

Managing locally stored scientific data with PASTA-ELN

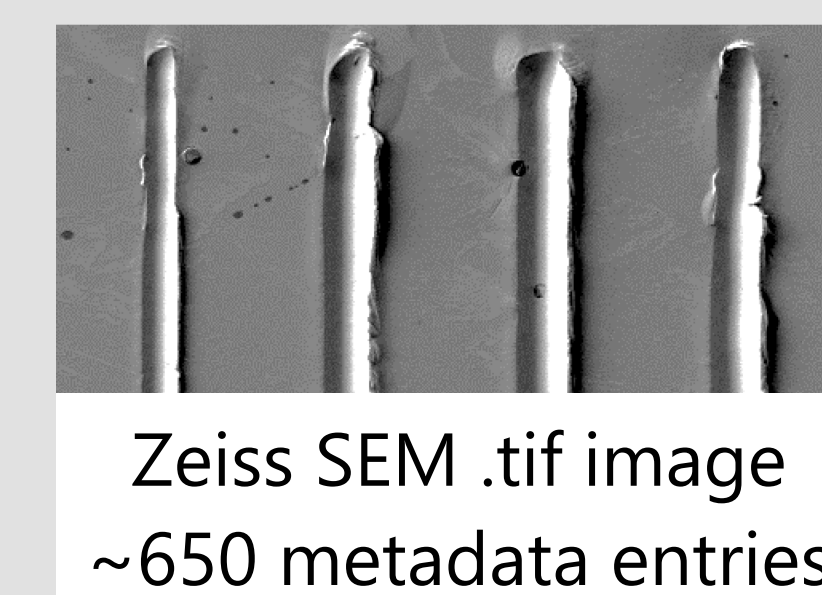
Hanna Tsybenko, Steffen Brinckmann, Ruth Schwaiger

Institut für Energie- und Klimaforschung, Structure and Function of Materials (IEK-2),
Forschungszentrum Jülich GmbH, 52428 Jülich, Germany

Contact: s.brinckmann@fz-juelich.de

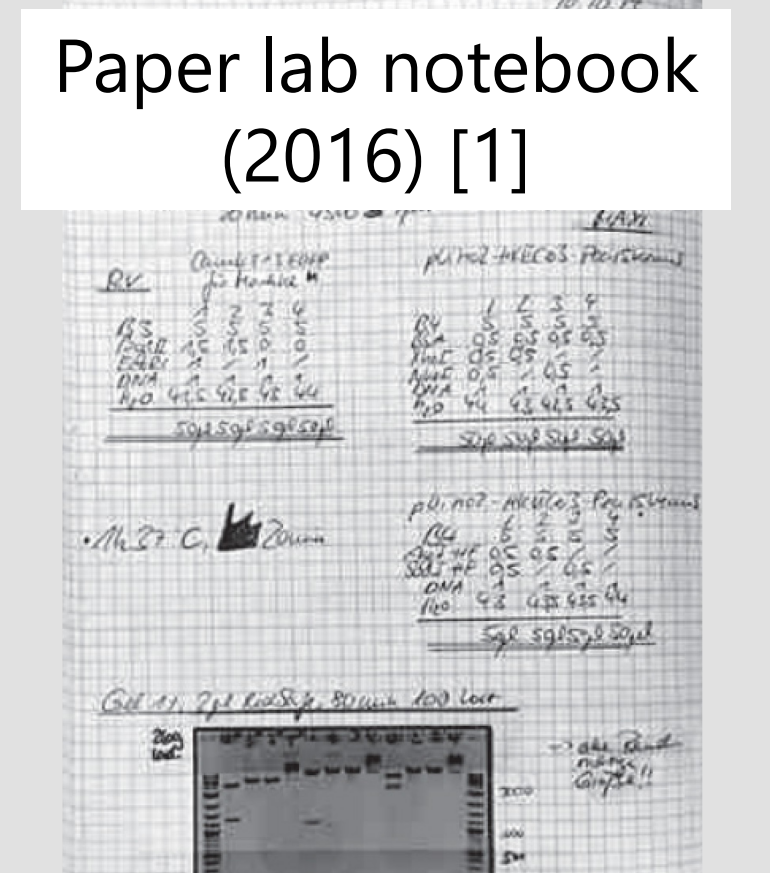
Challenges in experimental Materials Science RDM

- Hardware and software discontinued
- Data heterogeneous, stored via proprietary formats
- Analysis via locally installed vendor software
- Metadata entries often manually annotated



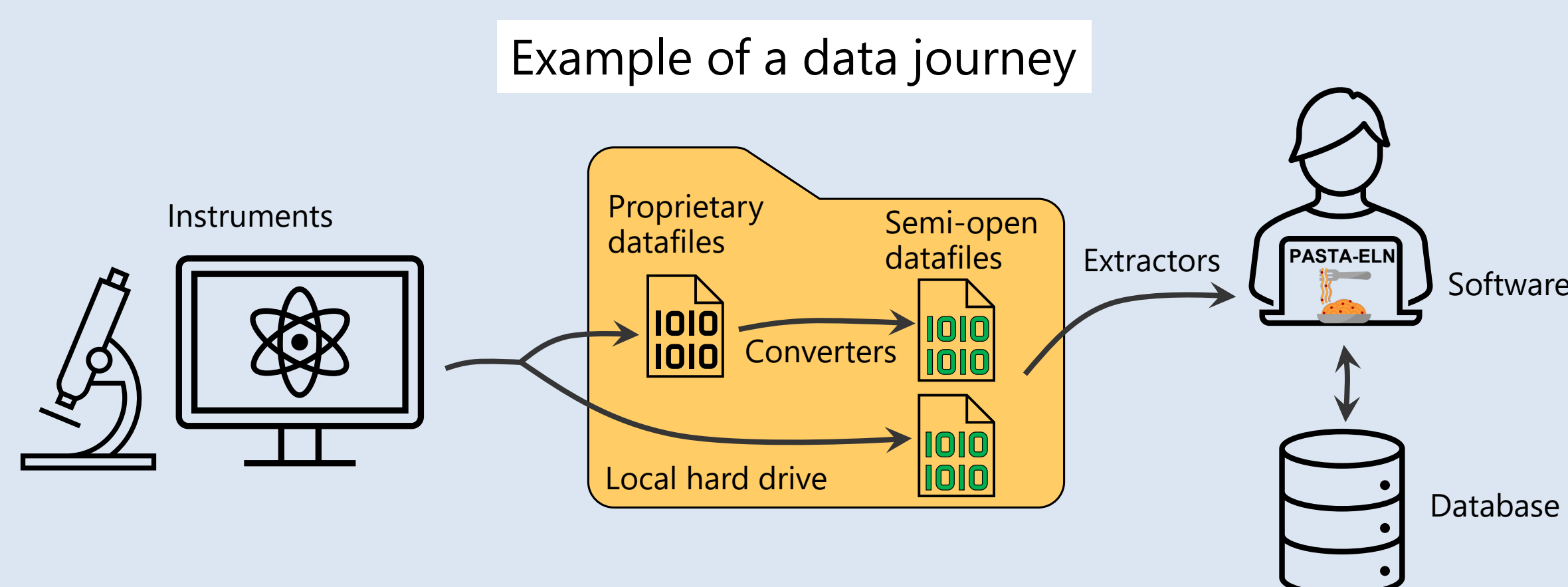
Metadata in spreadsheets

batch	-name	d _{max}	P _i [W]	t _i [us]	d _i [um]	d _{max} [um]	porosity xy [%]
1	AMT_0595	30	200	65	55	105	0.00%
6	AMT_1140	25	200			100	0.00%



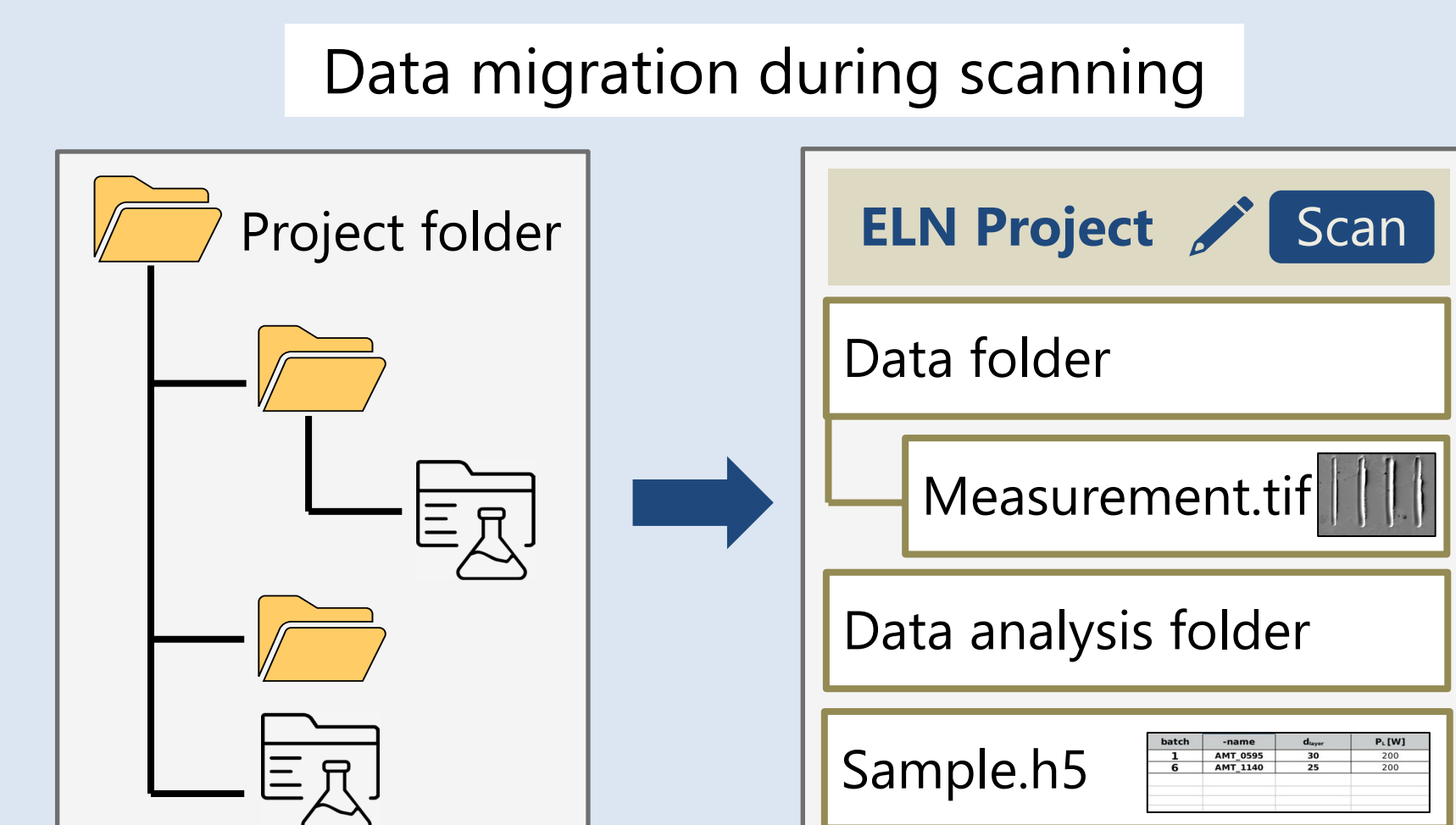
PASTA-ELN

- manages locally stored scientific data
- adaptable (extractors, hierarchy editor)
- stores metadata and project structure in CouchDB



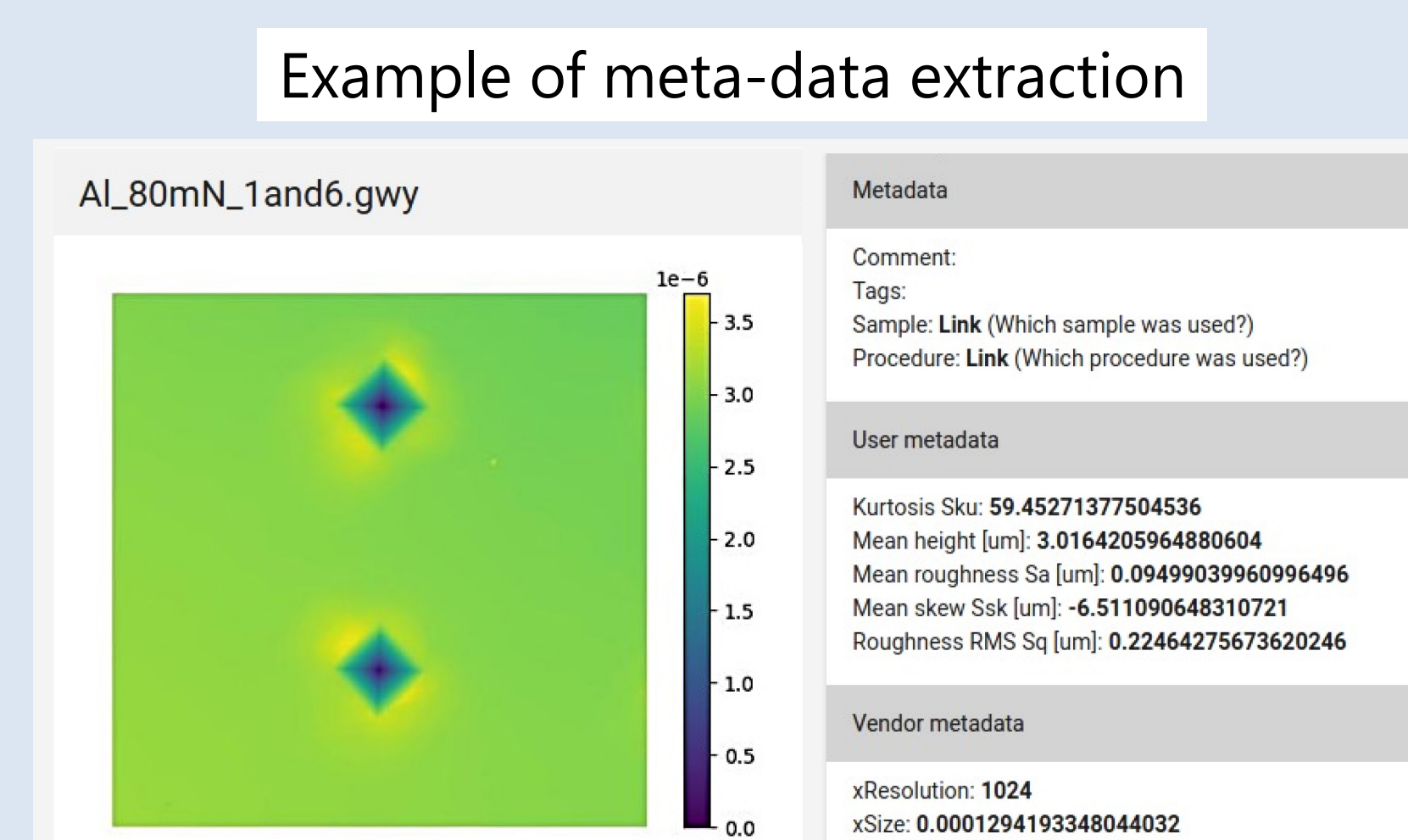
Data migration into the project

- Achieved by scanning the project directory
- Directory structure = data structure in notebook layout
- Easy to switch between analysis software and ELN



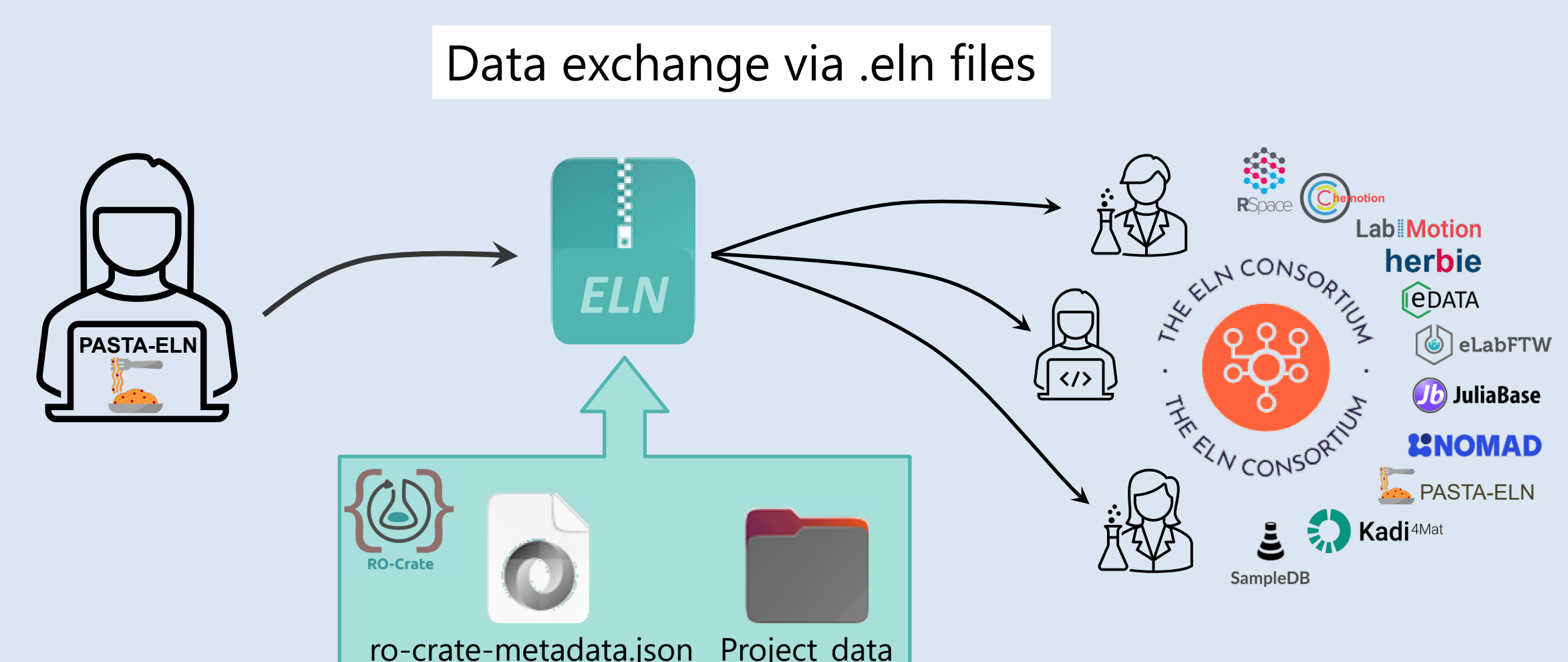
Automated metadata harvesting

- Extraction into the project via extractor scripts
- Available for both binary and converted files
- Instant previewing of metadata and analysis results



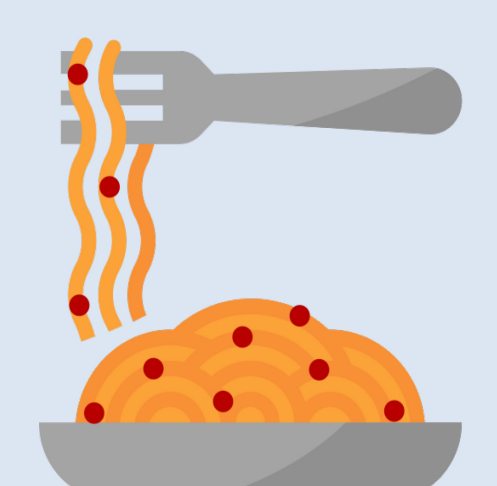
Interoperability between ELNs

- ELN Consortium: exchangeable file format
- .eln file = archive with all data and metadata
- RO-Crate [2]: metadata linked with research data



Take home message

PASTA-ELN provides the necessary functionality for managing scientific data transparently and consistently. Data accessibility through analysis software, its security and confidentiality are ensured. The software follows the principle of raw data being the origin of any research. Effective data archiving, sharing, and migration across platforms is achieved via a compatible exchange file format.



github.com/PASTA-ELN

Acknowledgements

The research has been supported by the German Research Foundation (Deutsche Forschungsgemeinschaft) within the framework of the NFDI-MatWerk project (National Research Data Infrastructure for Materials Science & Engineering, project number 460247524).

References

- [1] Dirnagl, U.; Przesdzing, I. (2016): A pocket guide to electronic laboratory notebooks in the academic life sciences. In F1000Research 5, p. 2. DOI: 10.12688/f1000research.7628.1.
- [2] Soiland-Reyes, S.; Sefton, P.; Crosas, M.; Castro, L. J.; Coppens, F.; Fernández, J. M. et al. (2022): Packaging research artefacts with RO-Crate. In Data Science 5 (2), pp. 97–138. DOI: 10.3233/DS-210053.