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MetaCook: FAIR Vocabularies Cookbook

One of the prerequisites for FAIR data publication is the use of FAIR vocabularies. Currently, tools for the collaborative composition of such vocabularies are missing. For this reason, a universal manual and software for user-friendly vocabulary assembly is being composed in the HMC-funded MetaCook project. The project includes 4 separate test cases from 4 labs across KIT and Hereon, which will help strengthen the software's universality and applicability to various domains.

The components described in MetaCook will be implemented in the form of multiple software tools. The first one, a Python-based web application called VocPopuli, is the entry point for domain experts. The software, whose first version is being developed at the time of writing, enables the collaborative definition, and editing of metadata terms. Additionally, it annotates each term, as well as the entire vocabulary, with the help of the PROV Data Model (PROV-DM) - a schema used to describe the provenance of a given object. Finally, it assigns a unique ID to each term in the vocabulary, as well as a hash-based ID the vocabulary itself.

The second software tool will facilitate the transformation of the vocabularies developed with the help of VocPopuli into ontologies. It will handle two distinct use cases –the from-scratch conversion of vocabularies into ontologies, and the augmentation of existing ontologies with the terms from a given thesaurus. Both software tools will be used by two semi-overlapping user groups: domain experts will input, edit, and discuss vocabulary terms in their area of interest, while vocabulary and ontology administrators will oversee the vocabulary creation, and ontology transformation.

Both the controlled vocabularies and the corresponding ontologies offer the possibility to enrich data documented in Electronic Laboratory Notebooks (ELNs). As the simplest solution, terms used within the ELN are linked to the IDs of the related vocabulary and ontology for an unambiguous definition. Additionally, an export of the defined schemes can be used to automatically create a structured form in the ELNs for documenting the described processes. The output from the developed tools will be exemplarily integrated into the ELNs Herbie and Kadi4Mat.

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Tools

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Vocabularies, Ontology, ELN, FAIR, MaterialsScience

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