DATA SCIENCE &
SCIENTIFIC COMPUTING

UNIVERSITÀ
DEGLI STUDI
DI TRIESTE

Designing and deploying a FAIR-by-design data pipeline and platform for electron microscopy laboratories

Research thesis in Data Management

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Outline

1. Data management challenges in electron microscopy
2. A possible solution: FAIR principles
3. Our infrastructure: LAME and ORFEO
4. Pipeline and platform design

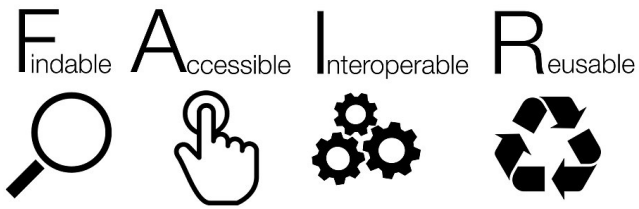
Electron microscopy and its data challenges

- **Electron microscopy (EM)**: probe matter at the nanometer scale.
- Techniques: TEM (internal), SEM (surface), STEM (combo + spectroscopy).
- Produces huge datasets: images, diffraction patterns, spectra.
- Issues:
  - Terabytes per session, proprietary formats, poor metadata.
  - Manual handling $\rightarrow$ lost context.
  - Hard to share and reuse.

Question: how to keep EM data usable and shareable in the long run?

A possible solution: FAIR principles

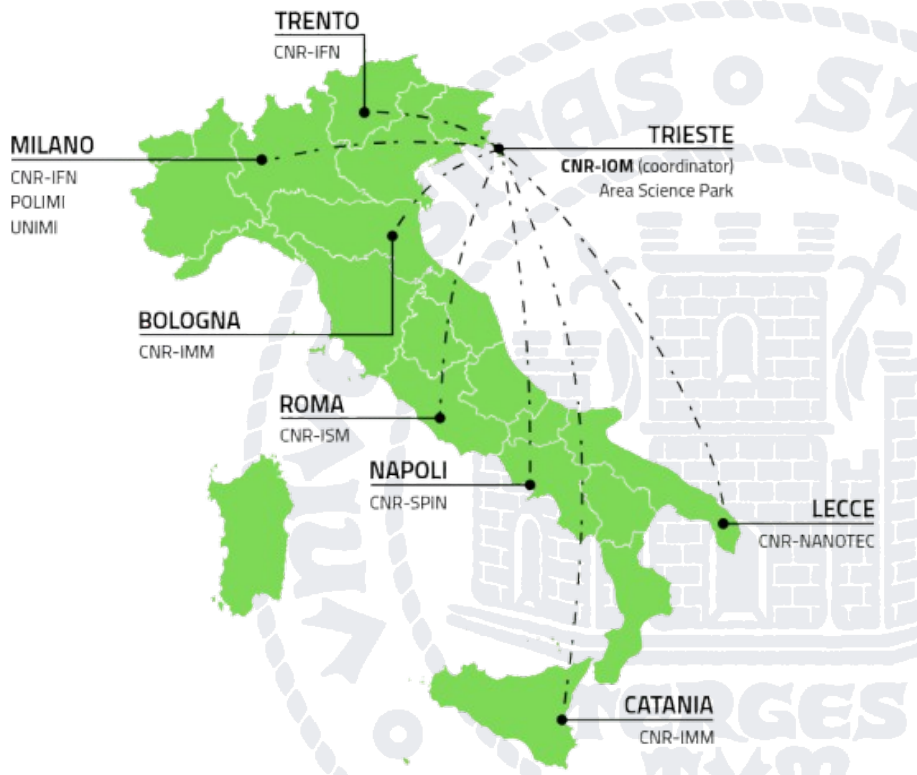
- FAIR =
  - **Findable**: unique identifiers, searchable metadata.
  - **Accessible**: stored on shared infrastructure, retrievable without manual copies.
  - **Interoperable**: common formats and vocabularies.
  - **Reusable**: provide context and metadata so data remain useful over time.
- **NeXus**: international standard on top of HDF5 for structured scientific data.
- **NXem**: NeXus application definition for electron microscopy.



NeXus

From principles to practice: NFFA-DI

- **NFFA-DI** = Nano Foundries and Fine Analysis – Digital Infrastructure.
- National initiative linking nanoscience labs across Italy.
- Mission: **FAIR data practices**, open access to advanced instruments, shared compute.
- My work contributes to this broader infrastructure effort.



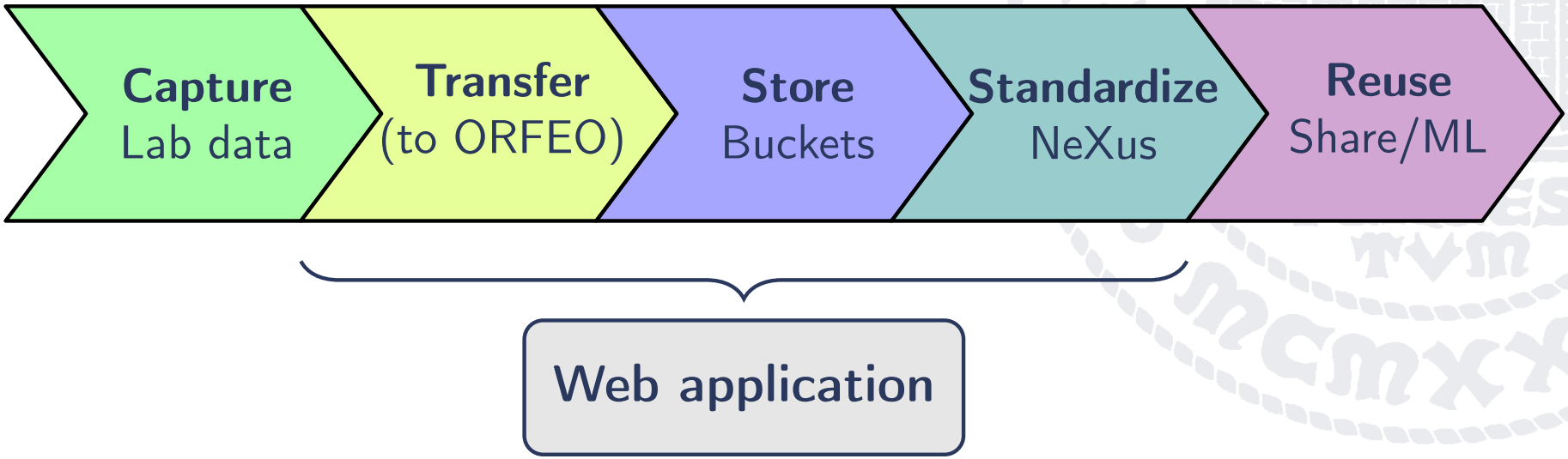
Source: `https://nffa-di.it/en/`

Our infrastructure: LAME and ORFEO

- **LAME**: advanced EM lab (opened 2022), with TEM/STEM and SEM; affiliated with NFFA-DI.
- **ORFEO**: datacenter providing storage, HPC, identity services. Core of the NFFA-DI digital infrastructure.
- **Current gap:** local storage, manual transfers, no smooth link to ORFEO.

Practical solution: a FAIR-by-design pipeline

- Bridges **LAME lab practices** with **ORFEO infrastructure**.
- Ensures data move **smoothly from capture to reuse**, without manual gaps.
- FAIRification happens at the **standardization step**.
- A **web application** orchestrates transfer, standardization, and storage.



Designing the web application

The infrastructure

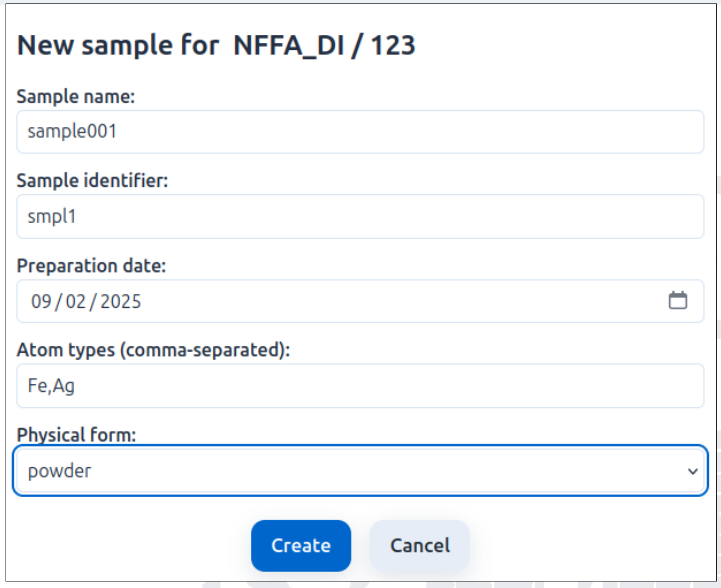
- **Authentik**: an open-source identity provider used for single sign-on (SSO)
- **Storage**: **Ceph**, a distributed storage system with the **RADOS Gateway** interface that organizes data as **objects** inside **buckets**.

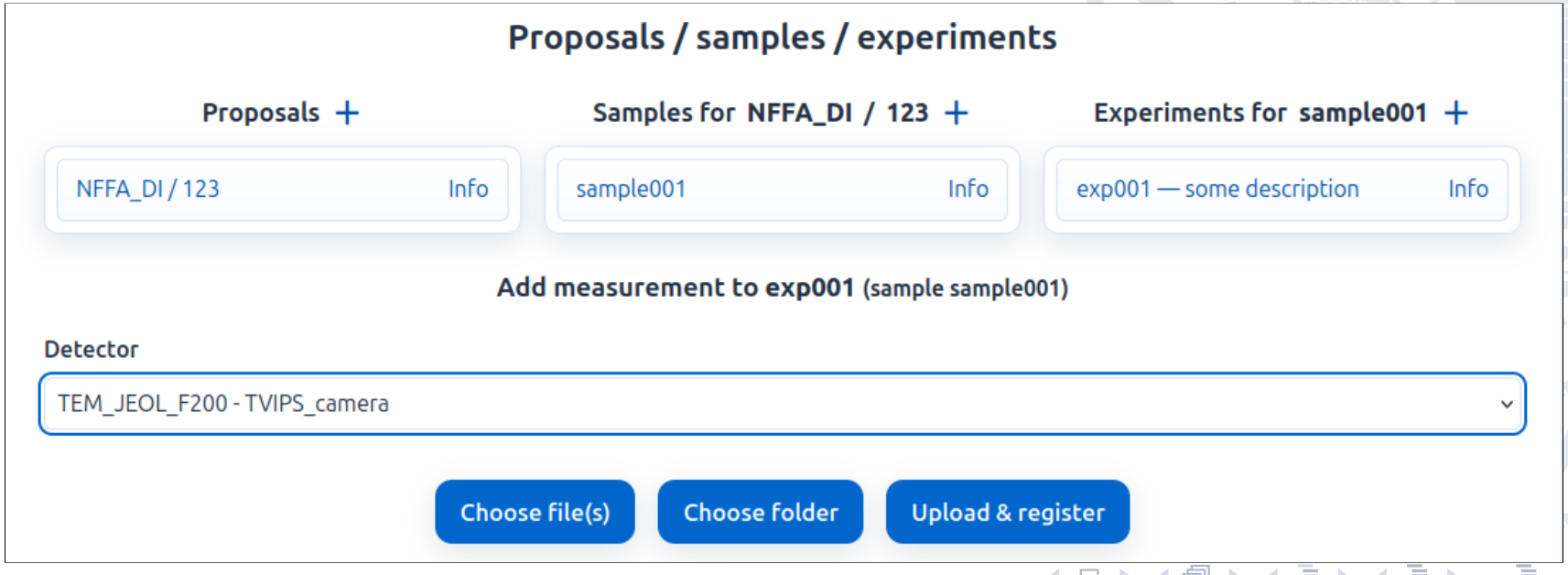
The application

- Built with **Django** and **PostgreSQL**, modeling research workflow as: **Project** / **Proposal** / **Sample** / **Experiment** / **Measurement**.
- Manages user identities through Authentik.
- Interacts with Ceph via the **Amazon S3 API**.
- Runs **background tasks** (NeXus conversion).

Using the web application

1. Log in with credentials.
2. Create a project, add samples and experiments.
3. Upload raw data files.





Testing & deployment: *VirtualOrfeo*

VirtualOrfeo is a lightweight digital twin of the ORFEO datacenter. It consists of multiple **virtual machines** and configuration files, simulating:

- storage
- identity
- compute nodes

The Django web application is packaged as a **container** and deployed inside the **Kubernetes (K3s) cluster**, integrated with storage and identity services as in production.

Conclusions

- **Pipeline**: from lab capture to FAIR data in ORFEO.
- **Webapp**: practical tool for projects, uploads, and NeXus conversion.
- **Validation**: tested end-to-end on VirtualOrfeo.
- **Impact**: reusable design for NFFA-DI and other labs.
- **Modularity**: the app can interact with **external services** (e.g. machine learning analysis, data management plan tools) through **APIs**, all testable within VirtualOrfeo.

Thank you!

Questions welcome.