



Contribution ID: 147

Type: INTERACTION

6. Workshop - From scientific terms to linked electronic lab notebooks –The workflow

Wednesday 6 November 2024 13:30 (4 hours)

In this interaction session, we will consolidate our talk on creating FAIR, rich and shared experimental (meta)data with a knowledge graph in mind. We will present the individual tools of the software workflow live and interactively, starting from vocabulary terms via ontologies to entering research (meta)data and sending it to another Electronic Lab Notebook (ELN).

A prerequisite for FAIR data publication is using FAIR vocabularies. Currently, tools for collaborative vocabulary composition are lacking. Our software tool, VocPopuli (developed in the HMC-funded MetaCook project), a Python-based web application, enables the collaborative definition and editing of metadata terms. Additionally, it annotates each term and the entire vocabulary using the PROV Data Model (PROV-DM), a schema for describing an object's provenance. Finally, it assigns a PID to each term and the vocabulary itself. The generated vocabularies are provided with a PID, contain data (defined terms) annotated with metadata (e.g., authors), and can be exported to SKOS and OWL. We present two exemplary ontologies (PolyMat and PolyLab, developed by Hereon and DLR Inst. f. Data Science) that can be expanded in VocPopuli.

Languages like OWL and SHACL within the RDF ecosystem support semantic enrichment and local conformance via validations, but can be tedious to apply. The ELN Herbie simplifies this process. It's a client-server web application that wraps an RDF triplestore, utilizing frameworks like RDFS, OWL, SHACL, and Schema.org. Herbie uses SHACL to create reusable web forms, turning a lab journal into a semantically rich knowledge base. It also supports RDF graph versioning and access management, allowing collaborative editing through a web interface or REST API.

ELNs are crucial for gathering analog metadata but face interoperability issues. With ELNdataBridge (from the HMC-funded ELN-DIY-Meta project), we have developed an API-based data exchange between the ELNs Herbie and Chemotion to enhance interoperability. The communication tool, a Python-based server application, uses API packages from both ELNs and an adapter for RESTful APIs. An administrator defines a synchronization key and maps data fields via a user-friendly web interface.

All presented software tools are open-source and can be applied to various research fields, as their development included experts from multiple scientific disciplines.

In addition, please add 3 to 5 keywords.

Please assign yourself (presenting author) to one of the following groups.

Please specify "other"

For whom will your contribution be of most interest?

Please specify "other"

Presenters: KIRCHNER, Fabian (Helmholtz-Zentrum Hereon); HELD, Martin (Hereon)

Session Classification: Interactive session