Towards structured data in electron spectroscopy

Heiko B. Weber and the FAIRmat team

Friedrich-Alexander-Universität Erlangen-Nürnberg

Outline

- The FAIRmat approach for making experimental data FAIR
- Application definitions and NEXUS
- MPES example

FAIRmat

RDM

Open data

Open access (~2001) to peer reviewed literature, being enforced by funding agencies

FAIR principles[1] (2016); statement at G20 summit in China[2]

Data as resource[3]: A European strategy for data (2020)

Expectations: DFG and other funding agencies expect FAIR data from us researchers

(funding is connected to FAIR data pledges)

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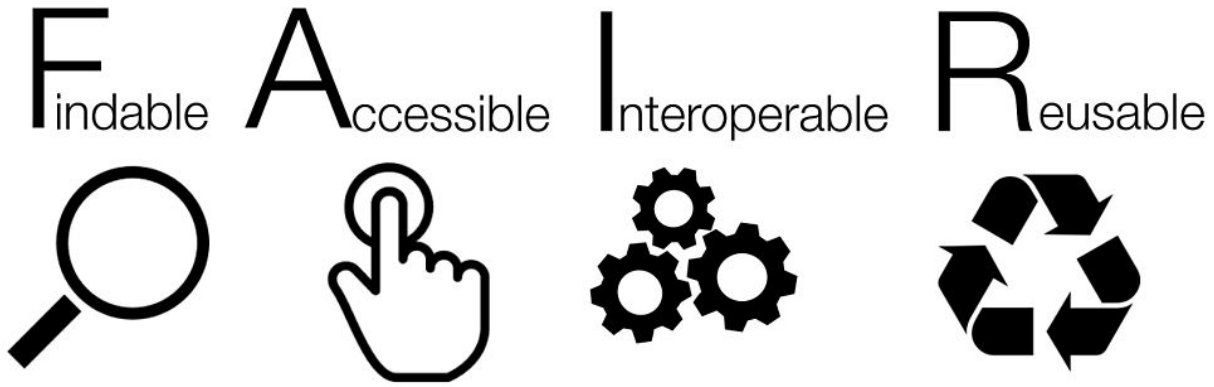
[1] Scientific Data 3, 160018 (2016)

[2] https://ec.europa.eu/commission/presscorner/detail/en/STATEMENT_16_2967

[3] https://ec.europa.eu/info/sites/default/files/communication-european-strategy-data-19feb2020_en.pdf

RDM

Underlying principles for open research data



Findable and **A**rtificial **I**ntelligence **R**eady

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RDM

FAIR data: benefit or burden?

Rich opportunities

- Big data opportunities in science
- Data analysis as novel discipline (besides experiment and theory)
- Accelerated materials discovery
- Enhanced data competence of scientists
- Reduction of misleading interpretations and fraud

Significant investment

- The transition to FAIR data demands for reorganizing scientists‘ workflow entirely

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Nationale Forschungsdaten-Infrastruktur (NFDI)

(polycentered bottom-up network)

1st round (10/2020)

- DataPLANT: Plant research data
- GHGA: German Human Genome–Phenome Archive
- KonsortSWD: Consortium for the Social, Educational, Behavioural and Economic Sciences
- NFDI4Biodiversity: Biodiversity, Ecology and Environmental Data
- NFDI4Cat: NFDI for sciences related to catalysis
- NFDI4Chem: Chemistry consortium for the NFDI
- NFDI4Culture: Consortium for Research Data on Material and Immaterial Cultural Heritage
- NFDI4Health: NFDI personal health data
- NFDI4Ing: NFDI for Engineering Sciences

2nd round (10/2021)

- BERD@NFDI: NFDI for Business, Economic and Related Data
- **DAPHNE4NFDI: Data from PHoton and Neutron Experiments for NFDI**
- **FAIRmat: FAIR Data Infrastructure for Condensed-Matter Physics and the Chemical Physics of Solids**
- MaRDI: Mathematical Research Data Initiative
- NFDI4DataScience: NFDI for Data Science and Artificial Intelligence
- NFDI4Earth: NFDI Consortium Earth System Sciences
- NFDI4Microbiota: NFDI for Microbiota Research
- **NFDI-MatWerk: NFDI for Materials Science and Materials Engineering**
- PUNCH4NFDI: Particles, Universe, NuClei and Hadrons for the NFDI
- Text+: Language and text-based research data infrastructure

3rd round (3/2023)

- FAIRagro: FAIR Data Infrastructure for Agrosystems
- NFDI4BIOIMAGE: National research data infrastructure for microscopy and bioimage analysis
- NFDI4Energy: National Research Data Infrastructure for Interdisciplinary Energy System Research
- NFDI4Immuno: National Research Data Infrastructure for Immunology
- NFDI4Memory: The Consortium for the Historically Oriented Humanities
- NFDI4Objects: Research Data Infrastructure for the Material Remains of Human History
- NFDIxCS: National Research Data Infrastructure for and with Computer Science

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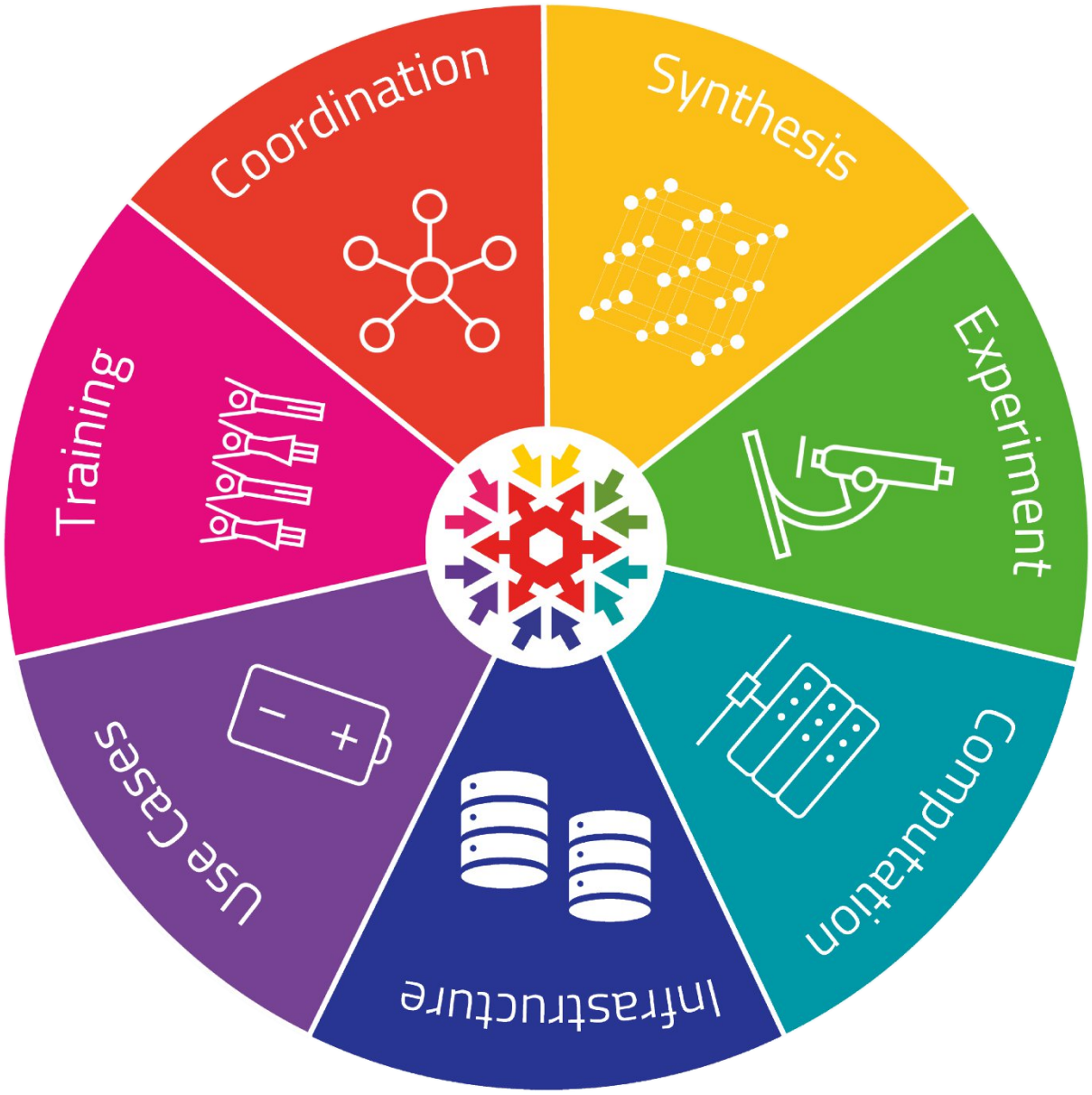
Experiment

FAIRmat



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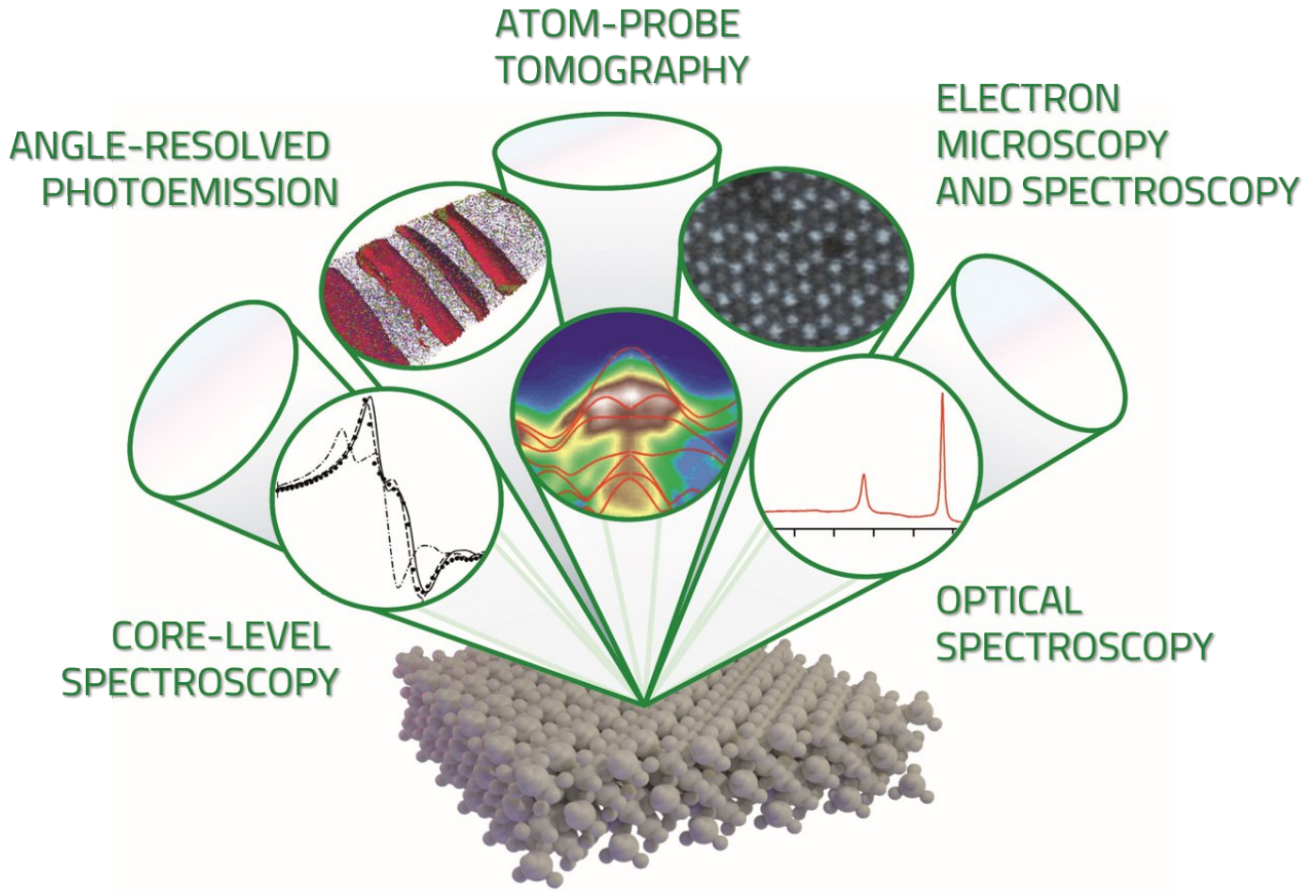
Experiment

Area B and its pilot experiments



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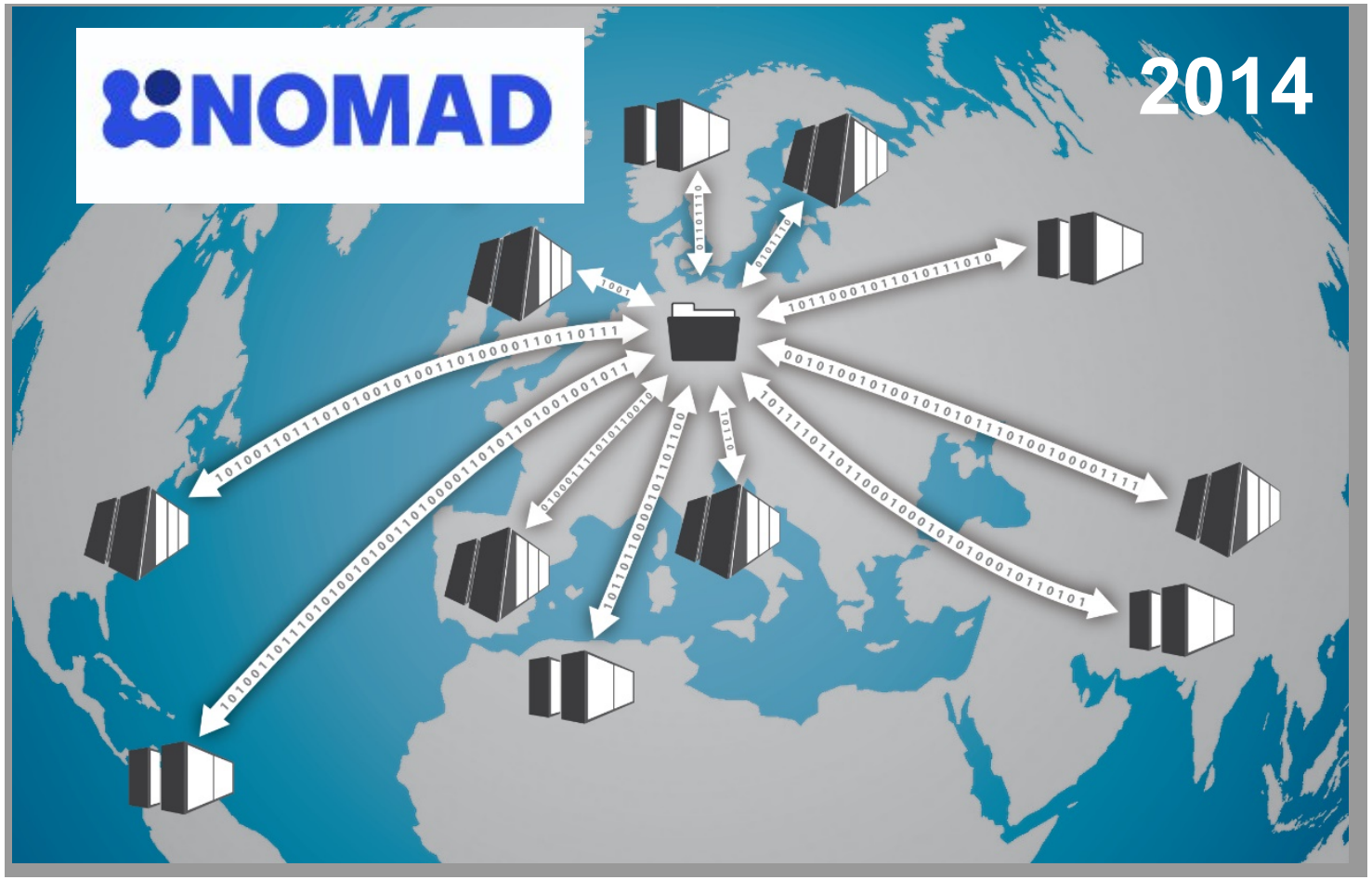
Forerunners

FAIRmat

Nomad repository

World's largest collection of computational materials science data



Make data repurposable

Recycle the waste!

The Novel Materials Discovery Laboratory

Forerunners

Computational Solid-state science

40 community software packages supported

Thus 40 parsers serve as *converters*

Normalized data in the NOMAD *Archive*

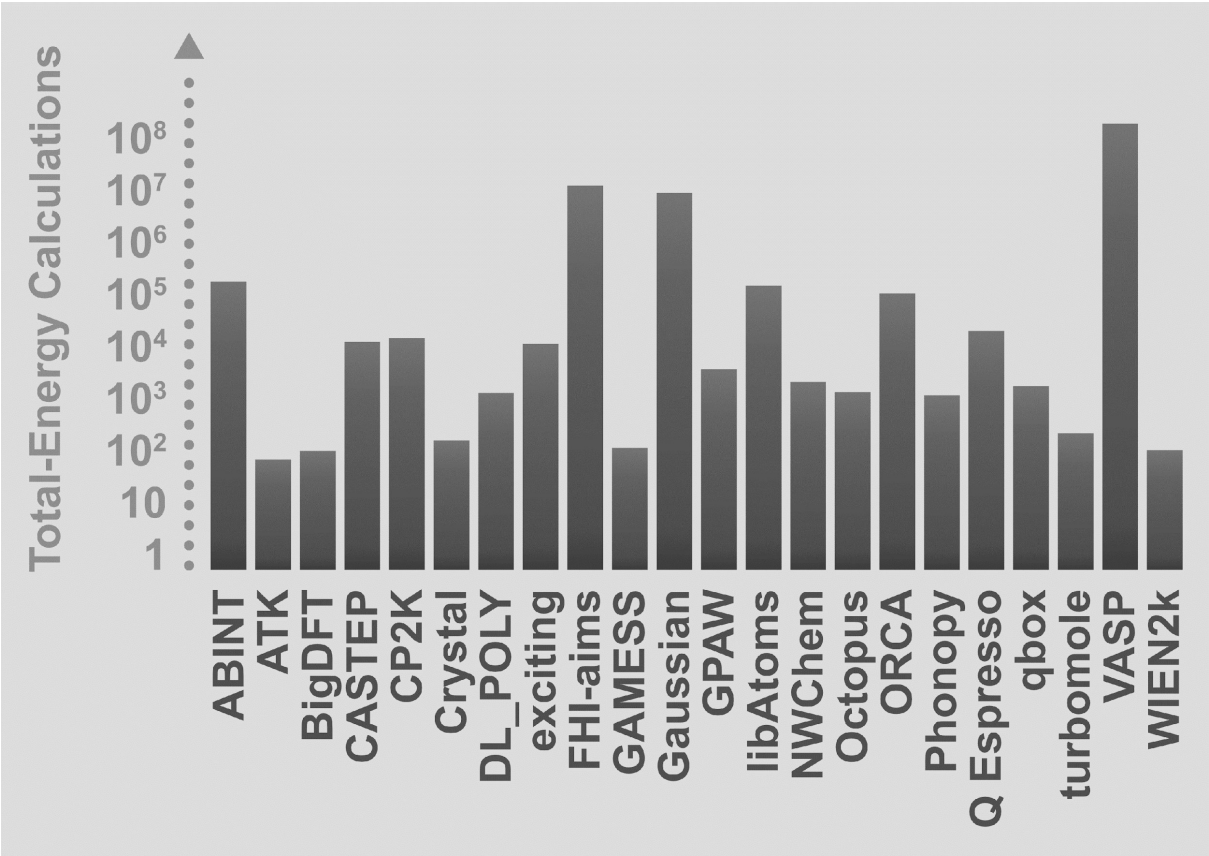
Same units, formats
>100 mio. calculations

billions of CPU core hours
at HPC centers, worldwide

Metadata items

several 1000

to uniquely describe all
the computed data



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Forerunners

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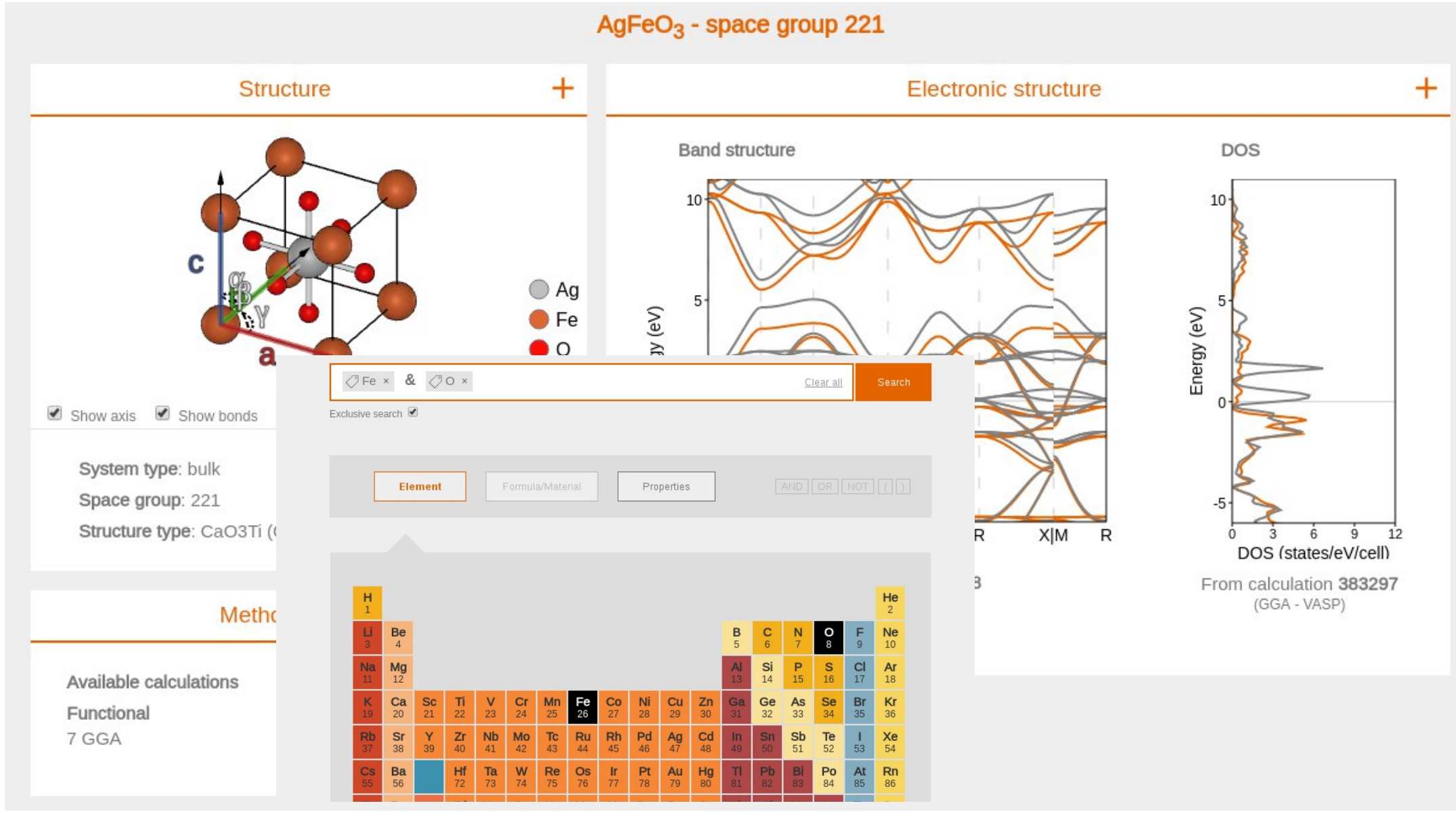
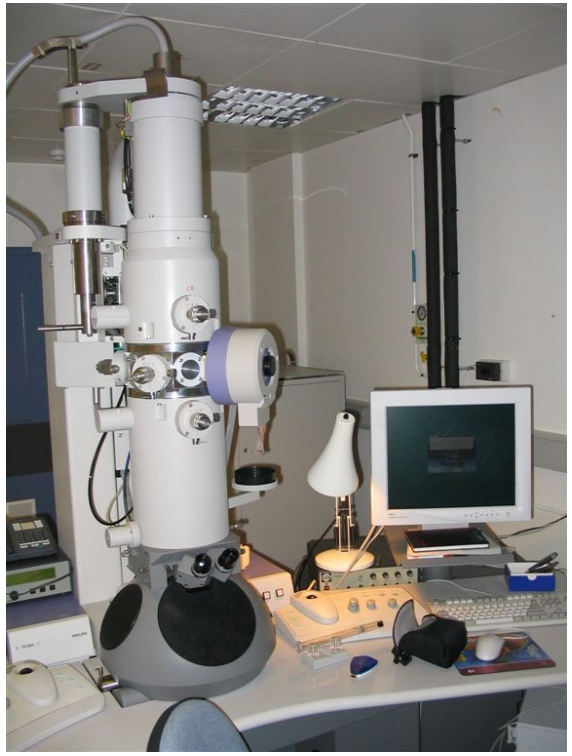
Added value – the NOMAD Encyclopedia

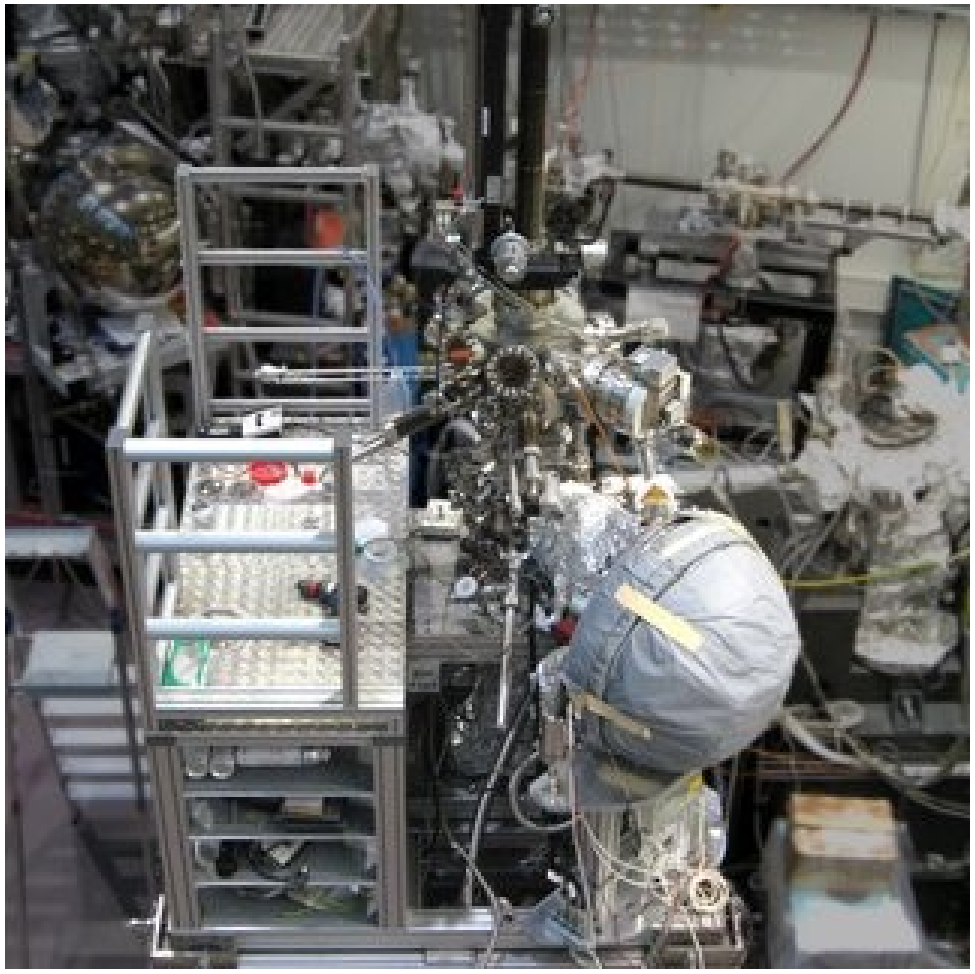


Experiment

Experiments

- Instrumentation
- Sample Preparation
- Sample Environment
- Monitors and Detectors
- Data Processing
- Notes





In comparison to large-scale experiments in physics,

solid-state physics is extremely heterogeneous.

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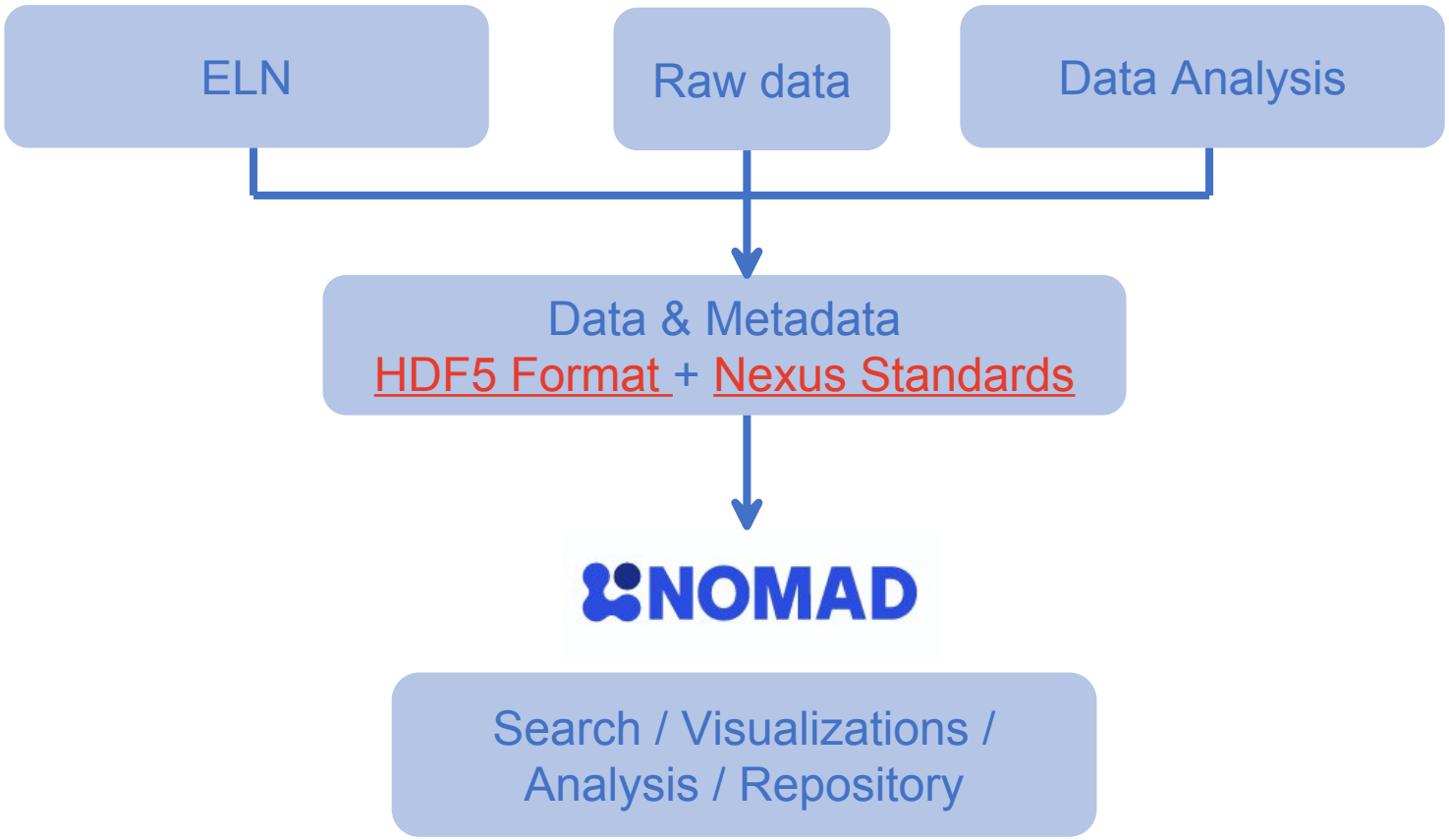
FAIRmat: experimental research data

Experiment



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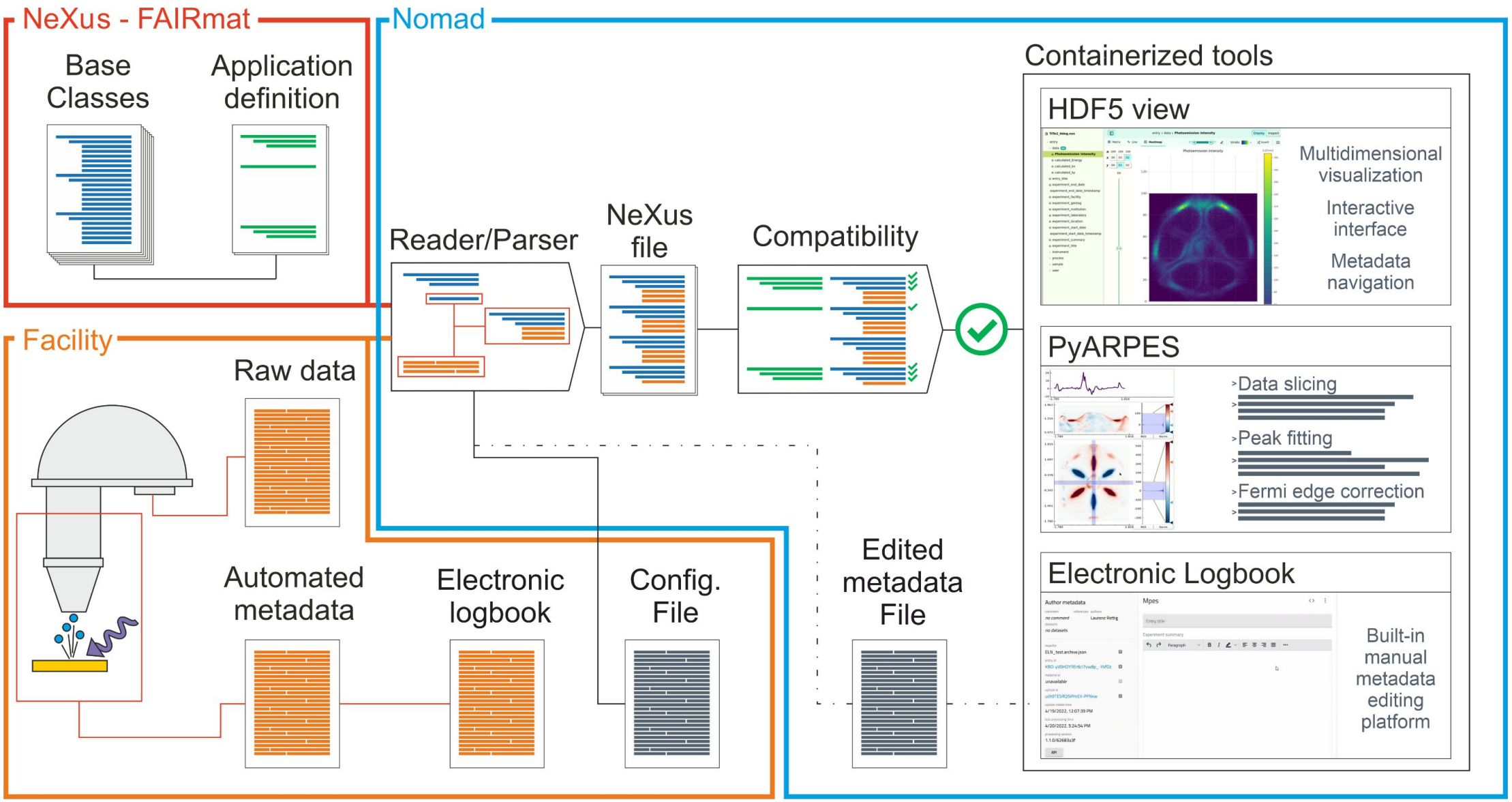
Photoelectron spectroscopy

What to do?



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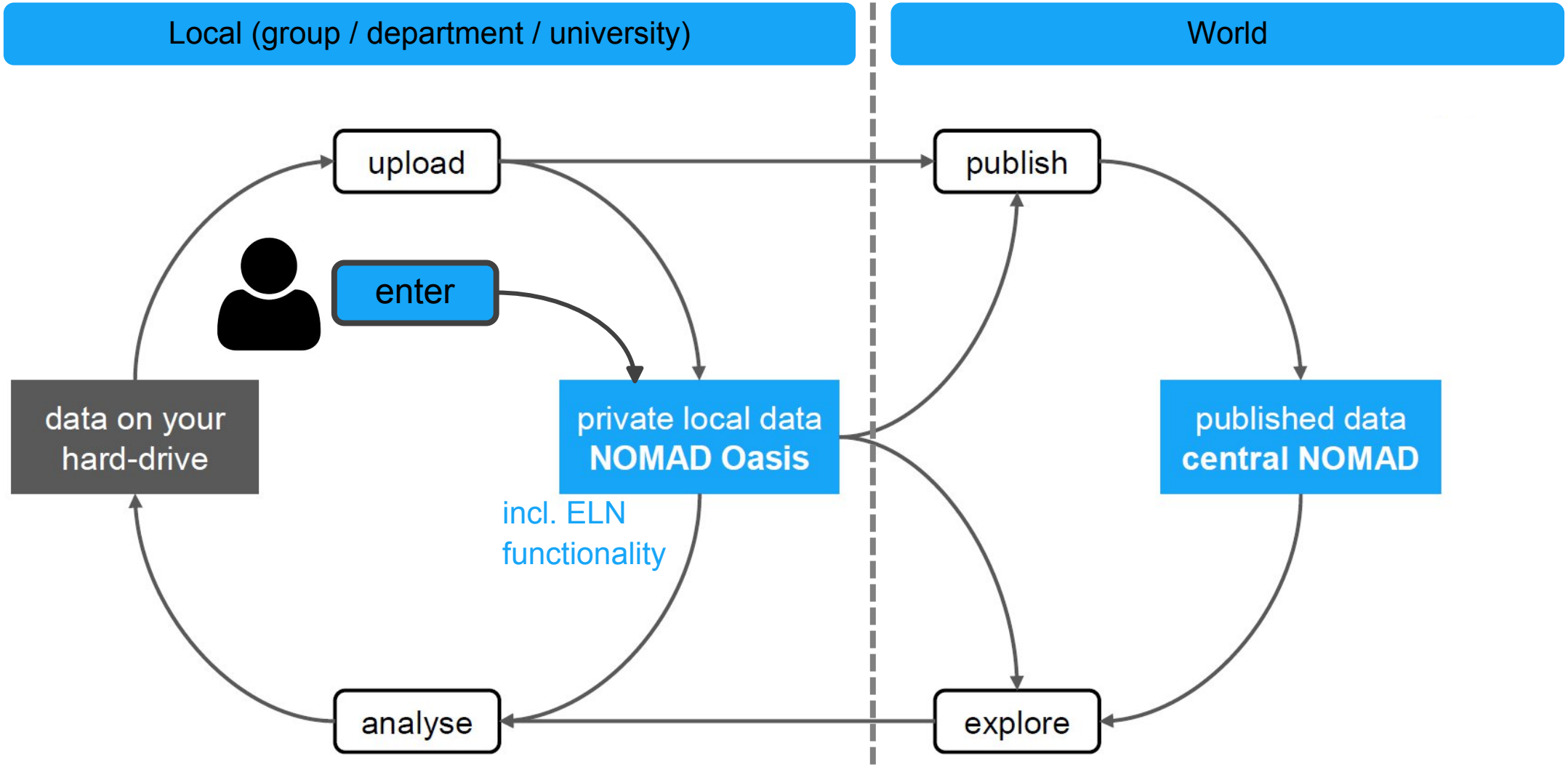
Local/global

NOMAD OASIS

NOMAD



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FAIRmat's fields of action for experimental physics

Experiment

- Configurable Lab Control Software
- Electronic Laboratory Notebooks (ELNs)
- FAIR-ready data management
- Community standards
- Involving technology partners
- Workflow in the NOMAD environment
- Broad data expertise

NOMAD CAMELS

NOMAD OASIS

NOMAD

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Application Definitions and the NeXus Standard

Sandor Brockhauser and the FAIRmat team

Center for Materials Science Data,
Humboldt-Universität zu Berlin, Germany

Data Modelling

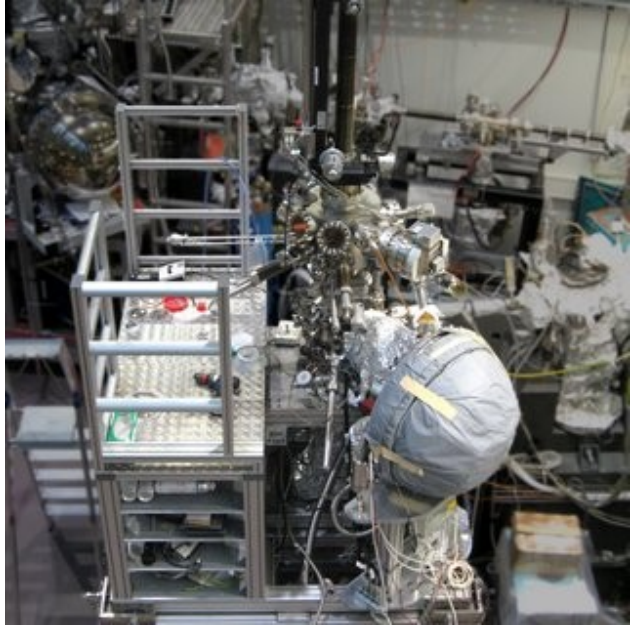
What to Model

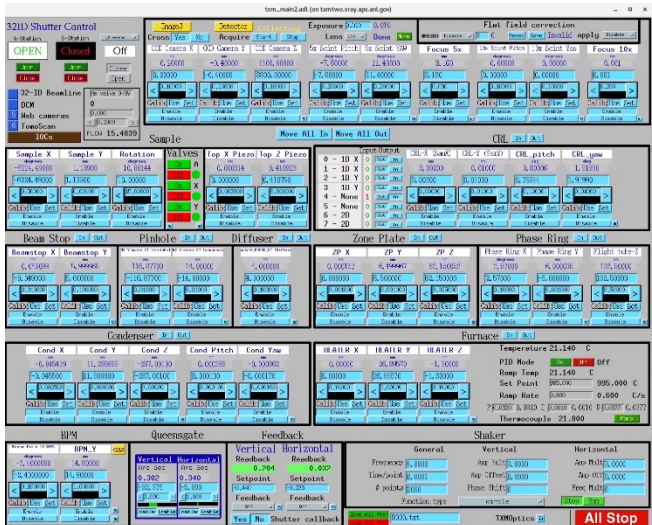
- **Experiment**
  - *Instrumentation*
  - *Sample* Preparation
  - Sample Environment
  - Monitors and Detectors
  - Data Processing
  - *Notes*

- **Observation**

in

- **Well-controlled environment**





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Data Modelling

What to Model

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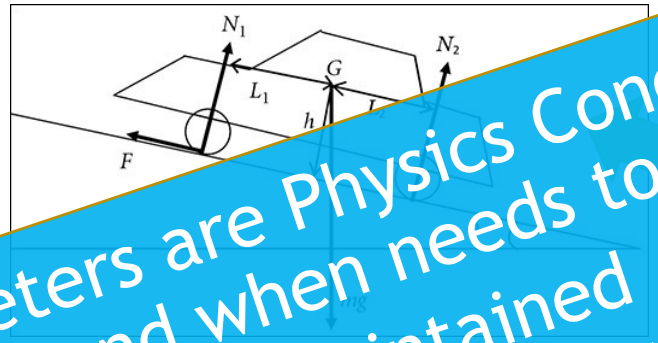
Experiment Data Models

Physics Model



Experiment Parameters are Physics Concepts to describe what and when needs to be
- Set or Maintained
- Measured or Calculated

Experiment
- start time, t_0
- duration, t
- distance, d

Slope
- angle, θ
- length, l

Car
- mass, m
- center of mass, $[G,h]$
- wheel positions, $[L_1,L_2]$
- force on wheels, $[N_1,N_2]$
- *resistive force*, F

Experiment Parameters

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Data Modelling

What to Model

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  - *Notes*

Conceptual Design Model

- ***Implementation independent Physics Model***
- *Note: Does not tell how exactly it is performed*

Samples:
- Composition
- Geometry
- History
- …

Sample Environment.:
- Temperature
- Pressure
- Magnetic field
- …

Instrument:
- ARPES experiment
- XRD
- XRF measurement
- I-V measurement
- …

Data Processing:
- Data correction
- Calibration
- Data reduction
- Scientific analysis
- …

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Data Modelling

Data-modelling for Reproducibility

- **Experiment**
  - *Instrumentation*
  - *Sample* Preparation
  - Sample Environment
  - Monitors and Detectors
  - Data Processing
  - *Notes*

Technical Design Model

- ***Implementation specific***
- *Not only Physics Model,*
  But also Technical Details

E.g.
what was the pressure in a chamber

how it has been produced and maintained

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Data Modelling

Data-modelling for Reproducibility

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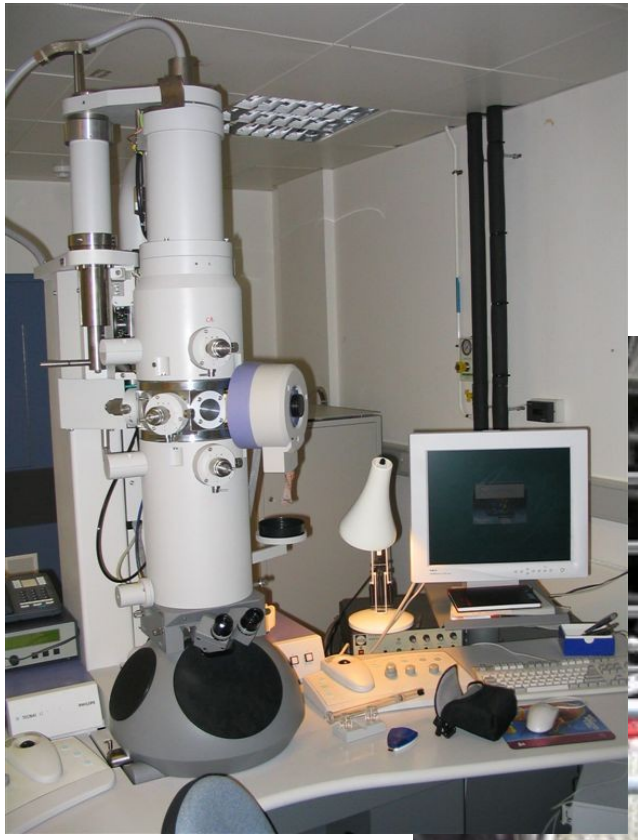

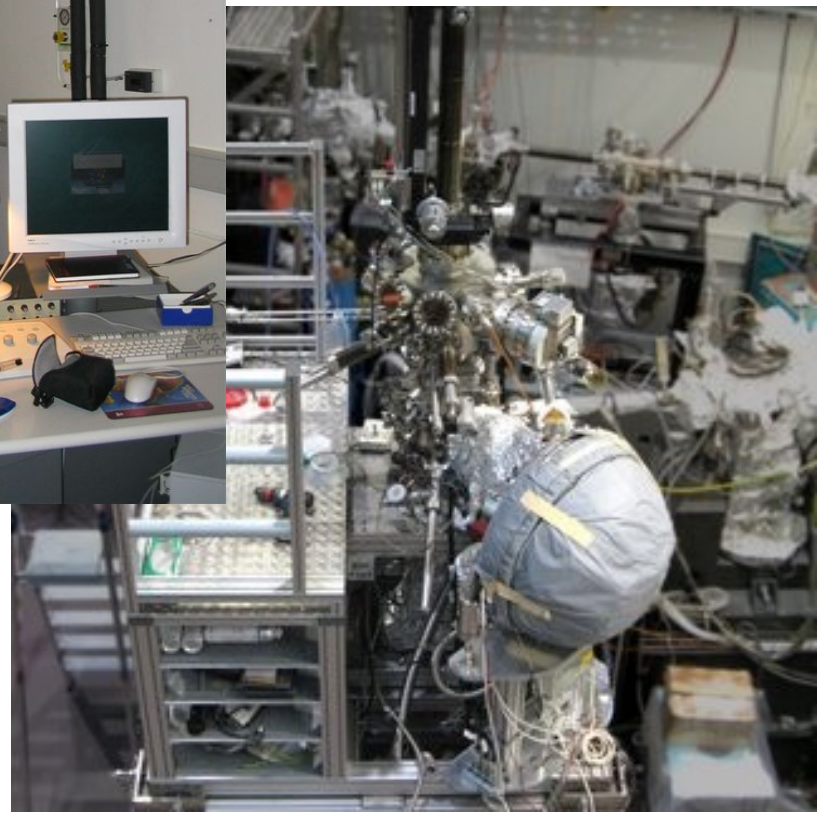

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Data Modelling

Data-modelling for Reproducibility

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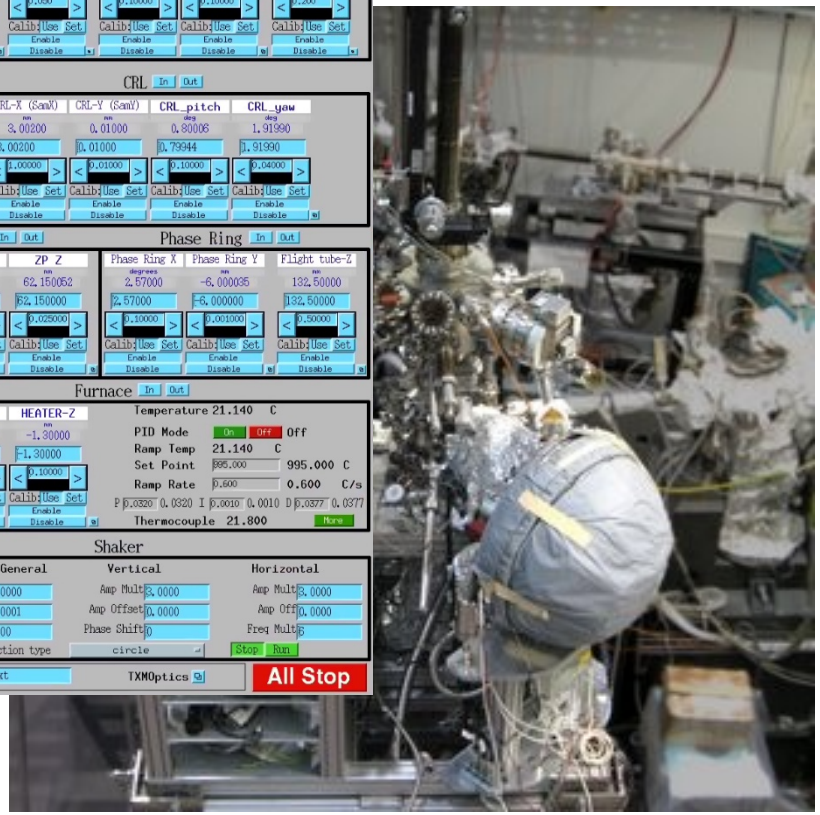

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Data Modelling

Data-modelling for Reproducibility

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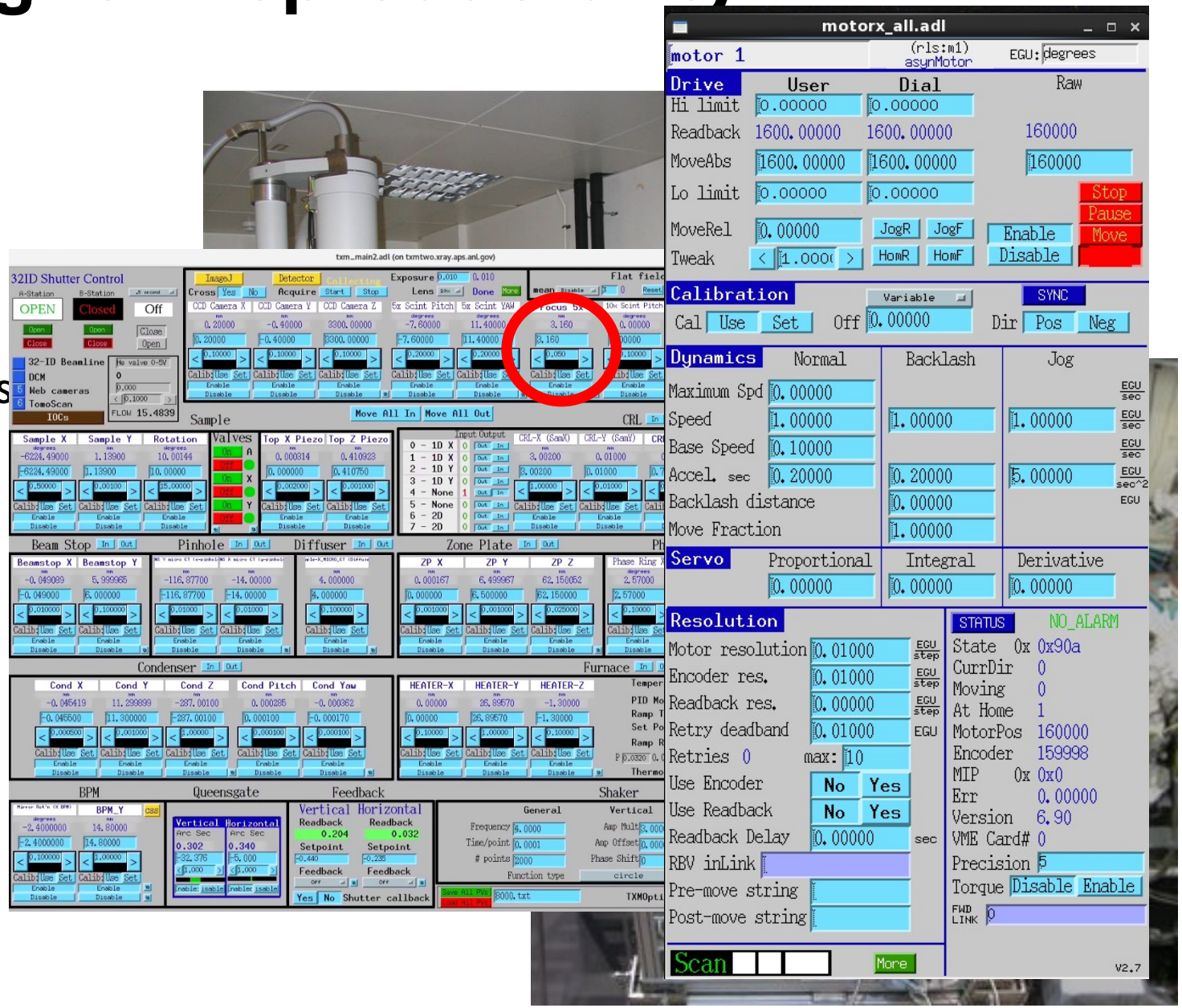

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Data Modelling

Data-modelling for Reproducibility

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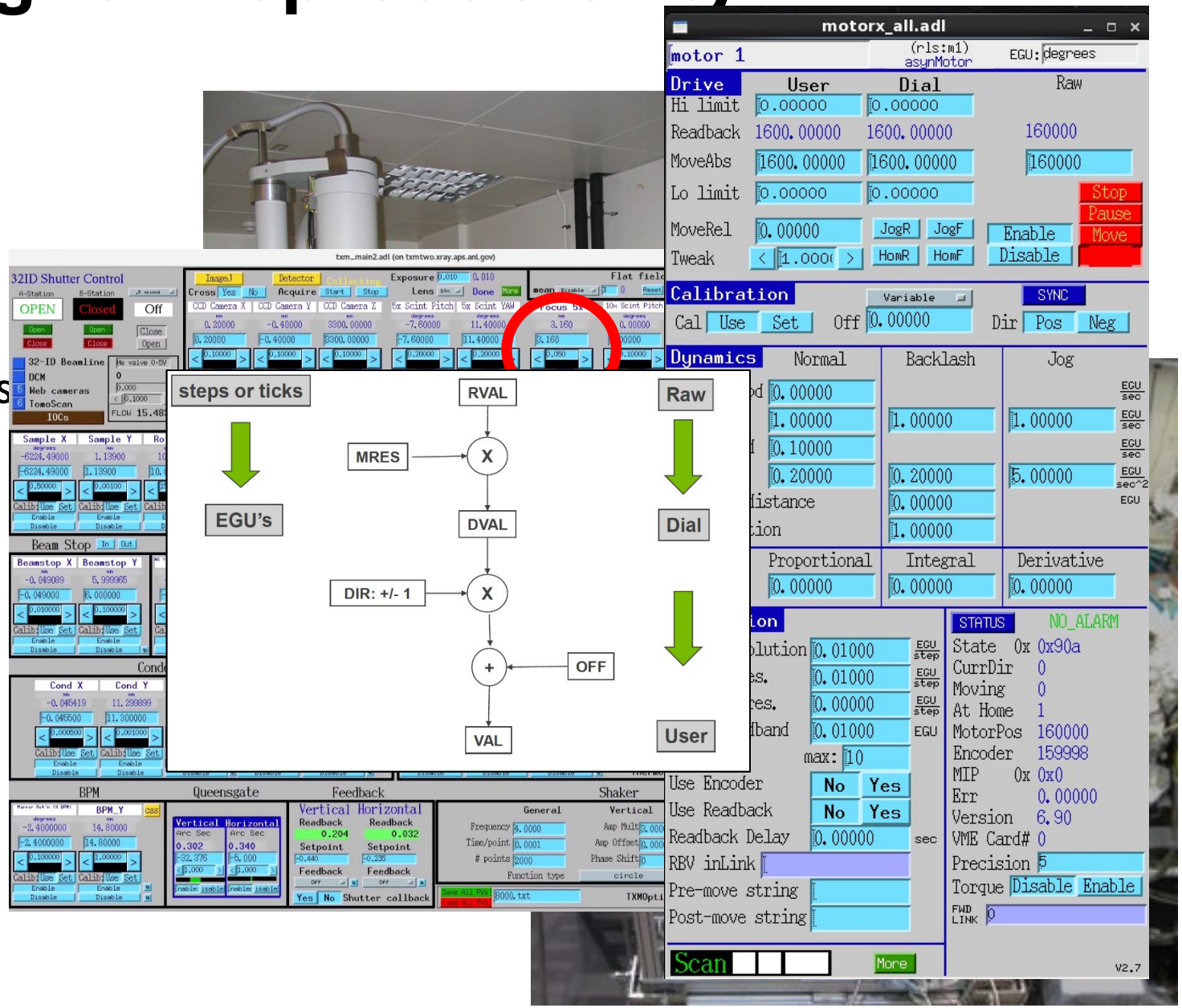
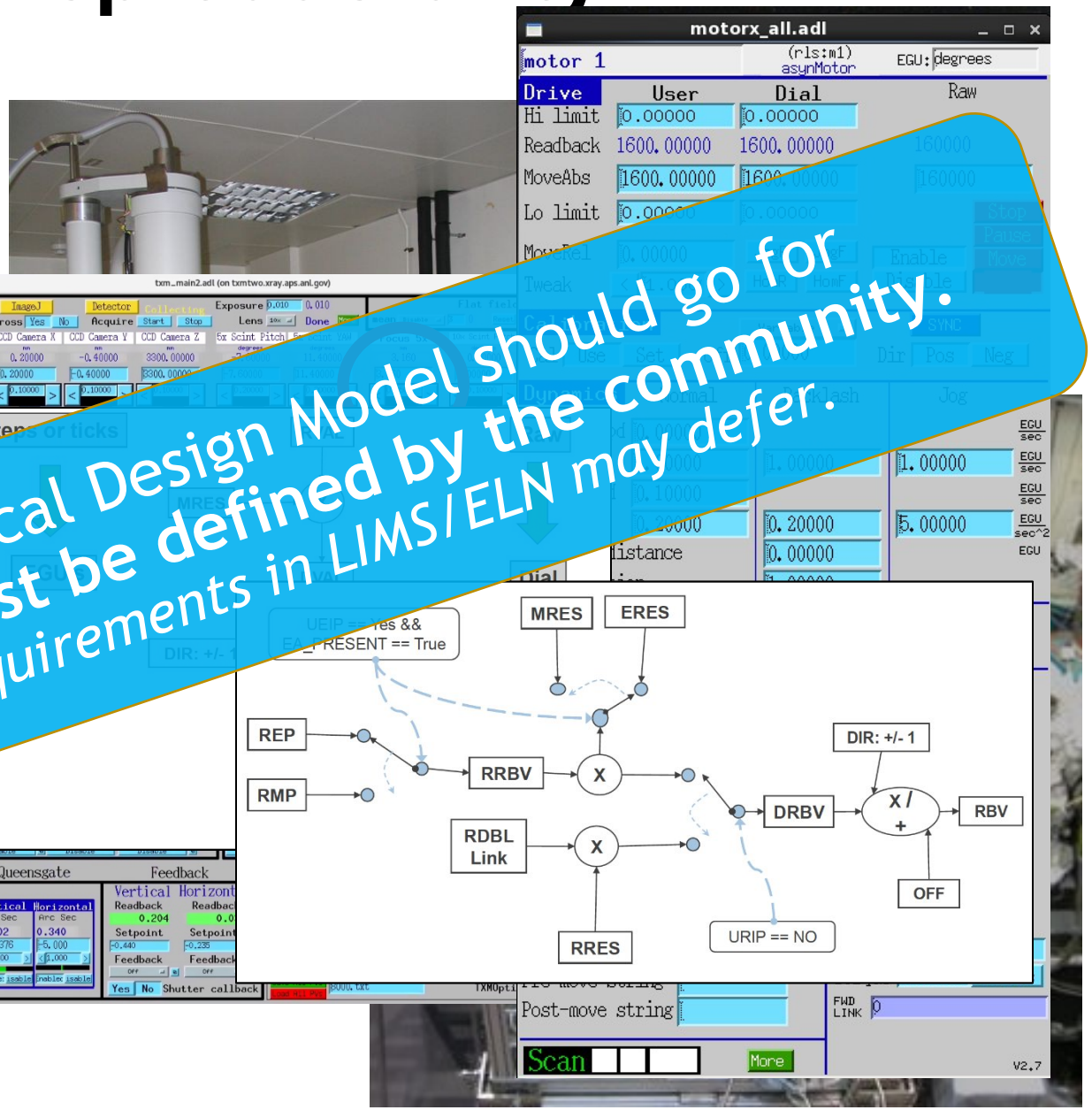


Data Modelling

Data-modelling for Reproducibility

- **Experiment**
  - *Instrumentation*
  - *Sample* Preparation
  - Sample Environment
  - Monitors and Detectors
  - Data Processing
  - *Notes*

How deep a Technical Design Model should go for reproducibility, **it must be defined by the community.** *Note that local requirements in LIMS/ELN may defer.*



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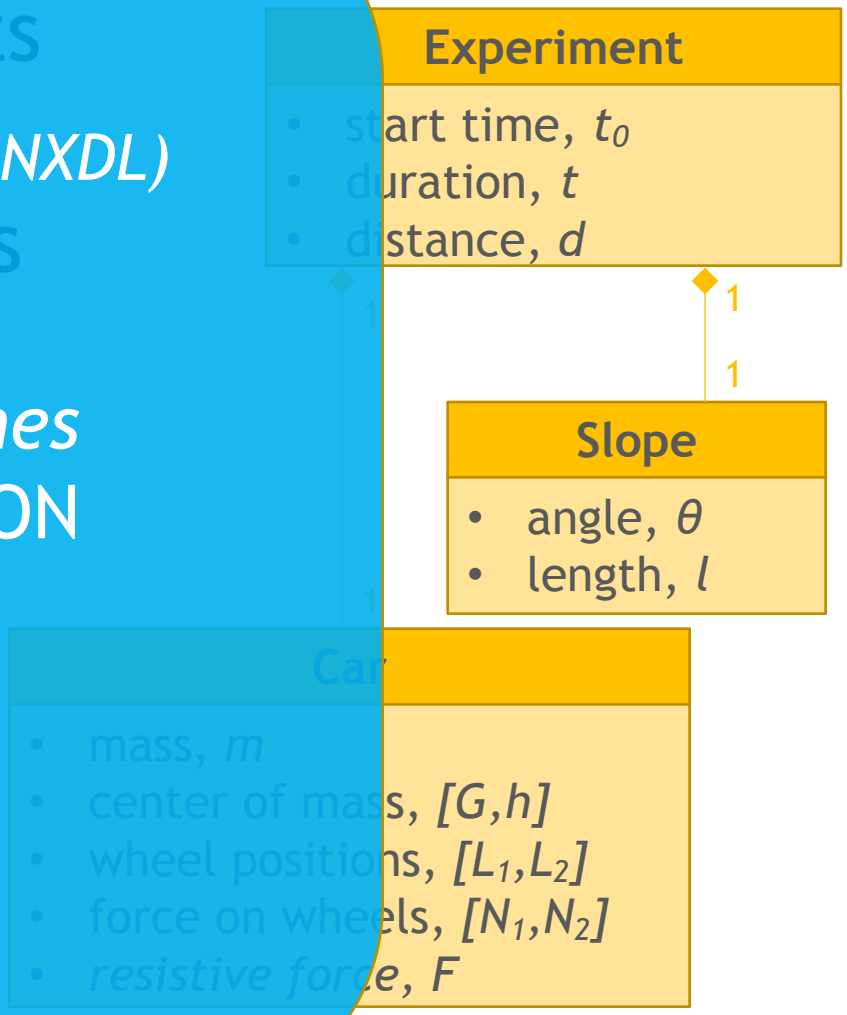
Data Modelling

Data-modelling for a Community

- Contr
- Clear
  conce
- Cardi
- Stand
- Comm
- Agree
- Commo

NeXus *https://www.nexusformat.org/*

- Extendable Data Modelling *(NXDL)*
- Automated documentation:
  HTML vocabulary - Humans
  OWL ontology OWL - Machines
- Community STANDARDIZATION process *(NIAC)*
- Tools
  - Verification and Validation
    NXDL *(schema)* ⟷ NXS *(data)*
  - Visualisation



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Standardisation

Data-modelling in NeXus

- Base Classes
  - NXinstrument, NXsample, NXprocess, NXuser NXnote
  - NXdetector, NXsensor, NXmonitor, NXbeam, NXmirror, NXgeometry,…

57

+106

- Application Definitions
  - NXarpes, NXxas, NXem, NXapm, NXmpes NXellipsometry, NXsensor_scan
    …

34

+38

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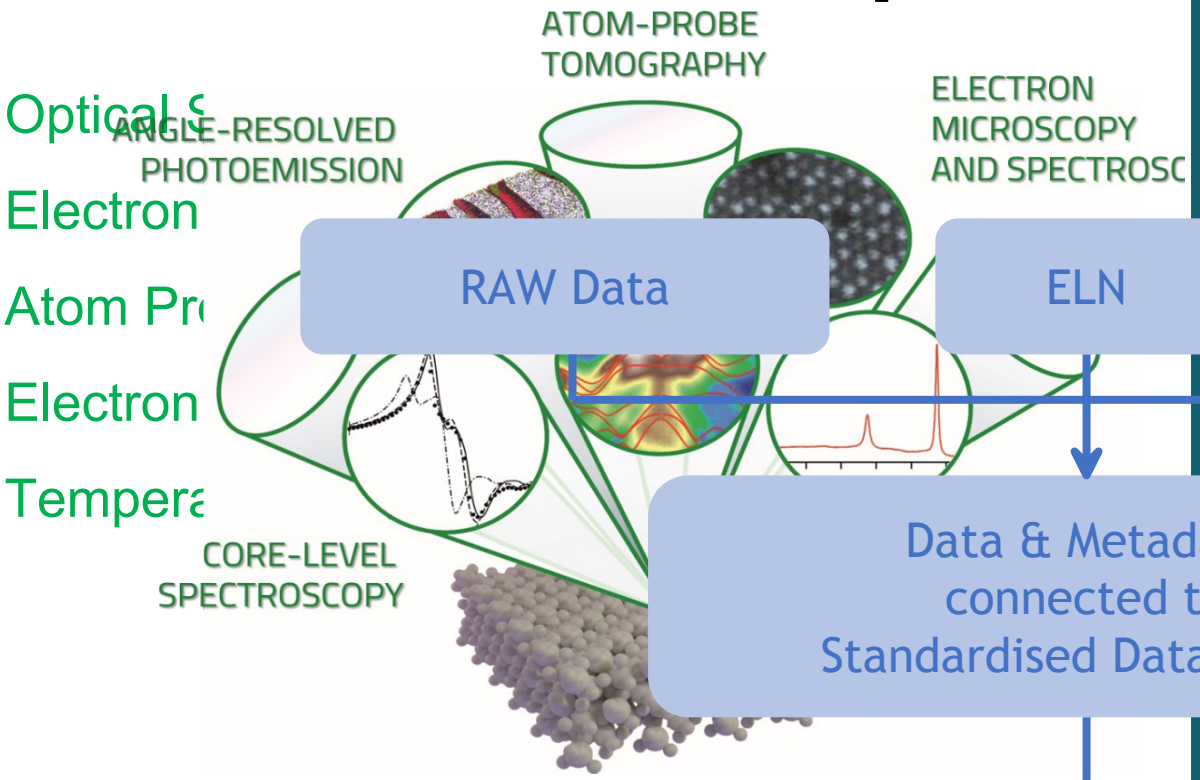
Techniques

Data Models for Experime



RAW Data

ELN

Data Analysis

Data & Metadata
connected to
Standardised Data Model

NOMAD
Search / Visualisation / Analysis

NeXus-FAIRmat

Proposal of NeXus expansion for FAIRmat data.

Watch

vigation

mat-NeXus Prop

s Documentation

Xus: User Manual

- Examples of writing and reading NeXus data files
- NeXus: Reference Documentation
- NeXus Community

Sample preparation

Nomad Remote Tools Hub (NORTH)

NXmpes

Status:

application definition, extends NXobject

Description:

This is the most general application definition for multidimensional photoelectron spectroscopy.

Symbols:

No symbol table

Groups cited:

NXaperture, NXbeam, NXcalibration, NXcollectioncolumn, NXdata, NXdetector, NXinstrument, NXmanipulator, NXnote,

title: (required) NX_CHAR

start_time: (required) NX_DATE_TIME

Datetime of the start of the measurement.

definition: (required) NX_CHAR

Obligatory value: `NXmpes`

@version: (required) NX_CHAR

USER: (required) NXuser

Contact information of at least the user of the instrument or the investigator who performed this experiment. Adding multiple users if relevant is recommended.

name: (required) NX_CHAR

Name of the user.

affiliation: (recommended) NX_CHAR

Name of the affiliation of the user at the point in time when the experiment was performed.

address: (recommended) NX_CHAR

Full address (street, street number, ZIP, city, country) of the user's affiliation.

email: (required) NX_CHAR

Email address of the user.

orcid: (recommended) NX_CHAR

Author ID defined by https://orcid.org/.

INSTRUMENT: (required) NXinstrument

energy_resolution: (required) NX_FLOAT {units=NX_ENERGY}

SOURCE: (required) NXsource

The source used to generate the primary photons. Properties refer strictly to parameters of the source, not of the output beam. For example, the energy of

https://fairmat-nfdi.github.io/nexus-fairmat-proposal/

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Roadmap

Data-modelling for a Community

- Initial Proposal with Examples
- Community Feedbacks
- Common Proposal with Technology Partners
- Standardisation

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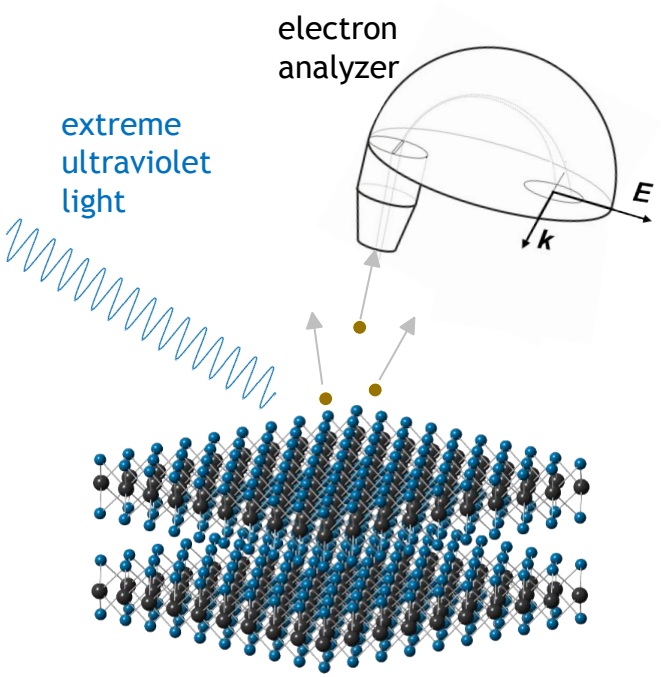
NXmpes: structure and example in NOMAD

Laurenz Rettig and the FAIRmat team

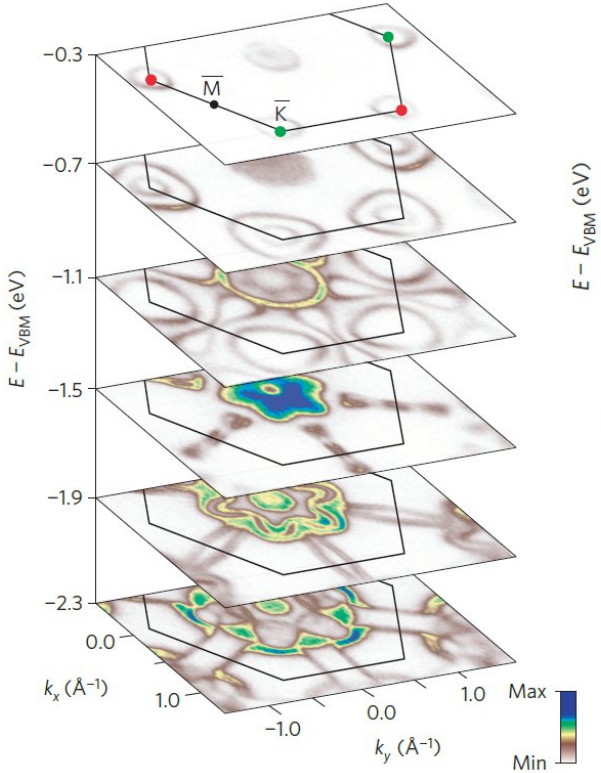
Fritz Haber Institute of the Max Planck Society, Berlin

Multidimensional photoemission spectroscopy

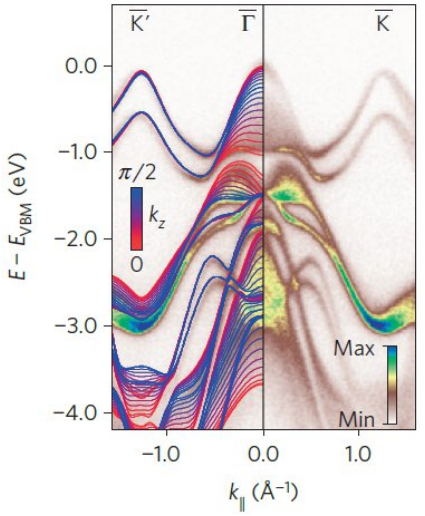
experiment



data: band mapping

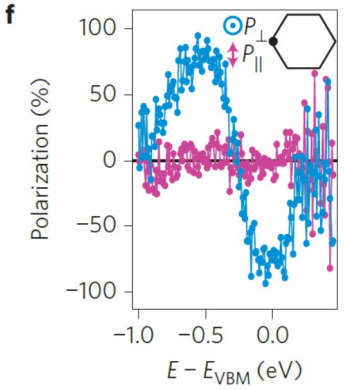


energy band dispersion



Also possible:

Spin polarization



Example: valence band structure of WSe_2
Riley *et al*, Nature Phys. 10, 835 (2014)

- momentum ***k*** *(k_x, k_y)*
- energy *E*
- spin ***S***

} "multidimensional PES" (more than 3D)

Schönhense et al., New J. Phys. 20, 033004 (2018)

Dataformat

FAIRmat

Dataformat

Extending the parameter space

$$I \rightarrow I(\mu_{mat}, E, k_x, k_y, S, t, \omega_p, \sigma, x, y, T, \ldots)$$

- Dependence on materials and preparation procedures (μ_{mat})
- Spin-resolving detectors: S
- Photon energy and polarization ω_p
- Electronic structure of **non-equilibrium states** (time-resolved ARPES): time t, pump/probe photon energy ω_p, polarization, …

à Dependence on sample parameters:
strain σ, sample position x,y, temperature T

- …

à huge parameter space
à Mostly only subspace both experiment-tally accessible and interesting

Goal to develop flexible, community-driven data + metadata format for such MPES data

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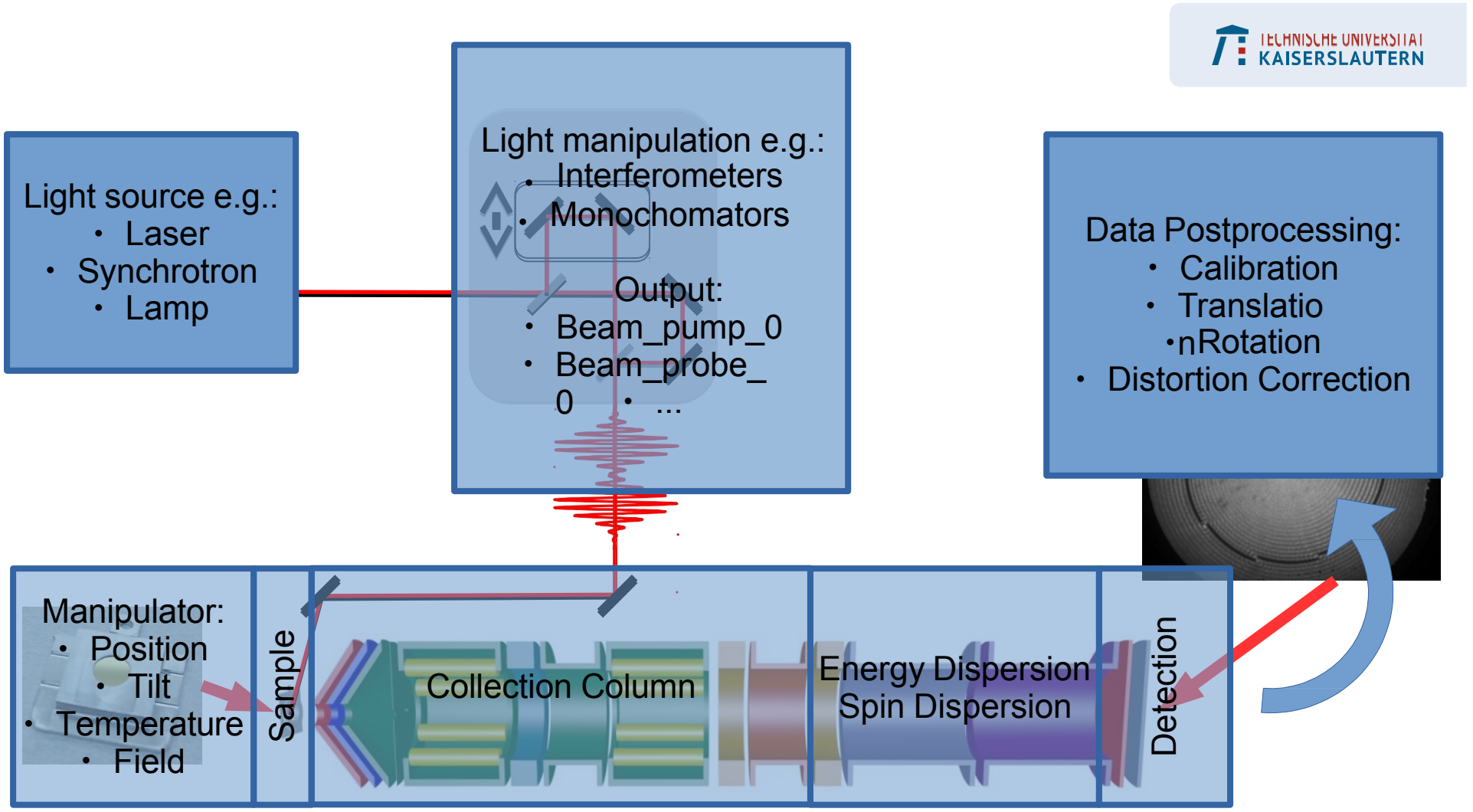
Dataformat

Ingredients of a photoemission experiment



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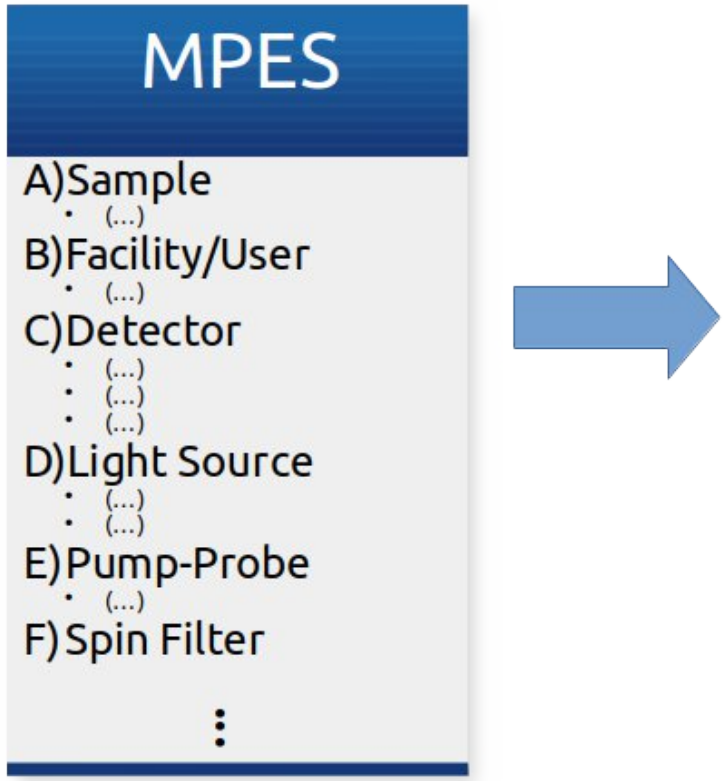
Hierarchy of application definitions

Universal MPES
metadata dictionary
(in NeXus: base classes)



Dataformat

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Dataformat

Simplify analysis

NeXus

Look-up Dictionary

Application definition

Facility

Raw data

Raw metadata

Parser

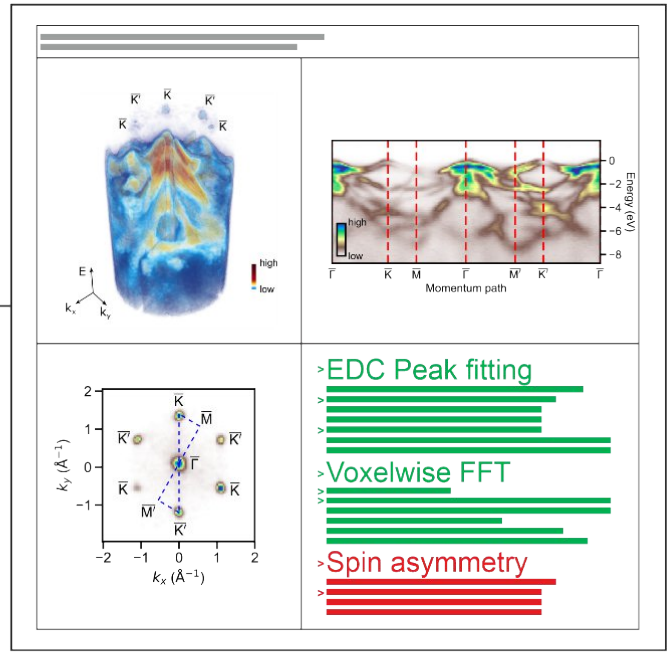
NeXus file

Compatibility

Hierar-chical structure, F.A.I.R. compliant

Modularity: a common platform deploys application-dependent tools

Automated access



Figures from: Xian, R. P. et al. arXiv:1909.07714 (2019).

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Dataformat

Application definition: NXmpes

Application Definitions

We created two new application definitions:

NXmpes:
A general appdef with minimalistic metadata requirements, apt to describe all photemission experiments.

Base Classes

We developed entirely new base classes:

NXelectronanalyser:
A base class to describe electron kinetic energy analizers. Contains the collective characteristics of the instrument such as energy resolution, and includes the following subclasses:

NXcollectioncolumn:
Base class to describe the set of electronic lenses in the electron collection column (standard, PEEM, momentum-microscope, etc.).

NXenergydispersion:
Base class to describe the energy dispersion sytem (hemispherical, time-of-flight, etc.).

NXspindispersion:
Base class to describe the set of electronic lenses in the electron collection column.

NXmanipulator:
A base class to describe the complex manipulators used in photoemission experiments, often with > 4 degrees of freedom, cryogenic cooling and other advanced features.

FAIRmat

https://fairmat-nfdi.github.io/nexus-fairmat-proposal

Application definitions and base classes

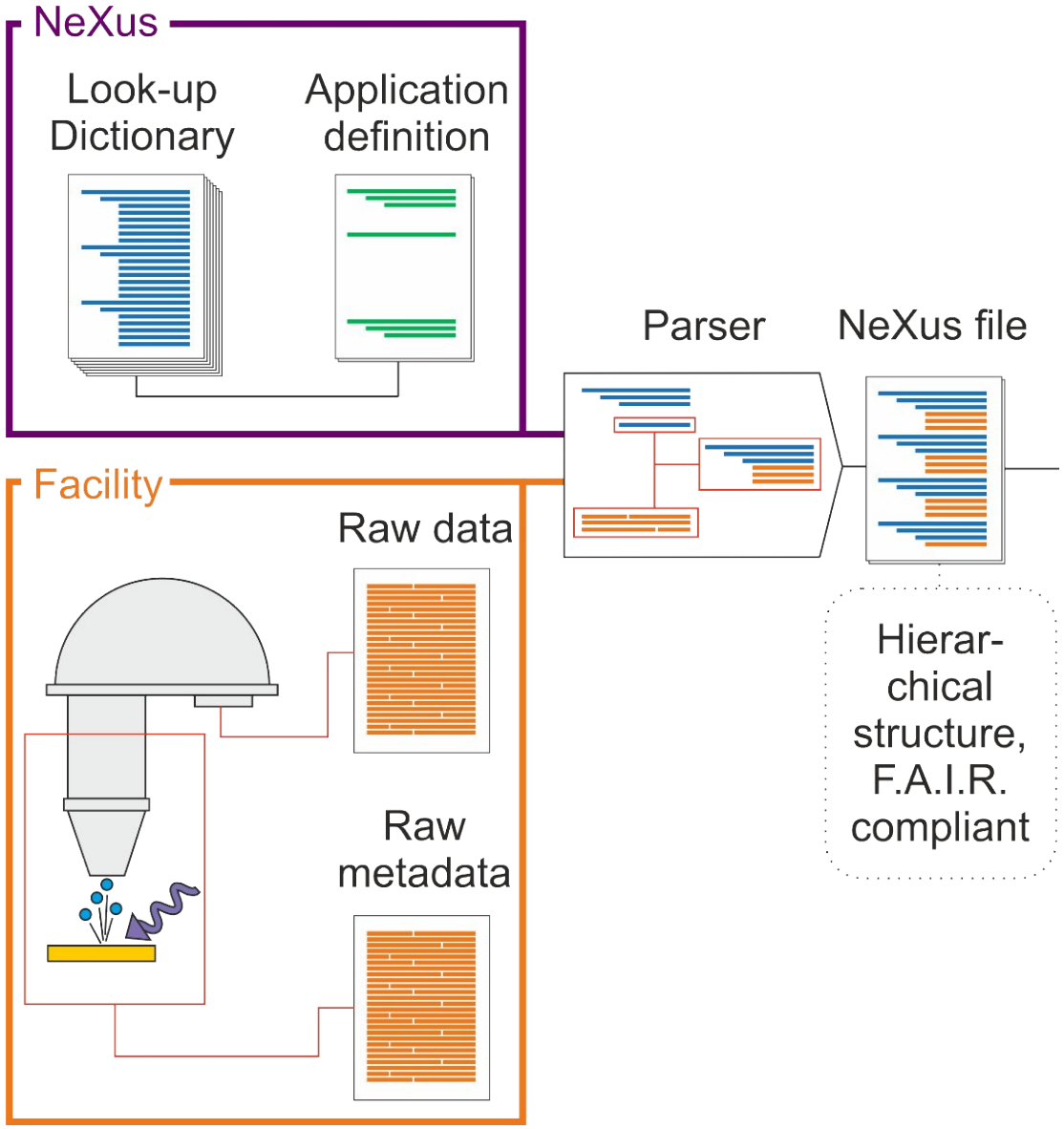
Dataformat

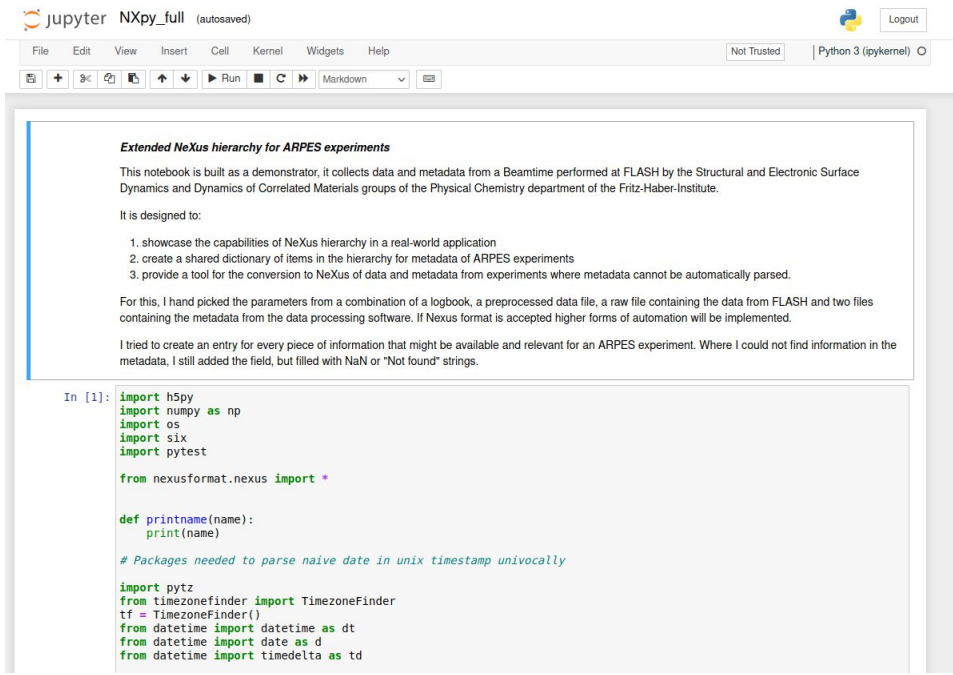
FAIRmat

Detailed discussion of base classes and application definitions tomorrow morning.

Dataformat

Practical examples





Converter/parser

- reads data + metadata from experiment
- Assigns them to the correct NXmpes paths
- Creates a verified NeXus file according to a provided application definition

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Reader + parser structure

Data.h5

- Volumetric data + axes
- Tree of metadata

config_file.json

```
"/ENTRY[entry]/definition": "NXmpes",
"/ENTRY[entry]/definition/@version": "None",
"/ENTRY[entry]/title": "@attrs:metadata/entry_title",
"/ENTRY[entry]/start_time": "@attrs:metadata/timing/acquisition_start",
"/ENTRY[entry]/experiment_institution": "Fritz Haber Institute - Max Planck Society",
"/ENTRY[entry]/experiment_facility": "Time Resolved ARPES",
"/ENTRY[entry]/experiment_laboratory": "Clean Room 4",
"/ENTRY[entry]/entry_identifier": "@attrs:metadata/entry_identifier",
"/ENTRY[entry]/end_time": "@attrs:metadata/timing/acquisition_stop",
"/ENTRY[entry]/duration": "@attrs:metadata/timing/acquisition_duration",
"/ENTRY[entry]/duration/@units": "s",
"/ENTRY[entry]/collection_time": "@attrs:metadata/timing/collection_time",
"/ENTRY[entry]/collection_time/@units": "s",

"/ENTRY[entry]/USER[user]/name": "@attrs:metadata/user0/name",
"/ENTRY[entry]/USER[user]/role": "@attrs:metadata/user0/role",
"/ENTRY[entry]/USER[user]/affiliation": "@attrs:metadata/user0/affiliation",
"/ENTRY[entry]/USER[user]/address": "@attrs:metadata/user0/address",
"/ENTRY[entry]/USER[user]/email": "@attrs:metadata/user0/email",
```

Python-based reader interprets data file, based on the information of the config file.
Additional information from other meta data sources.
A custom reader for each file type/technique, but a common infrastructure.

Dataformat

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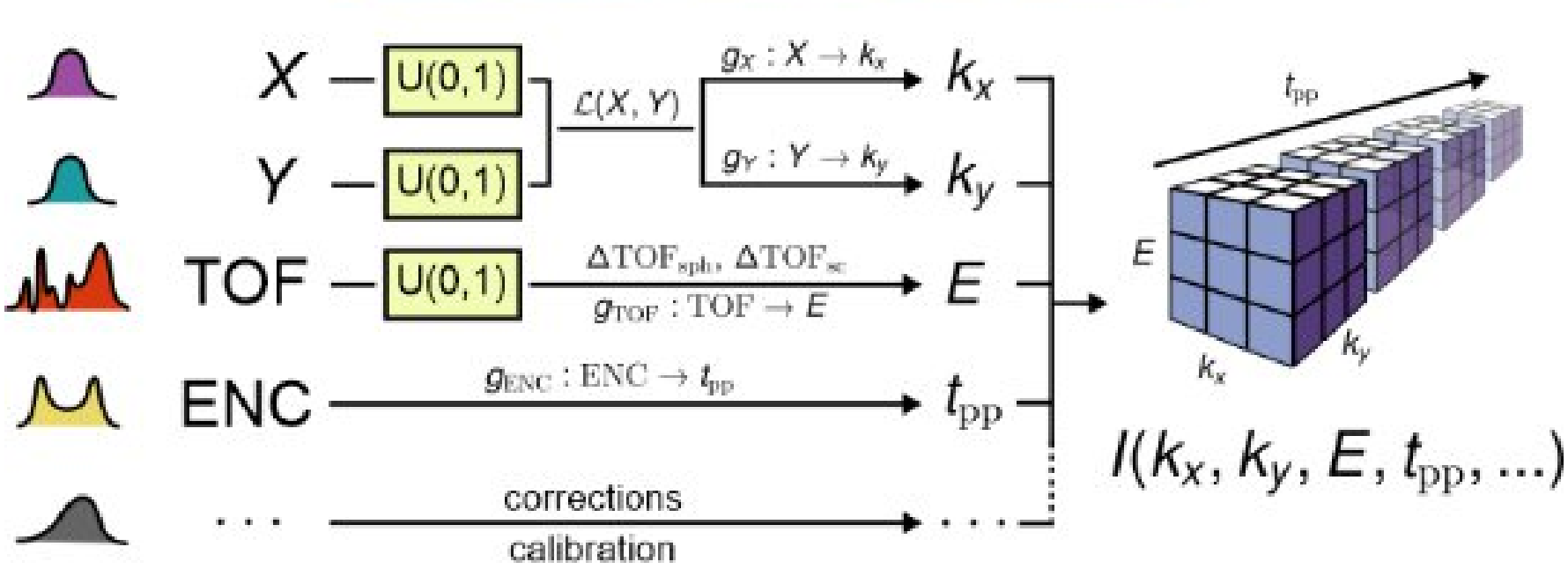
Dataformat

Single event data processing

Time-resolved Photoemission data, recorded with SPECS METIS 1000 momentum microscope.
Single-event data calibrated and converted into multidimensional volumetric data.



Xian, et al., Scientific Data 7, 442 (2020)
https://mpes.science/

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Practical examples

Dataformat

LIVE Example on NOMAD

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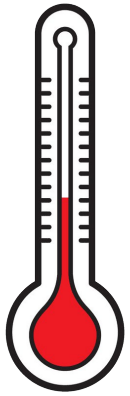
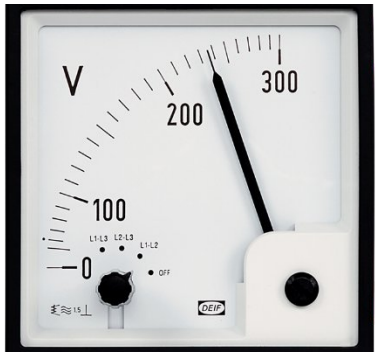
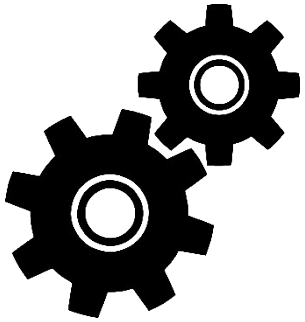
Sources of metadata

Machine-generated meta data:






Automated recording and assigning to respective fields

"Soft" meta data need structured user input
e.g.:

- User who does the experiment
- Name and composition of the sample
- …

Requires **structured electronic lab notebook** or **user interfaces**

Structured and configurable ELN capabilities available in NOMAD

Dataformat

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MPES reader infrastructure

Lukas Pielsticker and the FAIRmat team

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Data Converters

Storage of photoemission data

SURFACE CONCEPT

ThermoFisher SCIENTIFIC

FOCUS

scientaomicron

SPECS™

…

Problem:

- Each technology partner has its own file format
- Within a technology partner the file format can be different

→ How to go from vendor-specific format to structured NXmpes data?

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Data Converters

NXmpes readers - objectives

- Data- and vendor agnostic Nxmpes files
→ **Parsers, normalizers, and converters**

- Data curation and quality assessment
→ **Validation** against NeXus-FAIRmat application definitions

- Capture all **metadata** to produce valid NXmpes files
→ Instrument settings, ELN data, temperature/pressure logs, …

- Interoperability and repeatability
→ Calibration, transmission functions, etc.
→ Storing **raw, processed, and analysed** data

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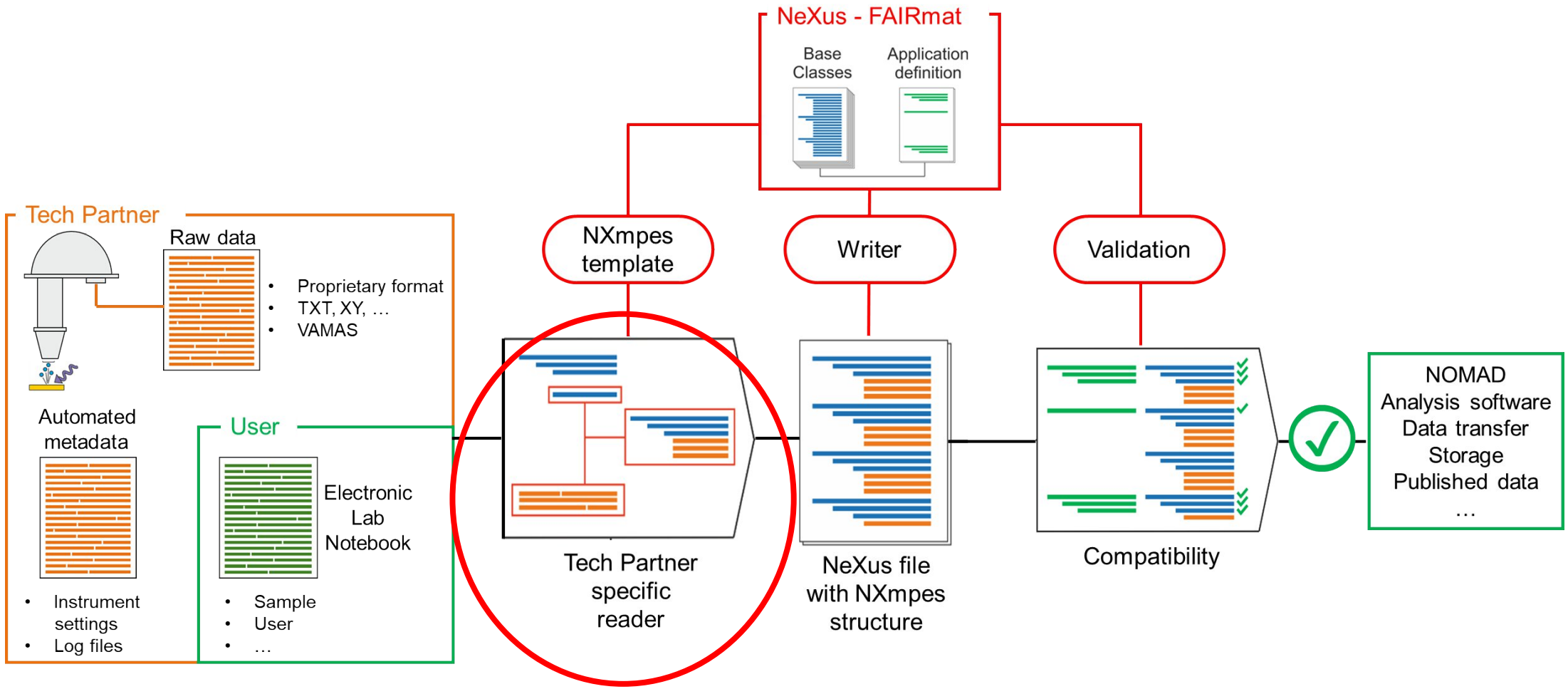
Data Converters

From vendor-specific data to NXmpes



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Data Converters

Link to technology partners and the community

Choice for technology partners

1. Full integration with native support to read/write NXmpes
2. Integrated option to directly export to NXmpes
3. Provide external parser to convert to NXmpes

What needs to be discussed

- Which (meta-)data would we like to store in NXmpes?
  → Discussion of MPES application definition (tomorrow, 9 am)
- Which are the limits of open data?
- Metadata sources
- Do the technology partners need support?

What we can provide

- Detailed description of application definitions
- Reader examples
- Validation infrastructure

NeXus-FAIRmat application definitions:
https://fairmat-nfdi.github.io/nexus-fairmat-proposal/

Example readers and validators:
https://github.com/FAIRmat-NFDI/pynxtools

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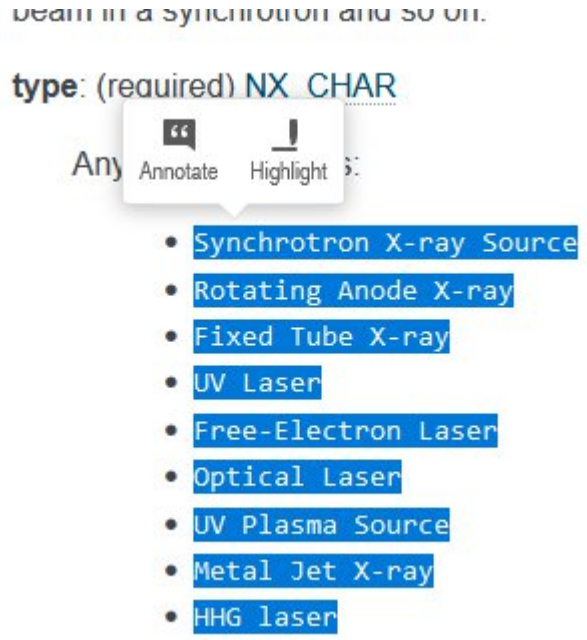
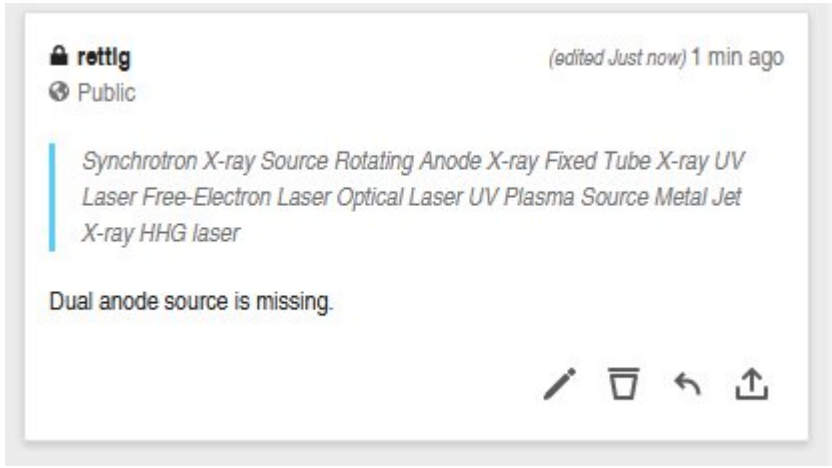
How to contribute further





We are very happy to integrate your input into the Nxmpes and base classes definitions!

https://fairmat-nfdi.github.io/nexus-fairmat-proposal

Dataformat

Discussion points and questions:

- Do our proposed definitions fit your use case? What is missing, needs to be changed?
- Requirement/optionality of parameters
- Which parameters can be provided, which not?
- How are “soft” metadata acquired e.g. in vendor software?
- What are legal constraints, IP restrictions?
- Interplay of user-specific data and instrumental metadata
- …

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