Data-Modelling Patterns for Experimental Characterisation

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FAIRmat

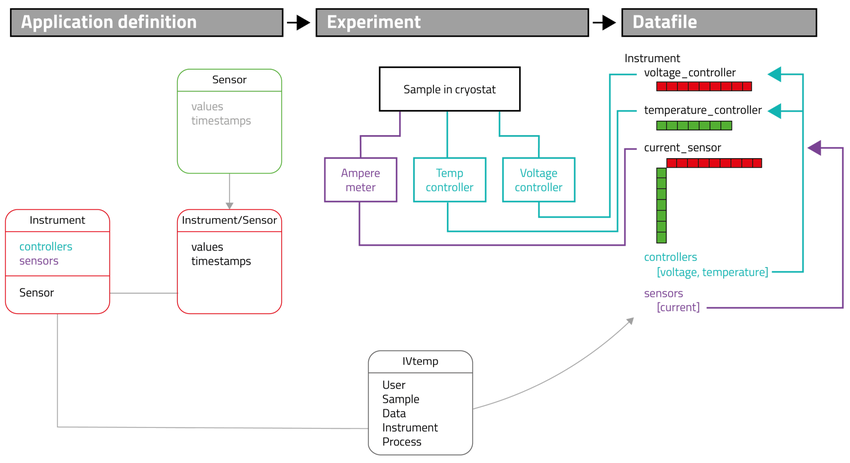
Necessity

- Scientific data are a signficant raw material of the 21st century.
- Most data are never used in publications.
- ***FAIRmat*** represents a broad community of numerous researchers from universities and leading institutions in Germany.
- To exploit the true value of scientific data, a **FAIR** – **F**indable, **A**ccessible, **I**nteroperable, and **R**e-purposable – data infrastructure (DI) is a must [1].

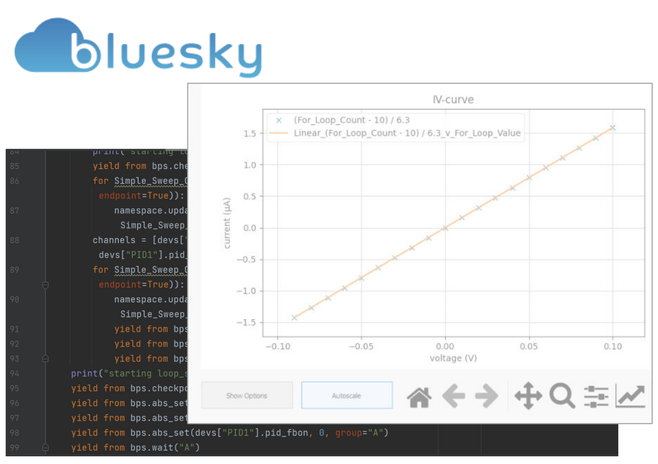
Objectives

- Build data handling and easy data modelling routines for experimental sciences.
- Building of a data-centric ontology for physical sciences, reaching out to chemistry, engineering, industry, and society.
- Usage of our metadata schema from our data infrastructure platform *NOMAD*.
- Keep compatibility with already established community standards, e.g., the *NeXus* format [2,3].

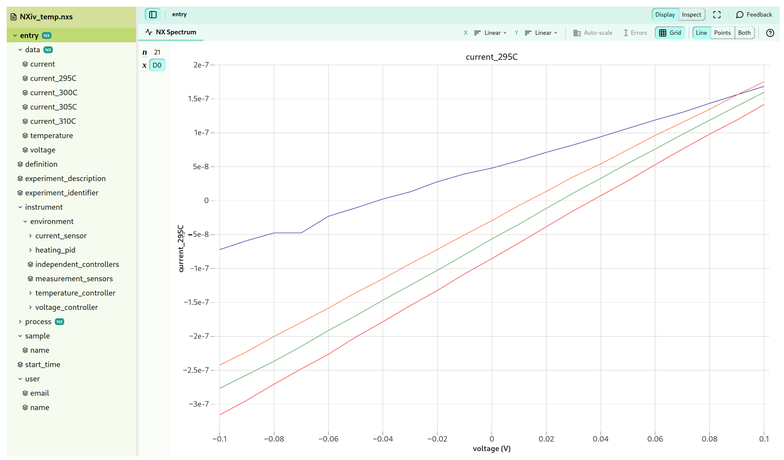
Data Modeling + Acquisition + Visualisation in IV_temp *(Temperature dependent IV measurement)*



Reuse of Sensor_Scan modeling arbitrary scan axes under Instrument. The fields independent controllers and measurement sensors refer to sensors acting as scanning axes or measured values.



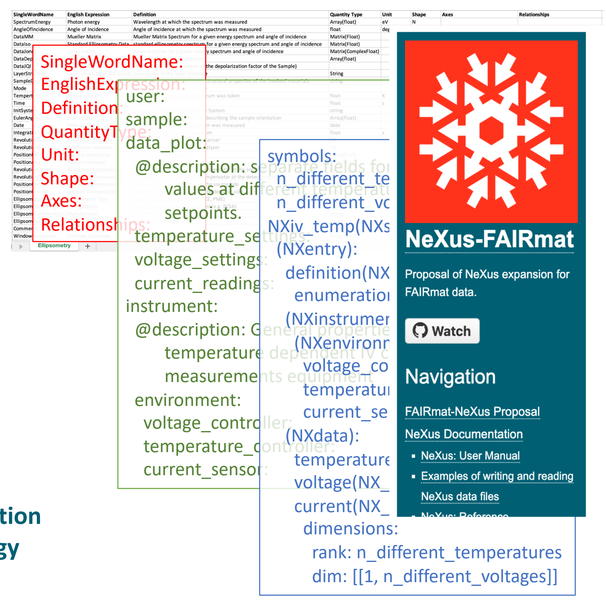
Control and Data Acquisition systems (*EPICS* / *Bluesky* [4]) can be configured to store data according to the specified data model. IV_temp is expressed in *NeXus* as NXiv_temp allowing standardized data stored in hdf5.



Generic visualization tool *h5web* provides plots automatically according to the specification in the data model. Temperature-dependent IV-curve measurements are plotted with different colors.

Generic data modelling patterns

- Physics Model
- Controlled Vocabulary
- Hierarchical modelling
- NeXus Definitions
- **Documentation and Ontology**



NXiv_temp

Status:

application definition, extends NXsensor_scan

Description:

Application definition for temperature-dependen

In this application definition, times should be spe

This is the application definition describing temp measurements. For this a temperature is set. Af sweep is performed. For each voltage a current perature is set and an IV measurement is perfor

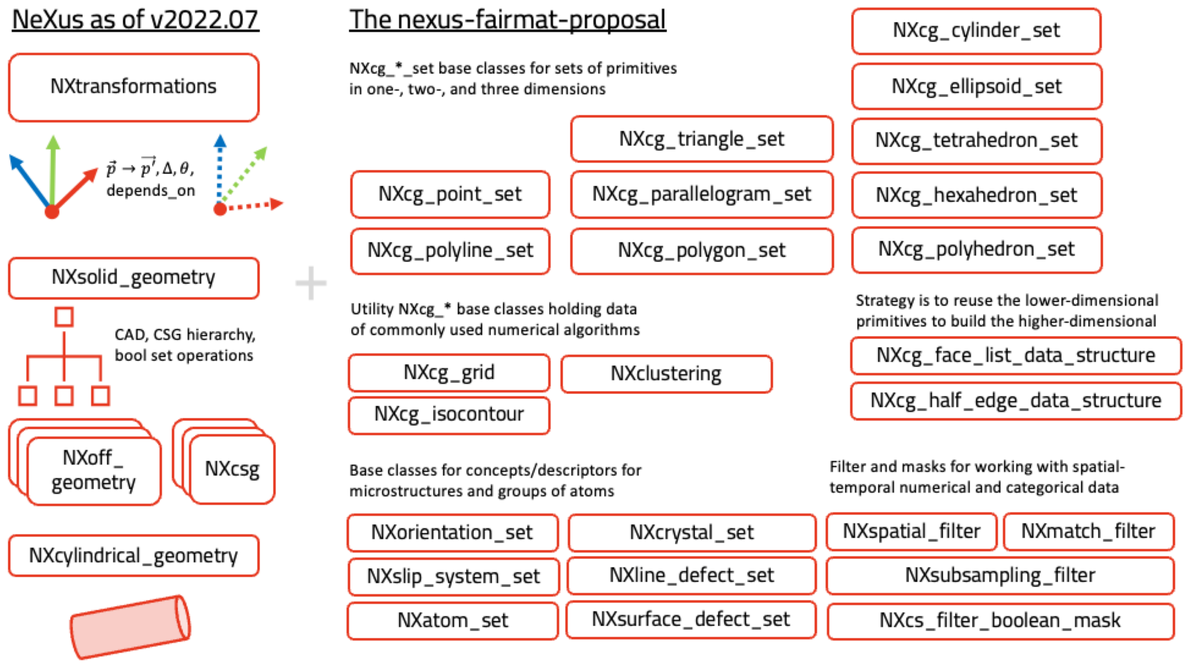
Symbols:

n_different_temperatures: Number of different experiment.

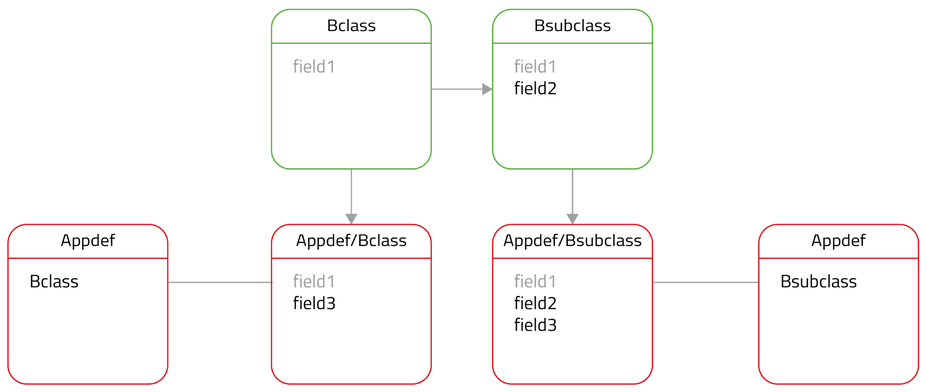
n_different_voltages: Number of different volta

Groups cited:

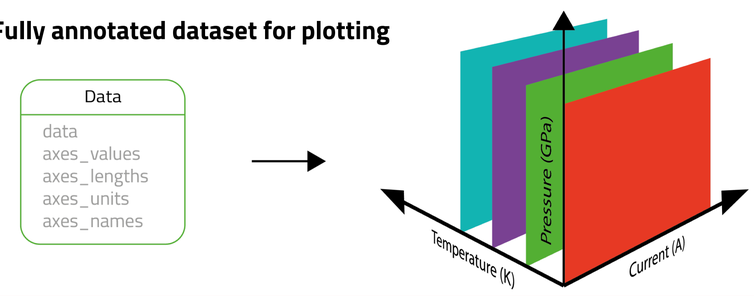
NXdata, NXentry, NXenvironment, NXinstrumer

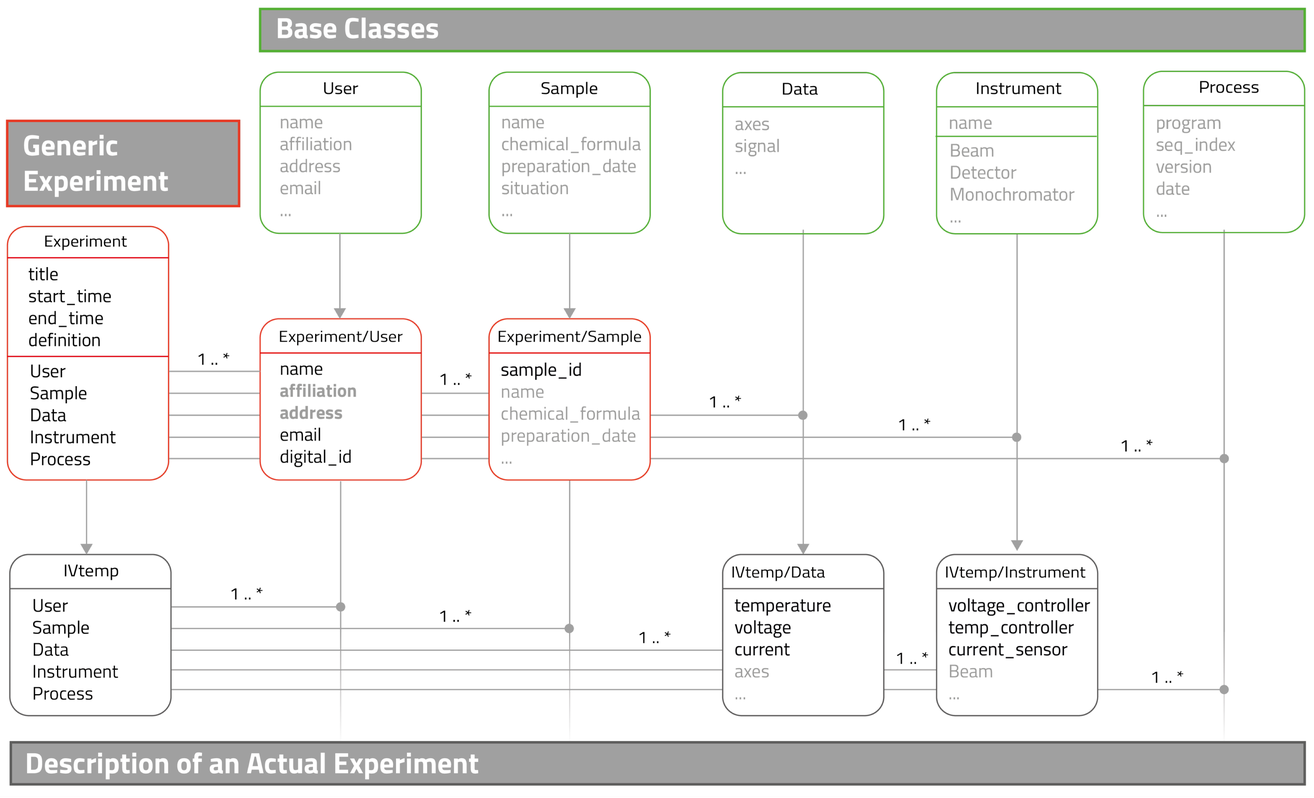


Inheritence in Application Definitions and Base Classes



Fully annotated dataset for plotting





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[1] M. Scheffler, *et al.*, *FAIR data enabling new horizons for materials research*, Nature Perspective 2022
[2] M. Könnecke, *et al.*, *The NeXus data format*, J. Appl. Cryst. (2015), 48, 301-305
[3] https://fairmat-experimental.github.io/nexus-fairmat-proposal
[4] https://blueskyproject.io