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Materials Data Science Ontology (MDS-Onto): Unifying Domain Knowledge in Materials and Applied Data Science

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Materials Data Science for Stockpile Stewardship

COE: US-Department of Energy-NNSA Award

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Purpose

Ontologies are used in the scientific community as a means to standardize concepts and terminology to facilitate data reuse

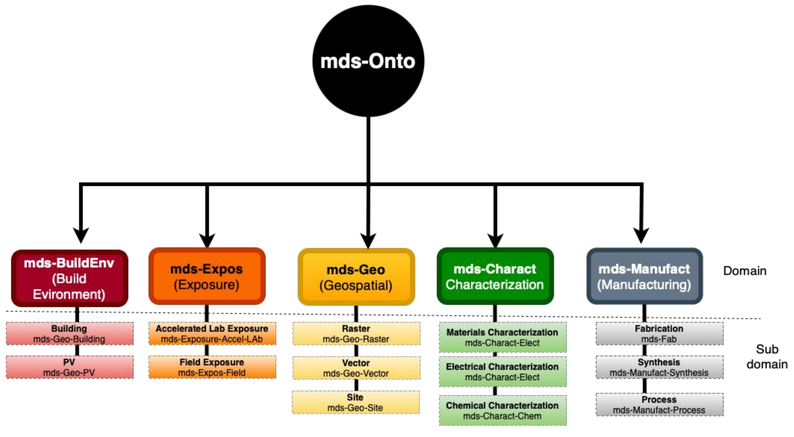
MDS-Onto Framework: Providing a comprehensive framework for ontology development, publishing, integration with the semantic web, and storage formats

R and Python packages: A user-friendly ontology creation and visualization tool that also allows for data and analysis to be annotated with robust metadata

MDS-Onto Framework

MDS-Onto Framework includes recommendations for ontology creation and development, how to FAIRify data, and platform for publishing created ontologies.

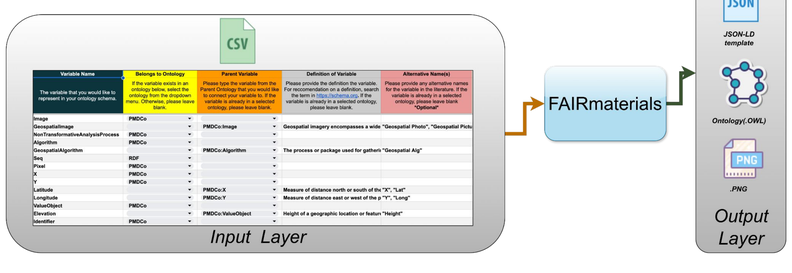
Application of MDS-Onto Framework: The creation of the MDS-Ontology, which encompasses 5 domains and over 30 subdomains in materials science and engineering.



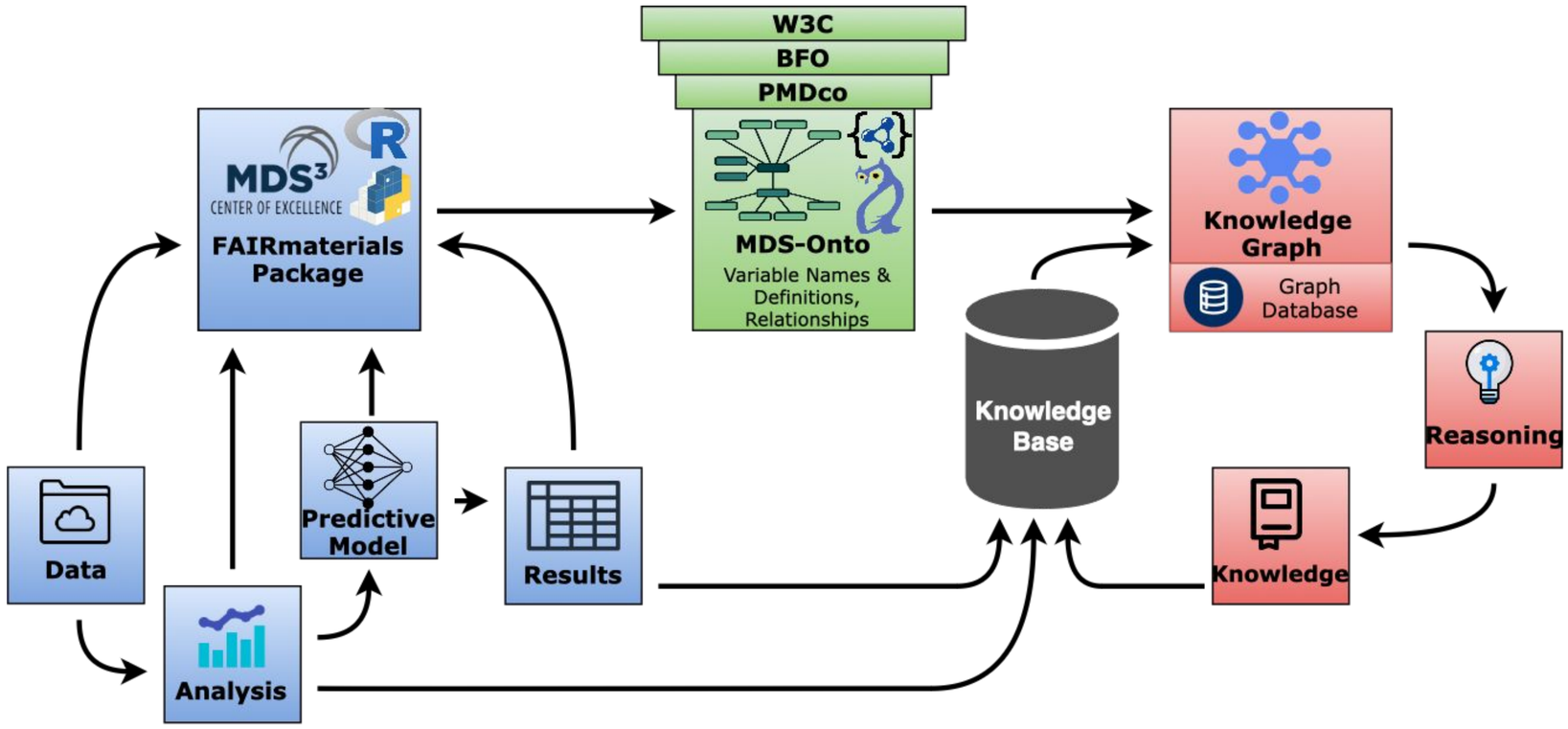
FAIRmaterials R and Python Package

`FAIRmaterials`[3] is a bilingual package simplifying the creation and visualization of ontologies.

The package converts simple and structured CSV inputs into rich, well-defined ontologies to support the process of data FAIRification[1].

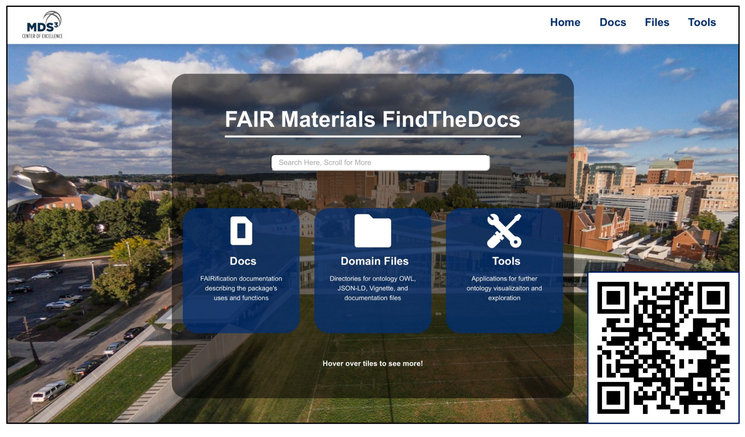


MDS-Onto Framework Workflow



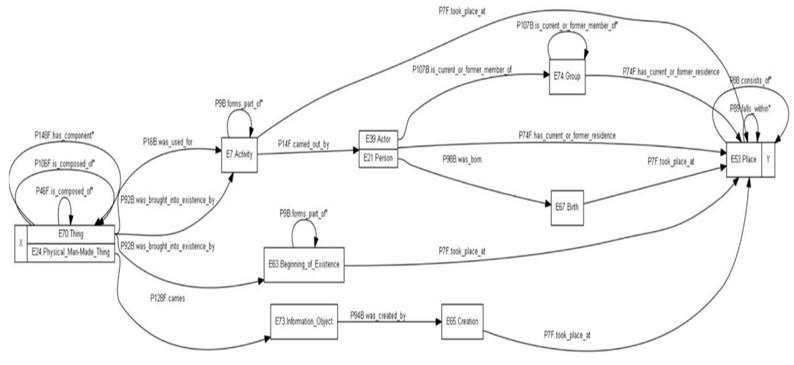
Find The Docs Website

Publishing ontologies is crucial for enabling new suggestions and integration into other researchers data. SDLE FAIR Materials FindTheDocs website, facilitates interoperability by offering an accessible interface for searching ontologies created via the MDS-Onto Framework.

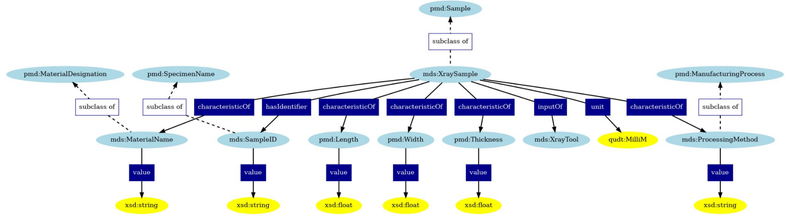


Knowledge Graphs

Knowledge graphs are networks where nodes represent concepts and entities and edges represent relationships between these concepts and entities. A neural-symbolic AI will act as a reasoner for query requests, and the knowledge base will be stored in graph database with ontologies as schema for organization.



MDS-Onto Framework Applied



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