
Herausforderungen bei der Arbeit mit Ontologien und deren Anwendung im FDM

Thüringer Kompetenznetzwerk Forschungsdatenmanagement: *Coffee Lecture*

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Agenda

1. Metadata for Research Data Management



1. Terminology Service



1. Overcome Data Silos with Ontologies



Metadata for Research Data Management

Intro

Research data is of inestimable value (*)

- *Empowers research*
- *Create innovation*

New research bases on existing research data (*)

- *Transparent*
- *Reproducible* } *Reusable*

Current situation in Germany (*)

- *Data is stored decentrally*
- *Stored temporarily*
- **Non-standardised metadata**
- *Varied quality*

Nationale Forschungsdateninfrastruktur (NFDI) establishes an infrastructure for high qualitative RDM to foster research reusability

nfdi Nationale
Forschungsdaten
Infrastruktur



(*) https://www.dfg.de/en/research_funding/programmes/nfdi/index.html

Metadata for Research Data Management

Current situation

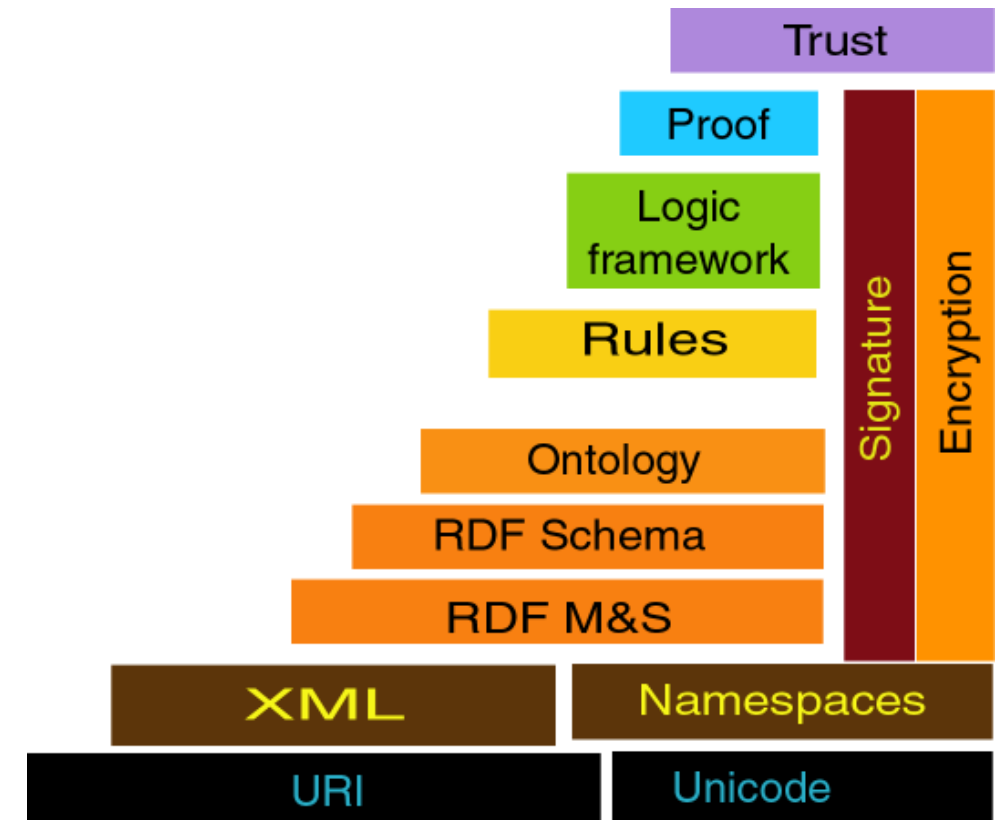
- Commonalities between **metadata** in **databases** and in the **library context, like**
 - **Structural:** Structure, organizational aspects (e.g. relation: scientific publication and supplementary data)
 - **Descriptive:** Creator, and keywords, ...
 - **Contextual Information:** Rights management, language, descriptions, ...
- **Used** in **databases** to: organize, integrate, govern, analyse, ...
- What about reproducibility? Contextual-**metadata**, can carry **reproducibility** relevant information
- ... requires unambiguous, **community specific** terminologies and expressive formalisms
 - **Content indexing.** E.g. micro- and macronutrients [*]
 - Soil scientists: *nitrogen, phosphorus, potassium, calcium, magnesium and sulphur*
 - Nutritionists: *carbohydrates, protein and fat*
 - **Workflow descriptions:** wet lab experiment, data-driven, input, output, configuration ...

[*] Jordan, I., Heil, E., & Keding, G. (2021). Coming to terms with terminology in agriculture-nutrition research projects: an interactive glossary. *Ernährungs Umschau*, 68(10), 198-203.

Metadata for Research Data Management

Current situation

- More **expressive** options
 - **Thesaurus:** semantically grouped terms
 - Writing and editing: get synonyms, antonyms, ...
 - Semantic text analysis: word definitions, ...
 - Knowledge Organisation and classification: classification of documents, ...
 - **Ontology:** formal representation of knowledge
 - Formalisation of knowledge: description of processes, ...
 - Semantic Interoperability: shared and machine processable information, ...
 - Decision support: inferencing, ...



Semantic Web Stack.

Taken from: <https://www.w3.org/2004/Talks/0611-sb-wsswintro/slide18-0.html>

Metadata for Research Data Management

Challenges with Ontologies

- **Domain specific** (Engineering, Culture, Chemistry, ...) and community specific
- **Evolving** continuously and dynamically over time
- Must be **accepted, developed and maintained** by a **designated community** (avoid isolated solution!). Includes i.e.
 - promotion (make community aware of its existence)
 - aligned with further metadata initiatives (moving away from silos)
 - applicable in RDM (in RDM practice)
- NFDI4Ing supports terminology development and use through introduction of engineering specific **Terminology Services** for Ontologies

Terminology Service

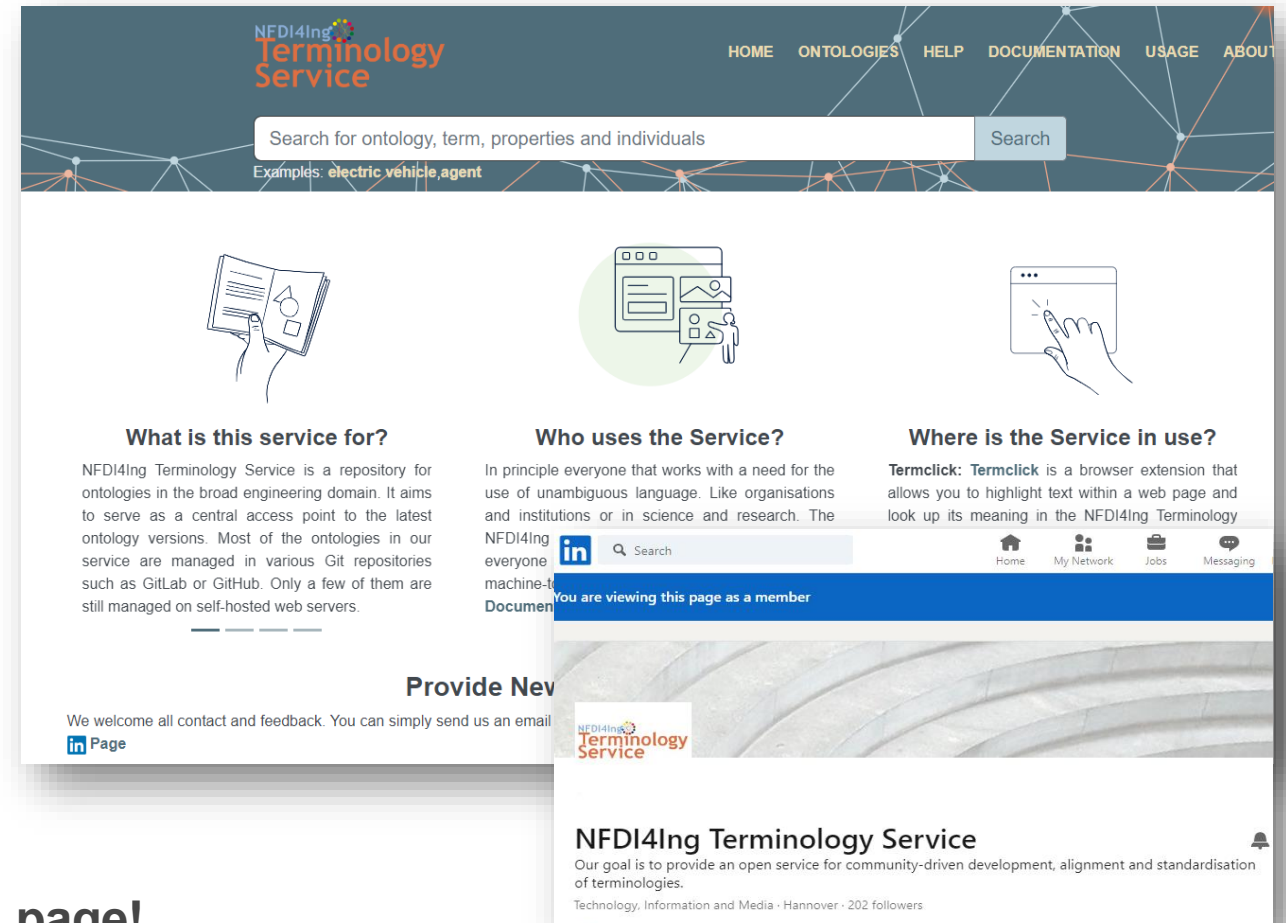
- In general: Our **Terminology Service** is a **web based platform** that support take-up and standardisation of Ontologies
- **Utilised as a**
 - **Developer (e.g. Back-End Services):** Data- and Knowledge Management tasks. I.e.
 - Content indexation with controlled vocabularies
 - Search: Query reformulation, term suggestion, ...
 - **Knowledge Engineers.** I.e.
 - Bundles ontologies of a domain
 - Provides meta data and statistics
 - Search for and within ontologies
 - Makes alignments visible
 - **Authors as dissemination point,** fosters awareness and alignment

Terminology Service

- **NFDI4Ing TS:** <https://terminology.nfdi4ing.de/ts/>
- **Some statistics**
 - 93 ontologies
 - ~160.000 Terms
 - ~12.000 properties
- **Functional service offer**
 - Free text search searching (for- and within ontologies)
 - Browsing and Filtering (by various metadata)
 - Visualisation
 - Issue tracker
 - Machine to machine communication (REST interfaces)



Stay up to date with our **LinkedIn page!**



Terminology Service



Browse Ontologies

Results Per Page sorted by

<p>cco All Core Ontology</p> <p>An import of all the Common Core mid-level ontologies into a single file so that content is easy to view. The All Core Ontology is not an ontology in the sense it contains no unique content. As such it should not be added to, but can be extended from.</p>	<p>1415 Classes</p> <p>338 Properties</p> <p>Loaded: 2023-07-05</p>
<p>atomistic Atomistic</p> <p>An EMMO-based domain ontology for atomistic and electronic modelling. Atomistic is released under the Creative Commons Attribution 4.0 International license (CC BY 4.0).</p>	<p>531 Classes</p> <p>84 Properties</p> <p>Loaded: 2023-08-23</p>
<p>bo Base Ontology</p> <p>This file contains the Base Ontology of oneM2M as specified in TS-0012</p>	<p>23 Classes</p> <p>42 Properties</p> <p>Loaded: 2023-07-05</p>
<p>bfo Basic Formal Ontology</p> <p>The upper level ontology upon which OBO Foundry ontologies are built.</p>	<p>35 Classes</p> <p>24 Properties</p>

NFDI4Ing Terminology Service

HOME ONTOLOGIES HELP DOCUMENTATION USAGE ABOUT SANDBOX

agent

Examples: electric, vehicle, agent

Filter Results 554 results found for "agent" Results Per Page

[Clear All Filters](#)

Type

- class 410
- property 126
- individual 18

Ontologies

- TEMA 125
- CCO 117
- SEPIO 39
- OEO 25
- DICL 23

[+ Show More](#)

[property] agent
http://www.w3.org/ns/prov#agent

Ontology: PROV

Also in: [estab](#) [mfi](#)

[class] Agent
http://purl.org/dc/terms/Agent

A resource that acts or has the power to act.

Ontology: [dcterms](#)

Also in: [dcterms](#) [STO](#) [ids](#) [MV](#) [MV](#)

[class] Agent
http://xmlns.com/foaf/0.1/Agent

Ontology: [FOAF](#)

Also in: [ssn:system](#) [SSN](#) [sosa](#) [EXTRUONT](#) [S4EHAW](#) [dr](#) [MODSCI](#) [ids](#) [ACO](#)

Terminology Service



The screenshot shows the web interface of the Terminology Service. At the top, there is a navigation bar with 'HOME', 'ONTOLOGIES', 'HELP', and 'DOCUMENTATION'. Below this is a search bar with the text 'Search in prov' and examples 'electric, vehicle, agent'. The main content area is titled 'The PROV Ontology' with the URL 'http://www.w3.org/ns/prov-0#'. There are tabs for 'Overview', 'Class Tree', 'Property Tree', 'Individuals', and 'Class List'. The 'Class Tree' tab is active, showing a tree structure with 'Activity' selected. Below the tree is a 'Jump to:' input field with 'Reset' and 'Sub Tree' buttons. The 'Activity' class details are shown in a table format:

Label	Activity
Synonyms	N/A
CURIE	N/A
Term ID	Activity
Description	An activity is something that occurs over a period of time and acts upon or with entities; it may include consuming, processing, transforming, modifying, relocating, using, or generating entities.
fullIRI	http://www.w3.org/ns/prov#Activity copy
SubClass Of	• Thing
category	starting-point
component	entities-activities
constraints	http://www.w3.org/TR/2013/REC-prov-constraints-20130430/#prov-dm-constraints-fig
dm	http://www.w3.org/TR/2013/REC-prov-dm-20130430/#term-Activity

The screenshot shows the Swagger API documentation for the Terminology Service. The title is 'TIB Terminology Service Documentation'. Below the title, there is a dropdown menu for 'Select a spec' with 'default' selected. The documentation lists several API endpoints:

- api-unavailable** Api Unavailable
- data-preparation-controller** The Properties, Terms and Individuals in a particular context such as an ontology or a classification
- hello-controller** Hello Controller
- individual-controller** The Individuals resources are used to list ontology individuals (instances) without a reference ontology
- ontology-config-controller** Ontology Config Controller
- ontology-controller** The Ontologies resources are used to list ontologies in this service

Overcome Data Silos with Ontologies

DM applications based on de facto standard ontologies



- **Simple Experiment:** *Semantification of Space Data – A feasibility Study*
 - Wikidata ontology: https://www.wikidata.org/wiki/Wikidata:WikiProject_Ontology
 - SpaCy pre-trained NER and Linking model



- **Data:** Planetary Data System 4 is a long term **archive** for **data products** from NASA's planetary missions

- **Approach:** Create **Knowledge Graph** and apply **federated SPARQL query**
 - Apply existing **SpaCy** model: entity extraction and linking (**Wikidata**)
 - **Federation:** PDS4 Knowledge Graph - Wikidata

- **Manually evaluated**

Query term	Record count	Concepts
Planet	20	Mars (14), Planet (5), Jupiter (1), Pluto (1), Neptune (1)
Solar System	20	same as 'Planet'
Superior Planet	20	same as 'Planet'
Vehicle	15	Spacecraft (15)
Vehicle*	20	Spacecraft (15), Lander (5)
Planetary Probe	5	Lander (5)

Overcome Data Silos with Ontologies

DM applications based on de facto standard ontologies



- Follow-up experiment: Train supervised **ML model to label text** with Ontology terms

- De facto standard: **Unified Astronomy Thesaurus (UAT)**

- > 2000 concepts
- Polyhierarchy
- 11 UAT Top concepts as Entity Types

- **Text categorisation**

- **Named Entity Recognition of UAT top concepts (11)**
- Train empty **SpaCy NER** model
- **First results**
 - Standard configuration
 - Precision: 80.86, Recall: 85.06 , F1: 82.65
 - Good, but needs improvement (distortion through “Others”)

- Kindly received **training data** from NASA *astrophysics data system* (ads)



Astrophysical processes	66.08	75.35	70.41
Cosmology	67.91	62.24	65.06
Exoplanet astronomy	51.10	80.78	62.60
Galactic and extragalactic astronomy	55.00	64.65	59.44
High energy astrophysics	65.45	57.86	61.42
Interdisciplinary astronomy	71.97	71.92	71.95
Interstellar medium	62.98	83.84	71.92
Observational astronomy	69.83	76.06	72.81
Solar physics	57.87	72.34	64.30
Solar system astronomy	69.78	72.89	71.30
Stellar astronomy	62.21	61.53	61.87
Other	98.18	99.23	98.66
Total	80.86	85.05	82.65

Overcome Data Silos with Ontologies

DM applications based on de facto standard ontologies

- **Positive example:**

*Thermally created scalar and vector Higgs portal **dark matter** masses are constrained and al this contains some of the example like the **Solar flares** is this working.*

- **Negative examples:**

*she recalled the thrill of exploring the abandoned **Mars** factory with her friends*

Annotation Service

The tool is intended to demonstrate the annotation of texts by reusing ontological resources in a prototypical way at first.

Status: We currently offer the annotation tool to support classification tasks by releasing entity recognition using the eleven parent terms of the **Unified Astronomy Thesaurus (UAT) ontology**.

Future Work: The tool will be extended successively with further functionalities. Among other things, this concerns the performance, the removal of the restriction to recognise only the 11 parent UAT terms, but also the transfer to other ontologies.

Enter Text *

Thermally created scalar and vector Higgs portal dark matter masses are constrained and al this contains some of the example like the Solar flares is this working.

Example Text: Thermally created scalar and vector Higgs portal dark matter masses are constrained and al this contains some of the example like the Solar flares is this working.

ANNOTATE **RESET**

Thermally created scalar and vector Higgs portal **dark matter** masses are constrained and al this contains some of the example like the **Solar flares** is this working.

UAT Terms

- [Galactic and extragalactic astronomy](#)
- [High energy astrophysics](#)

Overcome Data Silos with Ontologies

DM applications based on de facto standard ontologies

- **Challenge:** find words on the tip of the tongue
 - *Fear of spiders* → Arachnophobia
 - *Integrated Circuits* → Wafer or Chipset
- **Hypothesis:** Domain ontologies encode commonly accepted terminology for unambiguous information exchange, useful to train a Reverse Dictionary

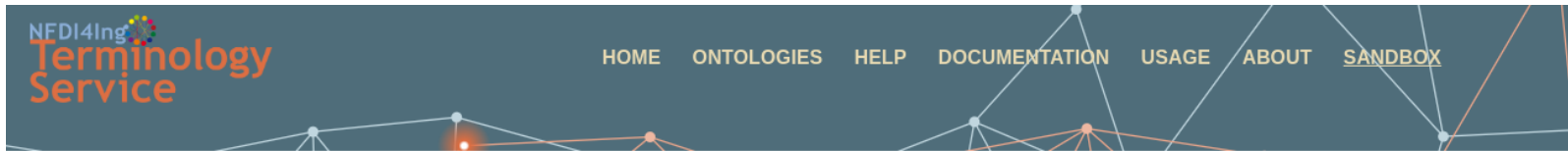


Dictionary vs. Reverse Dictionary

Look up words alphabetically to find their definitions

Start with a concept or an idea and try to find the word that best represents it

Overcome Data Silos with Ontologies



Reverse Dictionary

Welcome to the Reverse Dictionary tool! Simply type a word, phrase, or sentence into the search bar below.
 Press **Enter** to fetch **similar words/phrases**. Click on any word displayed below to explore further options. Press **Esc** to clear the search bar.
 The reverse dictionary model is based on textual components of the IEEE Thesaurus and all ontologies of the NFDI4Ing Terminology Services.
 The content obtained from these sources has not been changed, only pre-processed

Word2Vec Universal Sentence Encoder

liquid	particles	aerosol	system	solid	precipitation	cloud	lwe	phase	vapor	except	moist	mass
stratiform	fluvial	pressure	freely	ambient_aerosol	capture	brought	evaporation	condenses	ambient	warming		
cloud_base	rainout	reversible	equivalent	take	formations	partial	unaltered	stream	parcel	matter		
precipitating	floodplain	fly	composed	snowout	vertical	pulverized	widespread	taken	condensation	transition		
phases	particulate	condensed_water	ascend	fraction	transpiration	intermediate	atmosphere	circulated	pool	dry		
contact	sufficiently	gas	solids	mode	sinking	sum	influx	dried_aerosol	strike	dissolving	aspects	
formation	surface	formed	sublimation	rotating	absence	released	destroyed	sky	extraction	layer		
representation	including	total	mole	runoff	detritus	molecules	fallen	lagoon	highest	before_present		
transferred			density			aerosols			carrier			

Earth System Sciences

Query: *water droplets suspended in the air*

Overcome Data Silos with Ontologies

Pros and Cons

- **Pros**

- Means to standardize: **overcome language barriers**
- Model very **complex interdependencies** (reproducibility)
- Very **active field** research area

- **Cons**

- **Availability** is depending on domain
- **Hard to understand** as domain expert
- Still **not enough tooling** available

THANKS

