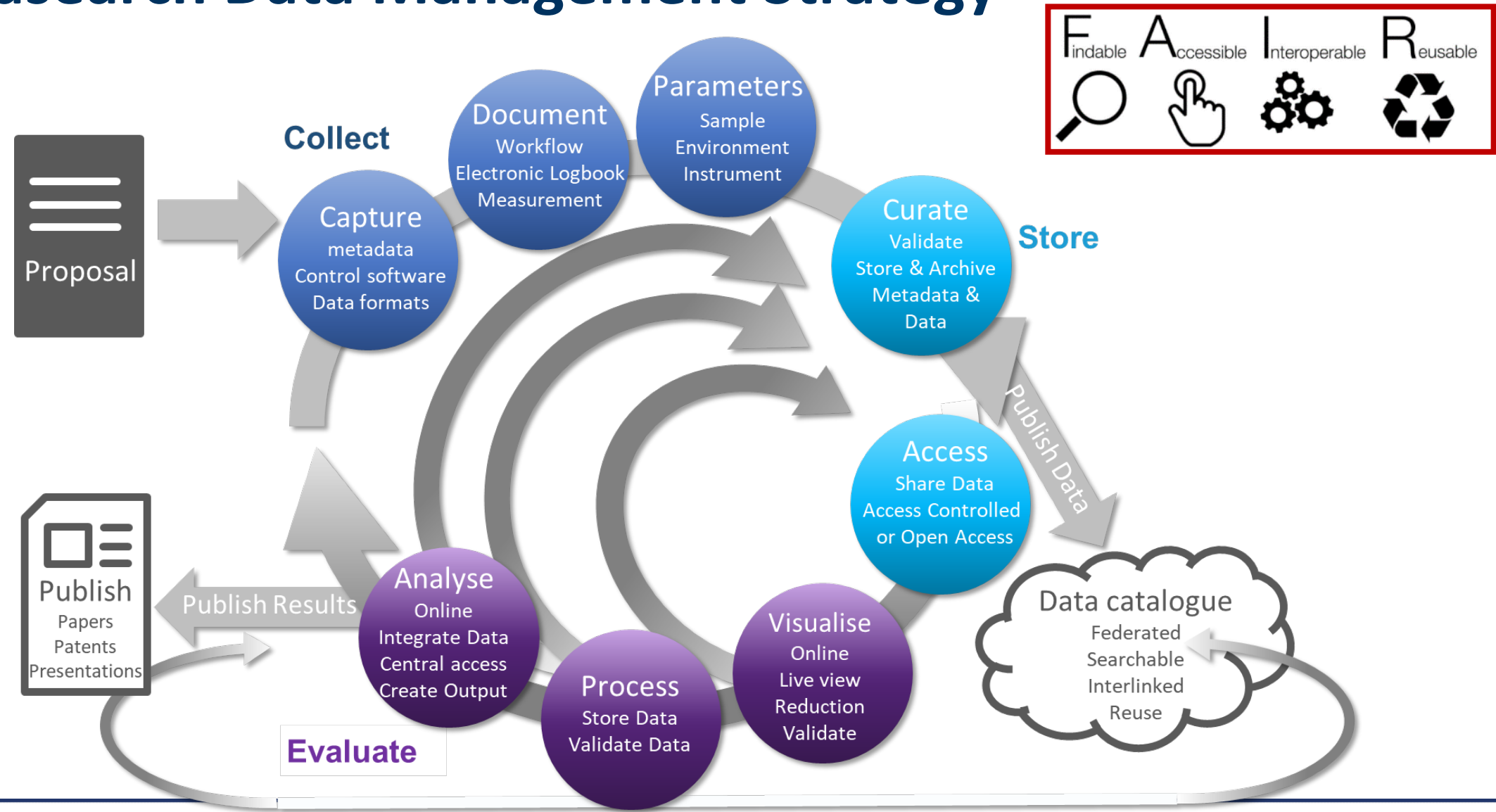
Research
domains



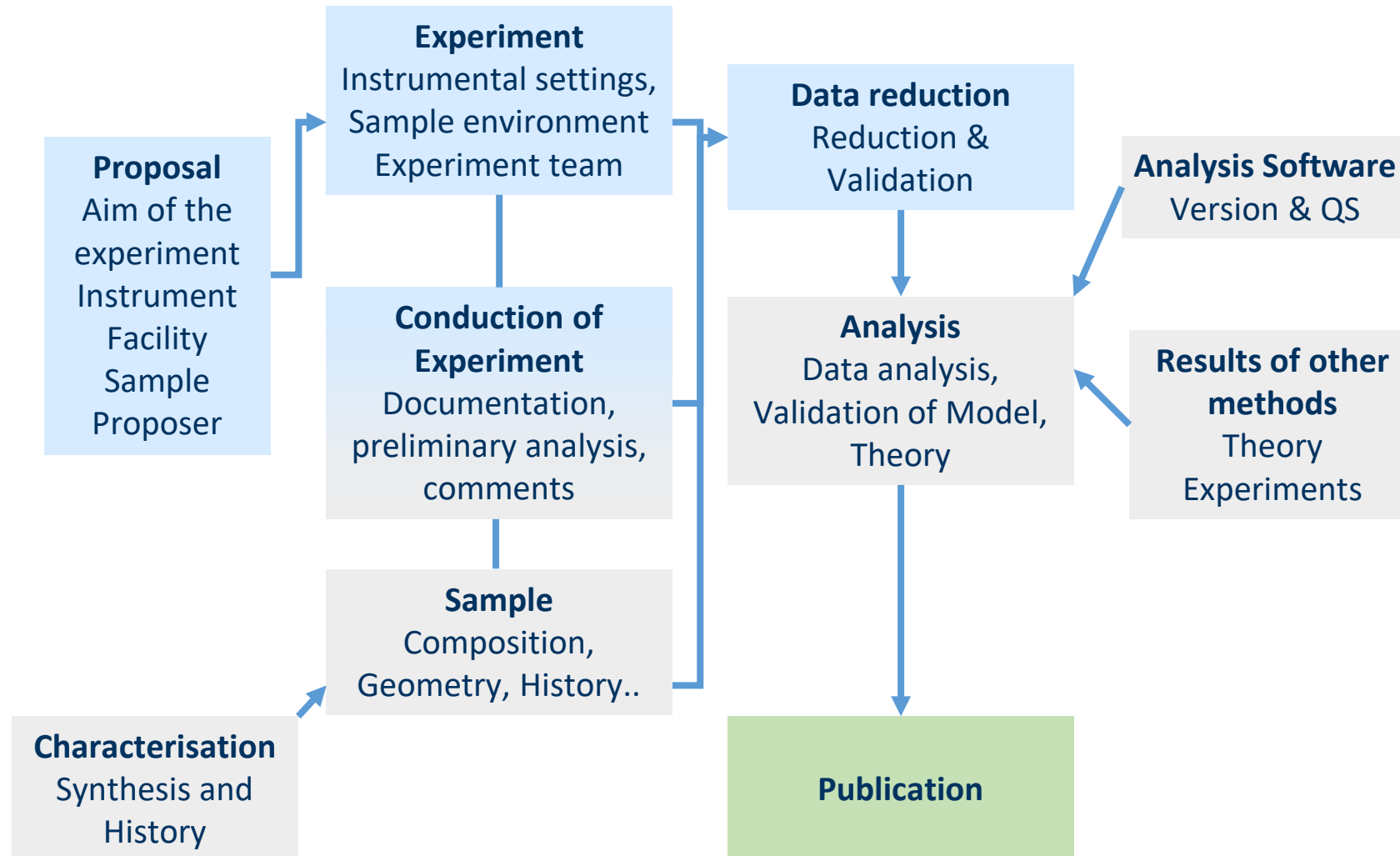
Analytic
methods



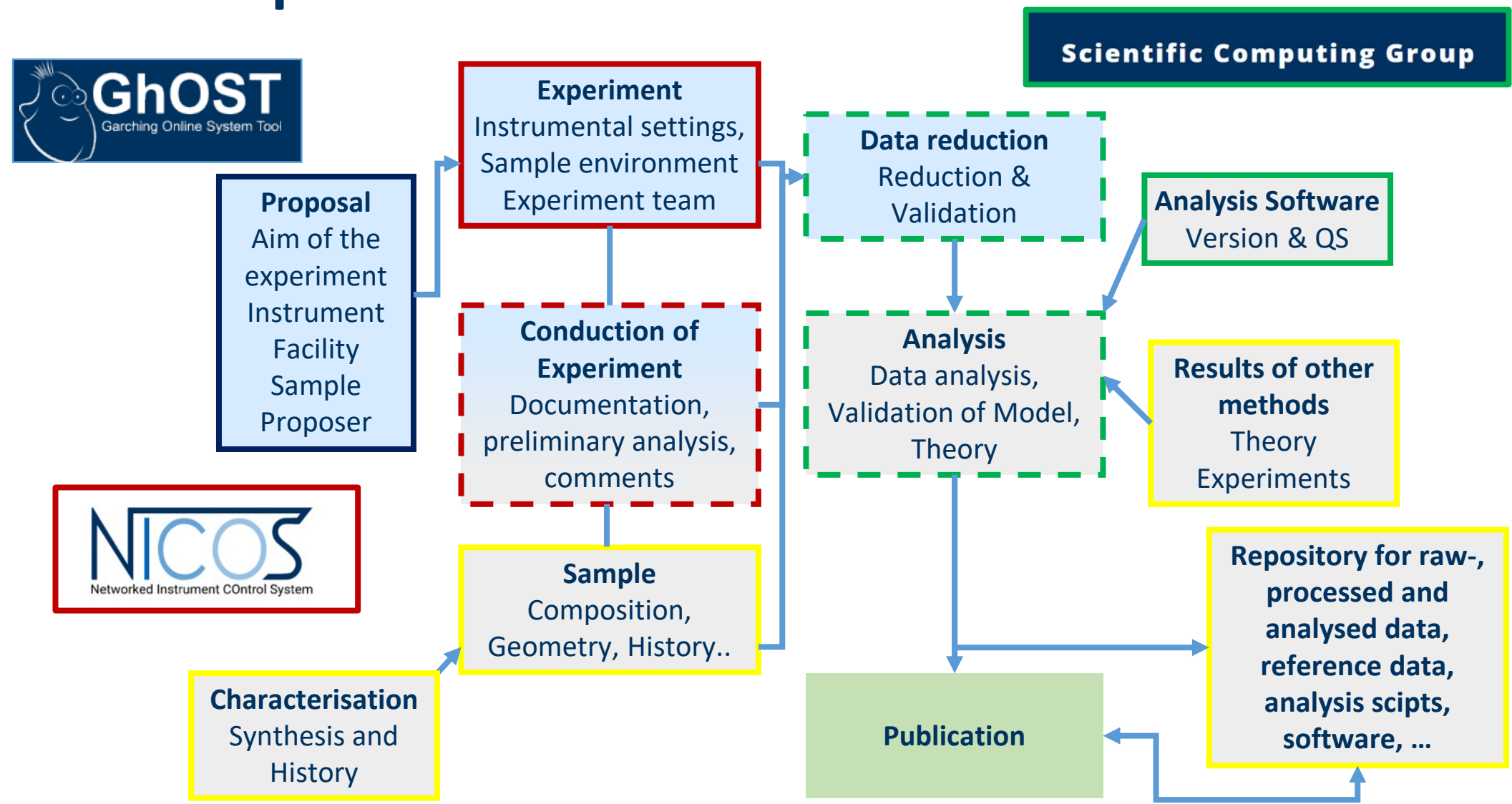
Research Data Management Strategy



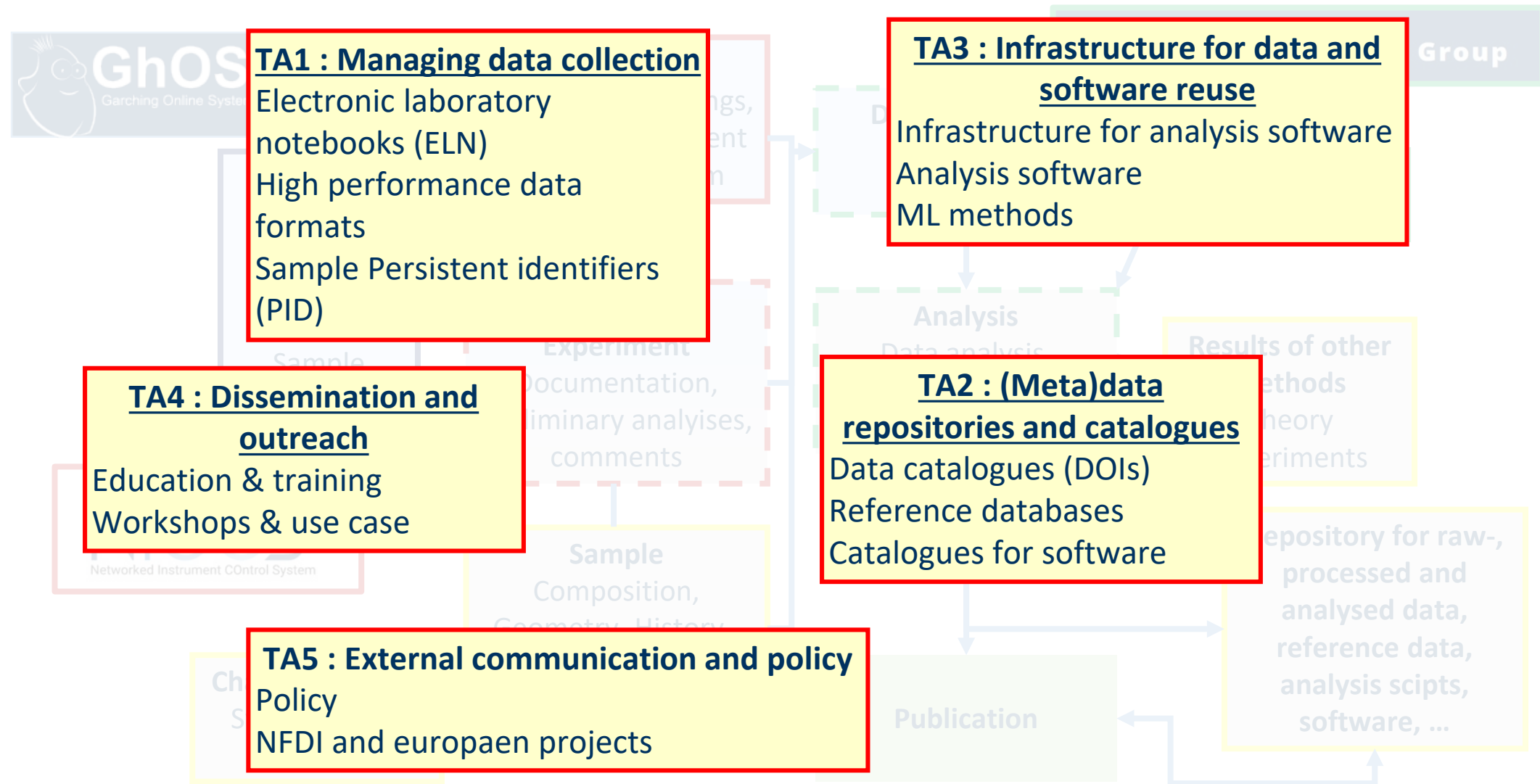
From Proposal to Publication



From Proposal to Publication



DAPHNE4NFDI



Task Areas 1: Managing data collection

Capture (meta)data as early as possible in electronic form

- Specification of metadata standards – application to use domain specific use cases, (further) develop PaN ontologies
- Link to Sample PID – sample metadata schemata (e.g. IGSN)
- Introduction of electronic Notebooks (ELN) (,contextual description / annotated data‘)
- Automatic capture of instrument / sample environment and sample data – conduction of the experiment
- Aggregate in harmonized, self-explaining data format (Nexus, OpenPMD)



ExPaNDS ontologies

Document Control Information

Settings	Value
Document Identifier:	D3.2
Project Title:	ExPaNDS ontologies
Work Package:	WP3

<https://zenodo.org/record/4806026#.YUh-kOdCRno>

Data Manager of Experiment : CXI / cxils2616

Logged in: holly Logout
Session expires in: 24:46:23

Experiment e-Log Run Tables File Manager Workflow

Recent (1 file)
Post
Search
Shifts
Runs
Attachments
Subscribe

Last messages: 100 Include runs Show deleted Auto-refresh 0/1 Refresh
39 messages, runs: 251 - 281 [Last update on: 2019-12-03 11:34:50]

Sort by: DATE CROUT BY DATE CROUT BY SHIFT CROUT BY TAG CROUT BY AUTHOR

Posted	Run	Length	Subject	Author
2018-10-29 14:43:56			Table of the number of lines for each run. All of the other parameters...	loglin
2018-05-28 10:46:55			Simulated powder pattern for 0.9 MeV at 137 mm	koz17
2018-05-28 04:08:26	272		DNA powder hits: single shot and sum of 12 hits	koz17
2018-05-27 09:02:58			End of experiment	rdm
2018-05-27 09:00:43	281	1:59	stop	DMA/RC

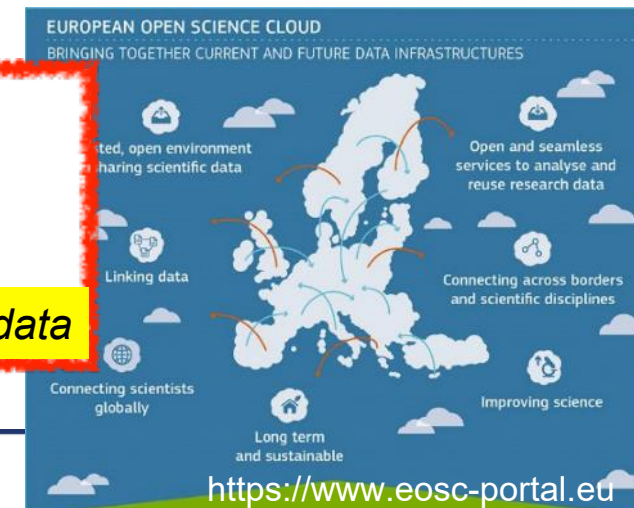
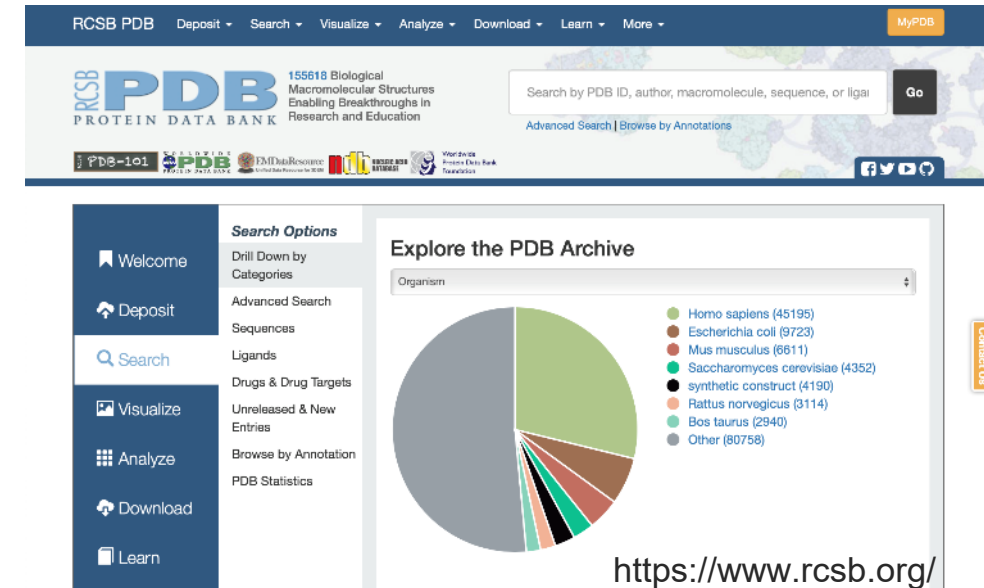
Electron and Photon beams

Parameter	Value	Unit
electron beam energy	12.3340	BEND.DMP1.480.B0ES
beam spot size	120.0000	EVNT.SYSR1.1CLUBHARATE
Particle N° electrons	< no data >	BPM5.DMP1.100.TMT.H
E-Beam	0.0000	SOC.SYSO.M0.A02B0

Task Area 2: (Meta)data repositories and catalogues

Searchable, federated data repositories

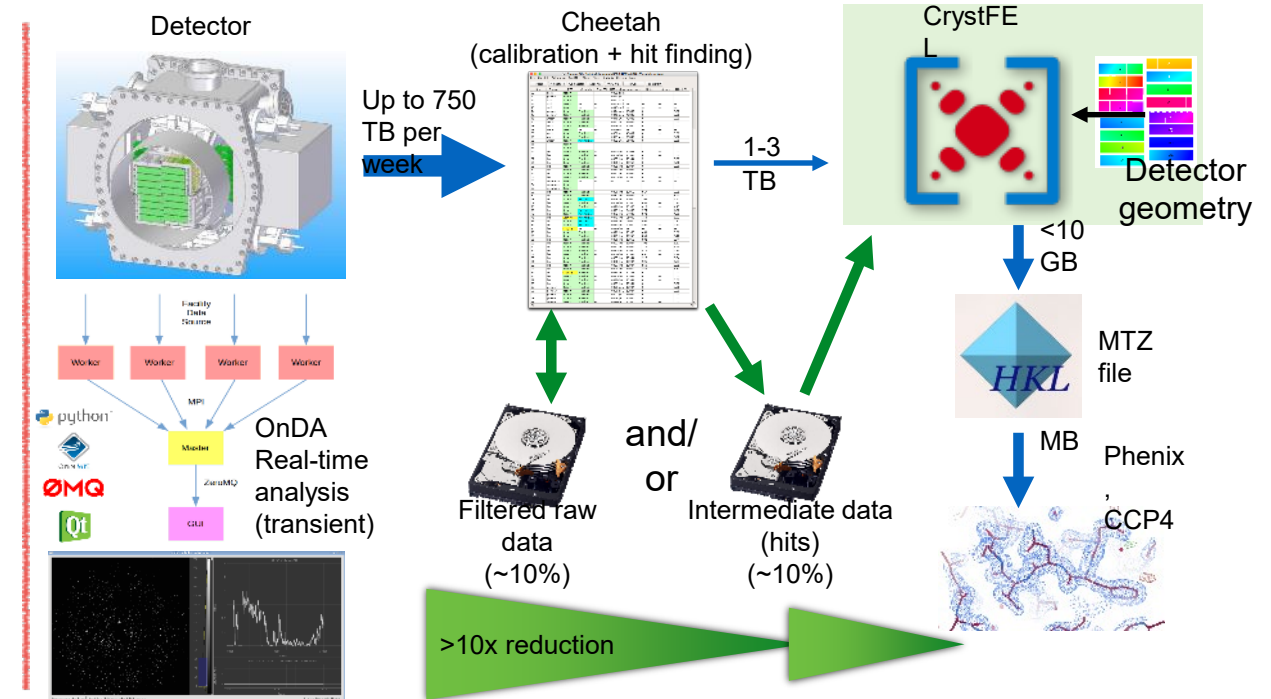
- Specification of metadata standards – application to use domain specific use cases
- Establish federated, interlinked data repository for participating facilities, DOI minting at MLZ
- Sample description and sample PID
- Repository for processed and analysed data
- Reference data bases
- Repository of analysis programs (e.g. <https://software.pan-data.eu/>)
- ‘Search data’



Task Area 3: Infrastructure for data and software reuse

„FAIR software“

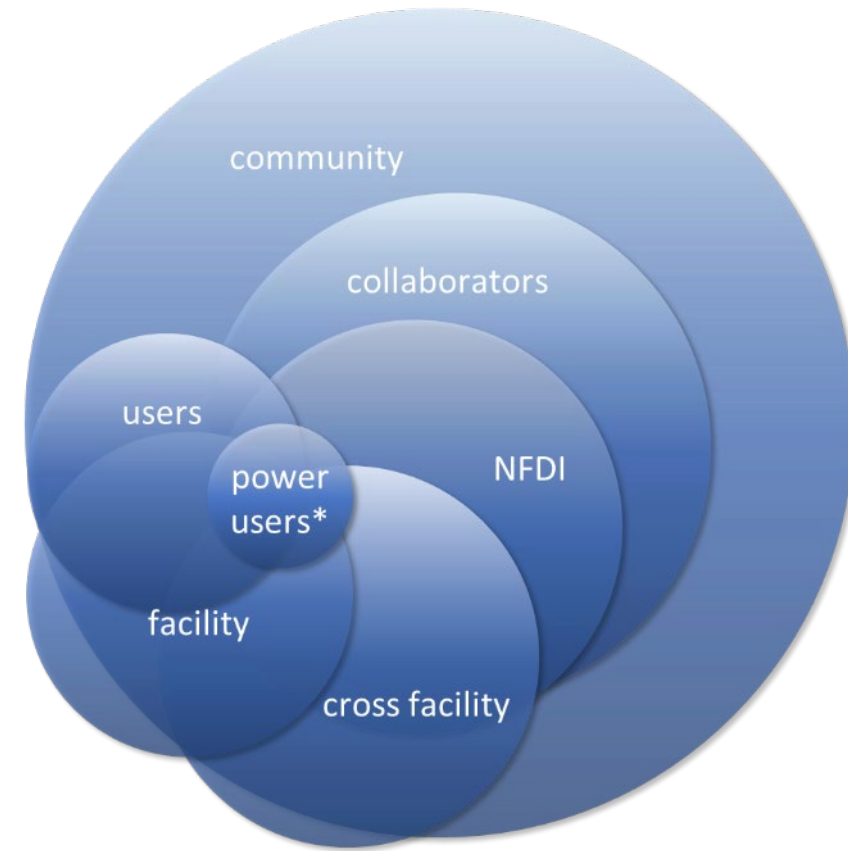
- Curate and deploy analysis software on cloud like infrastructures (currently frequently fragmented and diverse) for a number of use cases (tomography, EXAFS, small angle techniques, crystallography, tof-diffraction, interface to ML methods)
- Automatized data analysis chains
- AAI infrastructure
- Best practices for sustainable research software development



Task Area 4: Dissemination and outreach

The NFDI consortium as a role model and educator

- Workshops and community building - (meta)data definition and ontologies
- Discuss and Support use cases
- Young researches network – DAPHNE VISION
- Data management as part of the curriculum
- Connect society and industry to highlight developments
- Encourage to re-use



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Biomaterials- x-ray
imaging

Correlation
spectroscopy -
XPCS

Amorphous
materials for
catalysis

Soft matter and liquid
interfaces

Electrochemistry
& Catalysis

Proteins & Food
science

Correlated
electron systems
- spectroscopy

TOF diffraction

Chemical
systems – x-ray
absorption

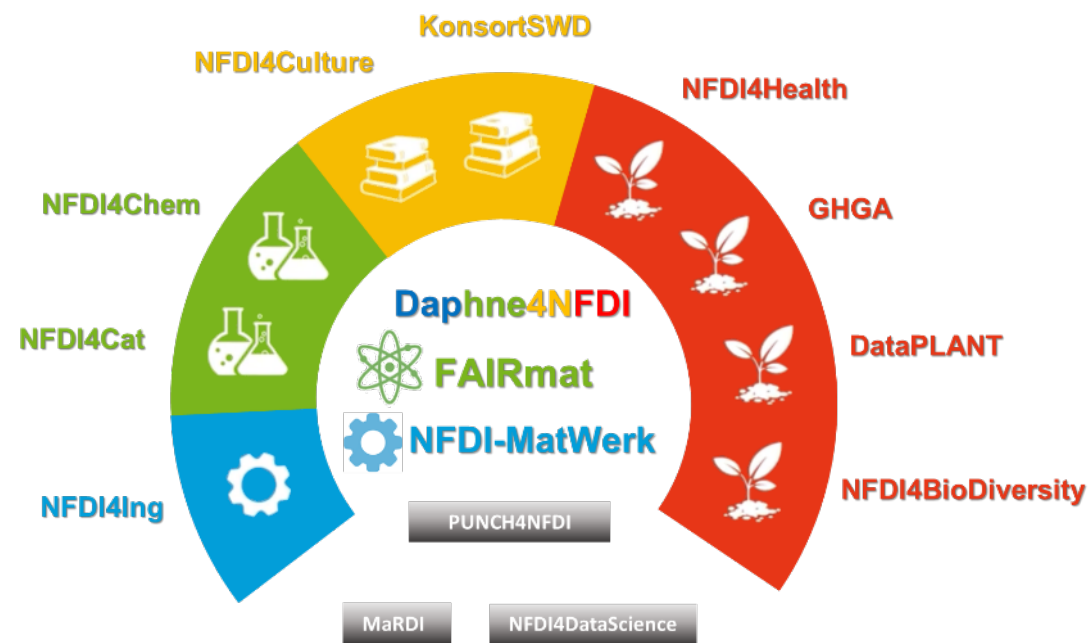
Magnetic structures

Energy materials

Task area 5: External communication and policy

Integration into the international research community

- DAPHNE is embedded in a worldwide network of > 30.000 synchrotron and neutron users
- Cross-consortia activities – interfaces and interlinkages to other NFDI consortia
- Organizational structures exists: European user organizations and facility organization
- Connects to European open science cloud X-ray and neutron data projects PaNOSC and ExPaNDS



DAta for PHoton and Neutron Experiments



- Project start 1st October 2021
- Initial duration 5 years
- Embedded in NFDI e.V.

Thank you for your attention!