NordDesign 2020
August 11-14, 2020
Kgs. Lyngby, Denmark

Research Data Management System for a large Collaborative Project

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Abstract

Data processing is an essential element of scientific work in engineering. The ongoing digitization in the engineering sciences generates more and more data, having a tremendous impact on the development and realisation of technological processes.
In large collaborative projects Research Data Management Systems are major assets to implement a research data management according to the FAIR data principles and to support scientist in their interdisciplinary research across multiple teams.
Based on the example of the Collaborative Research Centre 1153 "Process chain for the production of hybrid high-performance components through tailored forming", where an interdisciplinary team researches novel process chains for the manufacturing of hybrid components, an approach to organize the research data management process using a Research Data and Knowledge Management System and a domain specific vocabulary is being developed.

Keywords: research data management, vocabulary, design support system, knowledge management

1 Introduction

The engineering sciences consist of many sub disciplines with a broad variety of processes and methods generating, processing and analysing manifold research data (Sandfeld, S. et al., 2018). The heterogeneity of research data ranges from measurement data, observational data, data from simulations to images and videos. Methodical test procedures such as standard operating procedures, questionnaires, software used in simulations or data analysis can also be defined as artefacts of scientific research and should therefore be included under the term research data likewise. Findability, accessibility, understandability and reusability of data play a crucial rule in large collaborative projects, where data is exchanged between projects or along a process chain (Effertz, E., 2010). The diversity of data poses a major challenge. The data obtained is often not annotated in a standardized way. Concrete metadata standards for annotating the data are not in use. The overall goal of the implementation of research data management standards and workflows is to systematically make data findable, accessible, interoperable and reusable (Wilkinson, M.D. et al., 2016). The application and benefits of cooperative software systems for data management in collaborative projects have been investigated in numerous studies (Kapogiannis, G., & Sherratt, F., 2018), (Savolainen, J. et al., 2018), (Wang, W.M. et al., 2016). Strategic considerations are not limited to Research Data Management (RDM) systems. Beyond the management of data and provision of functionalities to support research and publication activities a holistic approach combines data and contextual information from the research process to ultimately enable researchers to take clear measures and to make knowledge based technical decisions. Such a combined Knowledge Management and RDM system should accompany all steps of the research process and enable their comprehensive documentation. Ideally, such a system allows to describe and to document research problems, hypotheses, applied methods and the data generated and analysed an integrated manner. Figure 1 summarizes this idea.

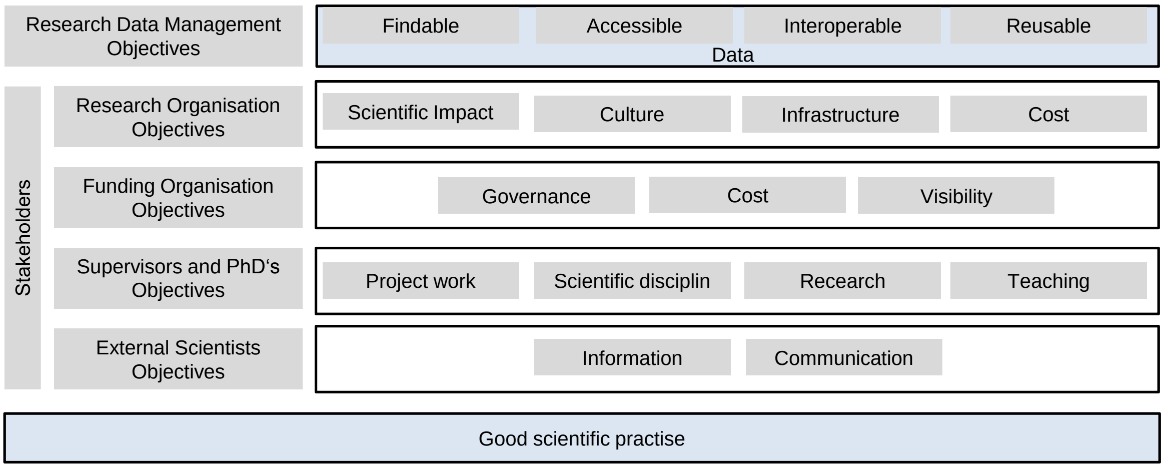

Figure 1. Research data management objectives.

The German Research Foundation promotes the awareness of research data by means of infrastructure projects embedded in Collaborative Research Centres (CRC) (Redöhl, B., 2016). The advised German National Research Data Infrastructure (NFDI) aims to link existing infrastructure components and services for an overarching, interdisciplinary and sustainable RDM (RfII, 2016). The NFDI4Ing consortium represents the engineering sciences and the requirements of the community (Schmitt R. et al., 2018).

In this publication we present identified requirements, challenges, the used methodology and possible solutions including a semantic approach for the functionality, architecture and implementation of RDM and Knowledge Management Systems based on our work in CRCs to foster the aforementioned cultural change.

We will discuss the following aspects and questions:

1. How to create awareness and work culture in dealing with research data in large collaborative projects?
2. What are the requirements to build a common understanding of the different data types in a large project?
3. How to implement intuitive RDM tools to support research data workflows between several projects?
4. How to develop a domain-specific vocabulary to semantically annotate research data?
5. How can new research questions be derived from existing data provided by a RDM system? How to turn raw and scattered information into useful ideas and research tools?

The answers to these questions enable strategic decisions on guidelines for project-wide research data management and corresponding working groups, the system architecture, the

choice of a RDM and Knowledge Management System, standards on data domain-specific vocabularies to describe data and information, and the choice of further data management tools that support the strategy at the level of hardware and software.
Section 2 of this publication describes the general requirements for RDM systems in collaborative projects and gives an overview of existing commercial and open data management systems. At the example of the CRC 1153, a description of the chosen strategies of the system architecture and the approach to implement the relationships between its elements is given in sections 3–4.

2 Requirements of a Research Data Management System

On the way to a successful implementation of a sustainable research data management one have to face numerous challenges. Data are increasing in volume, complexity, heterogeneity and speed of generation. The FAIR data principles aim to provide guidelines how to generate findable, accessible, interoperable and reusable data (Wilkinson, M.D. et al., 2016), (Mons, B. et al., 2017). The principle highlight the machine-readability of data as researchers rely more and more on computational support to deal with large and complex amounts of data. When discussing data, however, we must not overlook the context in which they were created, their meaning and the purpose of their production. Based on (VDI 5610, 2009), data are objective facts that cannot be interpreted without context and further background and are to be understood as "raw material". Information is structured data with relevance and purpose that can be contextualized, categorized, calculated and corrected. Knowledge is generated by semantically linking the information. In this way, knowledge is linked information that allows identifying relations, and making comparisons, qualitative judgments and decisions. The increasing level of abstraction from data to knowledge is described by the knowledge pyramid in Figure 2 (Ackoff, R.L., 1989).

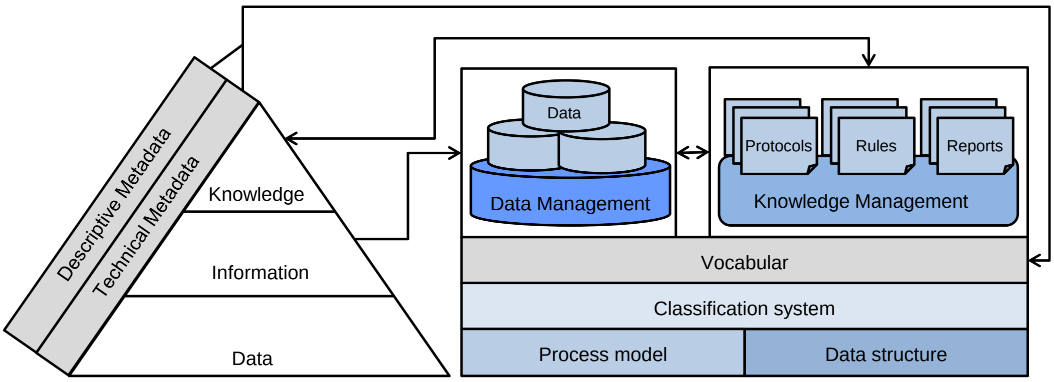

Figure 2. Relationships between data, information, knowledge.

If we apply these considerations to the implementation of RDM in large collaborative projects, new dimensions arise which must be included. On one hand individual subprojects often tend to organize their data and research documentation based on own standards. Often only selected data are stored in shared repositories. On the other hand the exchange and availability of contextualized, structured and categorized data between subprojects is essential in a joint research effort to generate information and knowledge. The contextualization can be achieved by classification and domain specific vocabularies to describe data. Interdisciplinary and interinstitutional collaboration, cooperation and communication between all subprojects are keys in the research and development process. A RDM system plays a central role in supporting the organization of these processes. The knowledge pyramid can therefore be matched with a RDM model (Figure 2, right side) and the corresponding RDM system described in the section 3.

The data in the RDM system ist organized and managed by identifying data structures, process models from which a data classification system and a domain-specific vocabulary are derived. The accompanying contextual metadata play an important role and cab be divided into two types: general metadata containing standard information, such as the date and place of the experiment or the person conducting the experiment and technical metadata like characteristic process parameters like gas flows, current range or welding time used in the experiments.

2.1 Industrial Product Data Management Systems

In industrial environments, Product Data Management (PDM) and Product Lifecycle Management (PLM) systems are used to organize the storage and management of data. PDM systems are applied to manage computer-generated models, drawing data and other documents within the development process. By extending functionality to the lifecycle view of a product, PDM is often considered as an important part of PLM (Feldhusen, J. & Grote, K.H., 2013).
Basic functions of PDM systems are document management, product structure management, project management and classification (Feldhusen, J. & Gebhardt , B., 2008), (VDMA, 2005), (VDI 2219, 2016). A PDM system supports the development of technical systems and ensures that everyone involved is at the same level of information. An overview of the current PDM systems on the market is given in (Ulrich, T., 2016). Modern PDM systems, as well as RDM systems, support the processing, analysis, archiving and subsequent reuse of system-relevant data in the development phase. What is missing, however, are unified interfaces and protocols for accessing and reusing data and feedback mechanisms to evolve subsequent generations of technical systems. Each data provider has its own service offerings and delivers data in various formats with different licenses and costs. In addition, commercial data providers are often limited to certain types of business in specific geographic areas of Europe and keep their data in isolated records. Apart from a few existing, internationally coordinated classification schemes, such as e. g. eCl@ss and efforts by the ProSTEP Association, the combination of these factors hinders interoperability and a better data value chain around enterprise information (Scheidel, W. et al., 2017). For the management of research data according to the FAIR data principles, these commercial systems therefore seem to be less suitable.

2.2 Open Source Data Management Systems

Alternative solutions for research data management, especially in the open source community, exist. The paper (Amorim, R.C. et al., 2017) presents an overview of several prominent RDM platforms that can be used by an institution to support part of its RDM workflow. One such a system for storing research data is the Comprehensive Knowledge Archive Network (CKAN, ckan.org). Major advantages of the CKAN compared to proprietary commercial systems are the connectivity via open-configurable interfaces (APIs) and the extensibility of the services via plugins and implementation of subject-specific vocabularies. Thus, the service can be supplemented by relevant tools, e. g. for the execution of software codes using Jupyter Notebooks or for the visualization of research data. Possible application areas of CKAN are demonstrated with the Leibniz Data Manager (datamanager.tib.eu). This includes a semantic description and linking of research data, other portals and preview functions for screening different data types to assist researchers in the selection of relevant data sets for their respective discipline. CKAN is used as Research Data Repository by Leibniz University Hanover.
For collecting and providing semi-structured information Wiki-based systems are widely used. Wikipedia is one well-known prime example and is operated via the open source

MediaWiki software (Krötzsch, M. & Vrandecic,D., 2009). Wikis have established themselves as Knowledge Management Systems in companies and in academia. With semantic extensions Wikis are able to store annotated data and semi-structured information e. g. protocols and process descriptions which can be queried and used for data aggregation in reports. The Semantic MediaWiki or OntoWiki (Frischmuth, P. et al., 2015) are such an extension using a machine-readable vocabulary, which provides the terminological basis across systems and thus promotes data interoperability.

3 Methodology

The goal of the data management system is to support project workflows and move from fragmented project-oriented to a common data management system.
Figure 3 summarizes the transformation from individually operating subprojects (indicated as SP A and SP B) with separate activities and data silos towards a collaborative research data management implementation with common data management guidelines and a central RDM system. The research data is to be stored and organized in a Data Management System, the information to contextualize the data is stored in a Knowledge Management System. Information can be the documentation of research activities as standard operating procedures, protocols of experiments, observation notes, or configuration settings of simulations. Relations between information can be described as sets of rules that allow automated generation of reports. The deduction of data structures their classification and the definition of a domain specific vocabulary support semantic annotation and cross-linking of data and Knowledge Management System and foster a common understanding of data across all subprojects. The mapping of data and their contextual information supports the discovery of new relations by joint comparison of data and descriptive metadata.

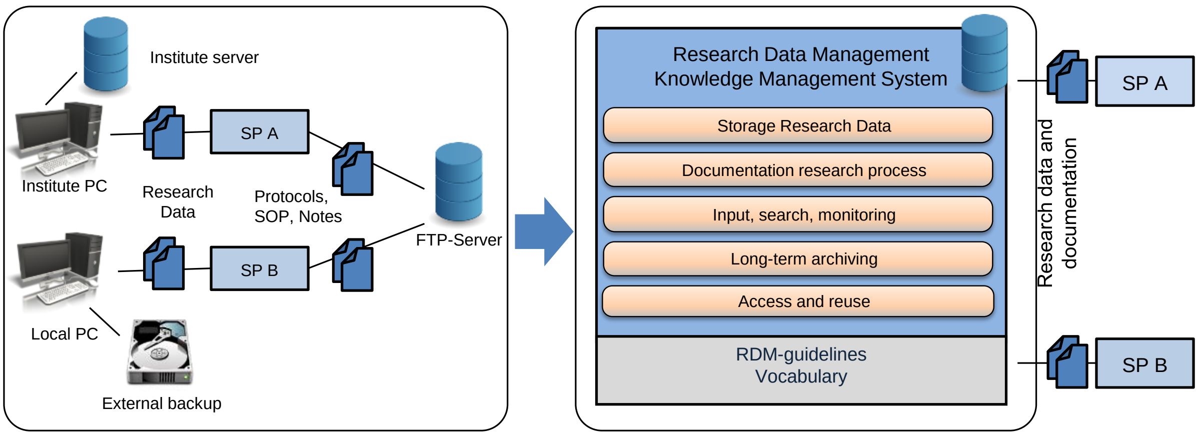

Figure 3. Transition from separate data storage to systematic Research Data Management.

In order to address the necessary tasks, the working group "Research Data Management" is introduced at the organisational level within the framework of the collaboratve project. The working group is lead by the information infrastructure subproject and includes participants from all subprojects. Based on an agile, empirical approach, several methods are used to collect information on processes and generated data in the subprojects and along process chains across several subprojects. Methods used include surveys, interviews and workshops and are chosen by the following criteria:

- online surveys allow a fast and easy mechanism to retrieve well formed data at low cost, but are not suitable for identifying implicit requirements;
- workshops allow to collect information about workflows and interactions of various stakeholders of the project to identify synergies and discuss the contradictions;

- interviews allow to identify implicit requirements and are well suited at obtaining specific information, requirements and to evaluate system designs.

While information about generated data, data types, formats and size can be gathered by surveys, interviews and workshops are suitable to collect information about cross-project workflows, interfaces and the habits of communication between researchers and project managers. The exchange and discussion in the workshops increase and deepen the common understanding of data and processes. These methods are suitable for identifying the requirements as well as for the evaluation of developed systems.

4 Use Case: RDM System for the Tailored Forming Technology

In developing data management systems for collaborative research projects, important aspects are empirical survey of research workflows to identify typical research activities of each subproject and information flows between the projects.

Here, we present RDM activities of the information infrastructure project of the CRC 1153 “Process chain for the production of hybrid high-performance components through tailored forming“. Within the CRC 1153, the development of novel process chains for the tailored manufacturing of hybrid components generates large amounts of data in various process steps (Behrens, B.-A., et al., 2016), (Siqueira, R., et al., 2019).

The CRC employs researchers from materials science, metal forming, machining, assembly technologies, tribology, construction, measurement technologies and others. The CRC is organized in three research areas with 17 subprojects, including two transfer subprojects, as well as an information infrastructure subproject and a central administration subproject. The research focus of project area A is the geometric design and manufacturing of hybrid semi-finished workpieces using different joining processes. Here, the selection and conditioning of suitable materials, modelling of the joining processes and their further development are the main research tasks. Project Area B is concerned with the processing of the hybrid semi-finished workpieces into finished components. The focus of the investigations is the design and development of various forming processes for the manufacturing of hybrid semi-finished components. Project Area C is devoted to the process design, expansion and future development for an evaluation and quality assurance of the individual production steps along the entire production chain.

4.1 Situation analysis and basic object recognition

In the initial phase, a workshop was held with participants from all subprojects to prepare the collection of system requirements. As a result, the organizational workflows and scientific aspects of the CRC were defined, discussed and agreed upon, and typical and CRC-specific scientific activities were identified. As a result of the workshop, the current situation in the project was analyzed. Data results from machine outputs, process simulations or subsequent analysis steps (Behrens, B.-A., et al., 2019). The generated research data, the corresponding documentation and the software applied represent important elements for a reproducible and a sustainable engineering research. These artefacts enable a comprehensive understanding of research questions that are investigated across the different production technologies and methods. The heterogeneity of the data generated by researchers poses a major challenge. The data obtained in initial data analysis is often not systematically structured and annotated, making it difficult to retrieve and access at a later date. Specific metadata standards or vocabularies for annotating the data are not in use.

The management of data from various sources and the assessment of their significance for previous and subsequent process steps within a process chain proved to be a major challenge. Ideally, all research data together with the respective components or samples should be passed on to the downstream processes so that an individual process design can be achieved on the basis of this data or processes of machine learning can be accelerated. The identified scientific activities in the field of mechanical engineering were taken as a basis for the classification of protocols in the Knowledge Management System. Basic objects and functions of the RDM system are depicted in Figure 4 at the example of one prototype part.

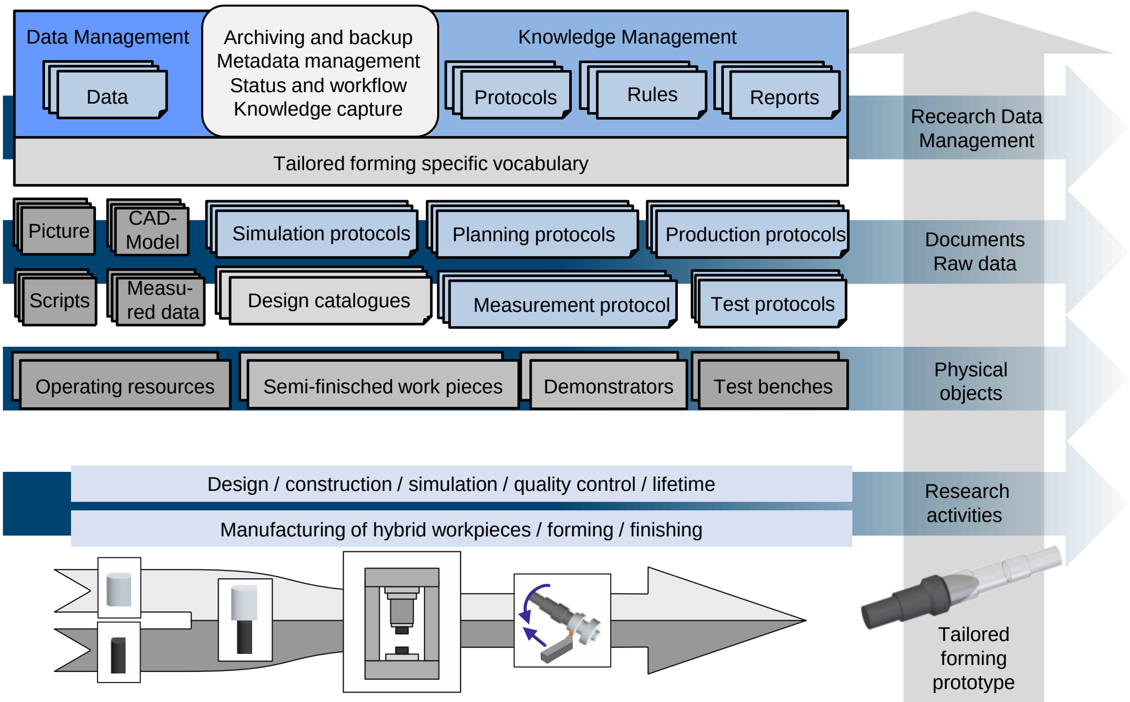

Figure 4. Basis objects of the RDM System.

At the beginning of the process chain, two mono material semi-finished metal parts are joined by friction welding, ultrasonic aided laser beam welding or lateral angular co-extrusion. In the next step, the resulting semi-finished workpiece is subjected to a metal forming process such as cross-wedge rolling, extrusion or die forging. Subsequently, the hybrid solid components are heat-treated and the geometry is finished in a machining process. Resulting, a high-performance component with locally adapted properties is available.

Object related data to be stored in the system includes, for example, data regarding materials, semi-finished workpieces, prototypes and test benches.

The first step involves an identification of project-specific research data, the corresponding workflow and analysis of the structure of protocols and reports.

The following approach was agreed upon to introduce a research data management:

- documentation of research activities and their results are entered into the RDM system in the form of protocols. The protocols are stored as semi-structured information based on identified data structures;
- the assignment of metadata allows to homogenize data and information described by the protocols and serve as a basis for the generation of automated reports;
- reports can be automatically generated based on queries and various filter options.

4.2 Identification of stakeholders and functions of RDM system

An important aspect for the implemention of the RDM system is the identification of user types and access right definitions. Besides, it is necessary to create project specific RDM guidelines. Discussion of these aspects was the aim of the second workshop. The identified stakeholders include project- and subproject leaders, researchers and PhD students, technical staff, students, external scientists and experts as well as industrial partners. Thus, a roles and rights management is relevant for the implementation of the RDM system. The results of the requirement analysis of the RDM system are given in Table 1. The system functions identified for implementation are classified into four categories: status monitoring, automated knowledge management, project administrative support and service functions.

Table 1. Functions of the RDM System.

Category	Function	Description
Service	▪ Data search on request ▪ Data visualization ▪ Export of data ▪ Export of reports	Generation of reports based on search queries for internal and external users
Administrative support for the entire project	▪ Adding and correction of information ▪ Information search ▪ Export of information	Storage and retrieval of information about project team, equipment, work meetings, conferences and publications
Status monitoring of semi-finished workpieces and of components	▪ Protocol creation and editing ▪ Sample localization in the process chain ▪ Creating reports about the workpiece's or component's status ▪ Creating reports by specified filters: subproject, component type, time interval, etc.	Within a single process chain, several subprojects work on the manufacturing of semi-finished workpieces and hybrid components, respectively. The monitoring of the status allows for process transparency and for quantitative and qualitative control of the scientific and technological processes
Automated knowledge management	Identification of stable processes and recognition of unexpected effects	Analysing and linking metadata into semantic constructs is intended to allow for ▪ an automated identification of information about efficiently functioning technological chains and ▪ to assist in testing hypotheses regarding the optimization of production chains and ▪ to search for new or unaccounted parameters and effects.

The implementation of these functions provide answers to the questions formulated in chapter one. Functions of the administrative and service category are designed to support basic research processes typical for most collaborative projects. The functions of the monitoring and knowledge management category allow a maximum benefit from the knowledge preserved in the system, to support information flows and joint work of subprojects, as well as to support and form scientific questions and hypotheses.

4.3 Identification of data structures

In order to identify data structures for each of the subprojects, surveys were organized to recognize data and protocol types and initial protocol structures. The implementation of a RDM System includes two parts: Data Management for the research data and Knowledge Management to collect contextual data in the form of protocols. These parts are realized by using the software CKAN and Semantic MediaWiki. A tailored forming specific vocabulary is developed to connect both systems. The protocol templates and metadata structures are unique for each subproject. Protocols may contain the following data types and formats: simulation models, simulation scripts, CAD models, various types of signals and machine data obtained during workpiece processing, testing and measurement; results in the form of text files, tables, diagrams and other graphical data. The results are stored in the Knowledge Management system in the form of various types of protocols, e. g. simulation, planning and test procedures.

The process of developing the RDM system is iterative and includes several steps at each iteration. Based on the identified objects and parameters of the tailored forming process

model, the second step classifies and aggregates these into data structures. Using these obtained results, the third step provides the creation of a classification system, which is to be applied in the fourth step to create a tailored forming technology specific vocabulary. The subsequent step uses the results of the first and second step, respectively, to adapt the RDM and Knowledge Management Systems to the requirements for storing and processing research data for the tailored forming technologies.
Individual interviews with subprojects were conducted for the purpose of further detailing, refining and standardizing the description of process parameters documented in protocolls, as well as coordinating and normalizing descriptive metadata. The results of the interviews were used to develop the tailored forming specific vocabulary.

5 Architecture of RDM System and Domain-specific Vocabulary

The semantic, machine-readable description of research data using a domain-specific tailed-forming vocabulary enables data and information from a wide variety of sources to be interpreted, processed and linked automatically. Considering the heterogeneous data of the various projects within the CRC the vocabulary enables the linking between datasets in the Data Management system CKAN and the Knowledge Management System Semantic MediaWiki. The vocabulary development can be described with a circular model in which the steps modelling, population and testing are repeated iteratively (Halilaj, L. et al., 2016).

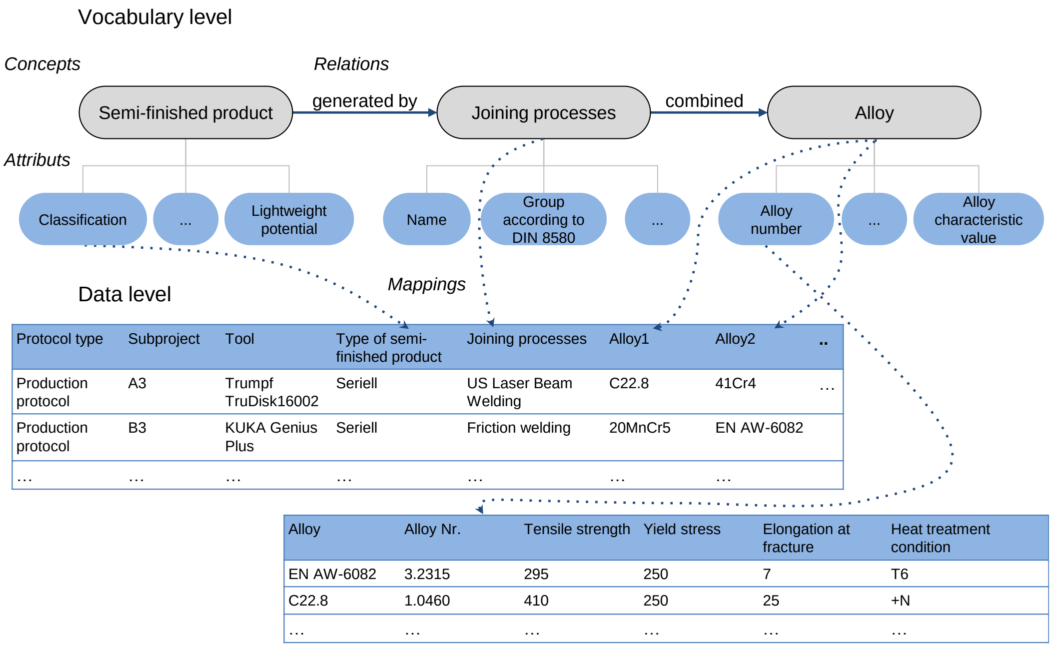

Figure 6. Example of tailored forming domain-specific vocabulary on the basis of RDF language.

By establishing relationships between objects, subjects, attribute sets and existing data structures specific to different subprojects, data mapping is carried out, which makes it possible to establish relationships between heterogeneous sources of data and information without restructuring. Identification, description and formation of relations between data are carried out in accordance with the following principles: all described entities receive unique identifiers, the Resource Description Framework (RDF) data model is used for data publication. An entity that is a subject in one relationship may be an object of another. Objects and subjects can be compared with sets of attributes (Figure 6). In this way content indexing of the data takes place via mappings by domain-specific vocabularies. Data mappings by vocabularies enable data integration and new explorations like semantic search or visualization, and establish a common understanding of data and capture domain-specific semantics. In order to verify the applied method and the resulting of domain specific vocabulary, a workshop was organized. The outcome of the workshop confirmed the validity of the chosen approach.

The process of creating the data management system consists of creating repositories for storing documents containing some terms and creating a specific ontology. The architecture of the advised RDM System is shown in Figure 7, enabling a sustainable, FAIR data management of extensive process data in different formats, volumes from all subprojects. The RDM system to store the research data is realized using CKAN. The capabilities of the RDM system are enhanced by an additional Knowledge Management System, which captures the context of the data generation, its relation and relevance for the process chain. A Semantic MediaWiki implementation is used for this purpose. Both systems are adapted to the domain-specific process models and data structures of the tailored forming technology so that researchers can use the system as intuitively as possible.

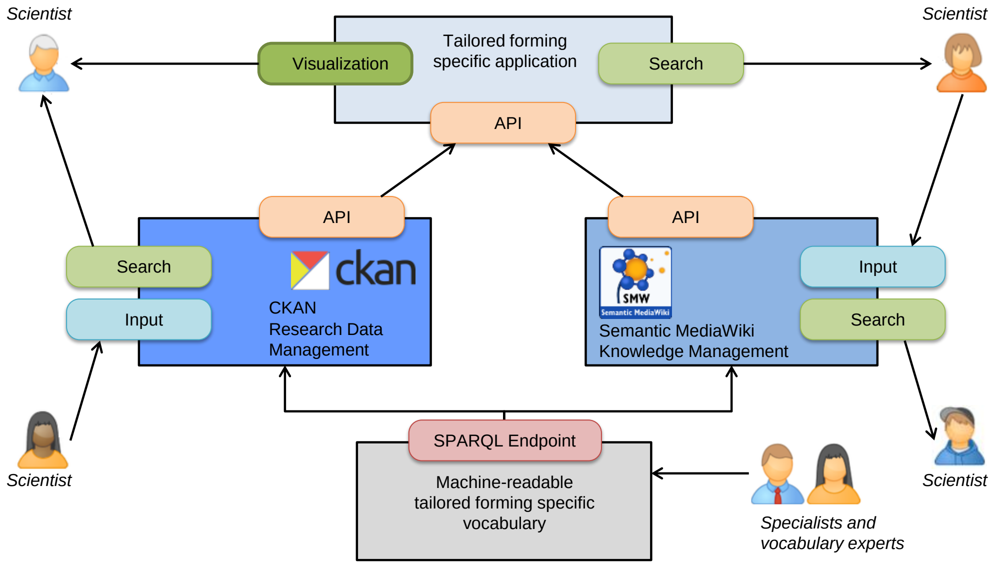

Figure 7. System architecture.

In addition, a vocabulary for semantic representation and thus for machine readability of the metadata and data structures in RDF will be implemented. The platform allows to import, export, curate, explore and process data directly via the web interface; alternatively also automatically via Representational State Transfer Application Programming Interface (REST-API) or SPARQL Protocol And RDF Query Language (SPARQL) endpoint.

6 Discussion and Conclusion

We described an approach for a RDM infrastructure consisting of a Research Data Management and Knowledge Management System and methods to develop a domain-specific vocabulary to be applied within a collaborative research centre. The proposed approach allows storage of research data in the Data Management System and storage of contextual information, documentation and research results in the form of standard operating procedures, research protocols, observation notes and generation of reports in the Knowledge Management System by all subprojects. A tailored forming specific vocabulary using RDF links both systems semantically together. The proposed infrastructure enables a common research data management according to the FAIR data principles across all subprojects of the CRC and common workflows for the exchange of data and information along the process

chain. Research data together with the respective physical components can be passed on to the next process step so that an individual process design can be made on the basis of all data generated for the process to this point. This approach ensures the quality of the process with an acceptable expenditure of time and resources.
The conducted workshops and interviews indicate that the RDM system and its planed functionality improve the understanding and transparency of data and processes investigated across the different production technologies and methods. Researchers confirm that the semantic annotation of data and process parameters helps to identify relationships and interdependencies between data and processes from different projects. However the success of this approach depends on the agreement of RDM guidelines and their consistent application by all stakeholders. In the end the proposed approach is, in the authors' opinion, applicable on an organisational level to any large research project. The identified system requirements and research workflows involving generated data and contextual data documented in protocols are typical for most projects. However, there are a number of project specific aspects like roles and rights management or data license models. Besides, each research project needs its own domain-specific vocabulary and adapted methods for its creation.

Acknowledgement

The authors gratefully acknowledge the support from the Collaborative Research Centre (CRC) 1153 "Process Chain for Manufacturing Hybrid High Performance Components by Tailored Forming", Project number 252662854 (INF), funded by the German Research Foundation (DFG).

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