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RESEARCH ARTICLE

Towards Improved Findability of Energy Research Software by Introducing a Metadata-based Registry

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Abstract. Research software in the energy domain becomes increasingly important for the analysis, simulation, and optimization of energy systems and supports design decisions in the required transition of energy systems to tackle the climate crisis. To make energy research software (ERS) more findable, it should be described with metadata following the FAIR (findable, accessible, interoperable, and reusable) criteria and be registered in a common registry. To this end, we present a concept for a metadata-based registry for ERS which should enable researchers to easily add new ERS as well as to find new ERS.

1 Motivation

In energy research, self-designed software is a basic tool for multiple purposes like visualization of processes and values, e.g., power quality [1], (co-)simulation of smart grids [2] , or analysis of transition paths [3]. Within an exemplified research cycle, this self-designed software is often a starting point and, therefore, fundamental for producing new research results while it also presents a result of performed research (see Figure 1).

Based on the definition of research software by Hasselbring et al. [4], we define energy research software (ERS) as software that is employed in the scientific discovery process to understand, analyze, improve, and/or design energy systems. With respect to the complexity of the software, ERS ranges from simple scripts and libraries, e.g., for python, up to full software solutions. Content-wise, it can for example visualize, analyze, and/or generate (artificial) data from energy (sub)components or grids in laboratories or the real world. Alternatively, it can also represent as a model particular energy (sub)components, energy (distribution) systems, and transition paths of energy use, distribution, conversion, and/or generation to analyze the design and/or control in simulations and optimizations.

Multiple models and frameworks in the energy domain have been developed in the last years. Partly, these have overlapping and similar features. Often new tools are developed without reusing the already existing ones. Due to the need for interdisciplinary research in the energy domain as well as the growing number of simulated components ERS will even become more complex in the upcoming years [5]. Therefore, a lot of time is spent on (re)developing software instead of doing research slowing down the progress in research.

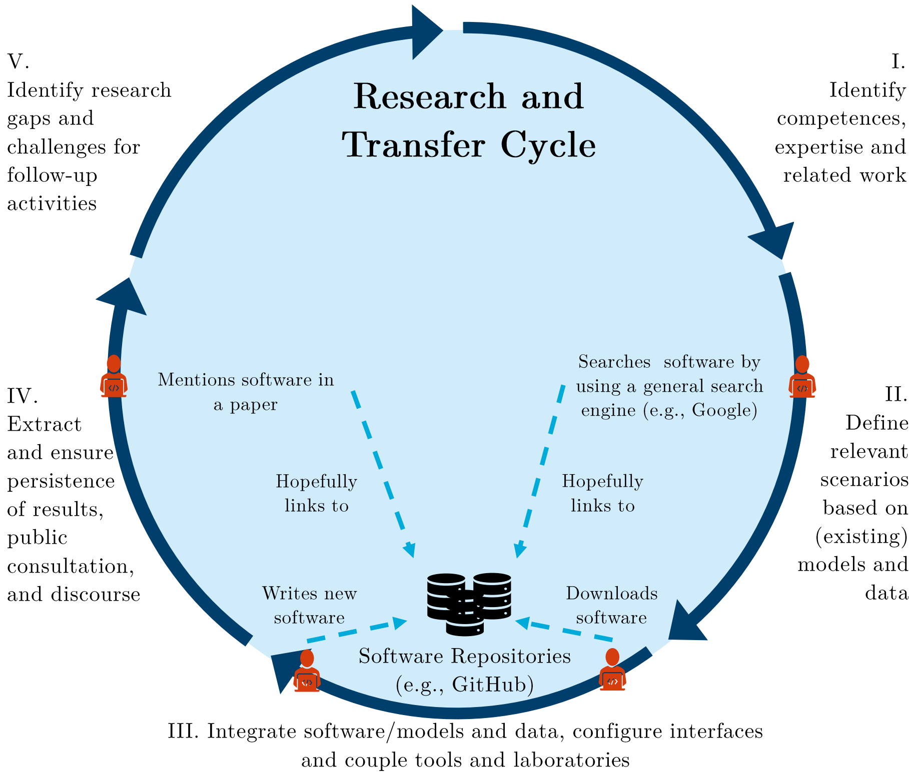

Figure 1: An exemplified research cycle of energy research with software usage

Different approaches to formulate FAIR criteria for research software show that metadata and repositories for these metadata, e.g., software registries, are key elements for FAIR research software [4], [6], [7].

Especially the findability of ERS can be increased by describing it with useful metadata and including it into a registry. Table 1 gives some examples for possible metadata elements with metadata for the co-simulation framework mosaik[1] as example instance. Together, good metadata and a registry are a first step for increasing the reuse of ERS and improving the research process in energy research.

For this goal, we propose a metadata-based registry for ERS based on a good metadata scheme. Our contribution are:

- We outline related work in the fields of metadata schemes for research software, metadata schemes in the field of energy research, and ontologies in the energy domain in Section 2.
- We introduce our concept of metadata-based registry for ERS in Section 3.
- We give an outlook of the further required work in Section 4.

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[1] `http://mosaik.offis.de/`, accessed 12.12.2022

Table 1: Examples for possible metadata elements based on the FAIR criteria with the software mosaik as example instance

Findability	Name	mosaik[1]
	Identifier	-
	Version	3.0
Accessibility	Link to repository	`https://gitlab.com/mosaik/mosaik`
Interoperability	Programming language	python
	Input/output formats	depends on used models
	Dependencies	-
Reusability	License	LGPL v3.0
	Link to documentation	`https://mosaik.readthedocs.io/en/latest/quickstart.html`

2 Related Work

Within this section, we give an overview on existing metadata schemes. First, we present current metadata schemes for research software in general or in other specific domains in Section 2.1. Second, we introduce metadata schemes in the field of energy research and engineering in Section 2.2. These are often designed for research data but can be used as foundation for a metadata scheme for ERS.

Since value vocabularies are an important part of metadata schemes, the third part (Section 2.3) outlines ontologies in the energy domain.

2.1 Metadata for Research Software

This section gives an overview of existing approaches for metadata schemes for research software. While some publications directly focus on metadata, others only introduce software ontologies, which can be used as metadata vocabulary for research software.

CodeMeta[2] is a community driven metadata standard for research software based on schema.org[3]. Various crosswalks to other metadata schemes already exist. CodeMeta contains multiple elements, some focusing on technical details like file size or supported operating systems and others including administrative information like license. The metadata standard does not have mandatory elements. It supports the use of URIs for authors and contributors as well as for licenses. The content specific metadata are limited to an application category and keywords.

For geosciences, Gil et al. introduced an ontology to describe research software, OntoSoft, with six categories: identify, understand, execute, do research, get support, and update [8]. They also developed an automated extraction tool for metadata and provided a registry for software metadata[4]. Garijo et al. expanded this approach by developing the Software Description Ontology[5] [9] with additional description for input and output data based on the Scientific Variables Ontology[6]. Also, they aligned their approach with CodeMeta and enabled publishing the metadata into an open knowledge graph including links to additional instances in the semantic

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2. `https://codemeta.github.io/`, accessed 12.12.2022
3. `https://schema.org/`, accessed 12.12.2022
4. `https://csdms.ontosoft.org/#home`, accessed 12.12.2022
5. `https://w3id.org/okn/o/sd`, accessed 12.12.2022
6. `https://scientificvariablesontology.org/svo/`, accessed 12.12.2022

Table 2: Overview of metadata scheme for research software

✓: fulfilled ✗: not fulfilled
(✓): ()partly) fulfilled

	Metadata scheme (s) vs. ontology (o)	Domain	Mandatory elements	Support for URIs	Use of domain ontologies as value vocabulary
CodeMeta[2]	s	General	✗	(✓)	✗
OntoSoft [8]	o	Geoscience	✗	✗	✗
Software Desciption Ontology [9]	o	Geoscience	✗	✓	✓
Software Ontology [10]	o	Bioinformatics	✗	✓	✓
biotoolsXSD [11]	s	Bioinformatics	✓	(✓)	✓

web like wikidata[7]. Additionally, they developed software to support researchers in the metadata creation and to find models[8].

In the domain of bioinformatics, the EDAM ontology describes general concepts. The Software Ontology (SWO) was developed to extend the EDAM ontology to describe software in this research field [10]. The SWO includes licenses, programming languages, and data formats as taxonomies. In contrast to OntoSoft, the use of the taxonomies improves the usability for semantic web applications and linking. Also for bioinformatics, Ison et al. developed the metadata scheme biotoolsXSD for the software registry bio.tools[9] [11]. The metadata scheme is expressed as an XML scheme containing 55 elements of which 10 are mandatory. The use of the EDAM ontology as value vocabulary is required for some elements like function, input, and output. The metadata scheme also contains software specific elements like programming language, license, and operating system for which the use of an ontology is not required.

Table 2 gives an overview of the diverse outlined metadata schemes and ontologies. While some metadata schemes are less extensive, like CodeMeta[2], others try to include value vocabularies to improve interoperability by using semantic web technologies. Some schemes include detailed domain knowledge based on domain ontologies like biotoolsXSD [11] or the Software Description Ontology [9].

2.2 Metadata in Engineering and the Energy Domain

In this section, metadata schemes for data and software in the engineering domain and especially in the energy domain are introduced, starting from the broad engineering perspective.

Schembera and Iglezakis developed the metadata scheme EngMeta for data in computational engineering which includes existing elements for technical and general descriptive information from DataCite, CodeMeta, and other relevant metadata schemes. They added additional elements for domain specific information. Controlled vocabularies and restrictions are available for multiple elements. Schembera and Iglezakis also presented a tool for automatic metadata

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7. https://www.wikidata.org/wiki/Wikidata:Main_Page, accessed 12.12.2022
8. http://models.mint.isi.edu, accessed 12.12.2022
9. http://bio.tools, accessed 12.12.2022

Table 3: Overview of metadata scheme for energy research software

✓: fulfilled ✗: not fulfilled
(✓): (partly) fulfilled

	Focus on models (m) vs. data (d)	Formalized metadata scheme	Based on existing scheme	Use of value vocabularies
EngMeta [12]	d	✓	✓	✓
Catalog of energy co-simulation components [13]	m	(✓)	✗	✗
openmod[11]	m	✗	✗	✗
Open Energy Metadata[12]	d	✓	✗	(✓)
Open Energy Platform factsheets on models[13]	m	✗	✗	✗

extraction and included the metadata scheme in a data repository based on Dataverse[10]. They validated their approach against common recommendations for good metadata schemes. [12]

Schwarz and Lehnhoff described a catalog of energy co-simulation components. They used a semantic media wiki to collect information on components and the Functional Mockup Interface (FMI) to add descriptions on the simulation interfaces. The elements of the catalog are usable as metadata scheme but are neither formalized nor described in more detail. [13]

The open energy modeling initiative (openmod) includes a list of energy models in their wiki[11]. For each model, administrative and descriptive metadata are listed, like license, link to a code repository, model class. The descriptive elements include detailed information on the models. The metadata scheme is not formalized and controlled vocabularies are neither used for the elements nor for the values.

The open energy platform introduces the open energy metadata[12] for data. The metadata scheme is designed for energy data and contains multiple elements. For a lot of elements, the use of controlled vocabularies is required, e.g., for language and license. The use of an energy ontology is not required for the description of the data but is planned as extension. The documentation of the metadata does not link to any existing schemes used for the design of the metadata scheme. Additionally, the open energy platform[13] includes information on models and frameworks. The metadata elements are similar to the ones of the openmod wiki and also not formalized.

Table 3 summarizes the most relevant metadata schemes in the engineering and energy domain. While EngMeta [12] presents a good broad metadata scheme in the engineering domain following best practices, a formalized metadata scheme for ERS is still missing. However, the open energy platform[13], the openmod wiki[11], and the work of Schwarz and Lehnhoff [13] present good starting points for developing a formalized metadata scheme for ERS.

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[10] `https://dataverse.org/`, accessed 12.12.2022
[11] `https://wiki.openmod-initiative.org/wiki/Open_Models`, accessed 12.12.2022
[12] `https://github.com/OpenEnergyPlatform/oemetadata`, accessed 12.12.2022
[13] `https://openenergy-platform.org/factsheets/models/`, accessed 12.12.2022

2.3 Domain Ontologies for Energy Research

Domain ontologies are necessary to improve the interoperability of the metadata by being used as value vocabularies. Wierling et al. [14] give a broad overview of ontologies in the energy domain. In the following, we only give a short overview and refer to Wierling et al. for further information.

Cuenca et al. introduced an approach to unify different existing ontologies in the energy domain [15]. They focused especially on ontologies for energy management applications in smart grids. Their ontology is called OEMA (Ontology for Energy Management Applications) and is formulated in OWL2 (Web Ontology Language 2[14]). It reuses existing ontologies and adds additional concepts. It has eight parts: infrastructure, energy and equipment, geographical, external factors, person and organization, energy saving, smart grid stakeholders, and units. The authors extended their work by introducing the Domain Analysis-Based Global Energy Ontology (DABGEO) [16]. To increase the reusability compared to OEMA, this ontology is constructed in a way that makes it easy to extend with application specific vocabulary. Using OWL2 DABGEO includes five parts: energy equipment, infrastructure, energy performance, energy external factors, and smart grid stakeholders.

Lefrançois presented the Smart Energy-Aware Systems (SEAS) ontology. It is a modular ontology published in Turtle[15]. The SEAS ontology contains the following modules: DeviceOntology, ForecastingOntology, OptimizationOntology, TradingOntology, and SmartMeterOntology. In the design process, he tried to follow the current best practices in ontology engineering. [17]

Booshehri et al. introduced the open energy ontology (OEO) as an ontology for energy systems analysis. The OEO is developed using OWL (Web Ontology Language[16]) and consists of oeo-modal, oeo-social, oeo-physical, and oeo-shared. The OEO includes concepts from other ontologies as the Financial Industry Business Ontology and the Unit Ontology. It can be used to annotate scenarios, factsheets, and data used in energy systems analysis. The ontology will be further developed on Github making it possible for everyone to contribute. [18]

Oppermann et al. introduced an ontology for EnArgus[17], the funding information system for energy research in Germany. The ontology aims to map the whole domain of energy research and is used to improve the search in a project database. The ontology is not yet publicly available but the authors see its publication as a future work. Also, the authors admitted that they followed less strict ontology engineering rules than the developers of the OEO. [19]

Fernández-Izquierdo et al. gave a good overview on ontologies in the energy domain and introduced an ontology for demand response to improve interoperability between demand response stakeholders. The ontology described in OWL is based on OpenADR[18], an open exchange model and global smart grid standard. The ontology is available on Github[19]. [20]

The Common Information Model (CIM) is a group of IEC standards and a domain ontology

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[14] `https://w3.org/TR/owl2-overview/`, accessed 12.12.2022
[15] `https://w3.org/TR/turtle/`, accessed 12.12.2022
[16] `https://w3.org/TR/owl-semantics/`, accessed 12.12.2022
[17] `https://enargus.de/`, accessed 12.12.2022
[18] `https://openadr.org/`, accessed 12.12.2022
[19] `https://github.com/albaizq/OpenADRontology`, accessed 21.07.2021

which can be used to describe multiple aspects in energy systems. The standard is mainly applied in the electric utilities sector and has a high industry focus. The description is given in the Unified Modeling Language (UML) and a conversion to OWL is possible by using the CIMTool[20]. [21]

There exist different ontologies for the energy (research) domain. It seems promising that one or a combination of multiple ontologies, for example of the OEO [18] and CIM [21], can be used as value vocabulary for describing ERS.

Overall, there exist good approaches for metadata schemes for research software in other domains like life science and geoscience, as shown in Section 2.1, which can be used as inspiration. The existing approaches for ERS often lack formalization, are not based on existing approaches and/or do not use value vocabularies like shown in Section 2.2. The last part of the related work showed that there exist multiple ontologies which can be used as value vocabularies for a metadata scheme for ERS.

3 Concept for a Metadata-based Registry for ERS

We introduce our concept for a Metadata-based Registry for ERS in Figure 2. As first step in the research cycle, researchers should be able to use the software registry in our concept to find relevant ERS for their research problem. All listed software should link to the responding software repositories (e.g., GitHub). We describe the registry in more detail in Section 3.3. After downloading the software researchers will use it as well as write additional software for their research. The new or extended software should be publish on any existing software repository. Then, researchers should be able to add the software to the software registry by using the metadata generation tool. It should extract as many information as possible from the software repository and, therefore, helps the researchers with creating metadata. We further describe the concept of the metadata generation tool in Section 3.2. Both the metadata generation tool and the registry are based on a common metadata scheme for ERS. Therefore, we first give more details on that in Section 3.1.

3.1 A Metadata Scheme for ERS

A metadata scheme for ERS should be usable for all different types of ERS to increase their findability. It is the foundation for the other two artifacts. A metadata scheme comprises elements describing the categories for the metadata, of guidelines for creating according metadata, of a syntax and of constrains for the metadata, e.g., ontologies as value vocabularies [22].

The metadata scheme should be developed as an application profile using existing methods like the approach of Curado Malta and Baptista [23]. It should be based on a domain model containing desired elements with short descriptions, examples, and their relations. These elements and their description should only be formulated in English to be usable by the international research community. The development of this metadata scheme for ERS should be based on an environmental scan [24] to incorporate existing approaches, especially the one in semantic-web compatible formats, like the general work on metadata for research software, e.g., CodeMeta[2], and the domain-specific developments like the metadata schemes of the Open Energy Platform[13].

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[20] https://wiki.cimtool.org/, accessed 12.12.2022

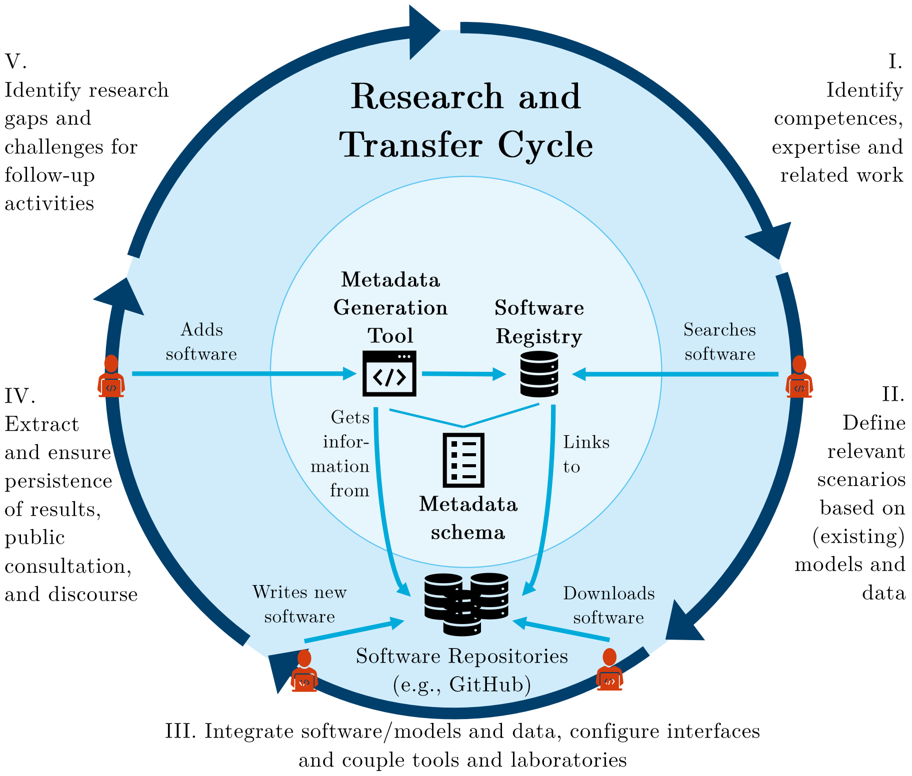

Figure 2: A metadata-based registry support the exemplified research cycle of energy research with software usage

For each element of the metadata scheme, it should be specified if it is mandatory or optional and if constraints exist, e.g., if the use of a controlled value vocabulary is required or not. Especially for the domain specific elements, value vocabularies should be used. It should be carefully analyzed if one or multiple ontologies, like OEO [18], can be integrated as value vocabulary.

The metadata scheme should be used by the registry and the metadata generation tool, as described in the following sections.

3.2 A Metadata Generation Tool

A metadata generation tool should support all researchers to create high-quality metadata for their ERS. It should lower the entrance barrier for creating metadata for all researchers in the energy domain without the need for a deeper understanding of the underlying technologies.

If the ERS is already in an open software repository like GitLab or GitHub, the tool should start by extracting as many metadata as possible from the repository. Mao et al. developed the framework SoMEF which already can extract a lot of metadata out of readme files [25]. The metadata will be mapped to the metadata scheme for ERS as described in Section 3.1. The tool should allow the user to add additional metadata as well as correct the automatic extracted ones. It should support the use of controlled value vocabularies as defined in the specification of the metadata scheme and should allow to integrate additional ontologies to include many links to other semantic web sources.

3.3 A Metadata Registry for ERS

A registry for ERS should help researchers to find the right software based on multiple search criteria, e.g., researchers wanting to do a grid simulation can look for a library or framework compatible with the models in a certain programming language they already use. For the development of such a registry, existing approaches from other domains like bio.tools[9] should be considered. The registry should be based on the new developed metadata scheme for ERS.

4 Conclusion and Outlook

There already exist a lot of ERS and even more ERS will be needed in the future. ERS is often developed without reusing existing software. One reason for that is that the existing software is not simple to find. The overall findability of ERS can be improved when ERS is registered in a registry with relevant metadata. Therefore, we introduced the concept of a **metadata-based registry for ERS** to enable this process.

We presented the state of the art in three parts. First, we described general approaches on metadata for research software as well as approaches focusing on research software in other domains. Second, we outlined metadata approaches in the energy domain where most current approaches focus on research data. The approaches already focusing on research software are not formalized and, therefore, do not meet our requirements. Third, we gave an overview on existing ontologies in the energy domain which can be serve as value vocabularies for a metadata scheme.

Based on the presented state of the art, we defined our concept consisting of three main artifacts. The metadata scheme for ERS presents the foundation and should be developed following best practices in metadata scheme development. It should include mandatory elements and value vocabularies. The metadata generation tool should assist researchers in creating metadata by extracting as many metadata as possible from different sources, e.g., GitLab or GitHub. The registry should be the place where ERS can be found. It should store metadata of ERS and should use advanced search technologies.

As future work, the different proposed artifacts will be developed and tested. Therefore, first a detailed requirement analysis will be performed as basis for the domain model of the metadata scheme.

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6 Roles and contributions

Stephan Ferenz: Conceptualization, Writing – original draft

Astrid Nieße: Conceptualization, Writing – review & editing

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