HELMHOLTZ

RESEARCH FOR
GRAND CHALLENGES

THE ROCK-IT PROJECT

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DESY. HZB Helmholtz Zentrum Berlin HZDR KIT

THE ROCK-IT PROJECT

remote, operando controlled, knowledge-driven, IT-based

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MOTIVATION

Strong need for further development of access and experiment schemes for more complex operando and in-situ experiments to

- **increase the resilience of operation against travel and working restrictions**
- **reduce the CO_2-footprint of the entire operation due to less travel requirements**
- **increase the efficiency by higher degree of automation (=> evaluation of larger exp. parameter spaces).**
- **attract more industrial users and as such contribute to the innovation cycle within Germany and Europe.**

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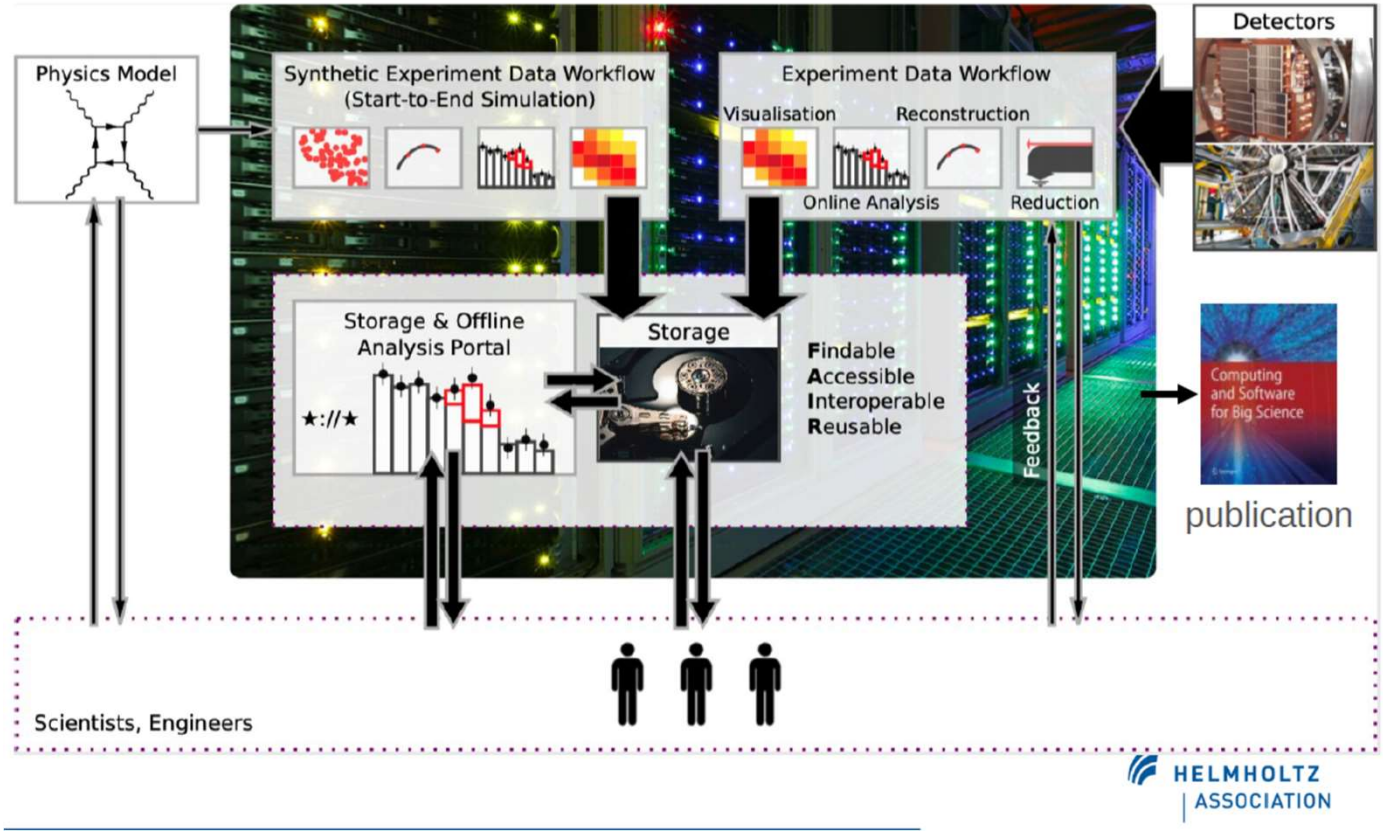
PROJECT AIM

Development of a holistic workflow for remote operando catalysis experiments at large-scale research facilities. Considering all aspects of experiment definition by the user, sample shipment, automated sample handling and measurement including online data analysis, remote control by the user, and data lifecycle management obeying the FAIR (Findability, Accessibility, Interoperability, and Reuse) data principles. Wherever possible Free and Open Source Software (FOSS) will be used and compatibility and integrability with the Helmholtz Federated IT Services will be ensured.

THE ROCK-IT PROJECT

full data lifecycle



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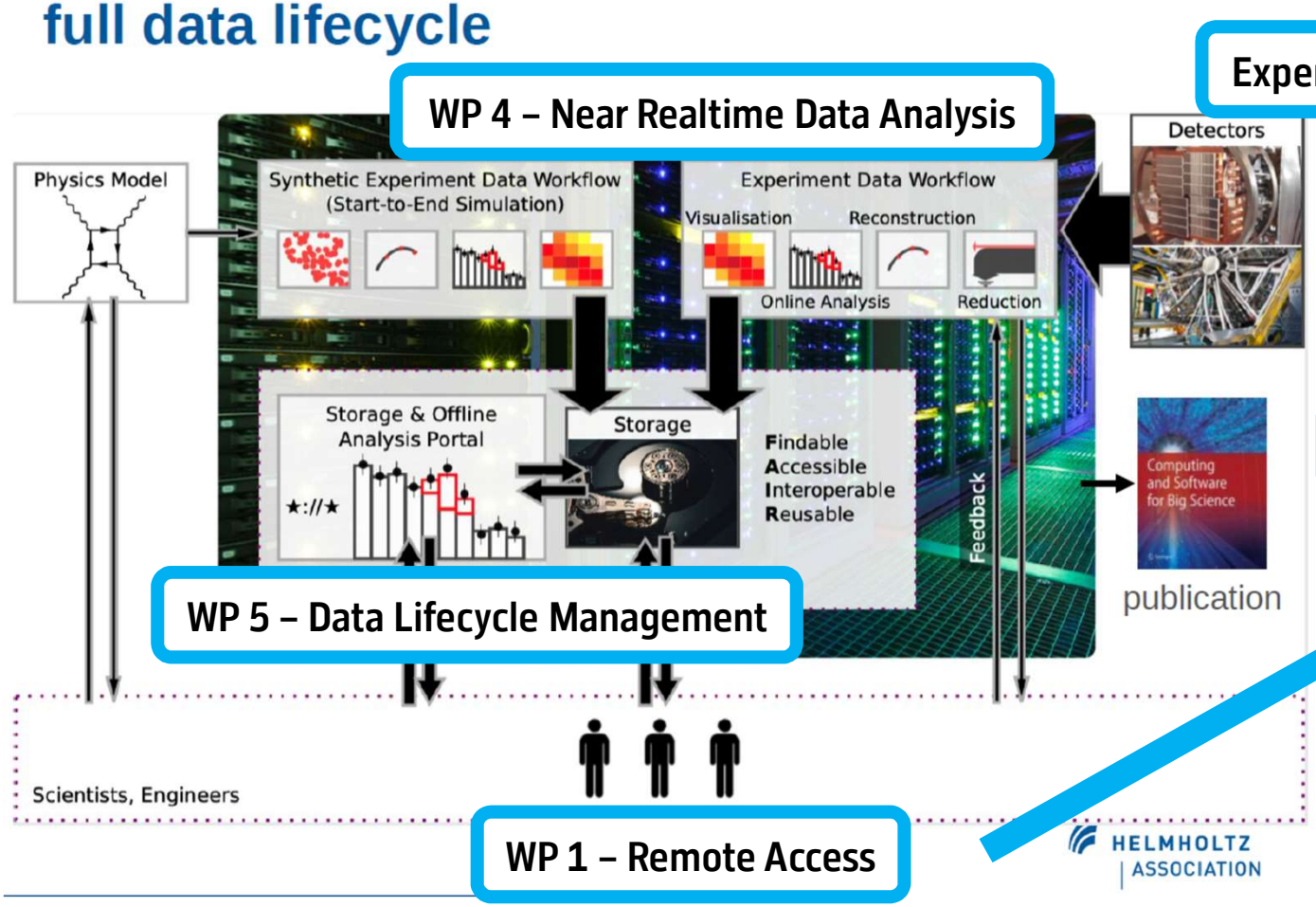
full data lifecycle



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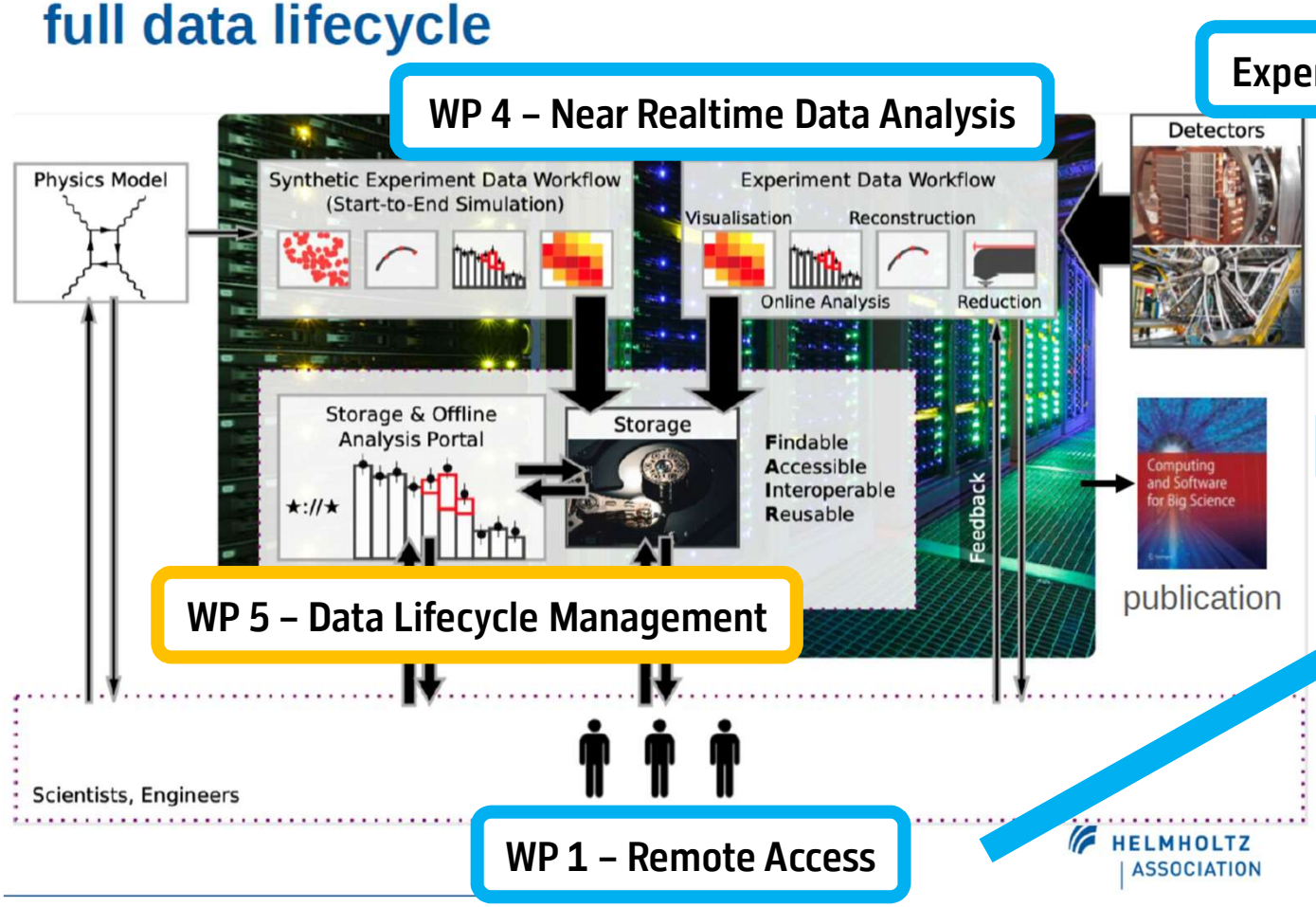
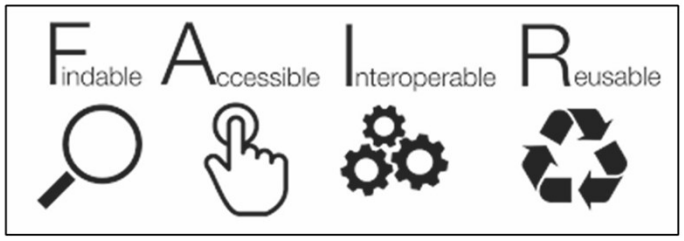


THE ROCK-IT PROJECT

work packages

WP5: DATA LIFECYCLE MANAGEMENT

- Data management based on FAIR principles building on German research data infrastructure (NFDI) projects, including DAPHNE4NFDI, FAIRmat, and NFDI4Cat
- FAIR ≠ Open: Protection of sensitive data
- Focus on standardizing metadata and data generation workflows, and on establishing best practices for electronic lab book usage



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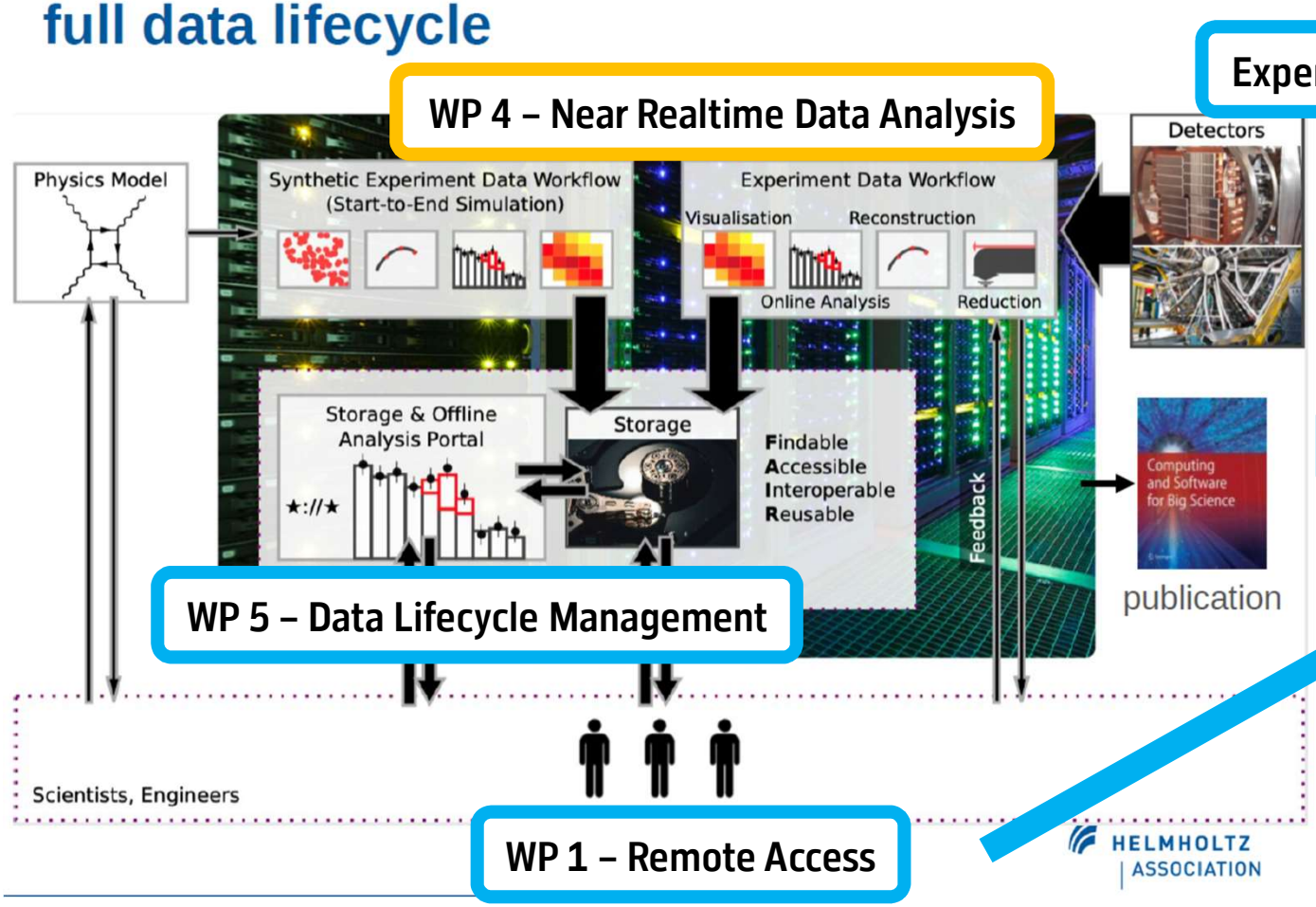

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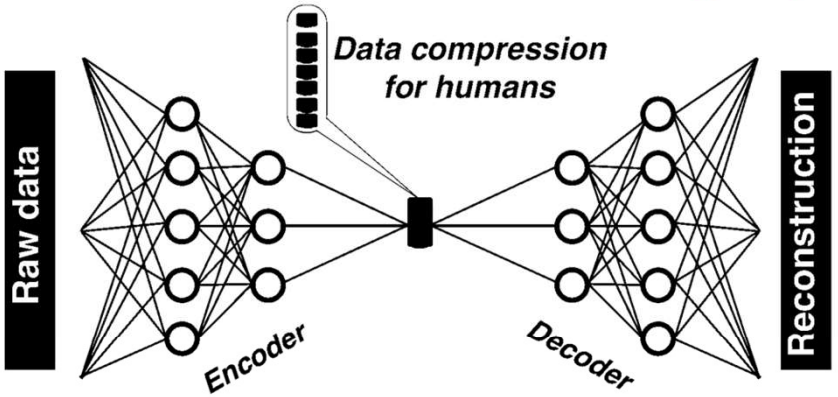
work packages

WP4: NEAR-REALTIME ANALYSIS (ML)



- Near-Realtime analysis: Optimization by looking at experiment outcome, optimizing data quality, allowing for in-transit data reduction, steering experiments towards optimum usage of measurement time and identify outliers
- Increase in efficiency and quality of data enabled through advances in machine learning (ML)

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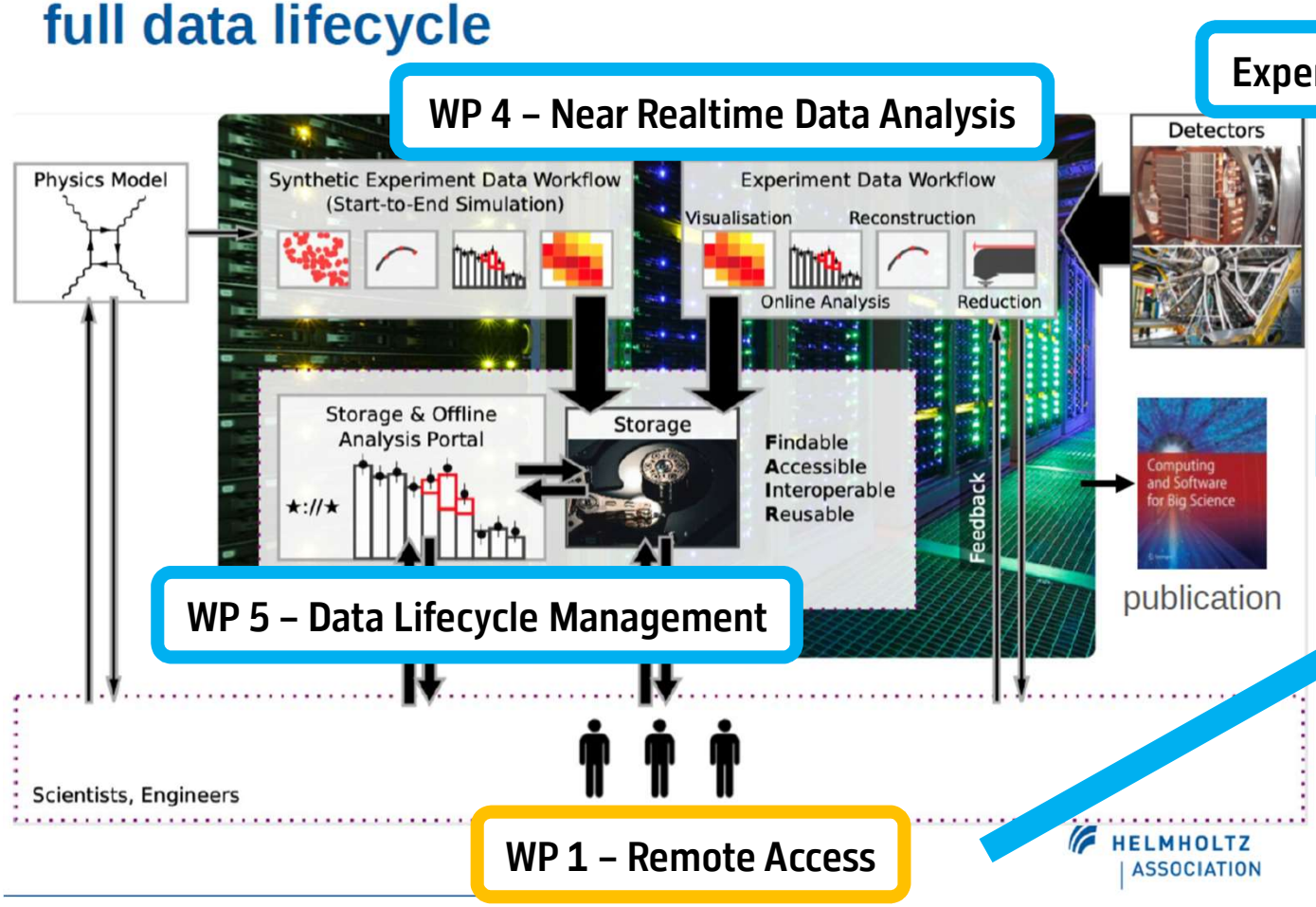
full data lifecycle



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work packages

WP1: REMOTE CONNECTION & SECURITY

- Modular concepts with defined, secured, and certified interfaces
- Compatibility with existing infrastructures, services (such as FAIRmat, DAPHNE4NFDI,...) and security policies
- Focus on usability in the development of remote-access software so that graphical interfaces are intuitive and easy to use for different types of users with different experiences and backgrounds

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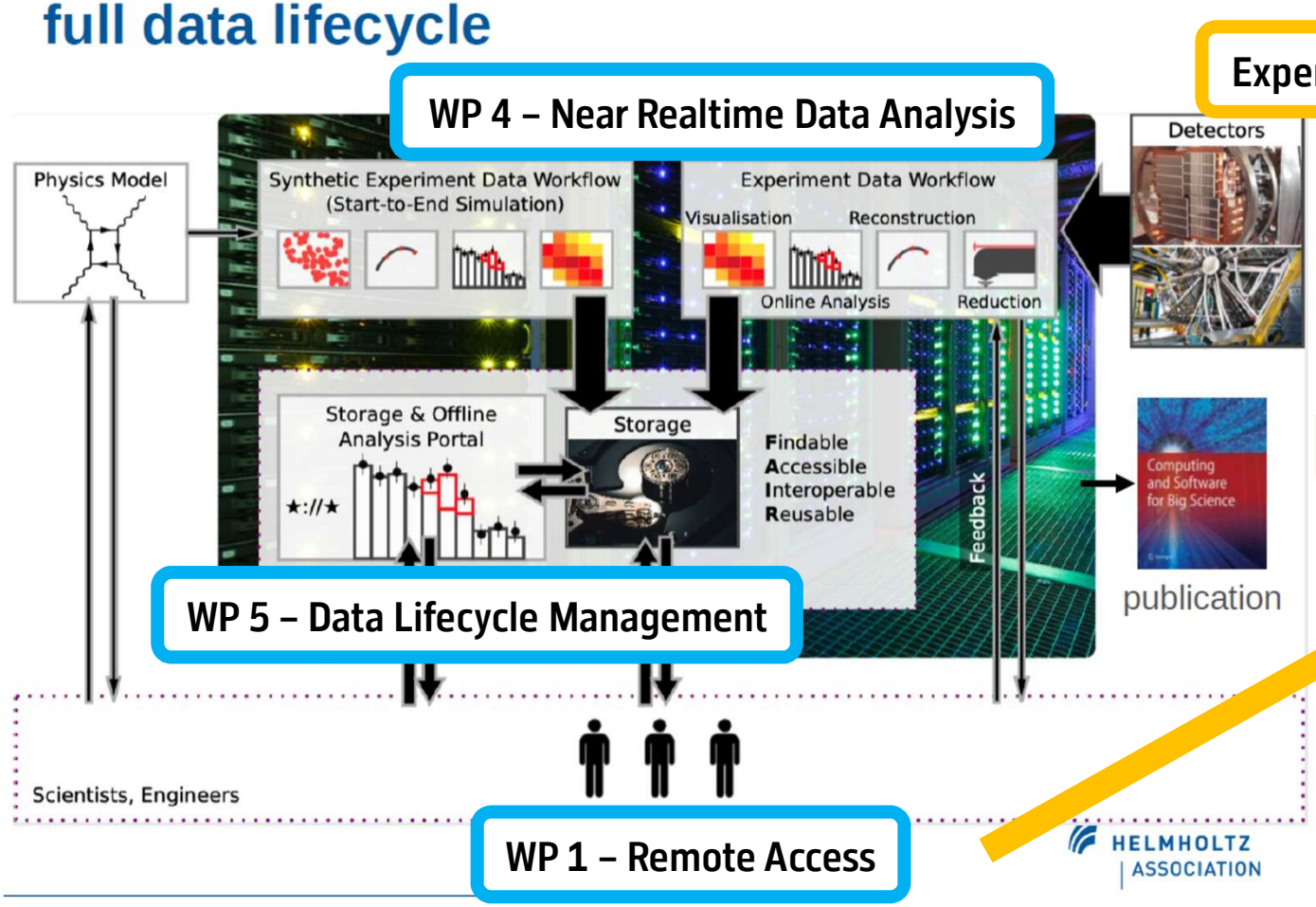
full data lifecycle



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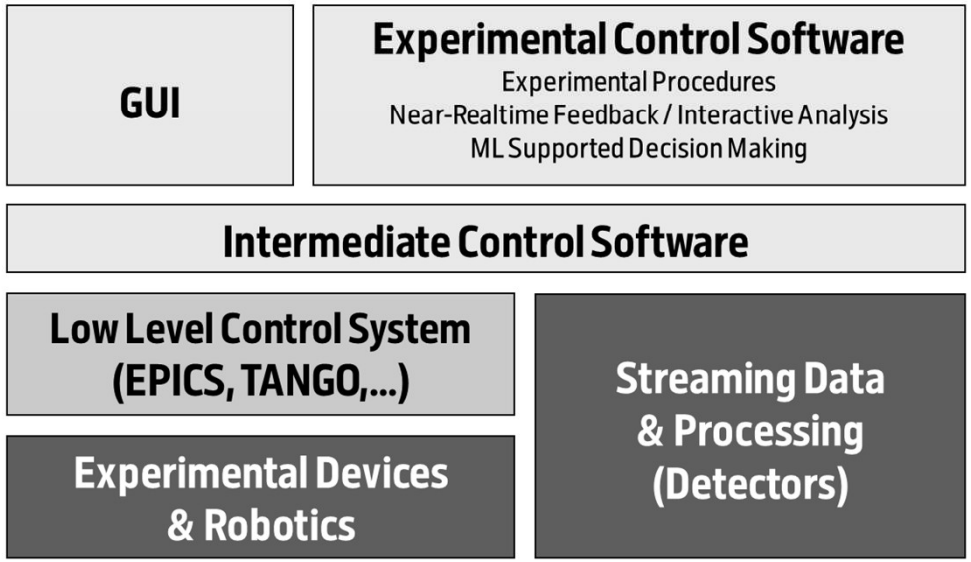
WP2: CONTROLS & AUTOMATION

- Experimental control software including a graphical user interface and providing the highest degree of automation
- Providing consistent "look & feel" at the synchrotron sources PETRA III, BESSY II, KARA, removing access barriers



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WP3: EXPERIMENT & ROBOTICS

- Tailored sample environments: Measure catalytic performance and get access to multimodal analytics
- Setup and control of exemplary reactor cells (for different samples and investigation methods) using robotic manipulators, realization of standardized gas supply and analysis infrastructure including quality control by automated reference measurements
- Aim: Full automation (robotic sample handling, gas supply and analysis infrastructure, metadata)

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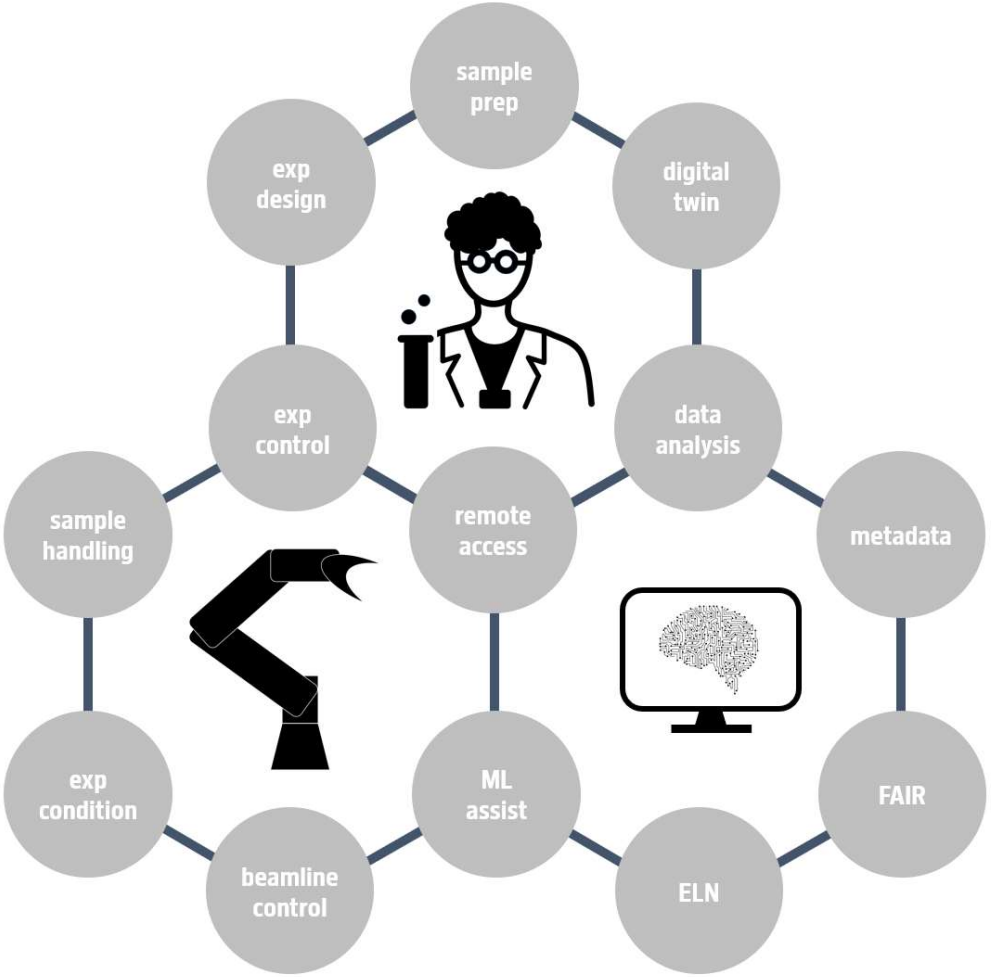
holistic workflow



ACKNOWLEDGEMENTS

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Thank you for your attention!