Session: Towards Implementations of Materials and Manufacturing Commons: Participants' Use-Cases

Data Structures and Tools for FAIR Synthesis data

Dr. Sebastian Brückner

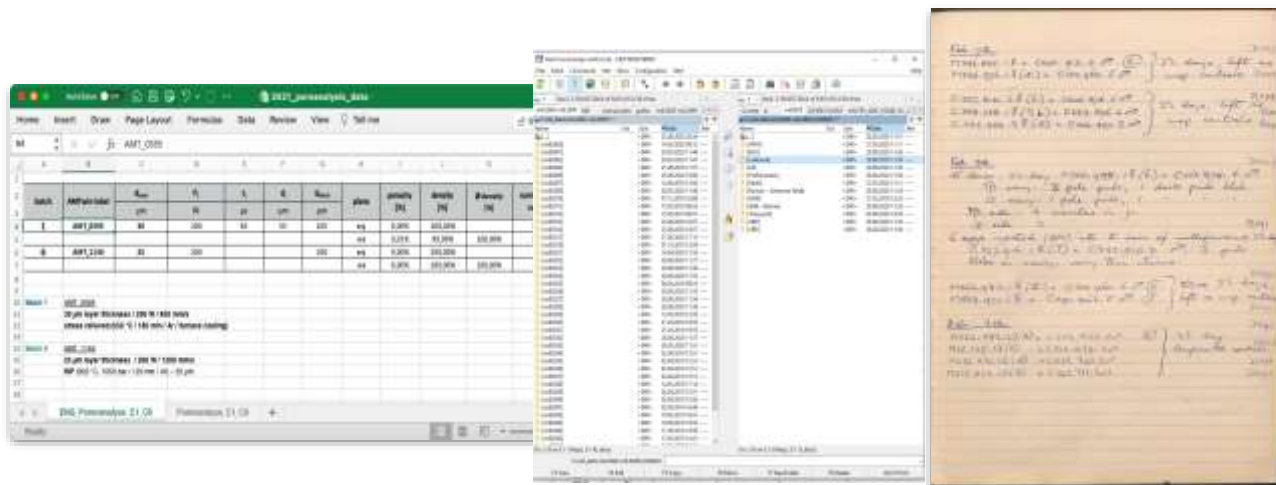*FAIRmat, HU Berlin, Zum Großen Windkanal 2, 12489 Berlin*
*IKZ Berlin, Max-Born-Straße 2, 12489 Berlin*

Use-case Introduction

* **FAIRmat** (NFDI Consortium): FAIR federated data infrastructure for solid state physics → **FAIR synthesis data**

* **From** unstructured data, no standards, no data sharing culture, no data skills…

* …**To** structured data → machine readable + shareable → **FAIR**

Spreadsheet Files   File Servers   Lab Notes

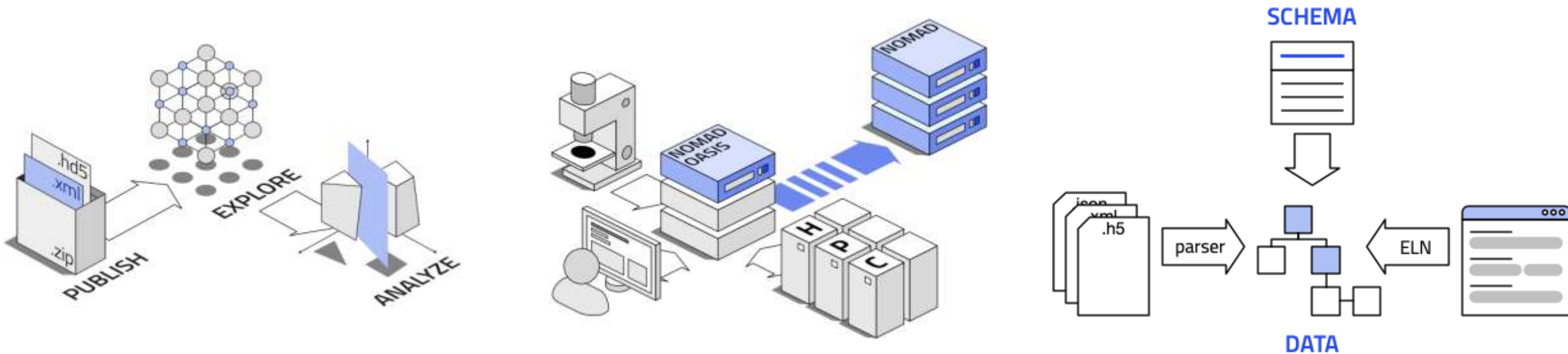Data Base

File Server

ML/AI

Electronic Lab Notes
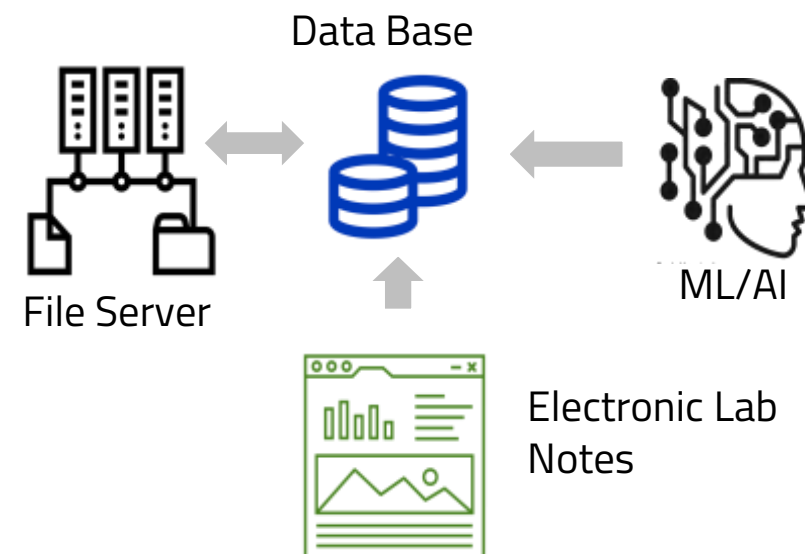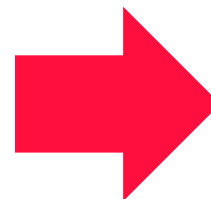
Benefits and Gaps

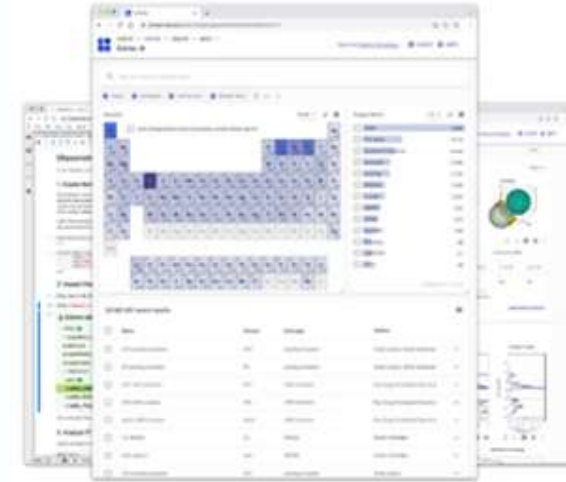a web-based software for FAIR research data management in materials science:

→Supports structured data

→Bottom up approach: input from users, support of community standards
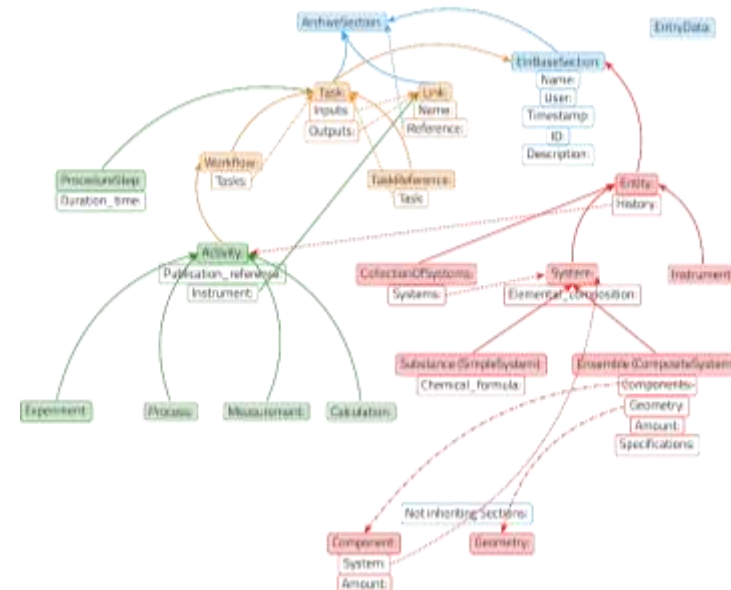
Future Development and Challenges

Towards a Standard / an Ontology

* **NOMAD** → platform/tool for FAIR data → fast implementat[ion]
  of our use cases/data structures

* **Data modelling** for synthesis and beyond, our steps:
  1. Flexible schema and base classes
  2. Composing application definitions
  3. Linking multiple archive files
  4. Workflows
  5. Base class hierarchy
     → **an ontology???**

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www.fairmat-nfdi.eu

https://nomad-lab.eu

https://github.com/FAIRmatNFDI/AreaA

-data_modeling_and_schemas