Deploying Kadi4Mat Workflows in Laboratory Environments for Reproducible and Guided Experimental Research

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Within the Kadi4Mat ecosystem, Kadi4Mat Workflows [1,2] support the systematic deployment of laboratory workflows by transitioning execution from previously exclusively local desktop systems (KadiStudio) to remote, containerized infrastructures, such as Docker and Kubernetes. This approach ensures controlled, scalable, and reproducible execution conditions across experimental runs. Interactions via a web interface allows workflows to be controlled and monitored on mobile devices at the point of experimentation. For procedural steps that require human intervention, the workflow provides predefined, structured input fields for capturing user inputs and observations during execution. QR code-based identification of samples and laboratory equipment further improves traceability and reduces manual transcription errors. Experimental data and associated metadata can be persistently stored in the Kadi4Mat repository, enabling comprehensive provenance tracking as well as reproducibility, reuse, and long-term preservation of laboratory research data.

As part of this framework, electrochemical corrosion measurements (e.g., OCP, polarization curves, EIS) are implemented as Kadi4Mat Workflows, enabling guided execution with structured capture of test parameters, sample history and electrolyte composition directly at the point of experimentation. The resulting raw data and metadata are stored persistently in the Kadi4Mat repository, providing end-to-end provenance and ensuring reproducible, comparable corrosion metrics across experimental runs and infrastructures.

Overall, Kadi4Mat Workflows extend electronic lab notebook (ELN) concepts from passive documentation toward guided experiment execution. By integrating structured data capture with workflow-driven experimental guidance, experiments are documented directly during execution rather than retrospectively. This approach embeds ELN functionality into everyday laboratory practice and supports reproducibility by design through the seamless coupling of experimental procedures, data, and metadata.

References

[1] Al-Salman, R. et al. (2023). KadiStudio use-case workflow: Automation of data-processing for in situ micropillar compression tests. Data Science Journal, 22(1).

[2] Griem, L., Zschumme, P., Laqua, M., Brandt, N., Schoof, E., Altschuh, P. and Selzer, M. (2022) ‘KadiStudio: FAIR Modelling of Scientific Research Processes’, Data Science Journal, 21(1), p. 16.