











FDO-Based FAIR-by-Design Upgrade of an Interdisciplinary Research Infrastructure for Nanoscience

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Abstract. The presentation describes the strategy of FDO-based generic digital workflows in nanoscience adopted for the data management upgrade at the Nanoscience Foundry and Fine Analysis Digital Infrastructure (NFFA-DI). The approach and framework improve the digital traceability of the workflow in the field of growth and structural characterisation of nano-objects and nano-structured materials in the context of condensed matter experiments by designing strategies for complete digitisation of the laboratories.

Keywords: Nanoscience, Condensed Matter Experiments, FAIR-by-Design Data Management, Digital Tracing of the Workflow, Generic FDO Workflow

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It is an acknowledged fact that modern scientific research requires more than just experimental instruments [1] or theoretical models to efficiently improve the description of reality. Here we present the strategy adopted for the data management upgrade at NFFA-DI (Nanoscience Foundry and Fine Analysis Digital Infrastructure). NFFA-DI is an Italian PNRR project for the upgrade of a distributed research infrastructure for nanoscience. It is the extension of NFFA Europe (European distributed research infrastructure) with an additional key feature i.e. a FAIR-by-design operating mode. NFFA infrastructure integrates nanofoundry laboratories (for atomically controlled growth and structural characterisation of nano-objects and nano-structured materials), Large-Scale Facilities (for fine analysis of matter based on radiation sources), and distributed theoretical tools (for condensed matter simulation).

In this framework, we designed strategies for the complete digitalization of the laboratories and for the digital tracing of the workflow concerning condensed matter experiments. Data are generated in an interdisciplinary environment and show a considerable variety in size, format, complexity and domain application. The main challenges we are facing in implementing an

efficient workflow are related to the interpretation and application of the FAIR principles in different contexts.

We introduced the concept of Fair Digital Objects in our project as a universal paradigm for the management of the generic digital workflow in order to fulfil the FAIR-by-design implementation principle. With this aim, sample production history and measurement output will be stored in FDOs, as well as the specifics and history of the experimental instrumentation. Experiments will be described by the information extracted from electronic logbook and collected in DOs. These will be attached to the measurement output to create datasets that are compliant with the specifics of FDO, and stored in a NOMAD Oasis repository, hosted by each infrastructure access-node. Along with the creation of the Data Management Plan for the NFFA facilities, we designed conceptual schemes for the implementation of a dedicated data management and storage infrastructure that will be implemented in the near future.

Our work is intended to address the issues coming from the fact that more than ever, the ability to collect, share and retrieve FAIR data has become critical to perform state-of-the-art studies. We believe that our use-case proves FDO to be a key-concept in shaping an effective FAIR-by-design data management system.

Data availability statement

Not applicable.

Underlying and related material

Not applicable.

Author contributions

Conceptualization (DA, IM, RA, GB, SC, RL, MP, AR, CA, GR); Data curation (N/A); Formal Analysis (N/A); Funding acquisition (N/A); Investigation (N/A); Methodology (N/A); Project administration (N/A); Resources (N/A); Software (N/A); Supervision (N/A); Validation (N/A); Visualization (N/A); Writing – original draft (DA); Writing – review & editing (DA).

Competing interests

The authors declare that they have no competing interests.

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