The ROCK-IT Project

Towards a Holistic Workflow for Complex Operando Experiments

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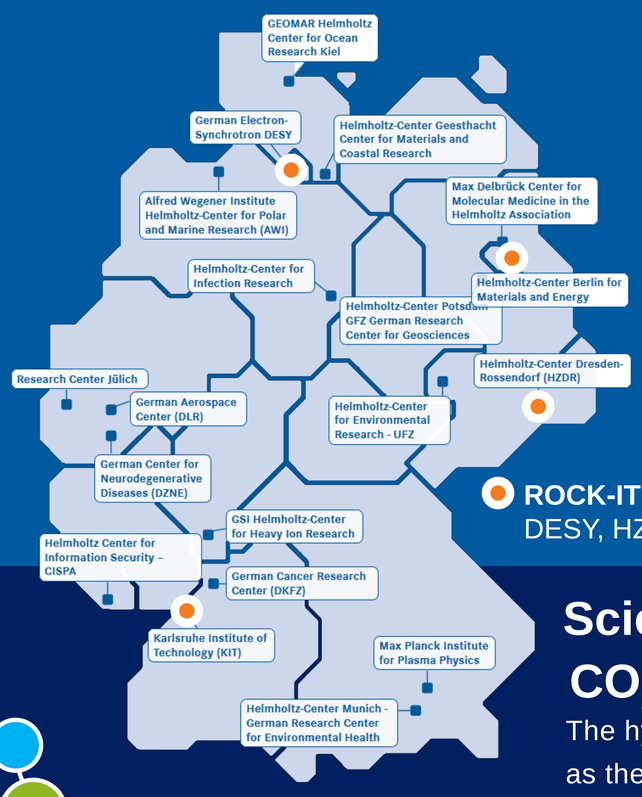
ROCK-IT (**R**emote, **O**perando-**C**ontrolled, **K**nowledge-driven, and **IT**-based) is a Helmholtz-funded project that aims to develop all the necessary tools for the automation and remote access of *in situ* and *operando* experiments, serving users of all experience levels. *Operando* catalysis experiments at synchrotron light sources, for which no automation exists so far, have been identified as a pilot development case within ROCK-IT.

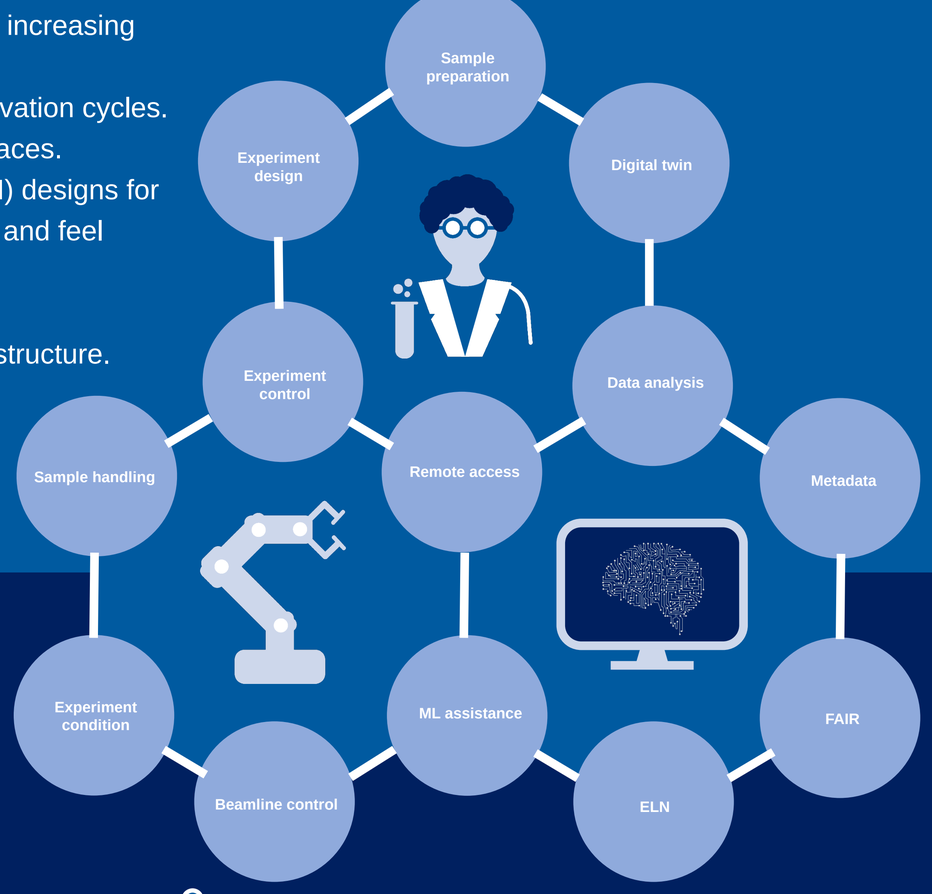


Helmholtz Centers map image source: https://upload.wikimedia.org/wikipedia/commons/3/3a/Map_of_19_member_centers_of_the_Helmholtz_association.png

ROCK-IT partners:
DESY, HZB, HZDR, KIT

ROCK-IT aims to

- Fill the gap of remote access & control for mail-in experiments among Helmholtz research centers.
- Develop standardized and modular solutions while increasing the resilience of facility operations.
- Improve the efficiency of usage and speed up innovation cycles.
- Increase standardization of components and interfaces.
- Create user-centered graphical user interface (GUI) designs for experiment control & analysis with a common look and feel among various institutes.
- FAIR data lifecycle management.
- Advanced cyber security to safeguard data & infrastructure.
- Attract more industrial users.
- Reduce the CO_2 footprint of user operations.

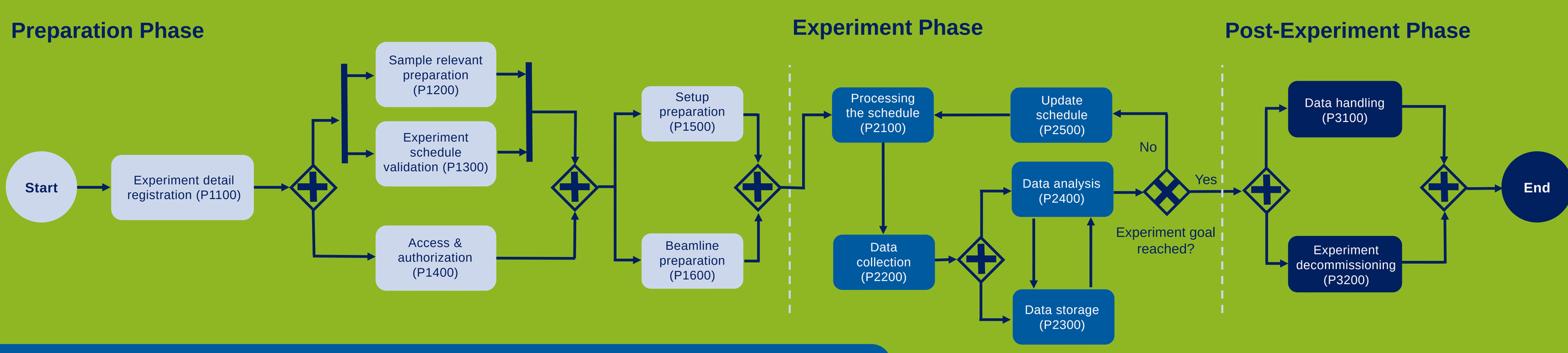


Science Case

$$CO_2 + 4\,H_2 \longrightarrow CH_4 + 2\,H_2O$$

The hydrogenation of CO_2 to methane (methanation) has been selected as the first catalytic reaction to be demonstrated in ROCK-IT. The main measurement technique will be x-ray absorption spectroscopy (XAS). Automated (robotic) sample handling and exchange are required to allow full remote control of the experiment. All reaction parameters (gas feed, temperature...) can be controlled by the user, scanned in an automated procedure, or explored in a collaborative ML-assisted way. ML will also assist in judging the quality of the data to optimize the measurement and use the beamtime efficiently.

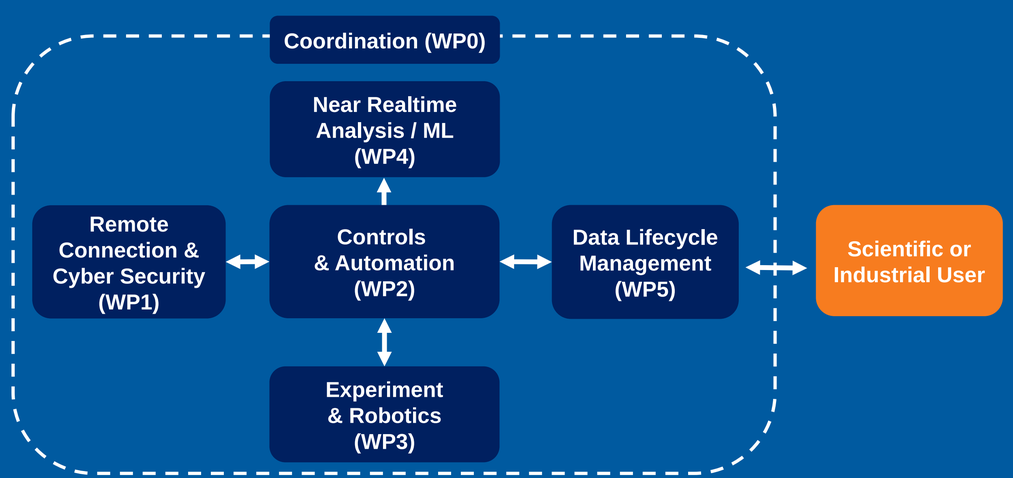
Workflow for Mail-in Remote-access Operando Experiments



Project Structure and Task Distribution

WP1 – Remote Connection & Security

- Providing secure network and data transfer based on modular concepts compatible with existing infrastructures and services (all centers are part of the HIFIS).
- Developing role-based permissions.
- Developed security concept (SeCo) based on the IT baseline protection from the German Federal Office for Information Security.
- Protection is based on confidentiality, integrity, and availability.



WP2 – Controls & Automation (Poster 60, 65 & 97)

- Implementing Bluesky as the common interface to instruments with different control systems.
- Developing a web-based user interface for experiment configuration, control, and monitoring (Daiquiri & REACT).
- Providing interfaces for machine learning and AI-assisted data quality and experiment control.
- Consistent "look & feel" of partner beamlines.

WP3 – Experiment & Robotics (Poster 97)

- Full automation (robotic sample handling, gas supply and analysis infrastructure, metadata)
- Providing tailored sample environments for operando catalysis experiments.
- Designing standardized reactor cells with robotic manipulation.
- Standardized high-level interface for sample environment automation (e.g. gas handling).

WP4 – Near-Realtime Analysis & ML

- Implementing near-realtime data analysis using ASAP::O.
- Heterogeneous data streaming and processing.
- Developing digital twins by leveraging surrogate models and machine learning (ML) inversion techniques to support beamline setup, preparation, and optimization.
- Enhancing data quality through advances in machine learning techniques.

WP5 – Data Lifecycle Management

- Developing data management architecture and plan (DMAP) following the FAIR principle.
- Providing the experimental data for users in standardized ways.
- Utilizing ongoing activities like NFDI projects *(e.g. DAPHNE4NFDI & NFDI4Cat), & Nexus.*
- Protection of sensitive data for (industrial) users FAIR ≠ Open.
- Establishing a metadata scheme for information exchange between electronic lab notebooks (ELN).

Acknowledgements

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rock-it-project.de

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