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Research Data Management Workflows for Multidimensional Characterization Techniques with NOMAD

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We present an overview of research data management workflows for multidimensional characterization techniques using the NOMAD platform. Our approach focuses on efficiently handling large-volume datasets, particularly in HDF5 format, and developing specialized NeXus application definitions for emerging characterization methods. We demonstrate how cloud-based analysis tools can be seamlessly integrated into the entire workflow, illustrated by examples from electron microscopy and multidimensional photoelectron spectroscopy. By leveraging customized JupyterLab environments and desktop-based tools in the cloud, this strategy supports efficient, advanced analyses that remain tightly integrated with the NOMAD data infrastructure, eliminating the need to relocate large datasets and enhancing data shareability. Furthermore, we show how instrument inventories and sample metadata can be linked to specific measurements, enabling robust traceability and a comprehensive history throughout the entire experimental lifecycle.

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