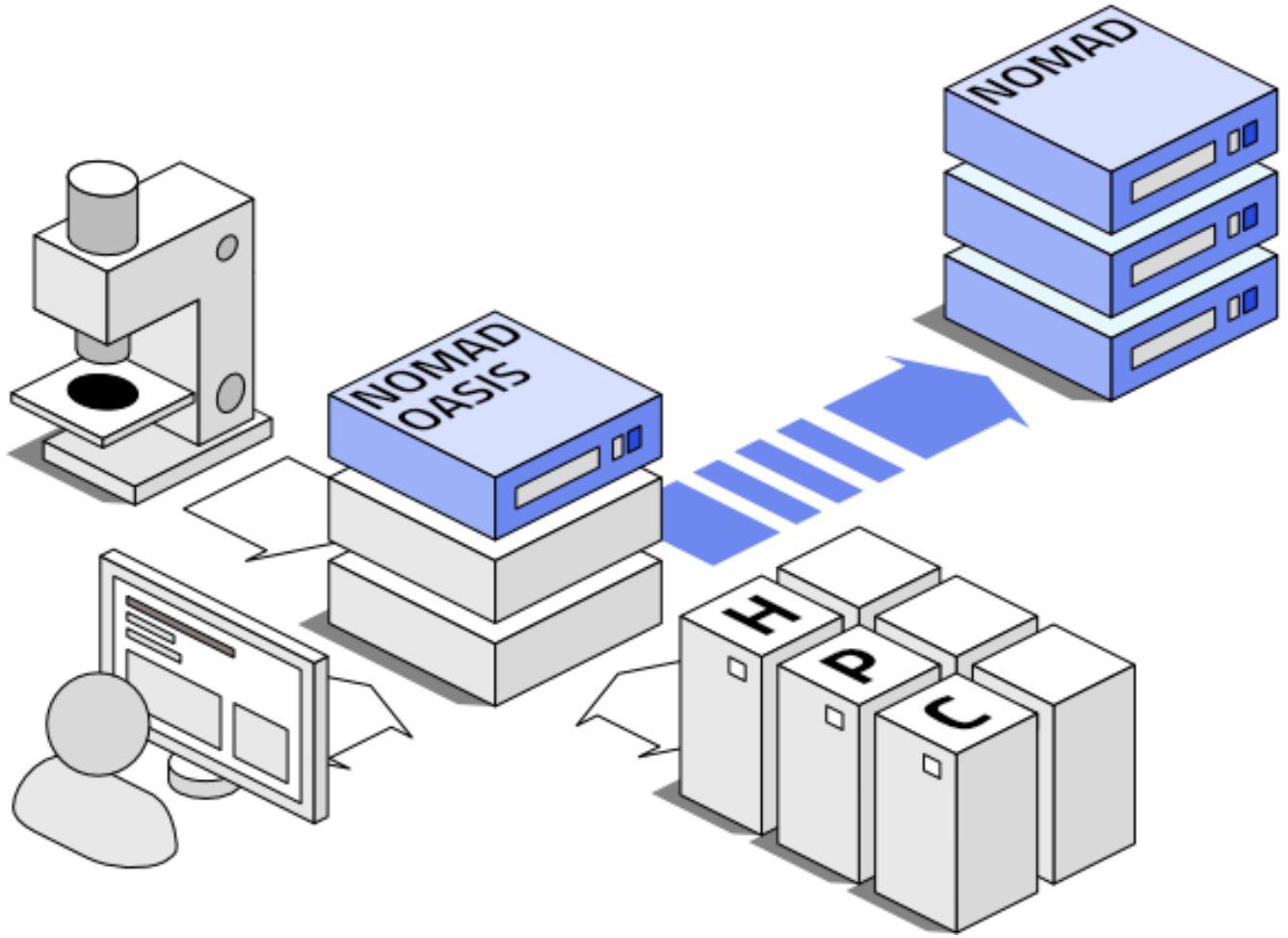


FAIRmat Tutorial 8:

Using NOMAD as an Electronic lab notebook (ELN) for FAIR data

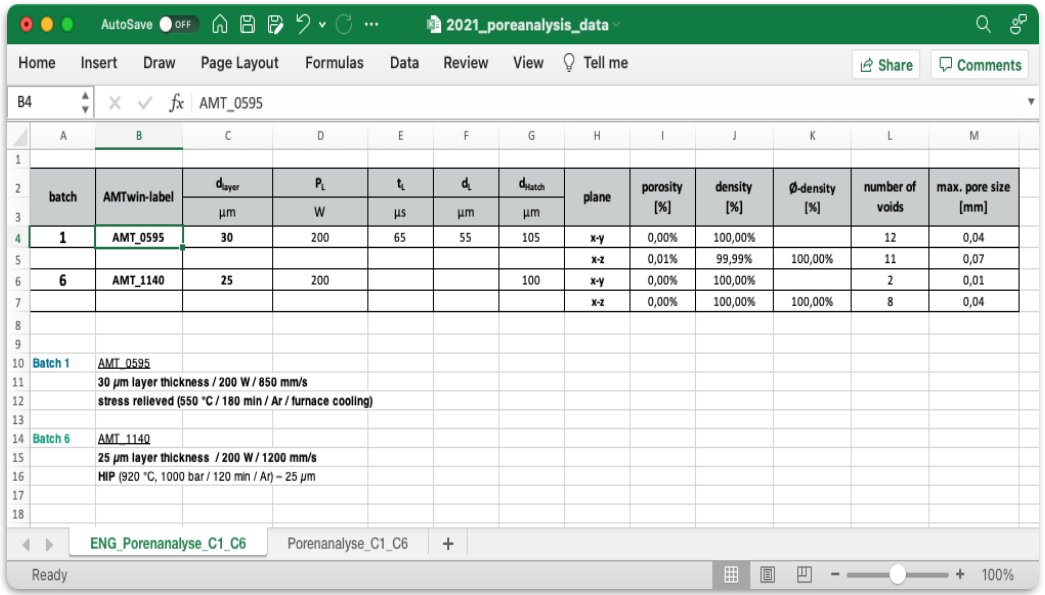
Organized by FAIRmat Area A Synthesis

Introduction

Present Situation in crystal growth

Motivation

Spreadsheet Files

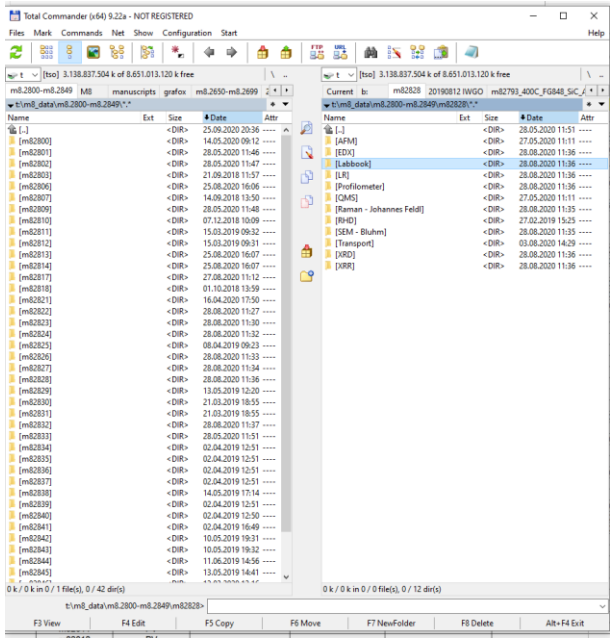


batch	AMTwin-label	d_{layer} µm	P_L W	t_L µs	d_L µm	d_{Hatch} µm	plane	porosity [%]	density [%]	Ø-density [%]	number of voids	max. pore size [mm]
1	AMT_0595	30	200	65	55	105	x-y	0,00%	100,00%		12	0,04
							x-z	0,01%	99,99%	100,00%	11	0,07
6	AMT_1140	25	200			100	x-y	0,00%	100,00%		2	0,01
							x-z	0,00%	100,00%	100,00%	8	0,04

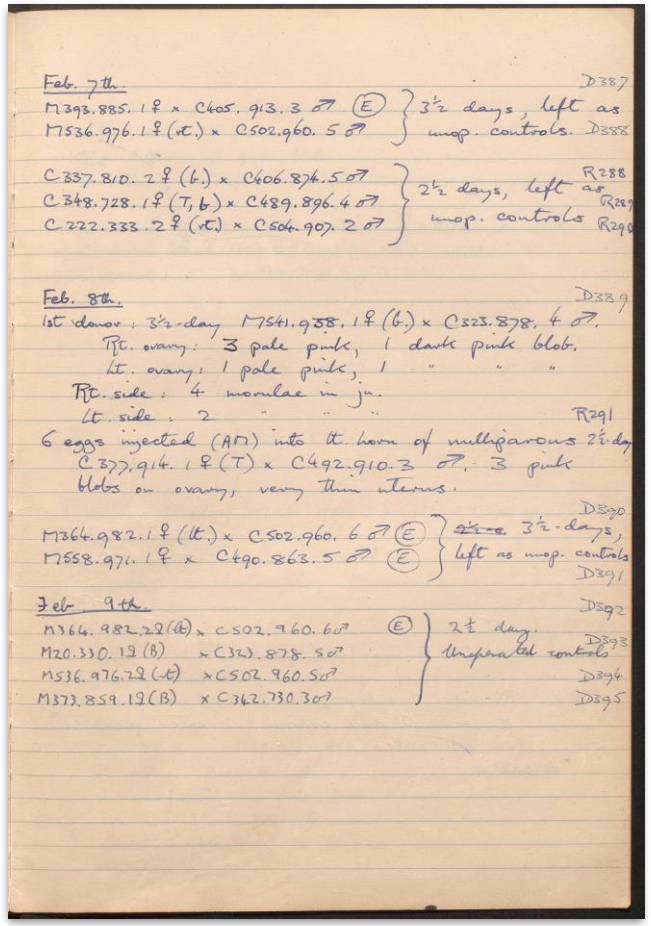
Batch 1 AMT_0595
30 µm layer thickness / 200 W / 850 mm/s
stress relieved (550 °C / 180 min / Ar / furnace cooling)

Batch 6 AMT_1140
25 µm layer thickness / 200 W / 1200 mm/s
HIP (920 °C, 1000 bar / 120 min / Ar) – 25 µm

File Servers



Lab Notes



→ Data are not accessible and findable

→ Data are not well characterized

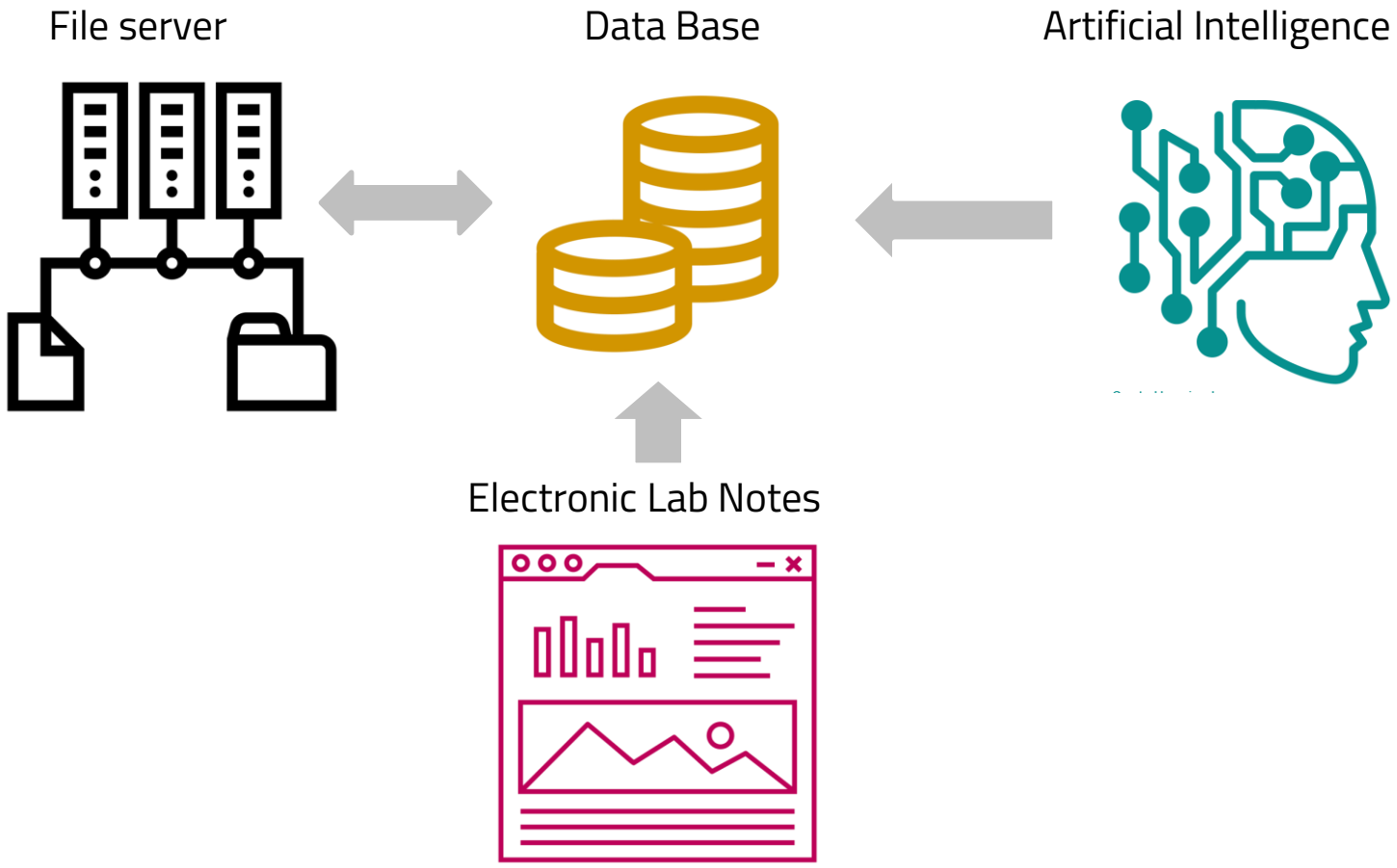
→ Data are not linked to other data

→ Data are not interoperable and reusable

→ Data are not machine-readable.

FAIRmat

Research data management (RDM) with Electronic Lab Notebooks (ELN) in NOMAD

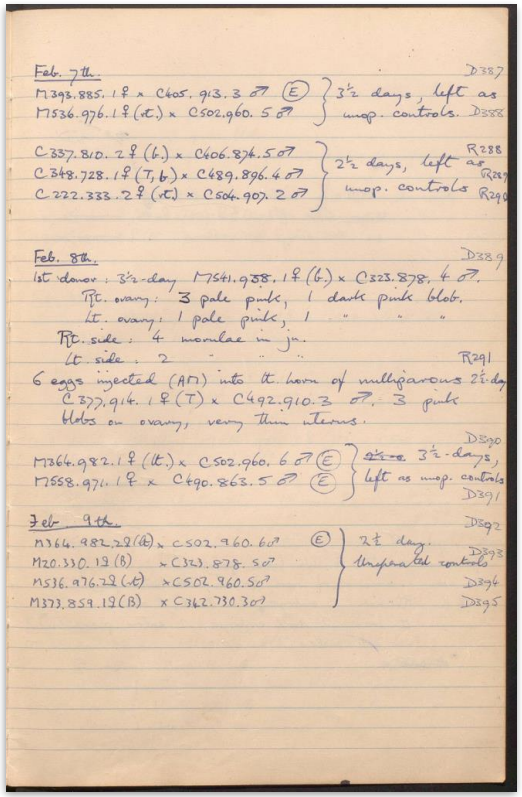


The ELN is an interface to a database
→ It is more then the simple electronic substitution of written lab notes!

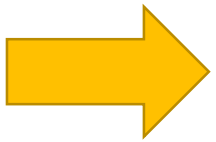
ELN entries require a **structured** approach of collecting data and a metadata structure

Electronic Lab Notebooks (ELN) in NOMAD: from analogue data to digitized data

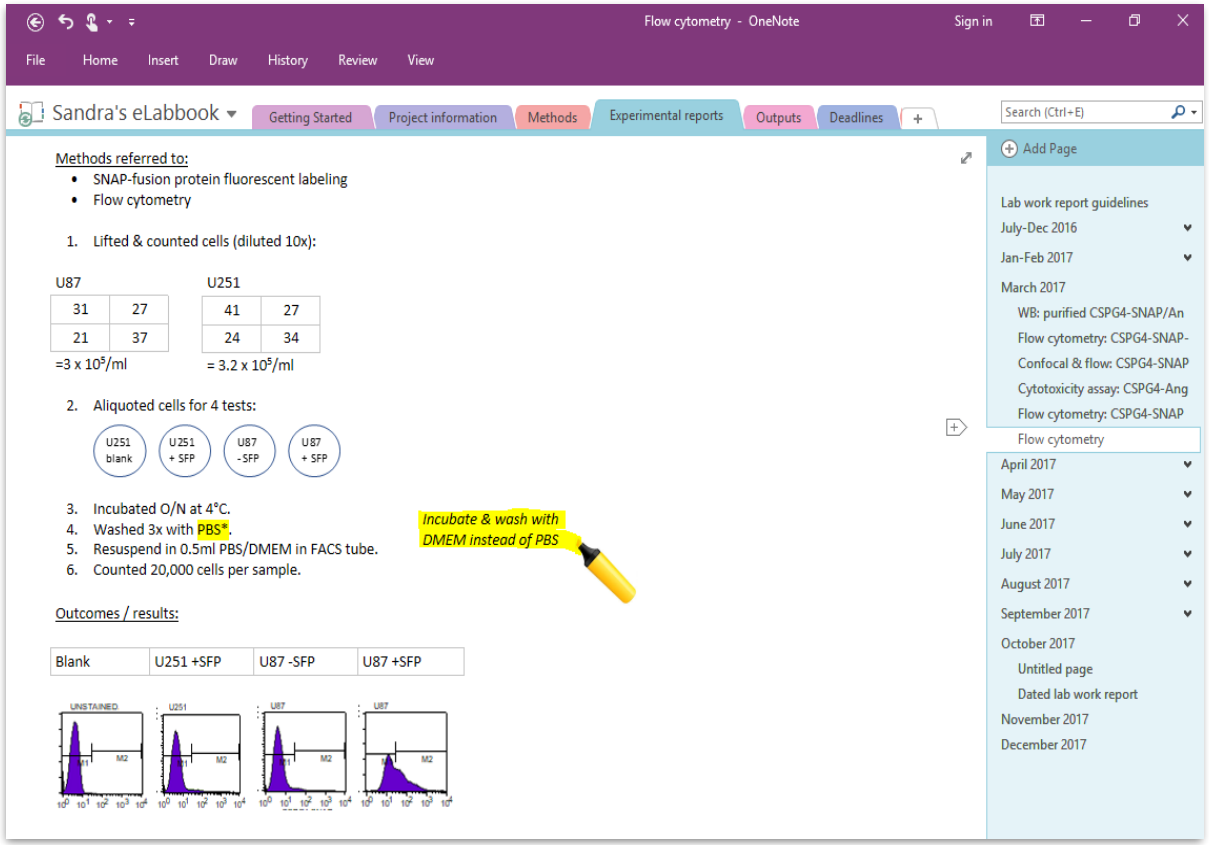
Motivation



Digitizing data



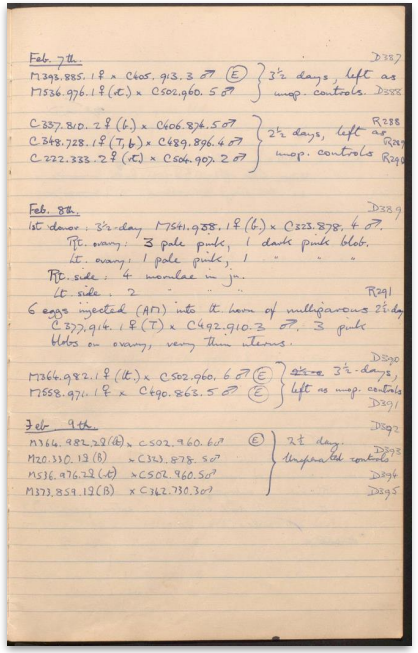
is not enough to make them machine-readable



FAIRmat

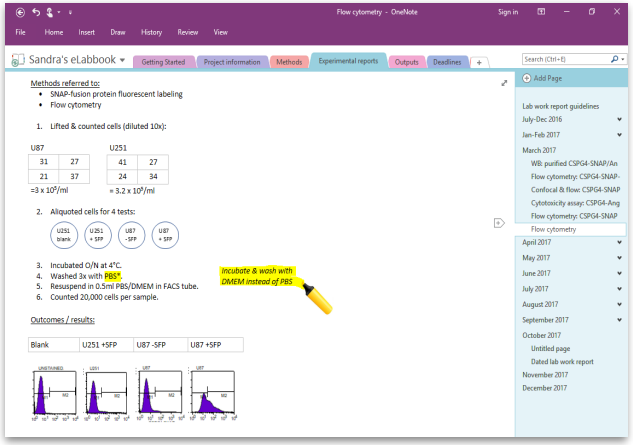
Electronic Lab Notebooks (ELN) in NOMAD: from analogue data to structured data

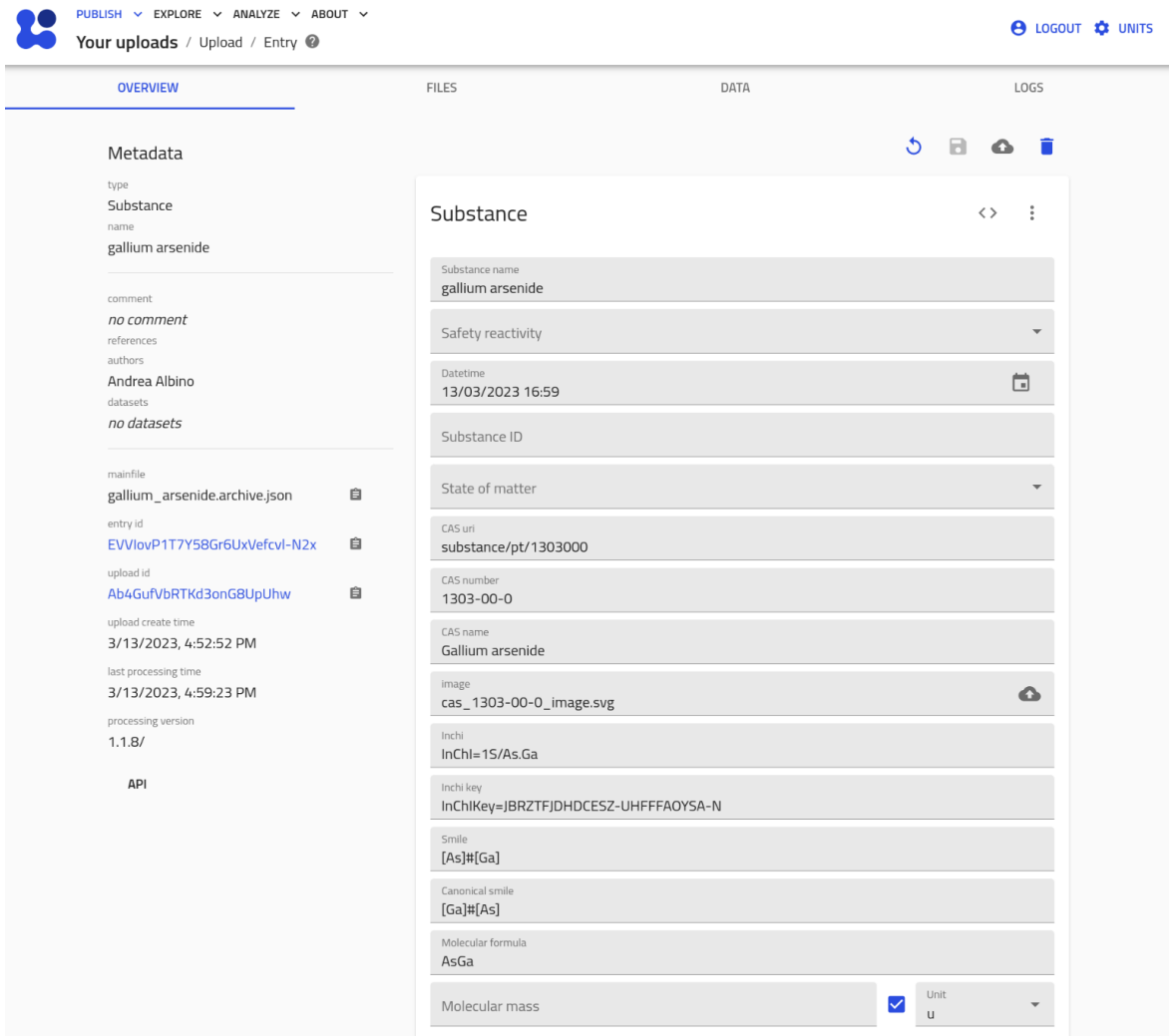
Motivation



Structuring data

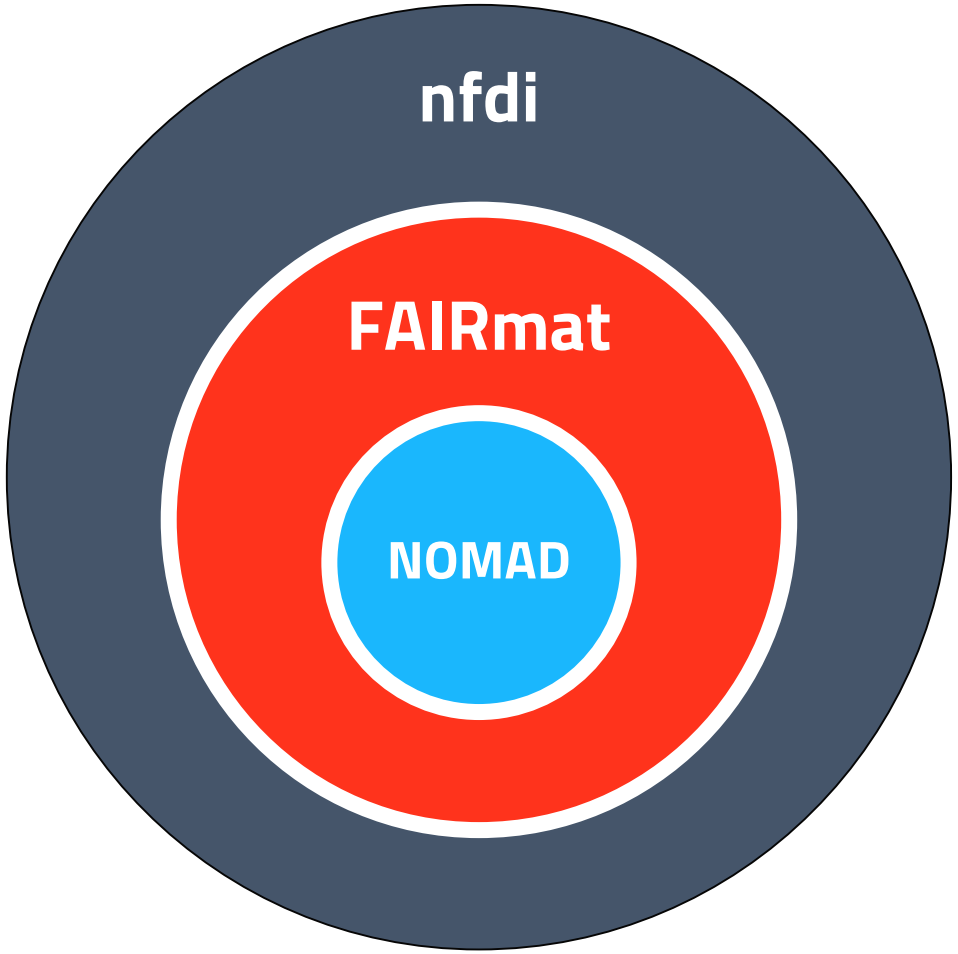
is required





FAIRmat

What are NFDI / FAIRmat / NOMAD



nfdi: Nationale Forschungsdaten Infrastructure, link
(national research data infrastructure)

FAIRmat: NFDI consortium for FAIR materials science data, link
(FAIR: findable, accessible, interoperable, re-usable)

NOMAD: A web-based service and software for managing FAIR materials science data, link
FAIRmat uses NOMAD to build a federated infrastructure of connected NOMAD installations

The FAIRmat Values

FAIR

Findable, Accessible, Interoperable, Re-usable

FAIR principles can transform every field of science

Bottom-up approach

Embracing the community

Development driven by the needs of scientists and already enjoys strong support from the community.

Open access

Use open processes to support a wide community

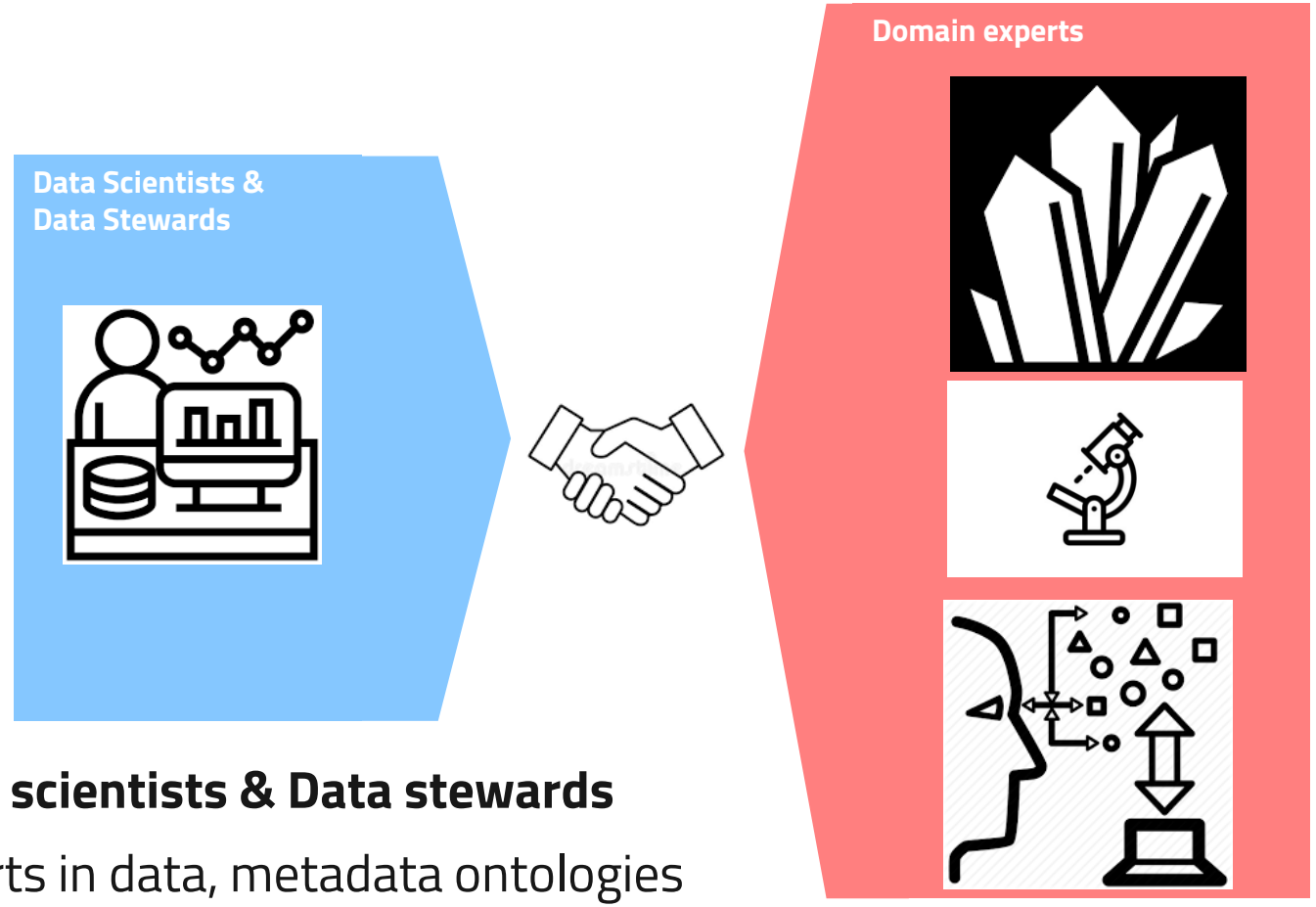
FAIRmat advocates for an urgently needed culture shift towards data sharing,
and stands for open access to scientific materials data and tools.

FAIRmat Approach

Strategy

Local Domain experts

→ define domain specific needs for data management



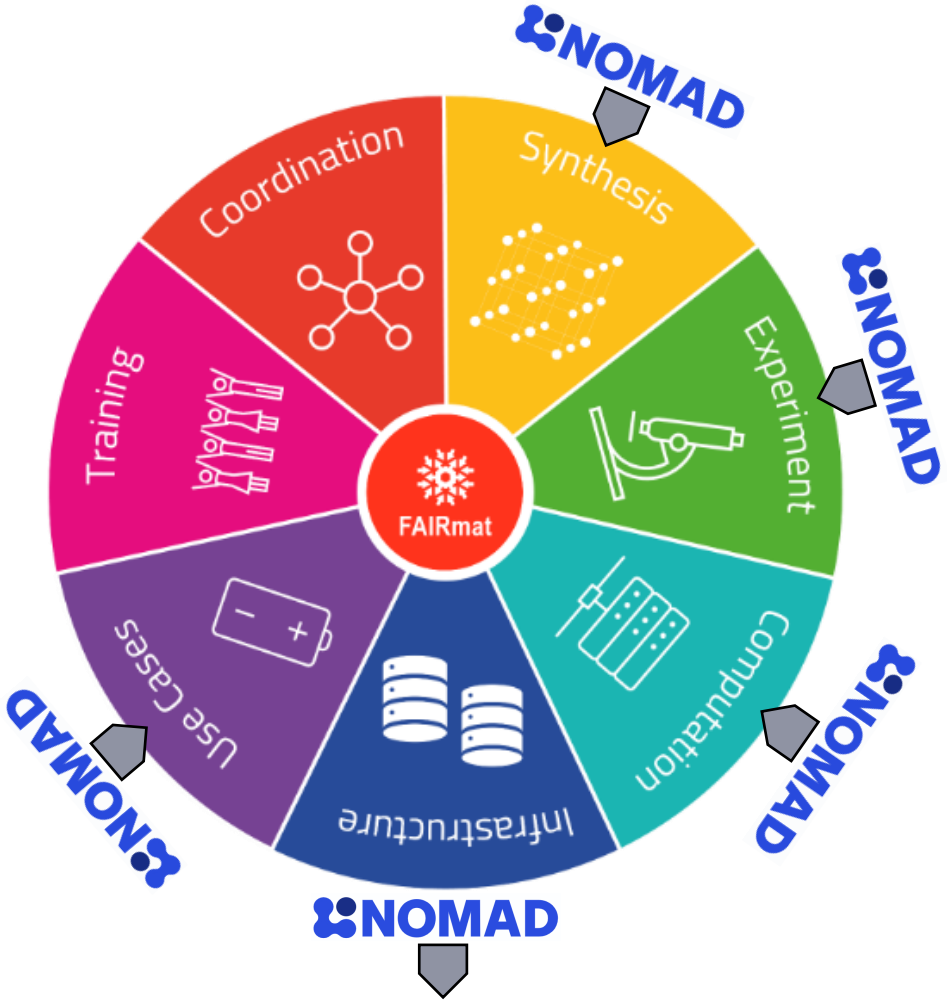
Data scientists & Data stewards

→ experts in data, metadata ontologies

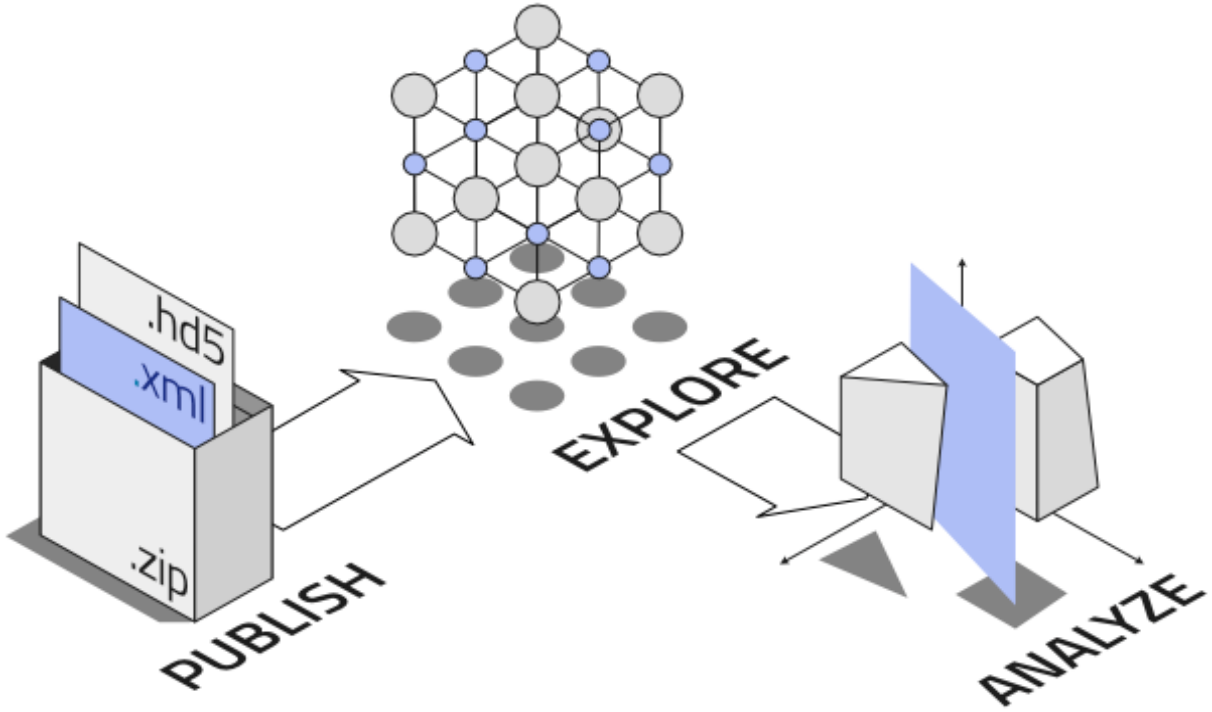
FAIRmat

What are NFDI / FAIRmat / NOMAD

FAIRmat is the NDFI consortium to build a FAIR federated data infrastructure for solid state physics



NOMAD is a web-based software for FAIR research data management in materials science

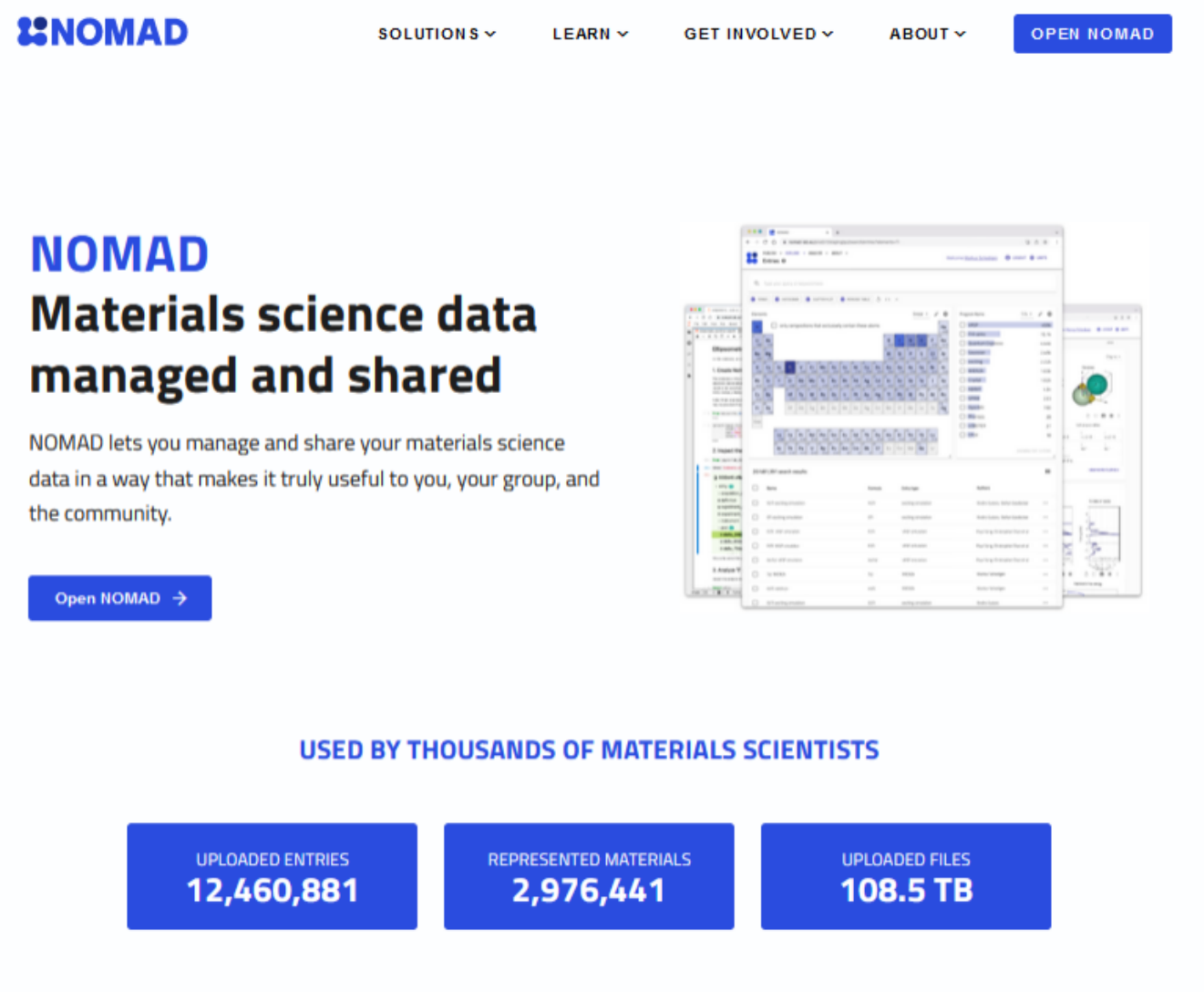


NOMAD

FAIRmat

FAIRmat

NOMAD webpage



https://nomad-lab.eu/

NOMAD

NOMAD

Drag & Drop

Upload file-by-file or zip
and upload whole directory structures.

Get a DOI

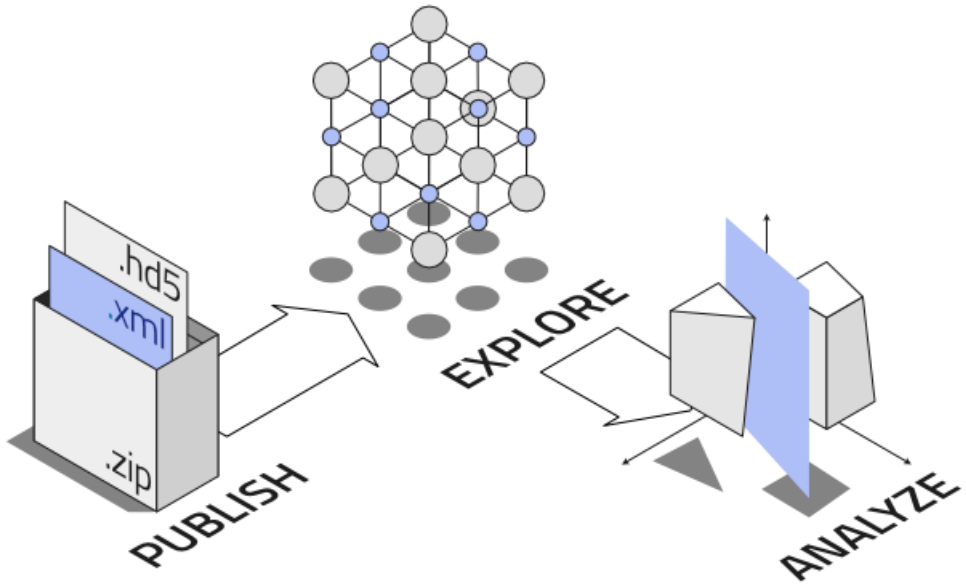
NOMAD allows you to publish and archive your data for free. Assign a DOI to uploaded datasets and reference your papers.

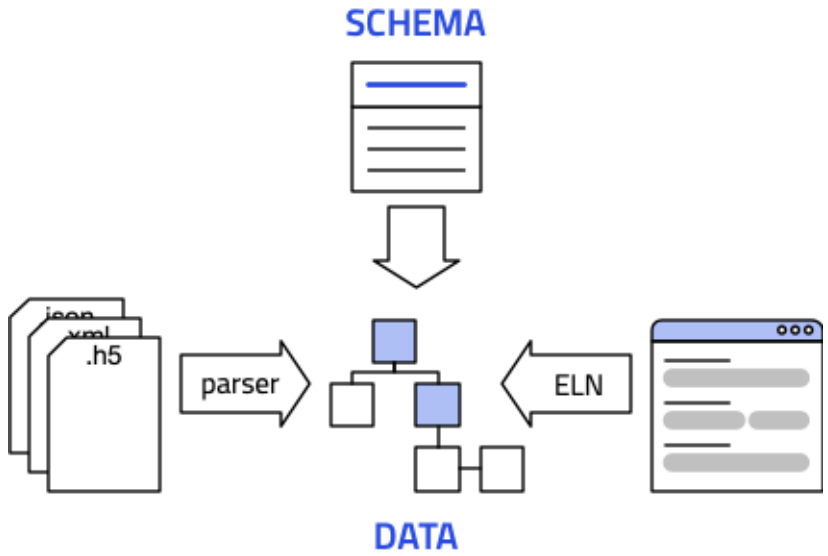
You Control Your Data

Not ready to publish? Organize data and collaborate in private first.

Ready to use Tools

Run Jupyter and other tools directly on NOMAD.





FAIRmat

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Run Jupyter and other tools directly on NOMAD.

NOMAD OASIS

Runs on your premises

Runs behind your firewall and inside your VPN. Use your own resources for processing and running analysis tools.

Custom ELNs

Extend and customize NOMAD's schema to create specialized editors to document your work.

Your own parsers

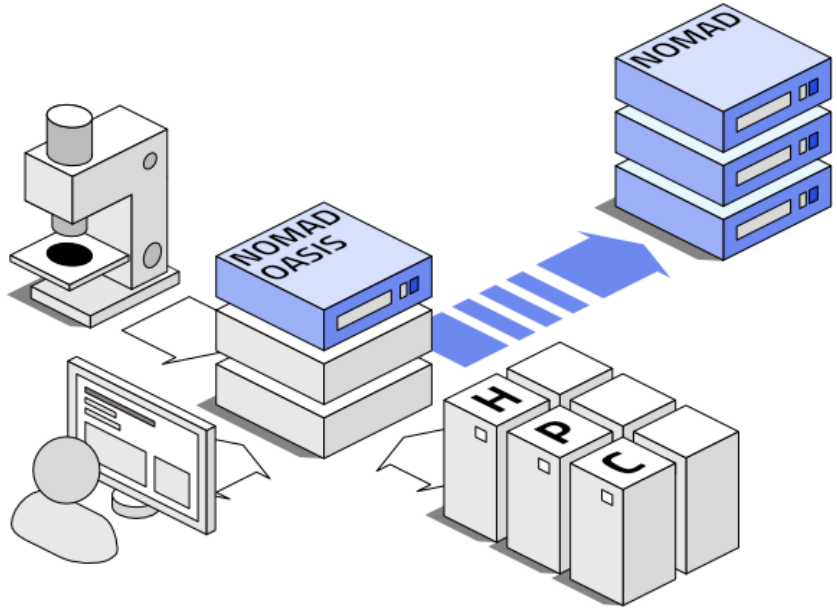
Support your own file formats. Add parsers and normalization routines.

Use your own tools

Add tools and notebooks that directly access and manipulate your data in NOMAD.

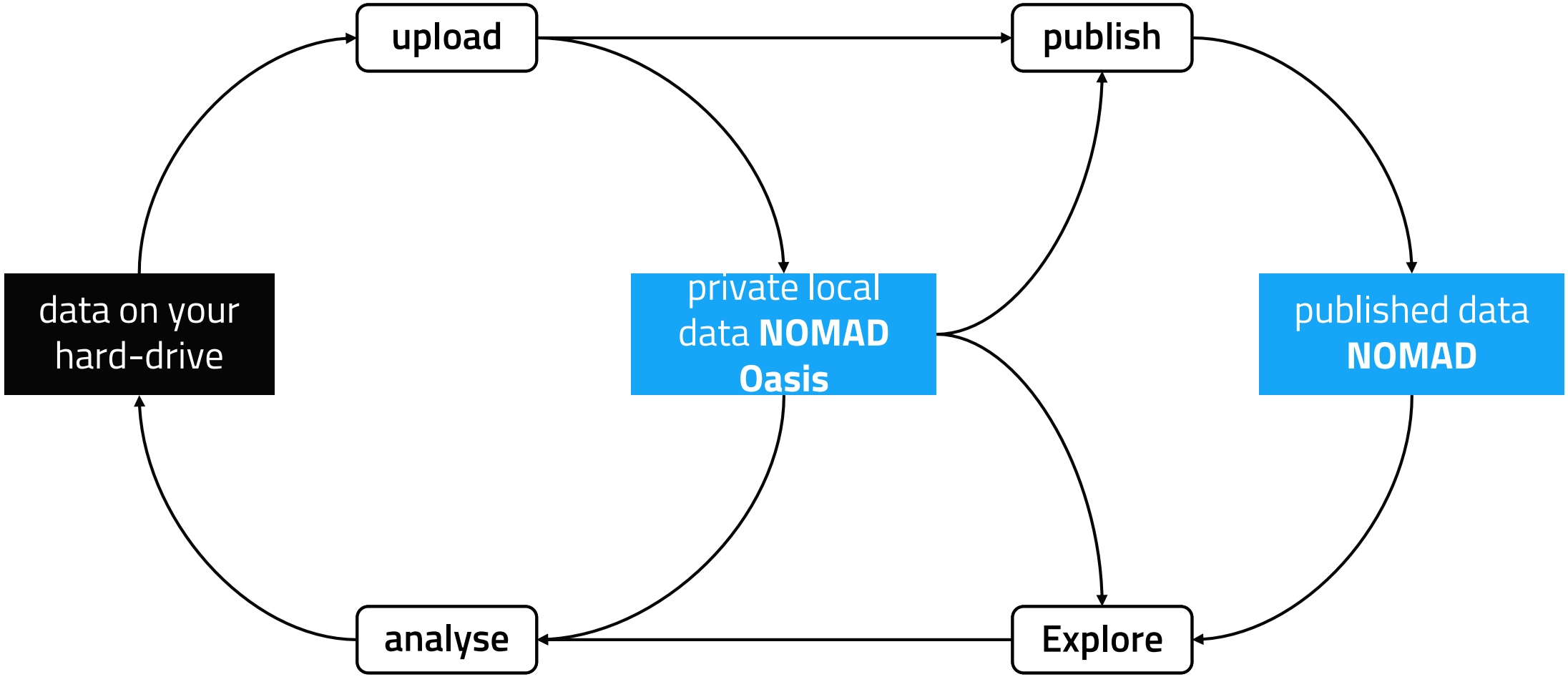
Publish selected data

Oasis will soon be connected to the public NOMAD service.



FAIRmat

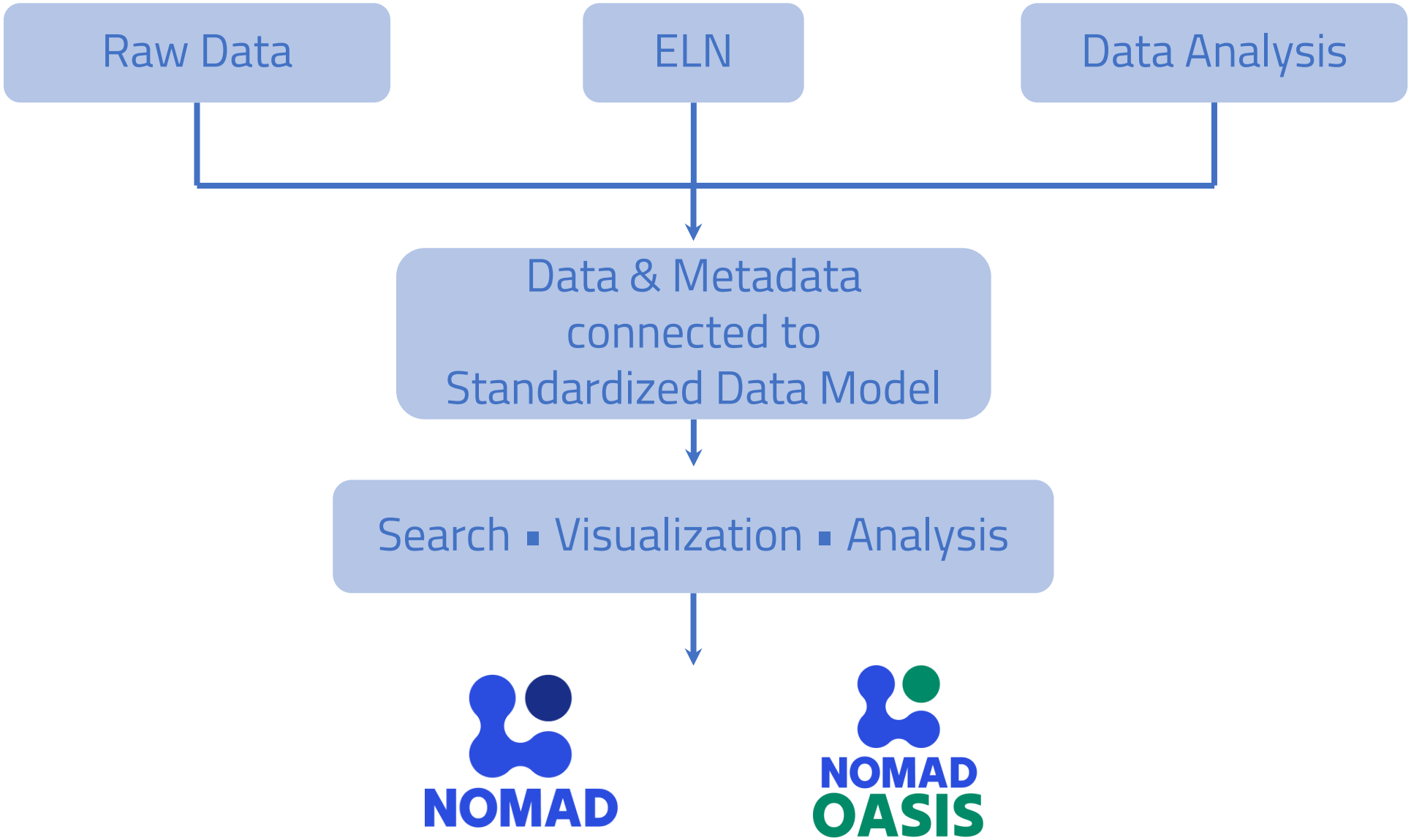
What is NOMAD Oasis?



NOMAD

FAIRmat

Research Data Management in NOMAD



FAIRmat Area A

Area A Team

Sebastian Brückner

Coordinator

Andrea Albino

Data Modelling
Implementation

Hampus Näsström

Data Modelling

Jose Marquez-Prieto

Implementation
Link to **Area E**

Florian Dobener

Infrastructure
Link to **Area B**

FAIRmat

Outline

Tutorial Outline

Time	Session	Speaker
14:00	1. Introduction	Sebastian Brückner
14:10	2. Vocabulary and Key Concepts	Andrea Albino
14:30	3. NOMAD usage (interactive)	Florian Dobener
15:00	4. Writing a Custom Schema (interactive)	Hampus Näsström
15:30	5. Reading Files with the Tabular Parser and Adding Plots (interactive)	Andrea Albino
16:00	6. Using Base Classes and References (interactive)	Hampus Näsström
16:30	7. Search your ELN data (interactive)	José Marquez

FAIRmat

Thank you!