

Materials Data Infrastructure and Ontology Development for Exemplary Reference Dataset

Yusra Shakeel¹, Angelika Gedsun², Sirieam Hunke³, Luis Ávila⁴, Mariano Forti⁵, Thomas Hammerschmidt⁵, Tilmann Hicke⁴, Jürgen Olbricht⁴, Birgit Skrotzki⁴, Rainer Stotzka¹

¹Scientific Computing Center, Karlsruhe Institute of Technology, Karlsruhe; ²Albert-Ludwigs Universität Freiburg, Freiburg; ³IT Center, RWTH Aachen, Aachen; ⁴Federal Institute for Materials Research and Testing (BAM), Berlin; ⁵Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University Bochum, Bochum

Our Goal

Conceptualize & implement a digital infrastructure for

- Shaping, storing, sharing
- Search, discovery, and usage of reference data

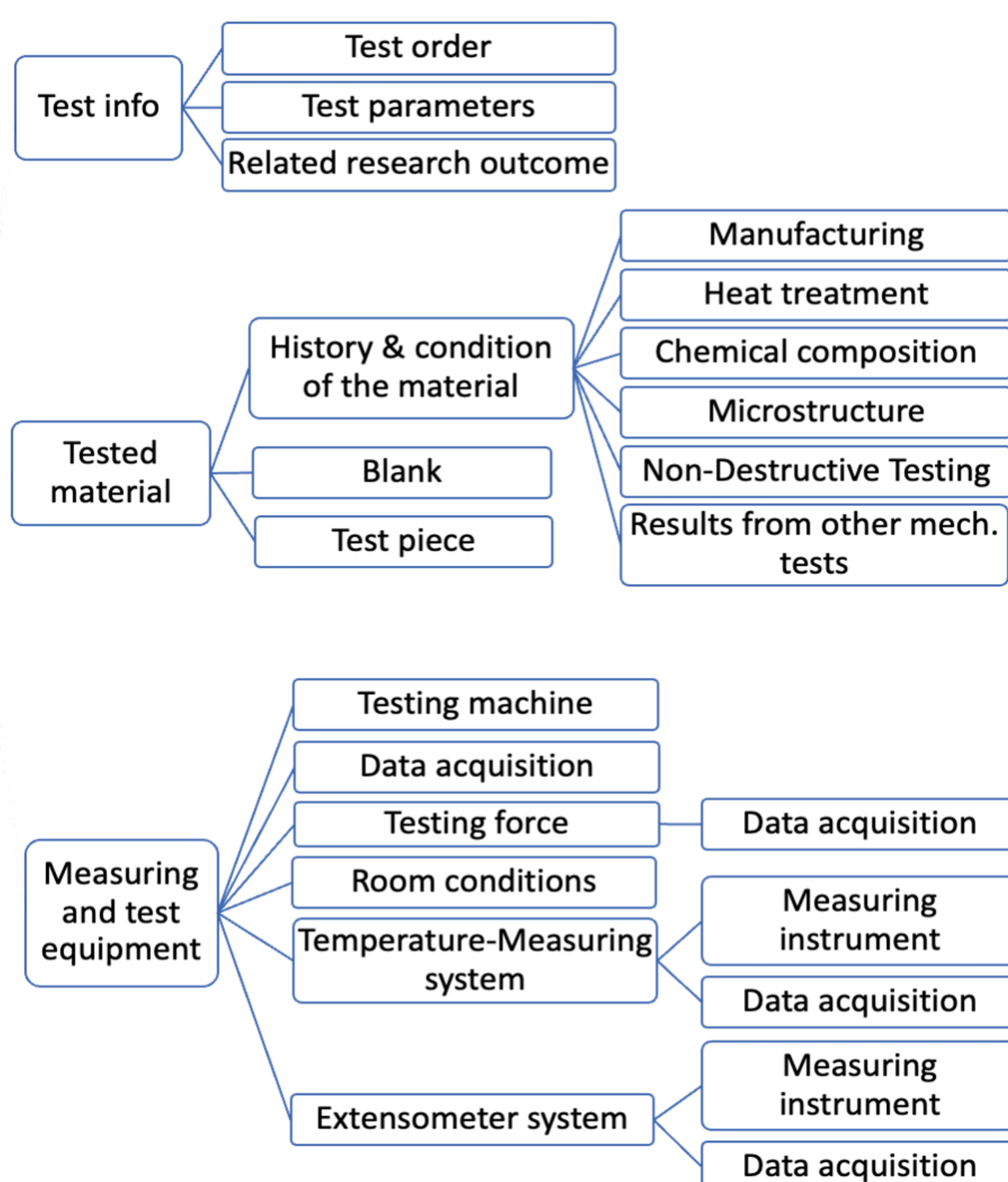
Key Takeaways

The infrastructure enables the researcher to:

- Validate a dataset as a reference dataset → Metadata schema
- Search/find data → FDO and instantiated ontology

Data Schema

- List use-case-related minimum requirements
- Usage of a defined **vocabulary**
- RDM to enhance documentation practices
- Serves as a template for other methods
- Used for shaping, sharing, and structuring data

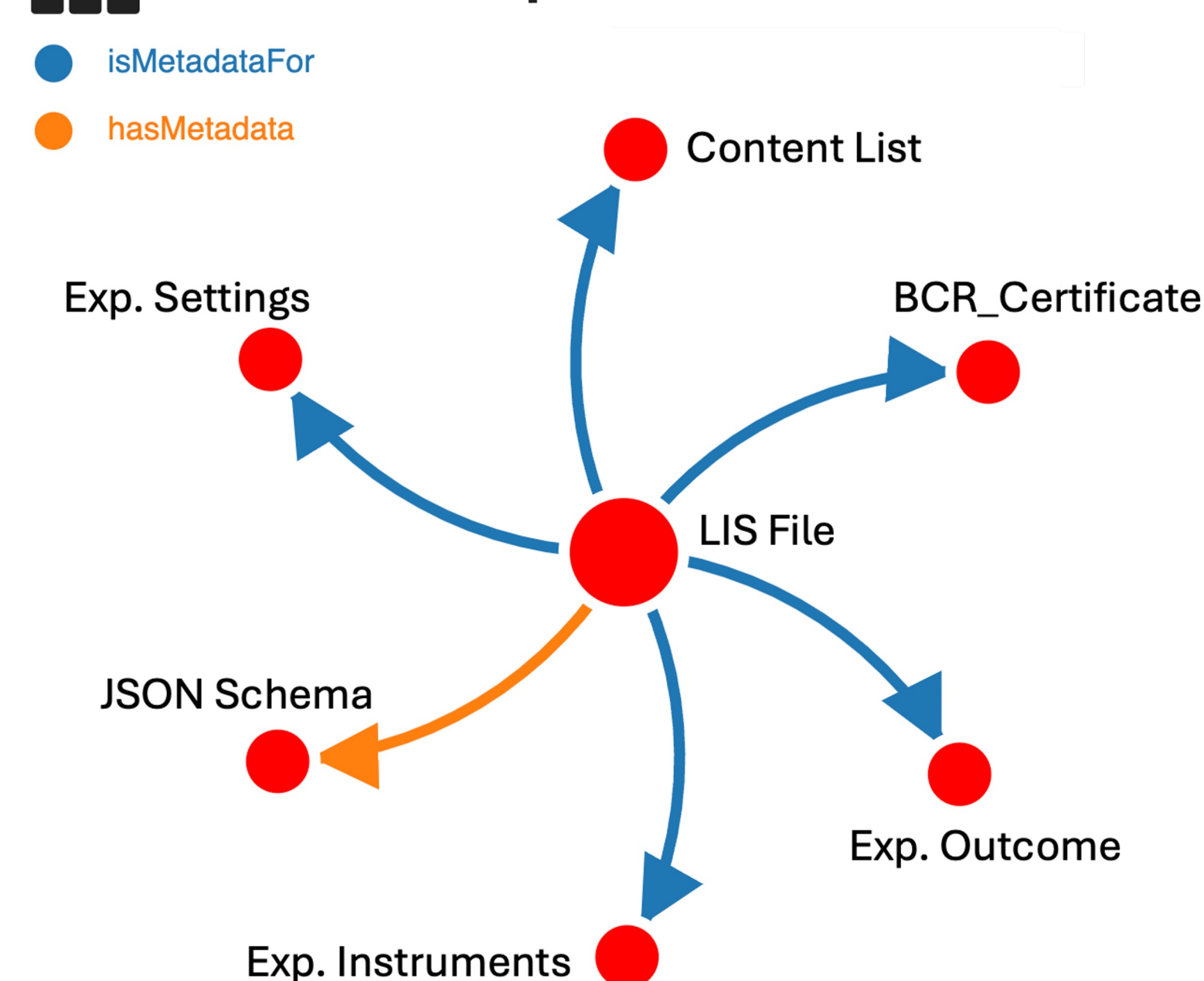


Data Discovery and Usage

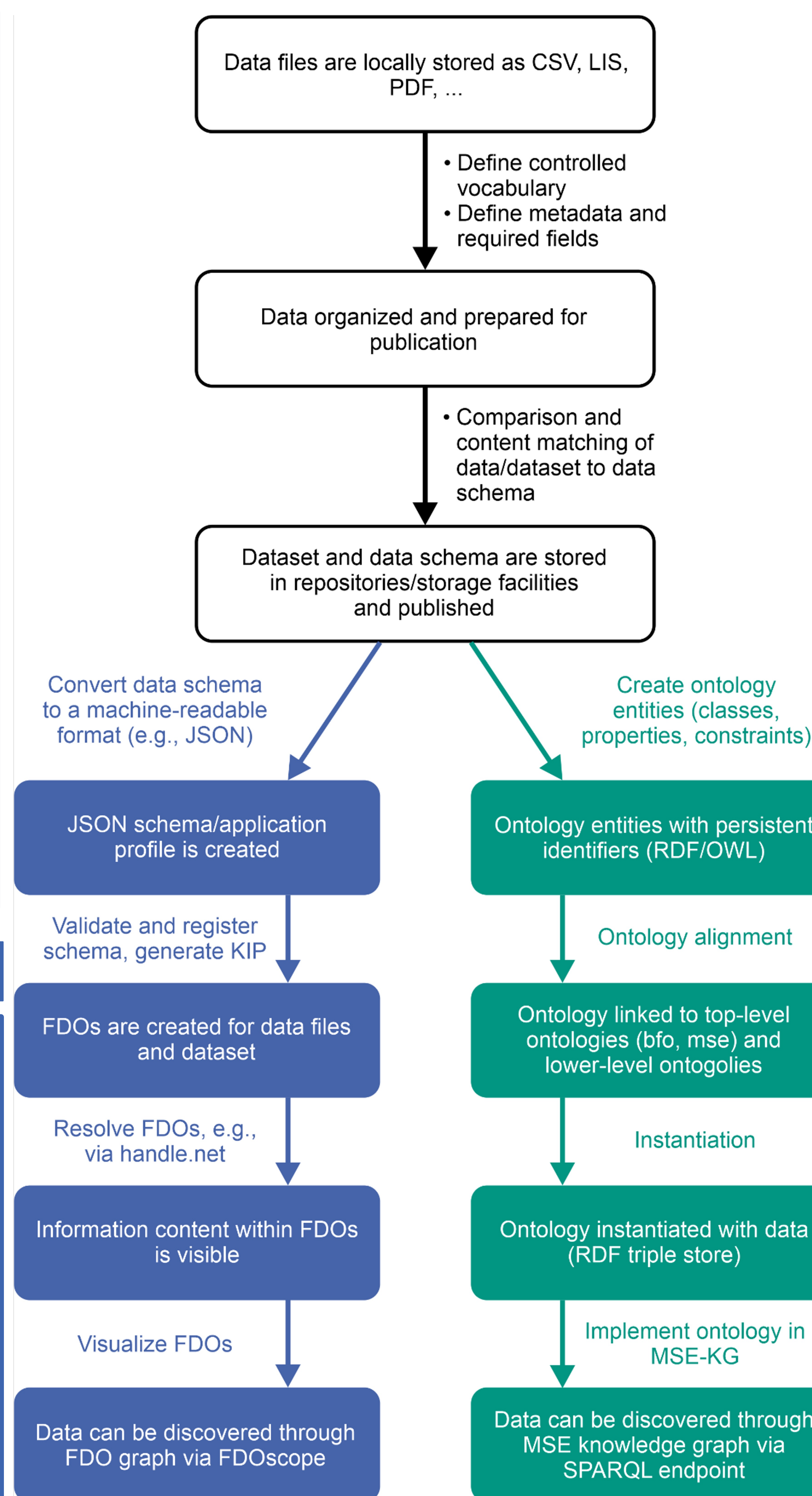
FAIR Digital Object (FDO)

- Globally accepted representation of research data that makes FAIR data not only machine readable but also machine actionable across scientific disciplines
- Allows a common view on all data artifacts independent of their scientific contents and metadata structures

FAIR DO Graph



Schematic View of the Data Journey

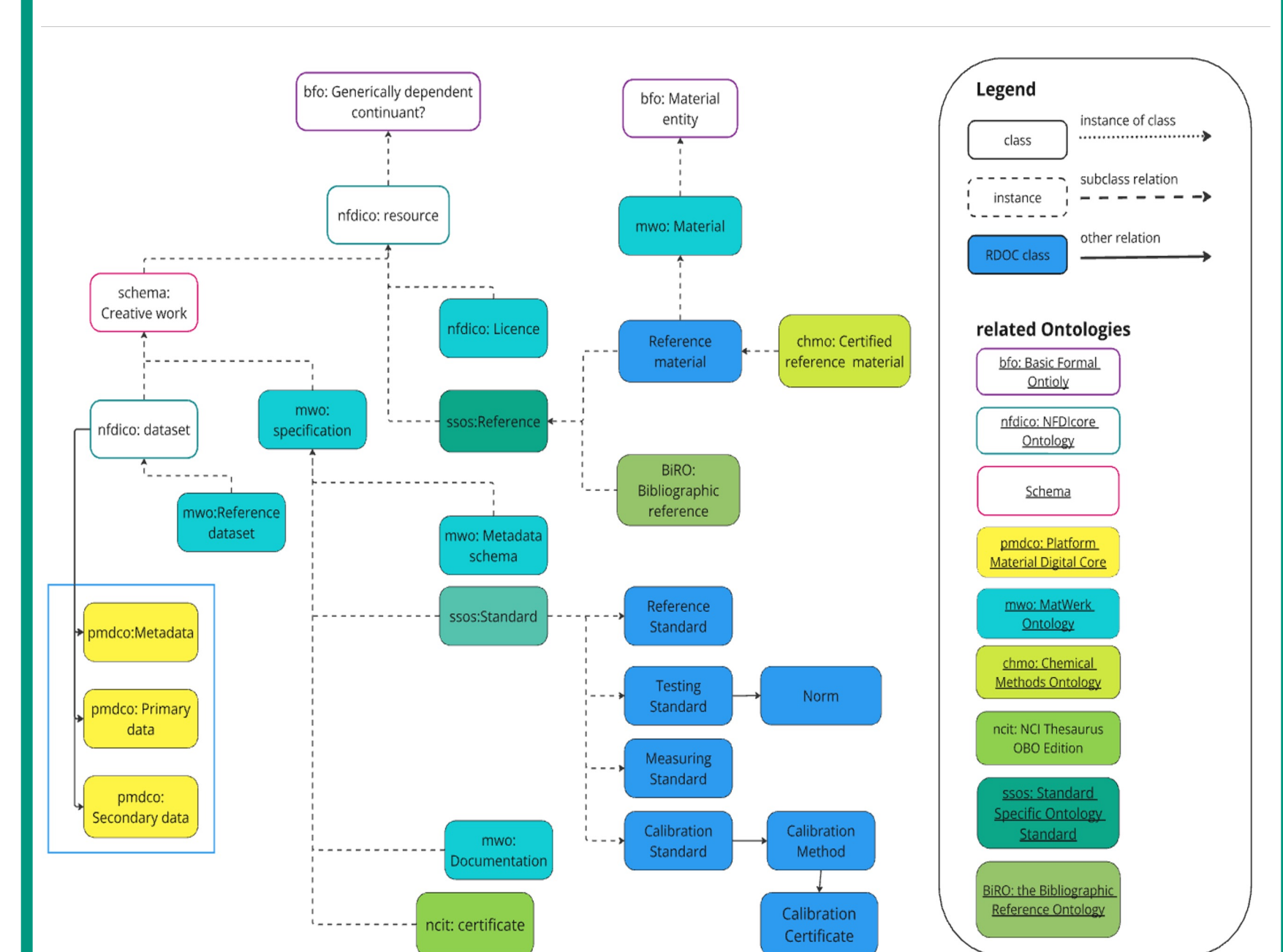


Possible usages of reference data

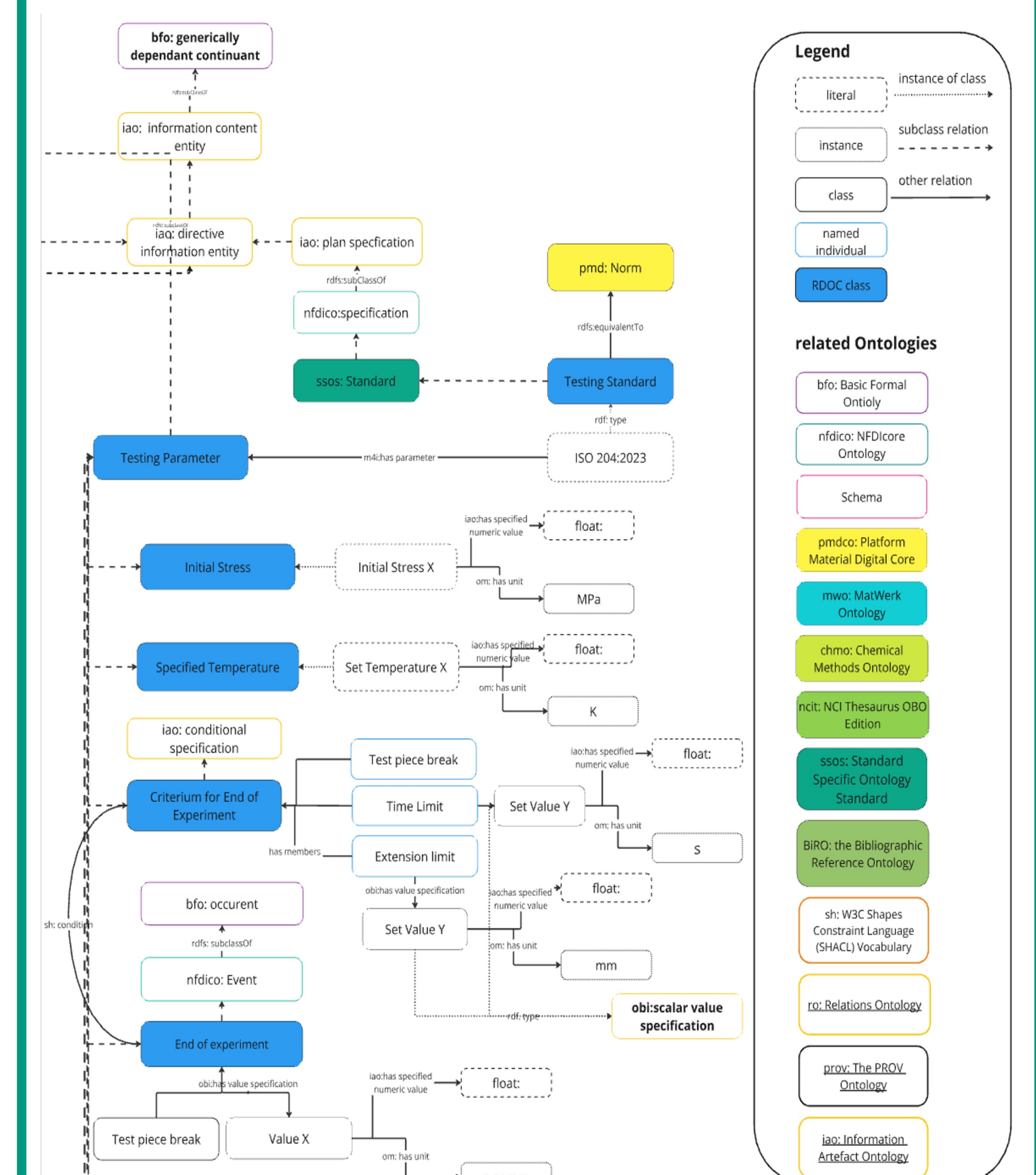
- Calibration of measurement devices, procedures or algorithms
- Comparison of data for interpreting individual measurement results
- Input for machine learning-based data analytics and for computational materials science (digital twin)
- Best practice examples for measurement and documentation procedures

Ontology Development

Concepts for a universal Reference Dataset



Concepts for a Reference Dataset for Creep Testing



- Instantiate ontology
- Integrate into MSE-KG
- Link to other resources in MSE community

