

# Kadi4Mat and the Kadi ecosystem

## A Virtual Research Environment for Materials Science

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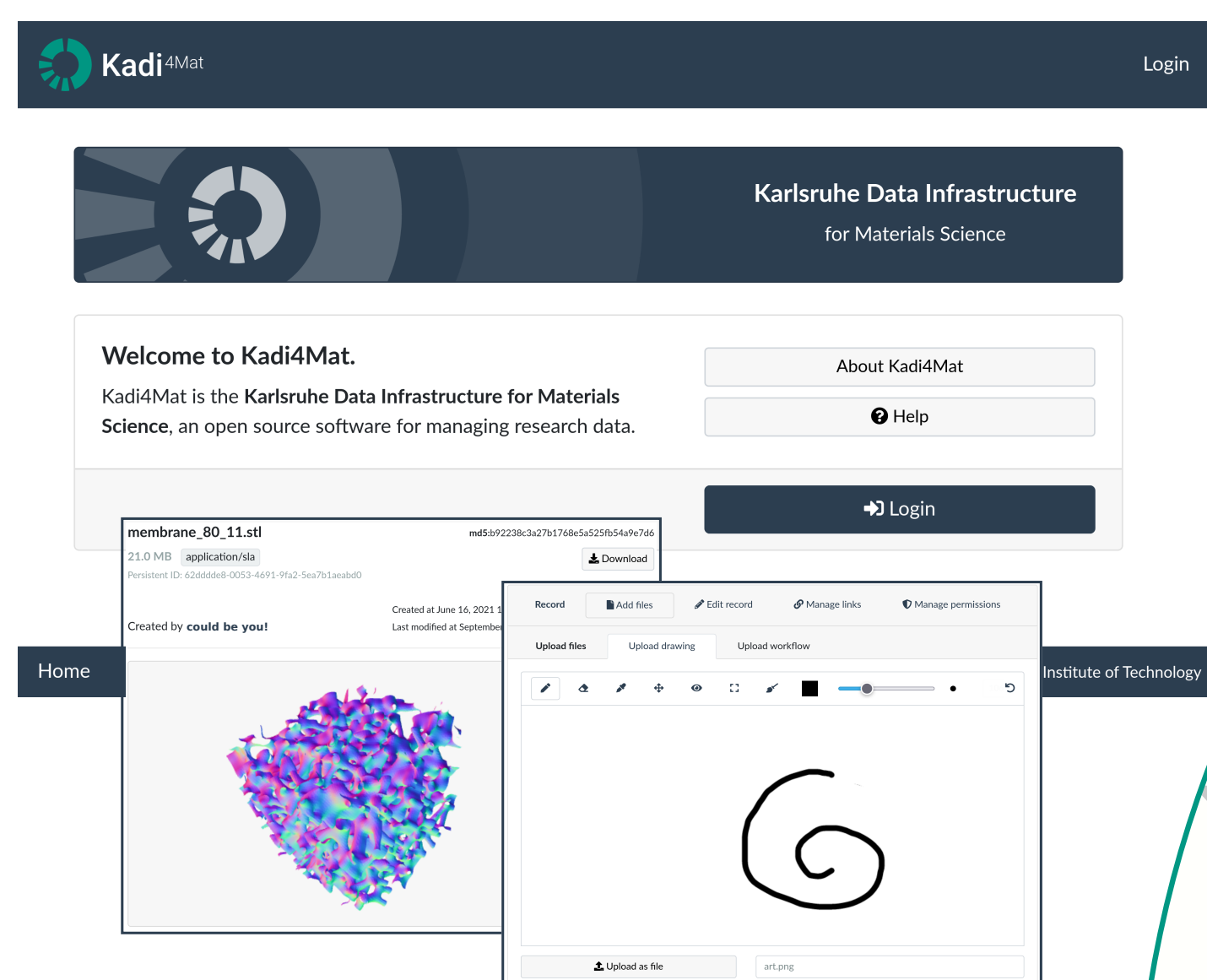
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### Introduction

Advancements in technology and the demand for tailored materials with specific properties and functionalities, keep increasing the complexity of materials science research. Managing the continuously expanding data from simulations and experiments will be unattainable without appropriate data science techniques. The structured preservation of research data and corresponding metadata is a fundamental requirement for conducting significant data analyses and facilitating result sharing. A suitable research data infrastructure plays an important role in achieving this aim. Our solution is Kadi4Mat, a comprehensive framework that integrates multiple modules collectively forming a versatile research data infrastructure.

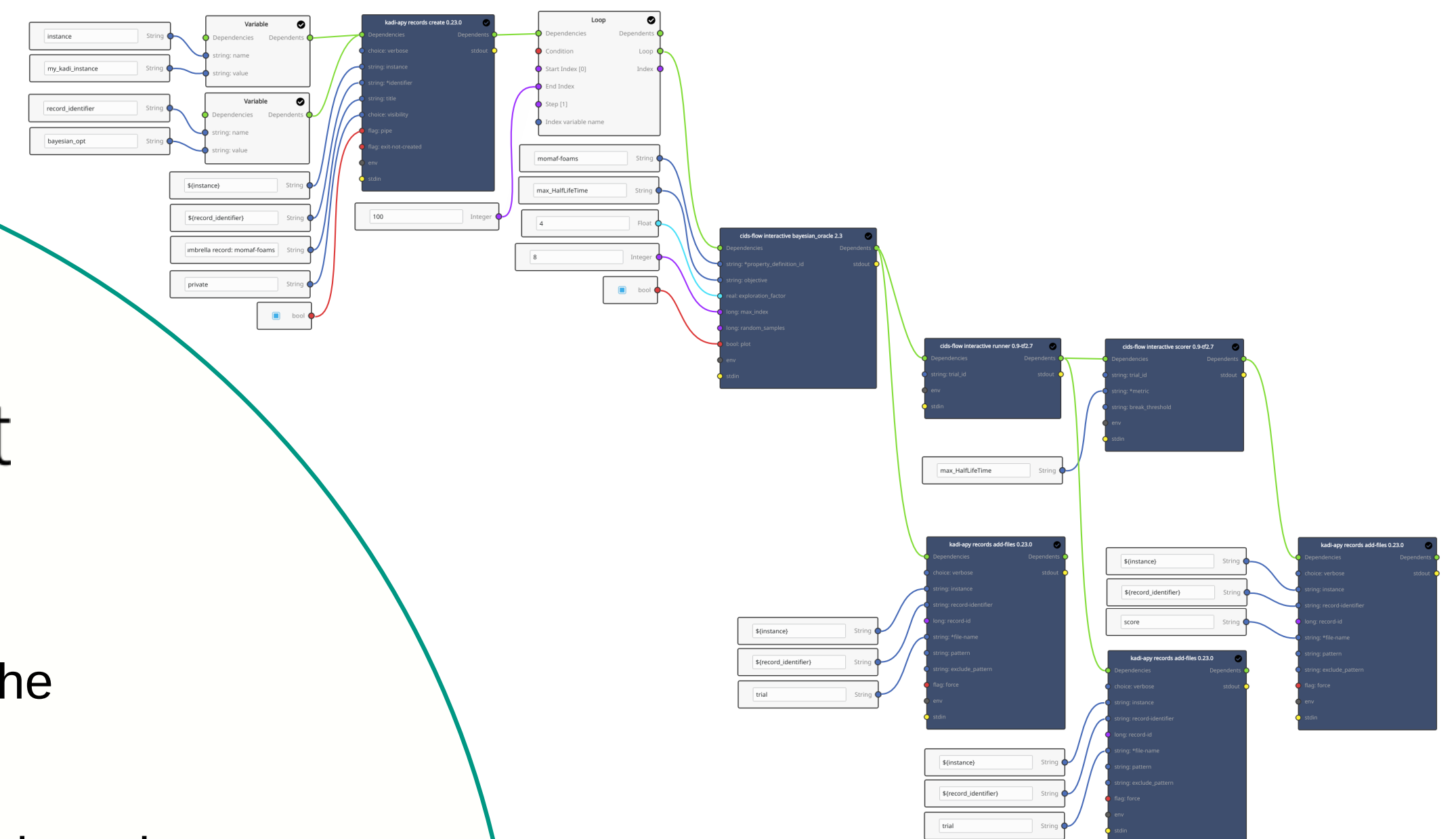
### KadiWeb

- General accessible web-based version of Kadi4Mat incorporating a classical ELN and a repository [1].
- Repository focuses on unpublished data that is to be analysed further.
- ELN component is focused on the automated and documented execution of heterogeneous workflows.



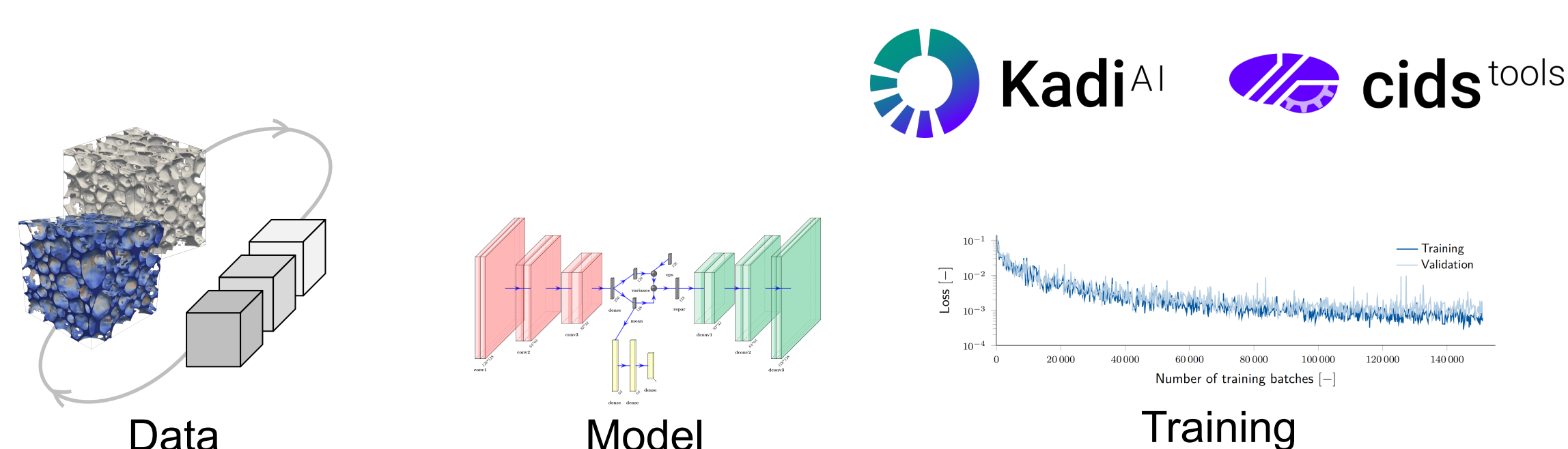
### KadiStudio

- Desktop-based application for formulation and execution of workflows [2].
- The application allows to design and execute node-based workflows that can also be used offline, by running as an ordinary application on a local workstation.



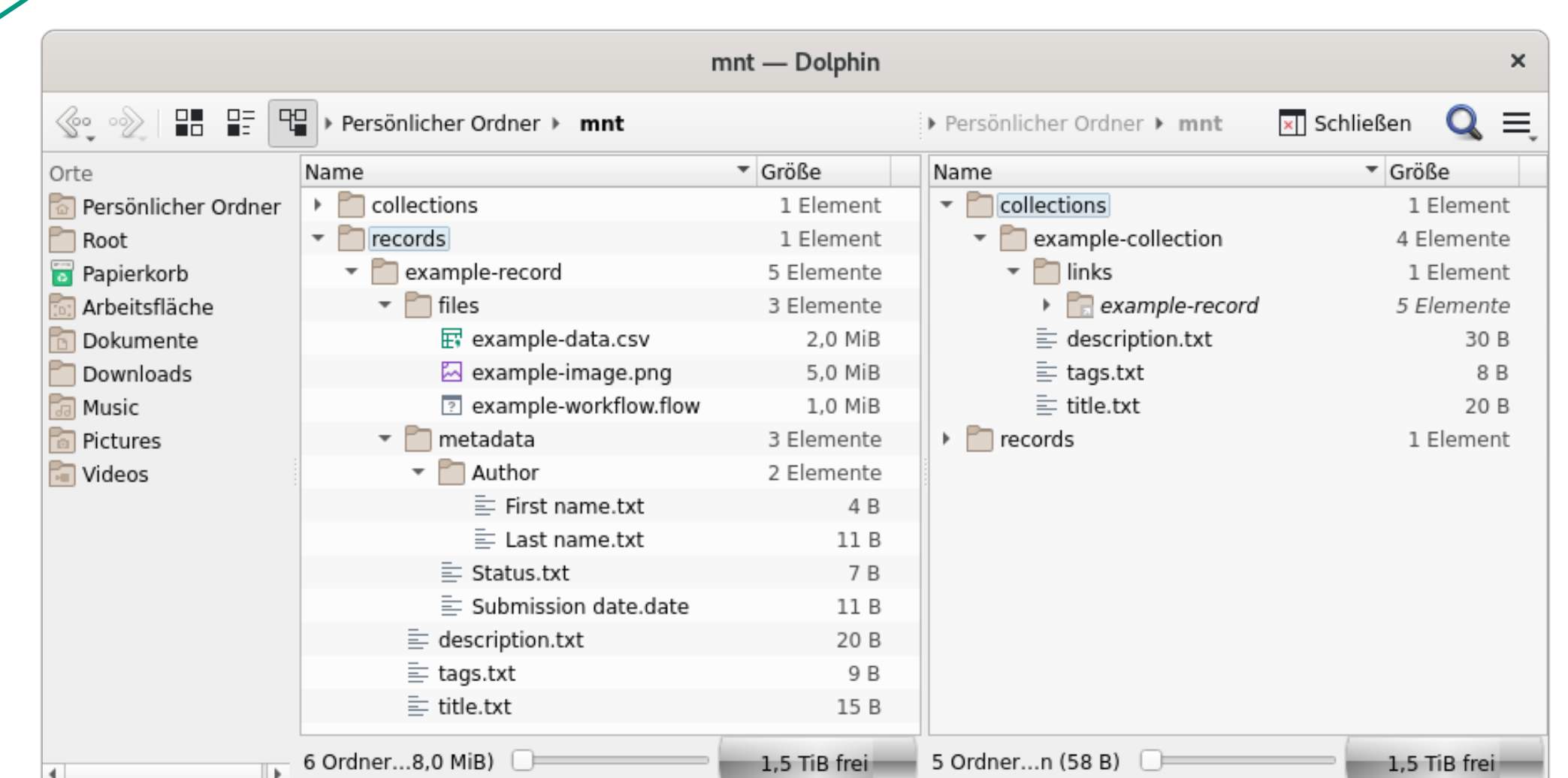
### KadiAI

- KadiAI and CIDS [3] are Kadi4Mat's interface and solution for integrated Machine Learning (ML) and Artificial Intelligence (AI).
- KadiAI provides an interface for AI projects, work packages, and process steps to integrate directly into the Kadi ecosystem.
- CIDS (Computational Intelligence and Data Science) is a Python based framework to efficiently implement AI models on datasets in Kadi4Mat leveraging libraries such as tensorflow and scikit-learn.



### KadiFS

- Integration of Kadi4Mat into a desktop environment to combine the advantages of Kadi4Mat and the work in the filesystem.
- Use the usual file system operations and/or any application to interact with the resources of Kadi4Mat.



FAIR storage of all data and processes in the research data infrastructure **Kadi4Mat**.

Modular and generic architecture that combines the two components **electronic lab notebook (ELN)** and **repository**.

Structures are equipped with **descriptive metadata** and stored within Kadi4Mat's repository.

Part of the Kadi ecosystem are **KadiWeb**, **KadiStudio**, **KadiAI** and **KadiFS**.

#### References.

- [1] Brandt, N., Griem, L., Herrmann, C., Schoof, E., Tosato, G., Zhao, Y., Zschumme, P. and Selzer, M., 2021. Kadi4Mat: A research data infrastructure for materials science. *Data Science Journal*, 20(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*, 19: XX, pp. 1–17. DOI: <https://doi.org/10.5334/dsj-2022-017>.  
 [3] Koeppel, A., and The KadiAI Team. CIDS: 3.1. 2023. 10.5281/zenodo.7524476.

#### Acknowledgement:

This work is funded by the Ministry of Science, Research and Art Baden-Württemberg (MWK-BW) in the Science Data Center MoMaF, with funds from the state digitization strategy digital@bw (project No. 57), the BMBF and MWK-BW as part of the Excellence Strategy of the German Federal and State Governments in the project Kadi4X and the support of the Karlsruhe Nano Micro Facility (KNMF, [www.knmf.kit.edu](http://www.knmf.kit.edu)), a Helmholtz Research Infrastructure at Karlsruhe Institute of Technology (KIT, [www.kit.edu](http://www.kit.edu)) within the program MSE No. 43.31.01. Furthermore, the authors would like to thank the Federal Government and the Heads of Government of the Länder, as well as the Joint Science Conference (GWK), for their funding and support within the framework of the NFDI4ing consortium, funded by the German Research Foundation (DFG) – project number 442146713.

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