

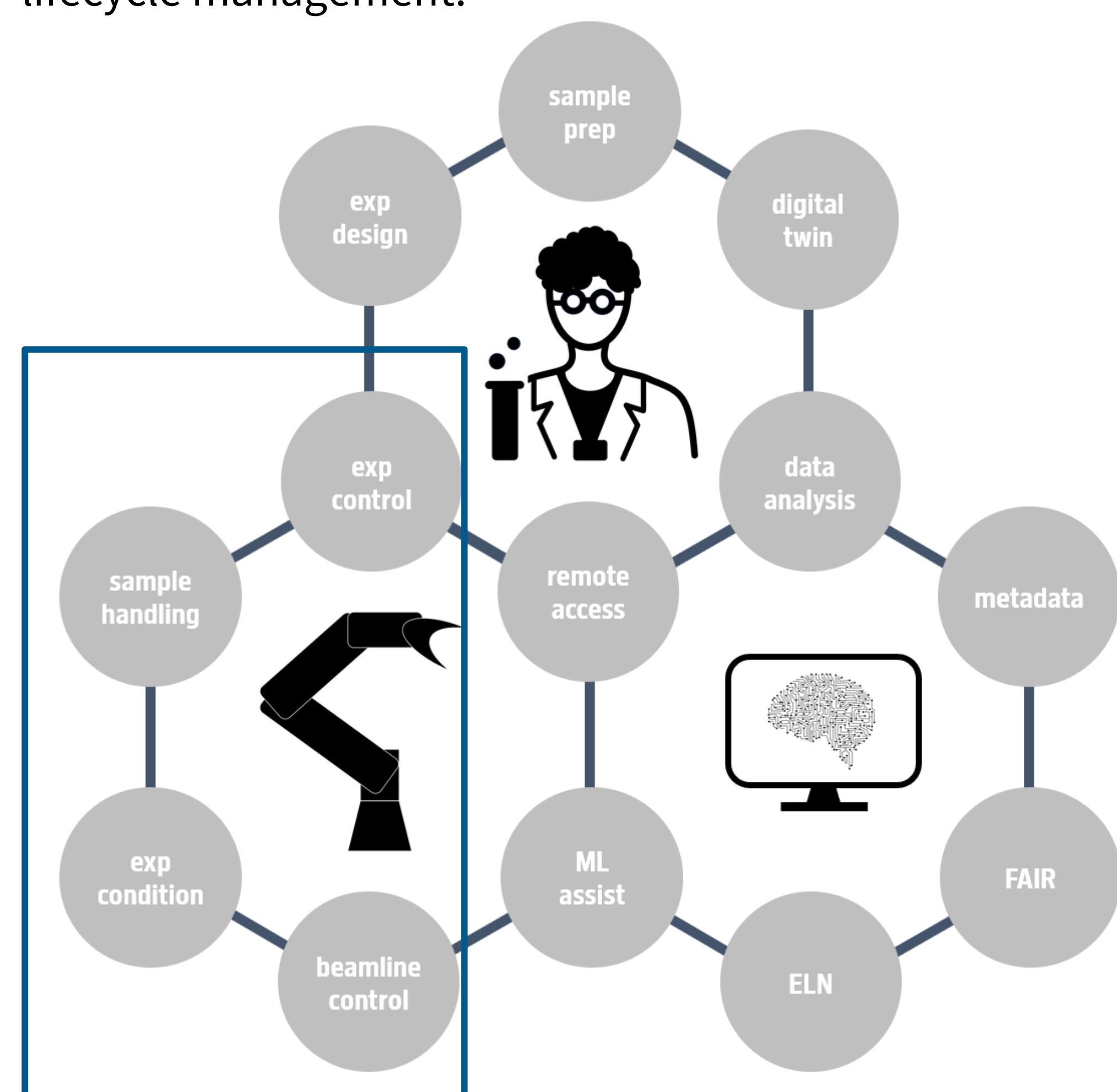
# ROCK-IT: Catalyzing innovation with EPICS, Bluesky at BESSY II MySpot beamline

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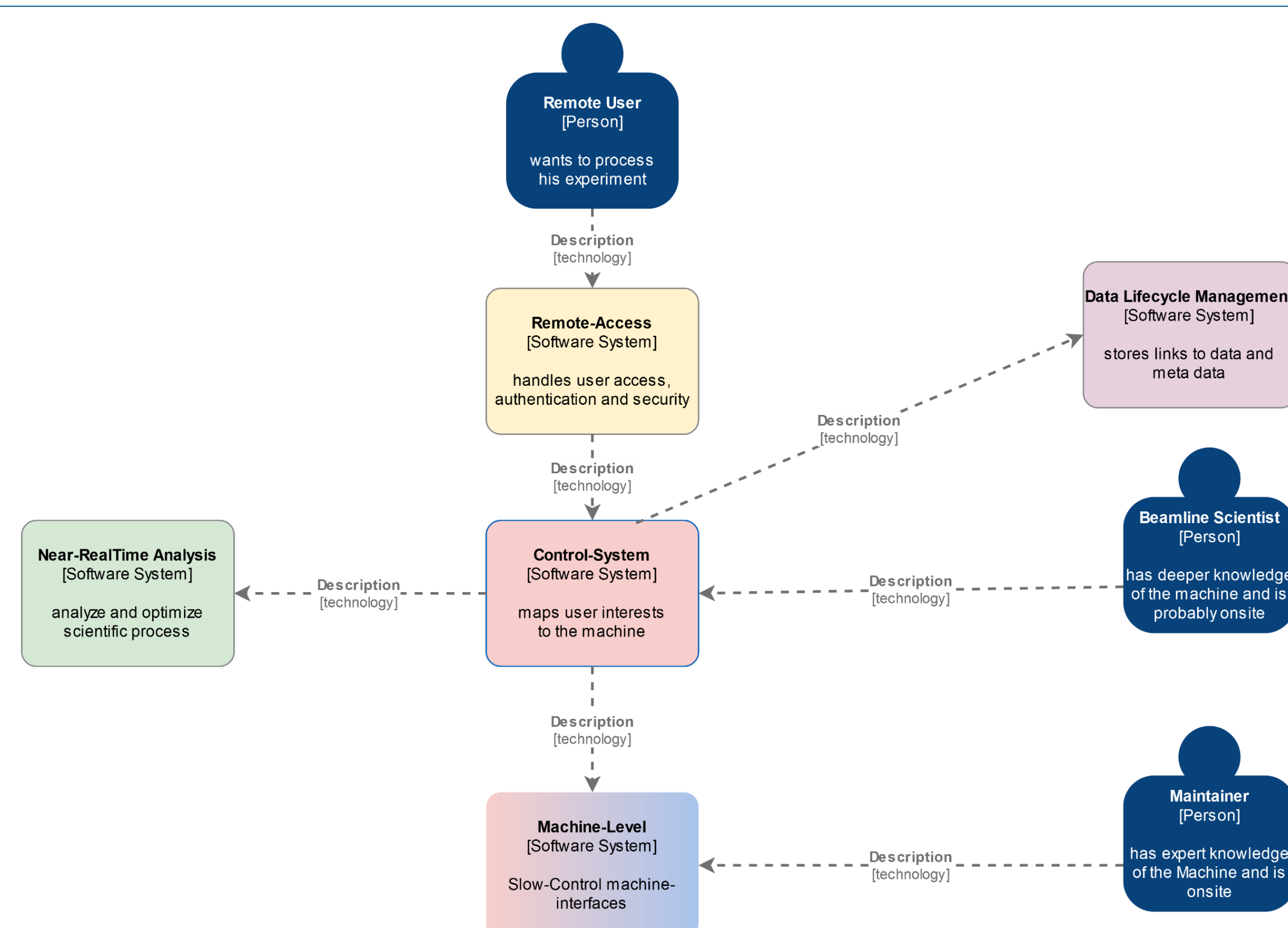
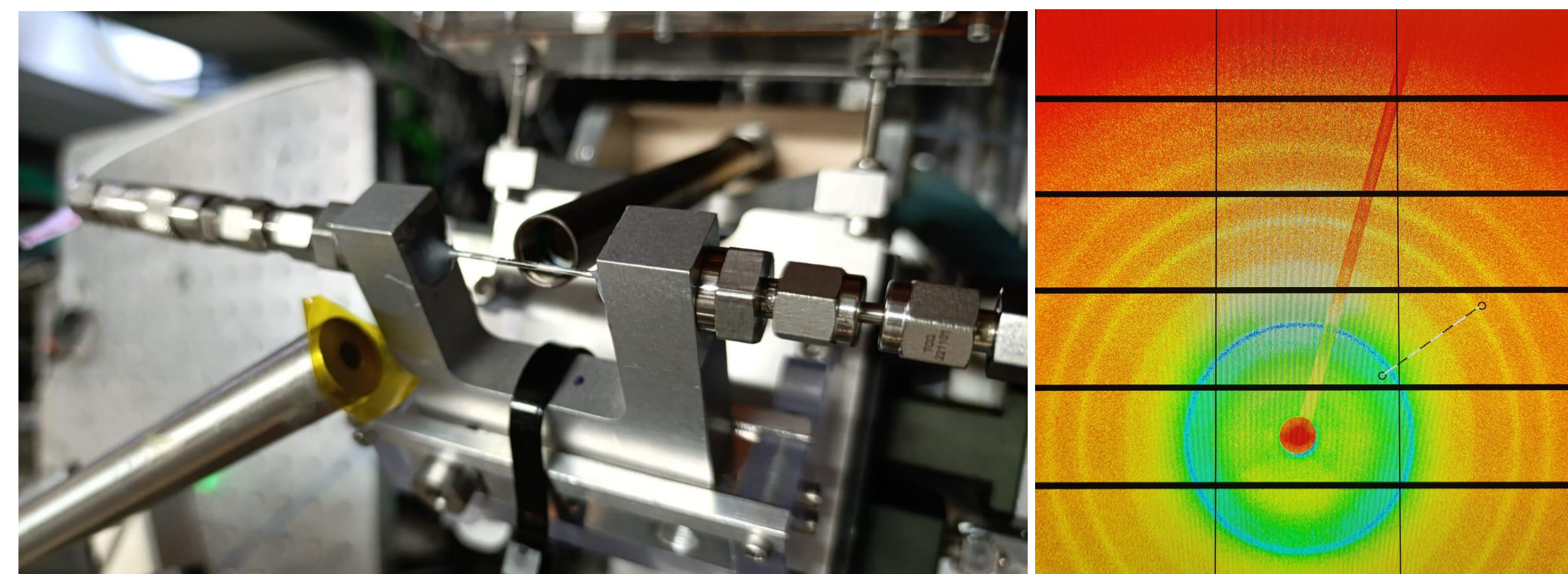
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ROCK-IT (Remote, Operando-Controlled, Knowledge-driven, and IT-based) is a project dedicated to creating user-friendly automated experiment environments with similar 'look and feel' at different facilities, aiming to reduce access barriers and accelerate innovation. Initially focusing on experimental techniques like macromolecular crystallography and standard powder diffraction conducted remotely. The ultimate goal is to make these tools transferable across various fields beyond synchrotron and neutron radiation applications, achieved through enhanced remote-access protocols, holistic experiment development, and the implementation of machine learning for automation and real-time analysis. One of the main pillars of the ROCK-IT is focused on automation and controls. The aim is to develop a top-level experimental control system with the highest degree of automation possible. This is achieved by unifying low-level controls like EPICS, TANGO, or SeCoP using Ophyd as an abstraction layer. Bluesky provides the specification and orchestration engine, that enables running complex experimental procedures. Moreover, the deployment of services follows the "Everything as a service" strategy. This contribution will outline the progress at the MySpot beamline, which was chosen as one of two demonstrators at BESSYII.

Development of a comprehensive workflow for **remote operando catalysis experiments** at large-scale research facilities, covering all aspects from experiment definition, sample shipment, automated handling and measurement, to online data analysis, remote user control, and data lifecycle management.

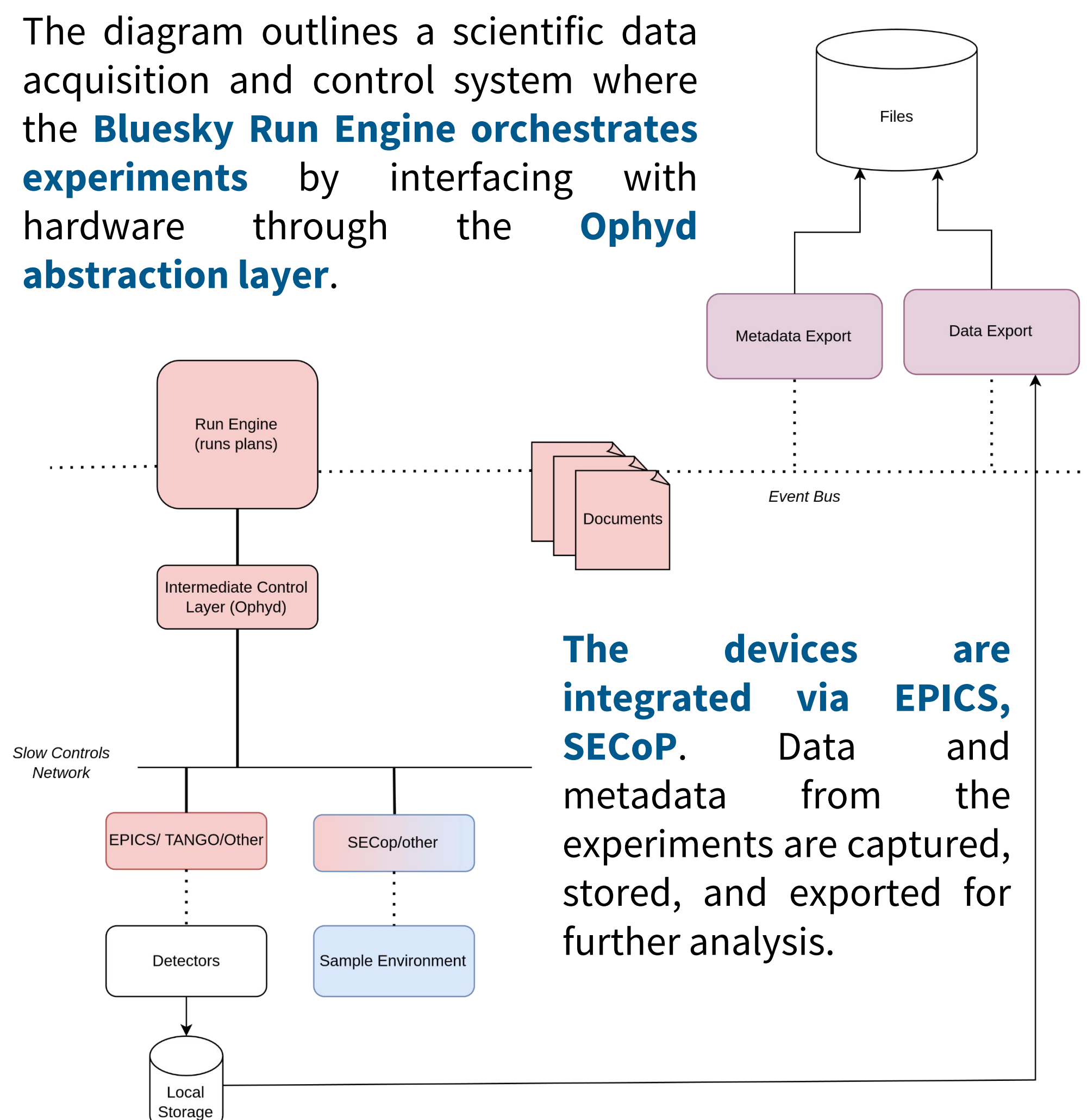


The experiment used high-resolution **X-ray powder diffraction at the BESSY II MySpot beamline** to capture detailed, real-time images of cobalt-based catalysts as they transformed, allowing for precise optimization of their performance to improve the efficiency of sustainable jet fuel production.



This diagram tells the story of a scientific experiment's journey. A **Remote User** begins by accessing the system, seeking to process their experiment. Their request flows through the Remote-Access system, ensuring **secure entry**, before being translated by the **Control System** to align with the machine's capabilities. As the experiment runs, the Machine-Level system manages the precise controls, while **Near-Real Time Analysis optimizes the process on the fly**. Behind the scenes, data is carefully managed and stored by the **Data Lifecycle Management** system, all under the watchful eyes of the **Beamline Scientist and Maintainer**, who ensure that the experiment runs smoothly.

The diagram outlines a scientific data acquisition and control system where the **Bluesky Run Engine orchestrates experiments** by interfacing with hardware through the **Ophyd abstraction layer**.



The devices are integrated via EPICS, SECoP. Data and metadata from the experiments are captured, stored, and exported for further analysis.

## RESULTS

- **Successful integration** of EPICS and SECoP controlled devices into Ophyd abstraction layer.
- Demonstrated the feasibility of performing **fully automated catalysis experiments** with custom Bluesky plans.
- Results and experiences from this catalysis experiment will help us **improve the reliability of hardware and software agents** for the next experiments in Q3/Q4 2024.

## ROCK-IT objectives

- Accelerating innovation cycles through **advanced robotics and software tools**.
- Facilitating user access to multiple German synchrotron sources with a **unified workflow**.
- **Reducing the CO2 footprint** by minimizing travel needs, allowing broader global participation.
- **Enhancing cybersecurity** to protect data and infrastructure.

## REFERENCES AND ACKNOWLEDGMENT

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## MORE INFORMATION

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