TUT 5: FAIR Research Data – Generation, Handling and Analysis within the FAIRmat Infrastructure

In many scientific fields, but especially in solid-state physics, comprehensive and homogeneous scientific data could pave the way for a completely new, data-driven research, often referred to as the fourth paradigm of science. New opportunities for science and technology, as well as for teaching and career paths are foreseeable. In reality, however, our field mostly provides extremely heterogeneous data. For this reason, the major funding organizations are calling for and supporting the conversion to FAIR (findable, accessible, interoperable, reusable) data. In solid-state physics, the consortium FAIRmat aims at developing concepts and solutions for this endeavor. This tutorial introduces the FAIRmat approach in four well-adapted contributions.

Organizers: Martin Aeschlimann (TU Kaiserslautern) and Laurenz Rettig (FHI Berlin)

Time: Sunday 16:00–18:15   Location: H 2013

Tutorial   TUT 5.1   Sun 16:00   H 2013
Experimental research data as a FAIR resource: Introduction and the FAIRmat approach — •Heiko B. Weber — Lehrstuhl für Angewandte Physik, Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

I will introduce the general framework of research data management and give an overview of FAIRmat's concepts on how to implement it in experimental solid-state physics. I will sketch how research data (collected by instruments) and metadata (collected in electronic laboratory notebooks and from instruments) can be consistently structured. Such harmonized data can be collected in local or worldwide hubs (NOMAD Oasis or NOMAD, respectively). On this platform one can search data, work with the data, compare data of different origin, and finally use it as repository. Implications for science and teaching, and for the solid-state physics community will be briefly discussed.

Tutorial   TUT 5.2   Sun 16:30   H 2013
Harmonization concepts for experimental research data: NOMAD and NeXus — •Sandor Brockhauser — Physics Department and CSMB, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

In order to achieve interoperability for data of different origin, a FAIR research-data platform for solid-state physics is created within FAIRmat, which we term NOMAD. It features flexible, but structured data modeling, allows custom data ingestion, while providing efficient search capabilities and online visualization of datasets. Several standard data formats are supported by NOMAD including the NeXus format [1].

In this tutorial, I will introduce NeXus as a community-driven data modeling standard for experiments. I will present the NeXus Ontology and discuss several examples of how a specific experimental community can extend it to cover their special needs. Finally, the integration of NeXus data from experiments into NOMAD will be introduced.

[1] https://www.nexusformat.org/

Tutorial   TUT 5.3   Sun 17:00   H 2013
How to build FAIR data pipelines for photoemission spectroscopy — •Florian Dobener — Physics Department and CSMB, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — Physics Department & Research Center OPTIMAS, RPTU Kaiserslautern,

Germany

Photoemission spectroscopy (PES) is presented as a use case for pioneering future research data concepts. We will show how FAIR research data can be organized and how we intend to create benefits for the scientists who participate. We will present an extensive and elaborated standard (NXmpes) for harmonizing PES data using NeXus. This tutorial aims to provide comprehensive guidance on how to establish a FAIR data pipeline within your laboratory using NXmpes in conjunction with the NOMAD research data management platform.

Our tooling integrates seamlessly with NOMAD's data management capabilities. Alternatively, it offers standalone tools for generating NXmpes files, facilitating their incorporation into custom data generation pipelines. Moreover, we present our strategy to collaborate with leading manufacturers of PES equipment to foster interoperability of NXmpes with their software solutions.

Tutorial   TUT 5.4   Sun 17:30   H 2013
Easy access to FAIR data generation for custom-built experiments with NOMAD CAMELS — •Alexander Fuchs — Lehrstuhl für Angewandte Physik, Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany

In this tutorial, I will introduce NOMAD CAMELS [1] as a standalone open-source measurement software targeted towards the requirements of experimental physics. It is designed to control instruments and to write and modify experimental procedures without the need of programming skills. CAMELS creates python code, which subsequently runs the measurement protocol, hence it can utilize powerful libraries and is widely extendable. CAMELS provides by default rich metadata and structured research data in a consistent way. With its NeXus output, immediate injection of FAIR data into NOMAD Oasis and NOMAD will be possible.

In this tutorial, I will explain the concept and capabilities of CAMELS, take the beginner's perspective and demonstrate how to start using it.

[1] https://nomad-lab.eu/nomad-lab/nomad-camels.html

Q & A with all Presenters (15 min.)