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Report D5.3
"Selection and specification of further cases"

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Report D5.3
"Selection and specification of further cases"

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Disclaimer

Executive Summary

OntoCommons project aims to provide an ecosystem of reference Top- Middle- and Domain ontologies and their alignments, as well as best practices and guidelines for ontology and tool development. The demonstrators are a cornerstone of these activities as they on one hand provide the requirements from an industrial perspective, on the other hand demonstrate the impact of the provided solutions.

The project began in 2020 with an initial set of 11 demonstrators and the first stage of the work has been completed with them. In the last quarter of 2021, we launched a campaign to acquire additional demonstrators to improve the variety of our industrial stakeholders in order to increase the quality of requirement collection and the impact of the results. This deliverable summarizes the results of the new demonstrator acquisition, which resulted in 11 new demonstrators. The demonstrators are described briefly with their key information extracted from the surveys and interview conducted with them. We also give an overall analysis of the demonstrator acquisition process, which shows the we fulfilled the criteria regarding the characteristics of the new demonstrators set by the project goals and expected impacts.

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1. Introduction

Demonstration is one of the cornerstones of OntoCommons project. The industrial stakeholders provide valuable input for the development of various building blocks of the OntoCommons Ecosystem and Roadmap. They also help us to demonstrate the impact of our work. The project started with 11 initial demonstrators and promised to expand them with new ones. To the end, we launched a campaign to acquire new demonstrators according to the criteria we built based on the expected impact of OntoCommons. As the result of this campaign, we acquired 11 new demonstrators from a wide range of NMBP domains (Nanotechnologies, Advanced Materials, Biotechnology and Advanced Manufacturing and Processing).

In this deliverable, we present the selection and specification of 11 new demonstrators. The selected demonstrators are provided with a survey to specify their use cases. The survey mainly asked about the main challenges, expectations, main scenario and the goals, ontologies and data sources considered to better understand the details of the use cases. The expected impacts of the OntoCommons Ecosystem in mind, we also asked demonstrators to provide a set of KPIs that they will use to validate their use cases and conducted a FAIR assessment in order to create a baseline for the validation of FAIRness improvement at the end of the project. As a result, we compiled our key findings and presented them in relation to the selection criteria, as well as a set of requirements that will be used as input for the other technical work packages of OntoCommons.

The deliverable is structured as follows: In Section 2, we describe demonstrators. We first present the selection criteria and an overall analysis of the selected demonstrators based on that criteria. We then continued with a concise specification of each demonstrator including key information about their use cases. In Section 3, we consolidated a set of requirements obtained from the demonstrators regarding ontology development, usage and tools as well as standardization. Finally, we concluded with a summary of the key points and a look at the future work. For the sake of readability, we provided individual detailed surveys filled by the demonstrators in the Appendix. We refer interested readers to see the details of each demonstrator and use case there.

2. Acquired Demonstrators

We launched a campaign between July and December 2021 in order to collect applications for becoming a demonstrator for the OntoCommons project. We have received 22 applications and among those we preliminarily selected 15 candidates. The following criteria from the OntoCommons Call for Demonstrators were considered for the selection:

- Relevance to the OntoCommons project topics. We expect use cases from NMBP domains.
- Representative coverage of various domains. Although use cases from any NMBP related domain are welcome, we aim to have diversity in the domains covered under these domains.
- Diversity in the technology requirements. We aim to cover a large, diverse range of challenges that can be solved with semantic technologies.
- Appropriate Technology Readiness Level (TRL). The demonstrators should have TRLs that are in-line with the expectation of the OntoCommons project (starting at 3-5 and targeting 6-7 for the end of the activity).
- Geographical distribution. The demonstrators shall be geographically distributed, to cover different EU and non-EU states, to ensure the representative collection of the requirements and awareness of the various national developments.
- Contribution to the goals of the project, cooperation potential with other work packages. The demonstrators will be selected considering the expectations towards their potential to contribute to various aims of the project, particularly, in different work packages. Thus, demonstrators working with various ontologies will be relevant.

As a methodology, we discussed the applications first within the work package working with the demonstrators, then we shared our initial selection with the project consortium. After a short feedback round, the selection was finalized. Among those 15, 11 demonstrator applicants responded to our initial contact attempt and we held a series of kick-off meetings with the demonstrators to explain to them the timeline of the project and the survey we created to collect the specifications of their use cases.

The remaining part of this section reports the results obtained from the surveys and interviews done with the newly acquired 11 demonstrators additional to the 11 demonstrators we had before. We will first provide our overall observations from the new demonstrators particularly in relation to the relevant selection criteria. Then we give brief descriptions of individual use cases.

2.1 Analysis of the Demonstrators w.r.t Selection Criteria

In the following we give a general overview of the key learnings from the demonstrators in relation to the demonstrator selection criteria we set for our open call, based on the conditions defined in the description of work.

2.1.1 Relevance to the project, domain diversity and coverage

All acquired demonstrators provide use cases that are related to the NMBP domains/verticals. The table below shows the distribution across domains. We managed to acquire demonstrators that work in 7 different domains:

Domain	Number of demonstrators
Manufacturing	5
Materials Development	3
Biotechnology	2
Life Cycle Assessment	2
Materials Processing	2
Material Characterisation	1
Materials Modelling	1

Note that, one use case may belong to multiple domains. Many use cases are in manufacturing domain which is not surprising, as there are many verticals involved in industrial manufacturing (e.g., chemicals, aircraft). From a diversity point of view we managed to touch 7 different domains including the ones like Biotechnology and Life Cycle Assessment, which we did not have among the initial set of demonstrators.

2.1.2 Diversity in challenges and requirements

The new use cases present many diverse challenges that can be addressed with ontologies and semantic technologies in a broader sense. The most popular challenges to be addressed are the following:

- Interoperability between different stakeholders and tools
- Size and heterogeneity of domains that makes ontology development more complex
- Lack of domain-specific ontologies for certain domains/verticals
- Data integration, harmonization and building knowledge graphs

There are many other challenges are mentioned such as scalability of reasoning, maintaining evolving ontologies, ontologies for NLP tasks and alignment between ontologies. The details of the challenges provided by each demonstrator can be found in Section 2.2. A more granular set of consolidated requirements is given in Section 3.

2.1.3 Appropriate Technology Readiness Level

We primarily target use cases that are in TRL3 to TRL5 level according to the EU definition of Technology Readiness Level (TRL)[1]. The demonstrators are expected to reach to TRL 6-TRL7 at the end of the project. The table below shows the distribution of demonstrator TRLs:

[1] https://de.wikipedia.org/wiki/Technology_Readiness_Level

Technology Readiness Level	Number of demonstrators
TRL3	4
TRL4	3
TRL5	3
TRL6	1

As seen above, the demonstrators are distributed evenly in terms of TRLs and mostly in the desired TRL.

2.1.4 Geographical Distribution

We acquired demonstrators from 8 different countries, which indicates a very good diversity as required in the selection criteria. The table below shows the geographical distribution of demonstrators.

Country	Number of demonstrators
Sweden	3
Germany	2
Brazil	1
China	1
France	1
Italy	1
Luxembourg	1
United Kingdom	1

One noticeable thing is that new demonstrators span across three continents. We have several countries that we did not have in the initial set of demonstrators such as Brazil, China, Luxembourg, and Sweden. This shows that our diverse geographical distribution goal is achieved.

2.1.5 Diversity of ontologies, tools and potential to contribute to the project

There are many different ontologies used or considered to be used which can be seen in Section 2.2. From the tools front, usual suspects like Protege are very common. A key point regarding the potential of contributing the various work packages of the project is that many use cases are involved with ontology development which means that they are good candidates for contributing to the development of reference ontologies that are part of the OntoCommons Ecosystem. Similarly, many demonstrators are developing in-house tools to work with ontologies, which makes them good candidates for providing input for the activities of WP4.

2.2 Use Case Specifications

In this section we provide a brief description and specification of the 11 new use cases. We give a brief description of each use case, then a tabular representation of key information about the use case, expected impact from the OntoCommons project and a diagram explaining the use case if available.

Additionally, a FAIR analysis of the use case a baseline is provided. The FAIR analysis is done based on the FAIR data maturity guidelines[2] and reported by the use cases via a survey[3]. Each principle is assessed in a scale between 0 and 4, where 0 refers to "not applicable" and 4 refers to "fully implemented".

2.2.1 UC12: Basajaun

Basajaun project builds two demo buildings and will be supported by a software platform. This platform would benefit from having a connection to an ontology layer and to related tools to cater for interoperability with and between supply chain domains and actors.

Buildings are going to be planned and built or renovated using innovative wood based materials and components. This is very important considering the great share of energy used by buildings and the urgent need to tackle the energy and climate crisis. How can the different actors (architects, construction companies, building owners, forest owners, process industry actors, manufacturers) in the value chain estimate and collaborate around important information about supply and performance of relevant indicators during the process? How can they know what is really making a difference in the value chain if there is no transparency and shared knowledge about the important key indicators? Some main aspects of this concern the verification and traceability of sustainable efforts along the value chain such as certification and other sustainability measures.

Use case owner / Country:	Paramountric / Sweden
Domain of application	• Value and supply chain for wooden building construction • Manufacturing • Processing • Materials development
Technology Readiness Level:	TRL2-TRL3
Data sources used:	• GIS data • Satellite data • Harvesting data • Transportation routes • Factory and manufacturing data

[2]https://www.rd-alliance.org/system/files/FAIR%20Data%20Maturity%20Model_%20Spezifikation%20und%20Leitlinien_FINAL.pdf

[3] Survey questions can be found here: https://ec.europa.eu/eusurvey/runner/b64d2bc9-28da-3347-332b-0dc6970789d3

	• Synthetically generated data (based on previous values) • Environmental Product Declaration
Ontologies considered:	• ifcOWL ontology[4]
Primary purpose of ontology usage	Interoperability between different actors in the supply chain
Main challenges with the ontology usage and development:	• Finding the most suitable ontology for a domain • Manual process of selecting ontologies or various part of ontologies.
Tools adopted:	• In-house development

Expected impact from OntoCommons

This use case needs state of the art principles and the best possible strategy for horizontal ontology development and alignment between actors (and domains) across supply chains. Expected is a solution that fits in the best possible way into European international standards and that can be applicable to the most important supply chains in manufacturing that concerns sustainability measures for saving energy, waste and climate. Expected is a balanced approach between abstraction and implementability to ensure feasible industry adoption, yet being flexible enough to extend into any domain. An overview of the application can be seen in Figure 1.

[4] https://standards.buildingsmart.org/IFC/DEV/IFC4/ADD2_TC1/OWL/index.html

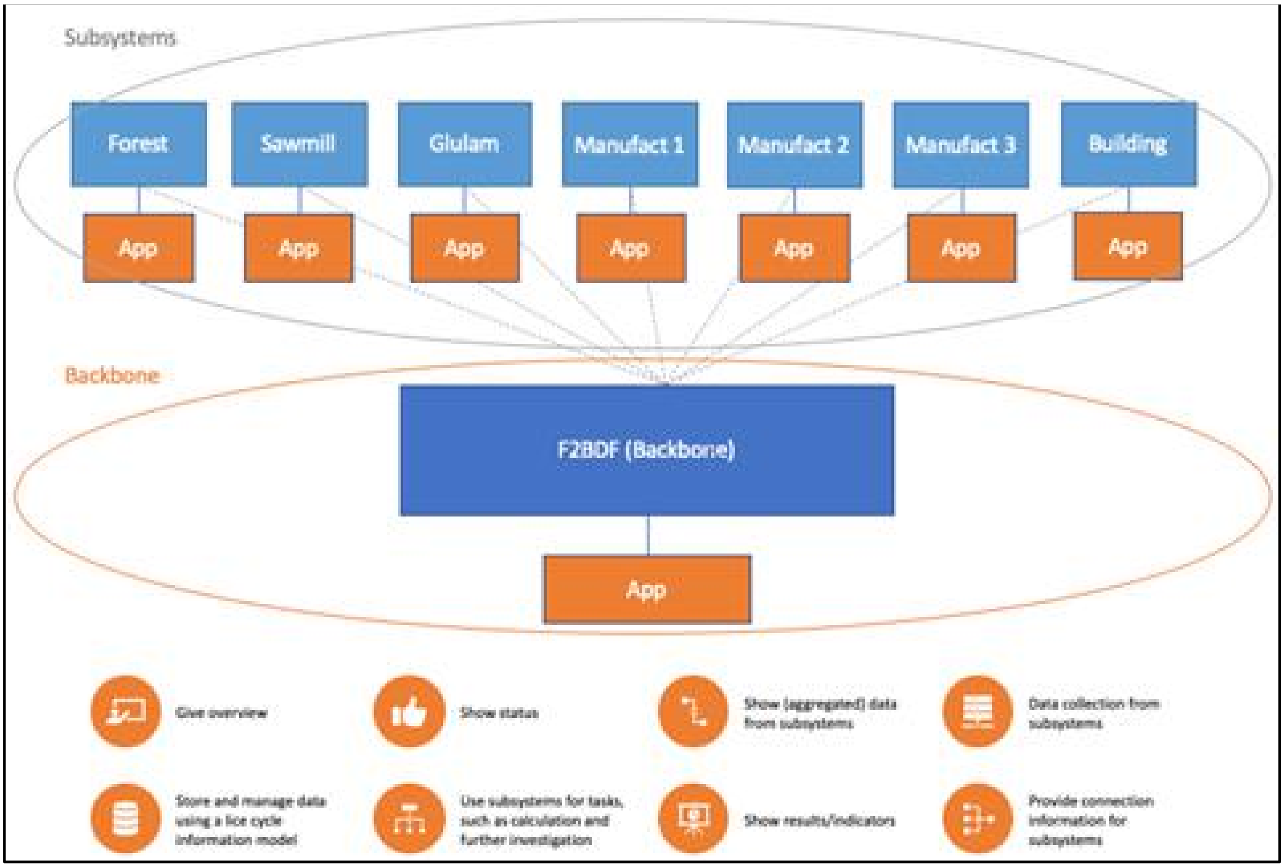
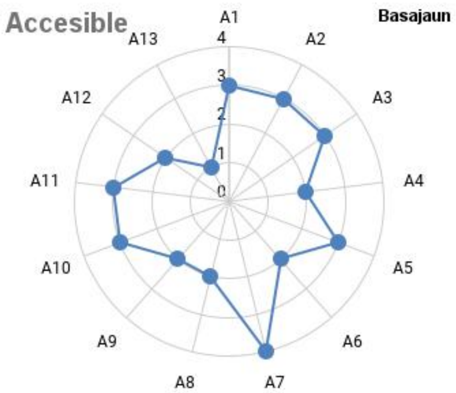
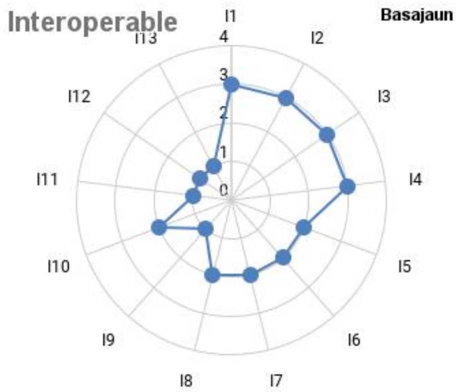


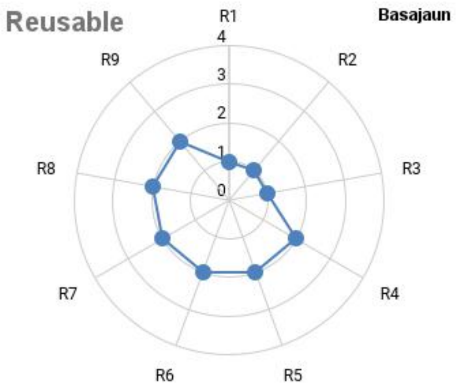
Figure 1 Overview of UC12

FAIRness assessment

The use case has no not applicable principle and many principles in Findable, Accessible and Interoperable dimensions are in the implementation stage. Given that the Reusable dimension is mostly in the planning phase, we expect a significant improvement as the use case develops further at that dimension.







2.2.2 UC13: Life Cycle Sustainability Assessment of a Chemical Product

BASF as a pilot of the ORIENTING project will be joining with a Life Cycle Assessment use case for chemical products. The use case will:

- Define the life cycle of the product, from extraction of raw materials to end of life fate and treatment (e.g., recycling, landfilling, incineration).
- Collect and analyse information about inputs and outputs associated with the life cycle of the product, such as consumption of resources, emissions, costs, information on social aspects.
- Calculate, integrate and interpret sustainability impacts through indicators addressing the environmental, economic and social performance of products, including also material criticality and circularity aspects.

Use case owner / Country:	BASF - ORIENTING Project / Germany and other EU countries
Domain of application	• Manufacturing • Life Cycle Assessment
Technology Readiness Level:	TRL4
Data sources used:	• Data from LCA software • Spreadsheets for Eco-efficiency
Ontologies considered:	BONSAI ontology Stavropoulos, T. G., Vrakas, D., Vlachava, D., & Bassiliades, N. (2012, June). BOnSAI: a smart building ontology for ambient intelligence. In *Proceedings of the 2nd international conference on web intelligence, mining and semantics* (pp. 1-12). An ontology developed based on the eILCD format[5]

[5] https://eplca.jrc.ec.europa.eu/LCDN/developerILCDDataFormat.xhtml

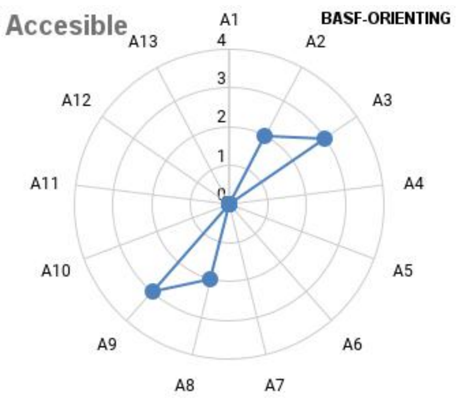
Primary purpose of ontology usage	Sustainability assessment with multi-dimensions
Main challenges with the ontology usage and development:	Data availability and data processing
Tools adopted:	• Protege • In-house development • Various LCA related tools (e.g., Gabi) • Excel

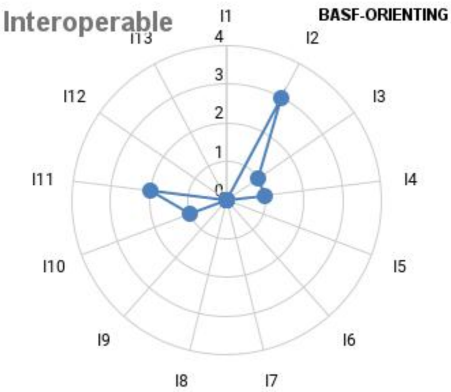
Expected impact from OntoCommons

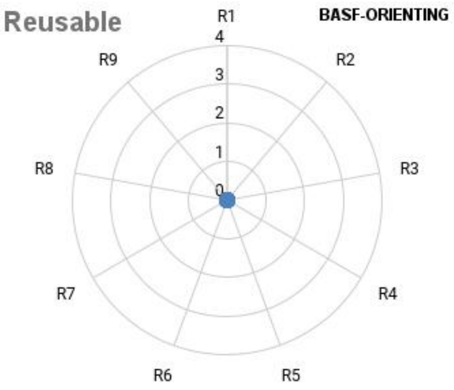
The demonstrator would like to learn how to facilitate, as far as possible, automation of calculations and sustainability assessments for chemicals.

Fairness Assessment

The demonstrator reports that many FAIR principles are not applicable to the use case. We will work this demonstrator closer in order to understand the reasons behind this situation and what steps can be taken to clear the roadblocks (e.g., not enough incentives, misconception of FAIR principles, concerns about data privacy).







2.2.3 UC14: Architecture design and ontology definition for Onboard Maintenance System of Aircraft

On-board Maintenance System (OMS) is one of the important systems in aircraft, it is responsible for fault diagnosis and prediction, as well as data collection and transmission. However, due to its complexity, modelling OMS is recognized as a tough task for the avionics development in aircraft design. Although SysML/UML are helpful in some parts, but they are unable to express physical and electrical layers of the system. So here the KARMA (Kombination of ARchitecture Model specificAtion) language is proposed to support architecture design and process definition of OMS with a model-based systems engineering approach.

The multi-architecture modelling language KARMA[6] is a semantic modelling language for a multi-architecture modelling approach. KARMA is expected to support descriptions and simulations of different architectural views of systems engineering. In our case, we plan to use KARMA to build OMS model though three perspectives: The reconfigurable process that helps for life cycle process definition and analysis, the integrated modelling framework that covers Mission, scenario, function, logical and physical layer of the SOI, and apply them into OMS modelling; **GOPPRRE ontology** is used to construct knowledge graph models which are generated from KARMA models. Design structure matrix table is used to define the interrelationships among model elements and requirements. ReqIF[7] is used to define the requirement items. The KARMA models, DSM tables, ReqIF requirement items are transformed to the ontology models which is defined based on BFO. Finally, some extra efforts will be made to interact with the existing SysML and Modelica models based on the ontology model for hybrid V&V consideration, which potentially will rebuild the ecosystem of M&S in Model-based System Engineering (MBSE) area.

The goal of the use case is to develop architecture model for the On-board Maintenance System of commercial aircraft and design the domain specific ontology for the PHM[8] system.

6 http://chinambse.com/RESEARCH

7 https://de.wikipedia.org/wiki/Requirements_Interchange_Format

8 https://en.wikipedia.org/wiki/Prognostics

Use case owner / Country:	COMAC BATR / China
Domain of application	Manufacturing Aircraft and aerospace
Technology Readiness Level:	TRL 5
Data sources used:	Aircraft OMS development
Ontologies considered:	GOPPRRE Ontology
Primary purpose of ontology usage	Represent the architecture models using ontology.
Main challenges with the ontology usage and development:	Interoperability among different modelling tools
Tools adopted:	MetaGraph 2.0

Expected impact from OntoCommons

Top level ontology to support aircraft design and manufacturing, particularly on model-based systems engineering and domain specific knowledge on fault detection.

Fairness Assessment

The assessment is currently in progress and will be reported by the demonstrator.

2.2.4 UC15: Monitoring human operators' safety and well-being via semantic data integration in an automotive manufacturing setting

This demonstrator use case constitutes part of our work within the H2020 ICT-01-2019 project CPSoSaware "Computing technologies and engineering methods for cyber-physical systems of systems" and will take place within the context of Trail #2 of the project "Human – Robot Interaction in the Manufacturing Environment". Trail #2 takes place in a car assembly line involving collaborating robots that assemble car chassis (e.g., welding, bolting). The process is assisted by human operators that intervene in specific parts of the assembly line to perform operations that robots cannot make.

Our aim in this use case is to develop a semantic data integration framework that will facilitate the monitoring of the human operators' safety and well-being as they are performing the requested operations.

A set of IoT sensors send their measurements to respective analysis components: (a) wearables (inertial measurement units, i.e., accelerometers and gyroscopes) for motion analysis and body tracking; (b) footage from static cameras analysed by computer vision components for estimating the operator's posture. The analysis outputs are fed into an ontology-based semantic Knowledge Graph (KG) through CASPAR (https://catalink.eu/caspar), a flexible semantic data integration framework, which will be properly extended for the purposes of the use case. The aim is to perform an ergonomic analysis of the operator's estimated posture to assess their well-being, and, potentially, reconfigure the robots' position to avoid long-term musculoskeletal problems and other health and/or safety risks. The goal of the use case is to assess human operators' ergonomic safety and well-being.

Use case owner / Country:	CPSosaware Consortium / Italy
Domain of application	Manufacturing Assembly Processing
Technology Readiness Level:	TRL 3
Data sources used:	Data from IoT devices
Ontologies considered:	SSN/SOSA
Primary purpose of ontology usage	As the uniform model for integrating inputs from heterogeneous sources.
Main challenges with the ontology usage and development:	Scalability of reasoning Lack of domain-specific ontologies
Tools adopted:	CASPAR framework (In-house development)

Expected impact from OntoCommons

We are looking forward to collaborating with OntoCommons experts in semantic technologies towards standardising the terminology and improving the cross-domain interoperability of our developed knowledge-based tools for scene analysis, posture recognition, and ergonomic assessment in a manufacturing environment. Our main expectation is to have a practical deployment of FAIR-compliant semantic knowledge representation and data integration in an industrial manufacturing setting. Testing the deployed solutions in additional industrial scenarios proposed by OntoCommons partners and/or affiliated stakeholders is also within our aims. An overview of the use case can be seen in Figure 2.

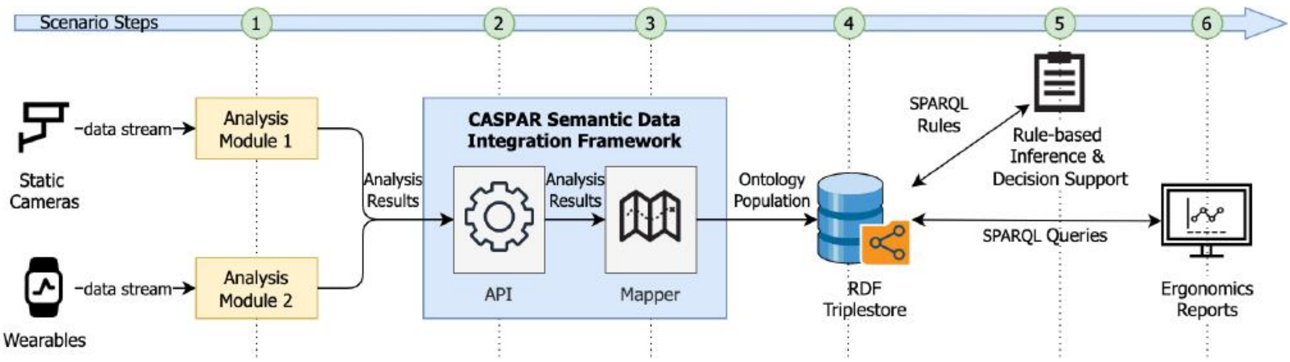
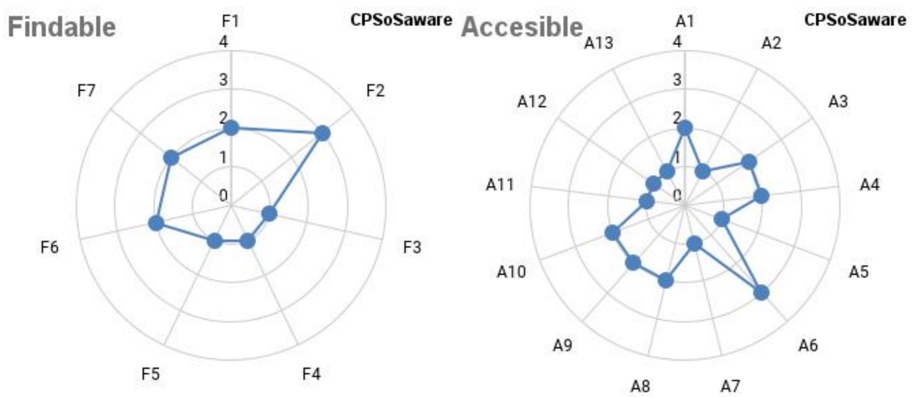
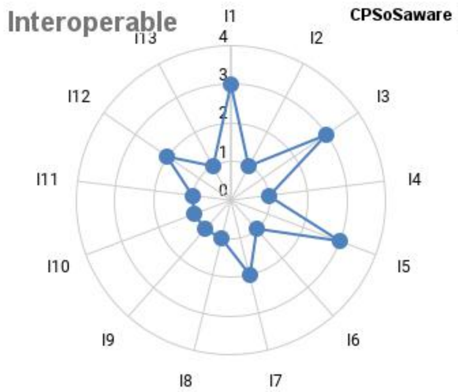


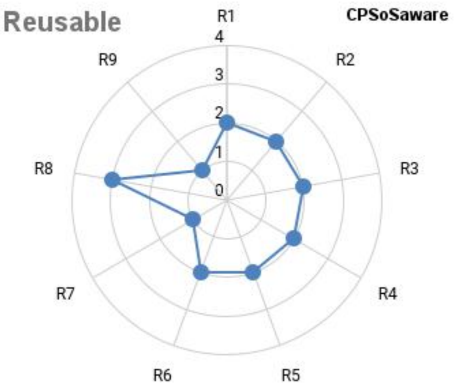
Figure 2 Overview of UC15

Fairness Assessment

Almost all principles in each FAIR dimension are in the planning phase except Interoperable. We expect significant improvements in every dimension as the use case develops. Nevertheless, there is reportedly no “not applicable” dimensions and we will engage closely with the demonstrator to identify the reasons that many Interoperable principles are not considered yet.







2.2.5 UC16: Food Knowledge Graph

The demonstrator would like to develop a proof-of-concept knowledge graph which is geared for additive or compound discovery in the sector of food processing or agri-science. An example could be using an ontology to link databases available from the European Institutions (such as the Additive Database from DG Sante, the substance database from ECHA, the PubChem database from NIH etc.) with the objective of discovering substitute compounds to be used as additives, as well as potential usage limits etc. The main goal of the use case is to keep ontologies in the knowledge graph consistent after updates and maintenance.

Use case owner / Country:	Dynaccurate SARL / Luxembourg
Domain of application	Biotechnology
Technology Readiness Level:	TRL5
Data sources used:	• https://echa.europa.eu/web/guest • Food additives[9] • Biocides[10] • Genetic information for organisms - such as probiotic cultures, yeasts etc.[11] • Allergens[12]
Ontologies considered:	FOODON Ontology[13]

[9] https://webgate.ec.europa.eu/foods_system/main/?event=substances.search&substances.pagination=1
[10] https://echa.europa.eu/information-on-chemicals/biocidal-products
[11] https://www.ncbi.nlm.nih.gov/genbank/samplerecord/#OrganismB
[12] http://www.allergenonline.org/databasebrowse.shtml
[13] https://bioportal.bioontology.org/ontologies/FOODON

Primary purpose of ontology usage	Representation of food and foodborne pathogens knowledge
Main challenges with the ontology usage and development:	• Generally speaking, any knowledge graph predicated on life sciences ontologies faces a major issue in management and remapping of those ontologies when the ontologies evolve to incorporate new terms etc. This is a generic problem in the life sciences. • Subjective mappings: Conceptual heterogeneity of different ontologies in a domain
Tools adopted:	• Protege • DyLink (In-house development) • Dynacurrate AI (In-house development)

Expected impact from OntoCommons

We would very much like to network with members of the OntoCommons team or wider community in the biotech sector so that we can learn more about end-user needs, receive feedback and also receive guidance on particular approaches. We can provide demonstrator without this support, but obviously it will be more relevant if we can engage with others beforehand. An overview of the use case workflow can be seen in Figure 3.

Figure 3 An overview of UC16

Fairness Assessment

The assessment is currently in progress and will be reported by the demonstrator.

2.2.6 UC17: Using iiRDS in the industrial internet of things (IIoT) with Siemens Industrial Edge

The demonstrator aims to create iiRDS[14] package prototypes and evaluate the customer view and content delivery

- Discuss with potential users
- Analyze and evaluate the customer benefits of an iiRDS delivery
- Estimate the effort, benefits and risks of generating and maintaining the data: for technical communicators and across teams
- Define requirements for a roll-out.
- Create a productive application of the prototype for EDGE devices

Use case owner / Country:	Siemens AG - iiRDS Consortium / Germany
Domain of application	• Manufacturing • Technical Documentation
Technology Readiness Level:	TRL6
Data sources used:	XML output from Siemens content management system SIPS+ Markdown files from GitHub PDF files Word
Ontologies considered:	• iiRDS Ontology[15] • Siemens extensions to iiRDS ontology
Primary purpose of ontology usage	• Use standardized vocabulary for enriching technical documentation content with metadata • Enable semantic search and search facets in content delivery portal • Enable targeted access and retrieval of content on Edge devices or from the Edge cloud based on use cases

[14] An ontology developed by the iiRDS consortium as metadata for technical documentation.

[15] https://iirds.tekom.de/fileadmin/iiRDS_specification/20190712-1.0.1-release/

Main challenges with the ontology usage and development:	• How to assign the metadata automatically using a linguistic tool in multiple languages (around 22 languages planned) • How to support 3rd party suppliers with their use cases
Tools adopted:	• Content management system (SIPS+) (customized Cosima system) • iiRDS converter • Linguistic engine (CLAT, Congree) • Delivery and content integration platform: c-rex

Expected impact from OntoCommons

- Ideas about general architecture / architectural framework
- Place iiRDS in the general architectural framework
- How to model terminologies as ontology > learn from other experiences/projects
- Participation in webinars, exchange best practices

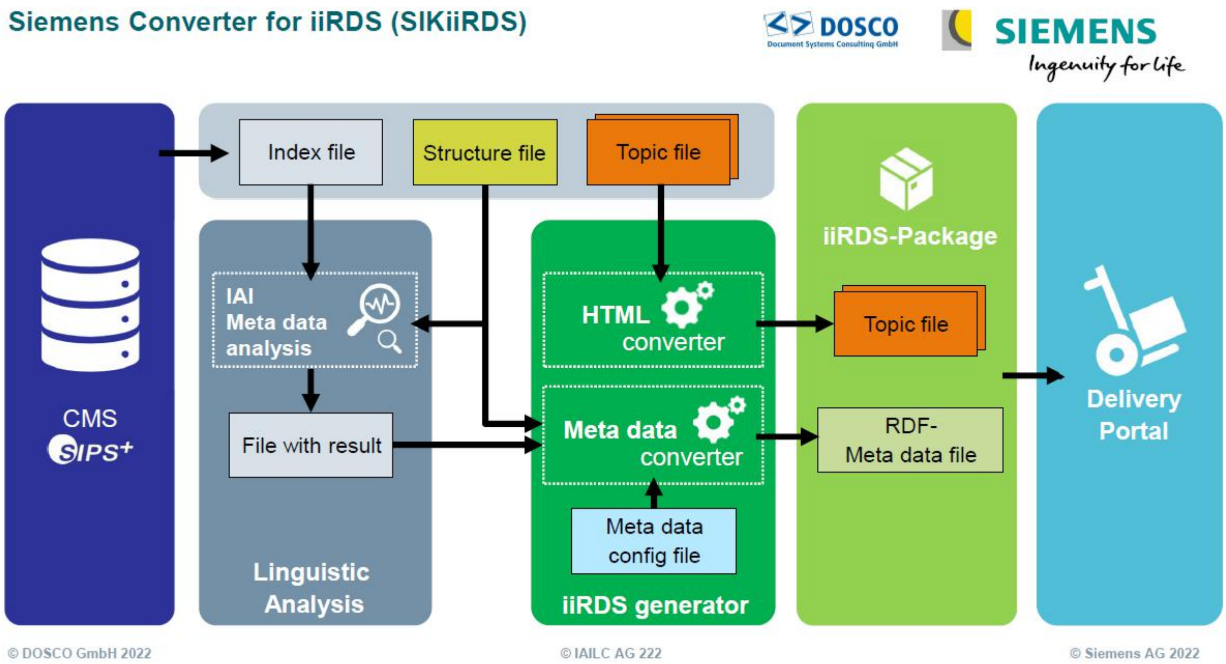
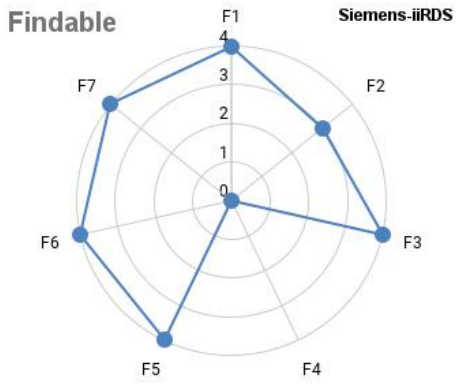
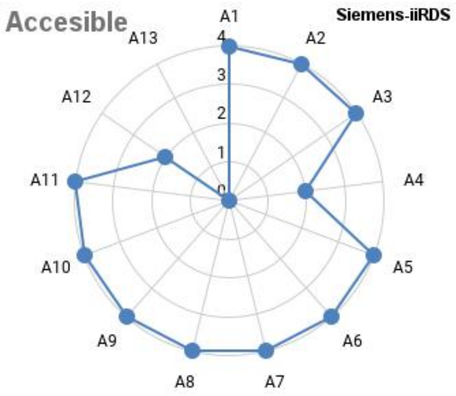


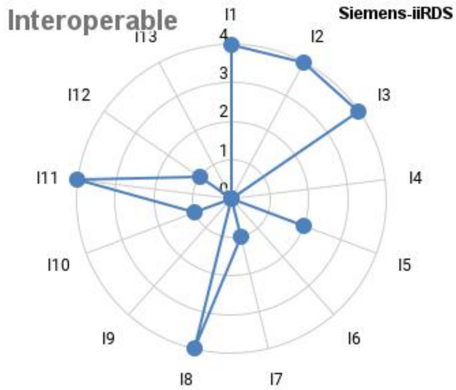
Figure 4 An overview of UC17

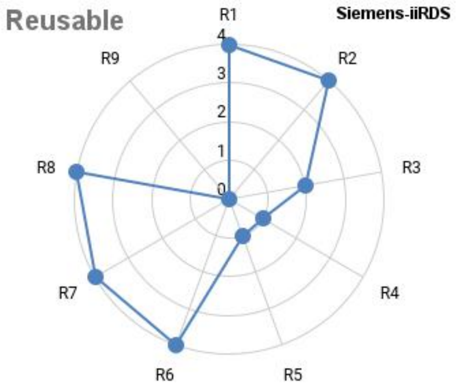
Fairness Assessment

The demonstrator implements Findable and Accessible almost completely, however, there is some room for improvement for Interoperable and Reusable dimensions. We will additionally further investigate the reasons behind some of principles being not applicable.









2.2.7 UC18: IKEA Knowledge Graph

IKEA holds a lot of knowledge and understanding of people's lives at home, needs, wishes, dreams, and problems, as well as solutions to those. This knowledge is spread out and stored in data silos. In order to serve IKEA's digitalisation transformation efforts, the IKEA Knowledge Graph sets as its goal to connect the data and make it usable throughout IKEA's services and systems.

Use case owner / Country:	Inter IKEA Systems / Sweden
Domain of application	Materials modelling Home-furnishing
Technology Readiness Level:	TRL4
Data sources used:	Internal data sources of IKEA
Ontologies considered:	In-house developed ontologies

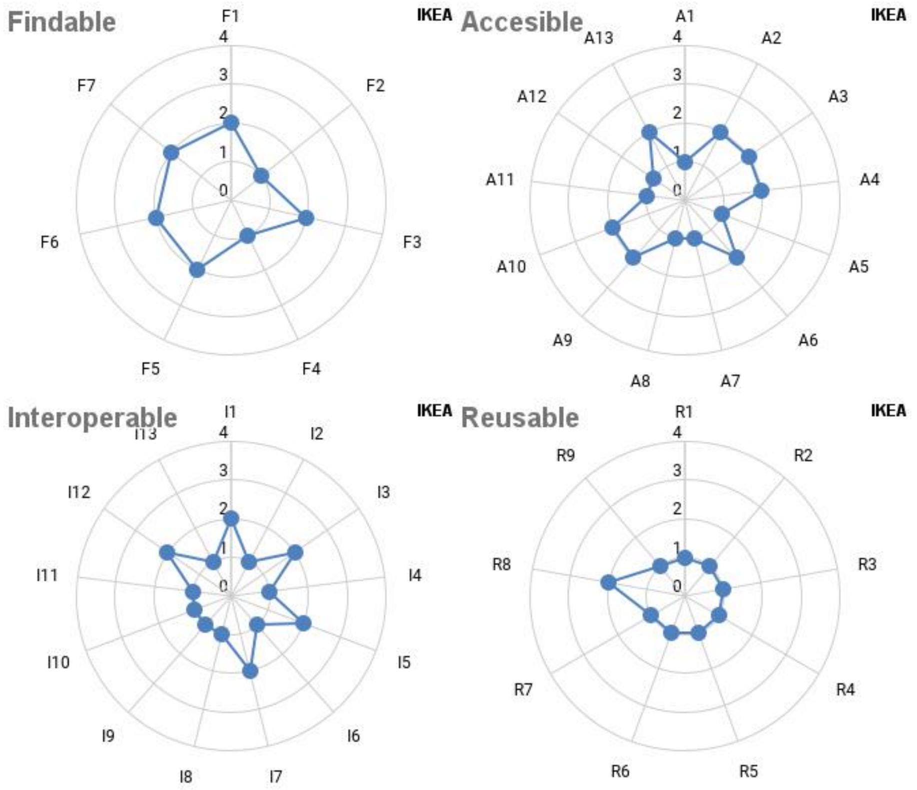
Primary purpose of ontology usage	In all use cases the ontology plays a central role in adding the IKEA Knowledge Graph and driving first identified use cases. Sometimes just to be able to maintain the vocabulary with proper governance process beats the maintaining of this information in excel.
Main challenges with the ontology usage and development:	Serving the ontologies via API endpoints requires a lot of software development work to set up a robust cloud-based platform for scalable storing and serving the knowledge graph and manage any deltas from stakeholder input or data sources.
Tools adopted:	• Frontend for authoring and discussing modelling changes (classes, properties) • Frontend for managing taxonomies • Visualisation of IKG • Visual editing • Suggest changes and review changes in all above mentioned tooling to enable governance

Expected impact from OntoCommons

- State-of-the-art ontologies and solutions
- Technical know-how regarding ontology usage and development

Fairness Assessment

The demonstrator has no not applicable principles and has the approximately same maturity level for Findable and Accessible dimensions. We will monitor the progress of the implementation of these dimensions as they are predominently in the planning phase. Interoperable and especially Reusable dimensions mostly are not being considered yet, and we will investigate the resaons behind this with a close engagement with the demonstrator.



2.2.8 UC19: Materials Databases Integration using the Materials Design Ontology

The Materials Design Ontology is used for semantic and integrated access to the computational materials databases in the OPTIMADE consortium, dealing with the heterogeneity of the databases in terms of underlying data models and use of terminology. The developed ontology will be used in ontology-driven data access and data integration for application in the materials design domain. Figure 5 shows an overview of how such an application would work.

Use case owner / Country:	Linköping University / Sweden
Domain of application	Materials Development
Technology Readiness Level:	TRL 3
Data sources used:	Databases in the OPTIMADE consortium
Ontologies considered:	Materials Design Ontology (MDO)[16] EMMO PROV-O[17]

[16] https://github.com/LiUSemWeb/Materials-Design-Ontology

[17] https://www.w3.org/TR/prov-o/

	CheBI[18] QUDT[19]
Primary purpose of ontology usage	Data integration Data structuring Data sharing
Main challenges with the ontology usage and development:	compatibility of MDO and top level ontologies, with EMMO as first candidate, regarding ontological commitment
Tools adopted:	Will be reported in the next stage

Expected impact from OntoCommons

Not yet specified.

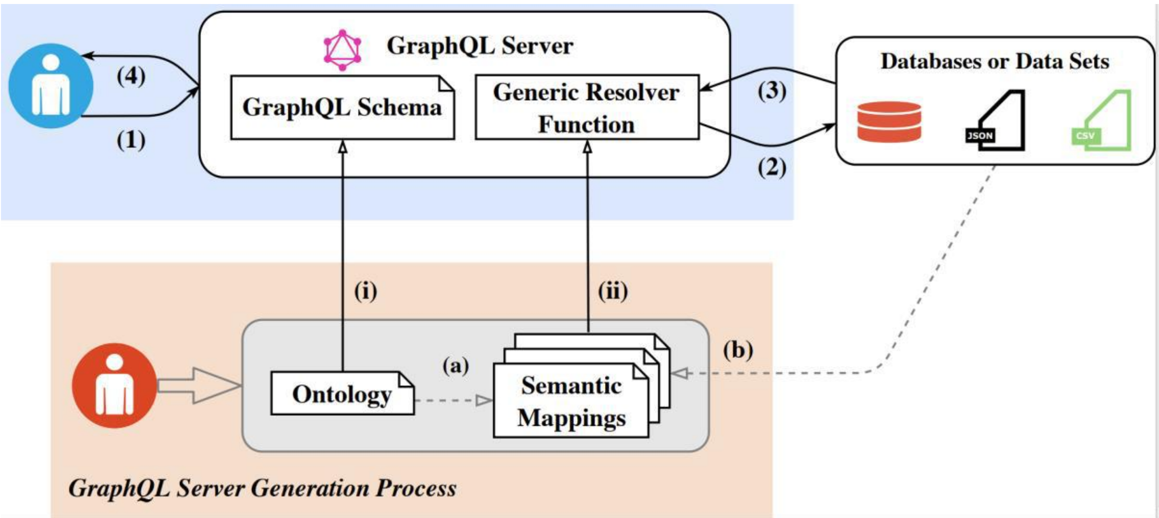


Figure 5 An overview of UC19

Fairness Assessment

The assessment is currently in progress and will be reported by the demonstrator.

2.2.9 UC20: Materials Characterisation Ontology

In the NanoMECommons project, the demonstrator is building an ontology of material characterisation to capture potentially any type of materials characterisation method and enable

[18] https://www.ebi.ac.uk/chebi/
[19] http://www.qudt.org/

harmonisation. The starting point is a human readable metadata called CHADA[20] and the work is to provide an EMMO compliant ontology. Current status is a scope and mapping to EMMO[21].

Use case owner / Country:	Goldbeck Consulting Ltd / United Kingdom
Domain of application	Materials Characterisation
Technology Readiness Level:	TRL 3
Data sources used:	Materials Characterisation experiments data
Ontologies considered:	EMMO Domain ontologies related to materials, manufacturing, software Mechanical Testing Ontology[22]
Primary purpose of ontology usage	Harmonize the documentation of characterisation procedures in a machine-readable way, exploiting structured information through taxonomies, overcoming the limitations of free text documentation and heterogeneous terminology.
Main challenges with the ontology usage and development:	Non-specified
Tools adopted:	Open Innovation Environment[23]

Expected impact from OntoCommons

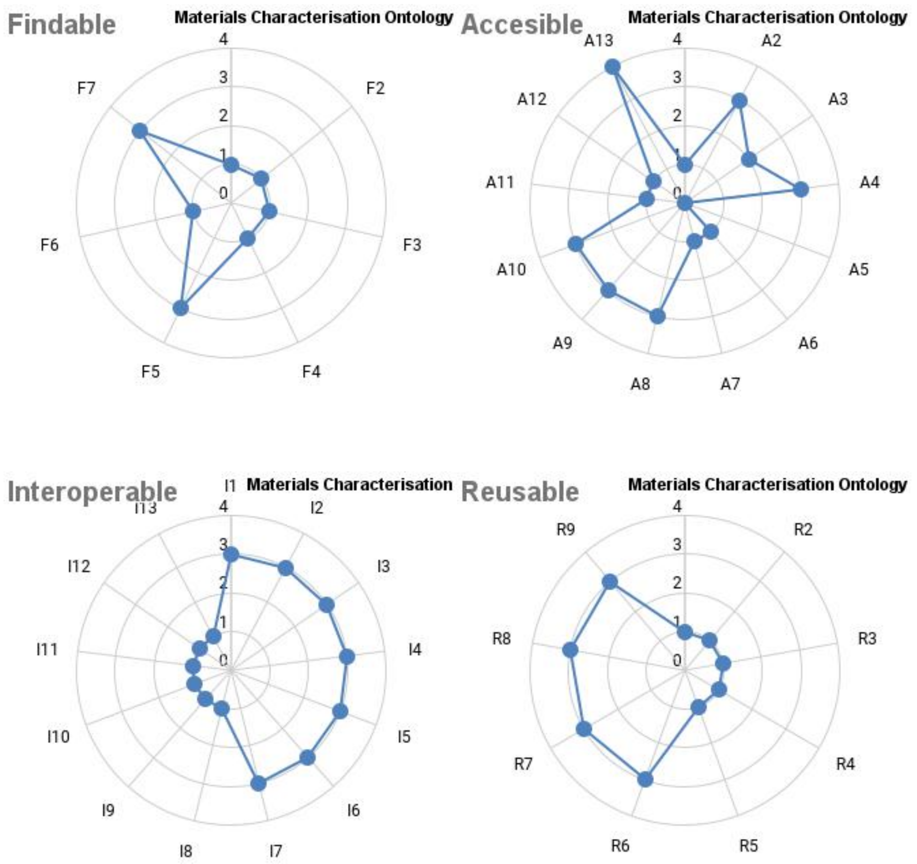
The demonstrator would like to utilise OntoCommons recommendations for ontology development and implementation and ensure TLO/MLO compliance.

Fairness Assessment

The demonstrator has a very heterogeneous maturity level for each dimension. There are no fully implemented principles; however, a majority of the principles, particularly in Interoperable dimension

[20] https://zenodo.org/record/2636609
[21] https://emmc.info/emmo-info/
[22] https://github.com/emmo-repo/domain-mechanical-testing
[23] based on https://github.com/simphony/osp-core

are in the implementation phase. Therefore there is still a development room in terms of the implementation of FAIR principles and we will monitor the progress in the next stage of the project.



2.2.10 UC21: Lubricant Designer

SCIENOMICS is developing a platform of virtual experiments for sustainable materials and product development. These virtual experiments integrate materials and process simulation technology.

Interoperability is a limitation factor and therefore SCIENOMICS is seeking to adopt the relevant ontologies that would allow the communication between different simulation engines which are involved in a virtual experiment.

In this demonstration case we will develop and demonstrate (a) the technology of our platform and how it is possible to easily create user interfaces and (b) using domain ontologies it is possible to develop value-adding workflows. The demonstration case will show, on a practical level, how to develop a Designer for lubricants that fulfil both materials and use constraints. Figure 6 shows an overview of the use case.

Use case owner / Country:	Scienomics SAS / France
Domain of application	Materials Development

	Materials Processing Life Cycle Assessment
Technology Readiness Level:	TRL 4
Data sources used:	Engine data provided by SimTech providers DIPPR[24] Open data provided by end users about processes
Ontologies considered:	Materials Design Ontology Various domain ontologies for engines, products and processes
Primary purpose of ontology usage	Interoperability
Main challenges with the ontology usage and development:	Existing Ontologies will not cover all needs of the project, extensions will be needed for all scenarios
Tools adopted:	Neo4j Protege GraphQL

Expected impact from OntoCommons

Scienomics expects access to the standards provided by the OntoCommons project. Scienomics also expects this case to benefit from the wide networking opportunity of the project and the ontology expertise available.

[24] https://www.aiche.org/dippr

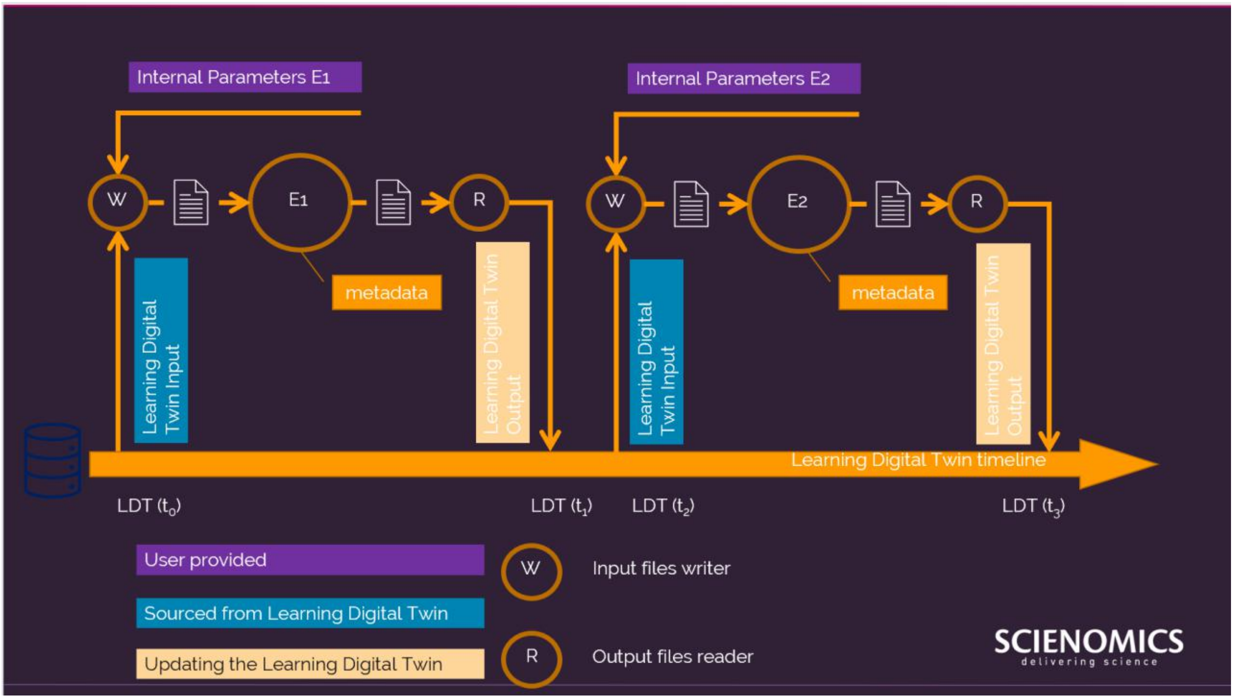


Figure 6 Overview of UC21

Fairness Assessment

The assessment is currently in progress and will be reported by the demonstrator.

2.2.11 UC22: Automated production of a nutrient solution for soilless culture application.

Automated production of a nutrient solution is of paramount importance for soilless culture applications, e.g., hydroponics agriculture techniques. This can be accomplished by monitoring the environment and remote controlling a sequence of processes. The use of heterogeneous IIoT devices equipped with different sensors and actuators allows this to happen. These devices can use distinct communication protocols and data structuring, which increases interoperability problems. The demonstrator is developing an industry 4.0 oriented ontology, based on the IEEE 1872 international standard to mitigate these problems.

Use case owner / Country:	UFRGS / Brazil
Domain of application	Biotechnology Agriculture
Technology Readiness Level:	TRL 5
Data sources used:	• IoT devices • Synthetic data generated by simulations

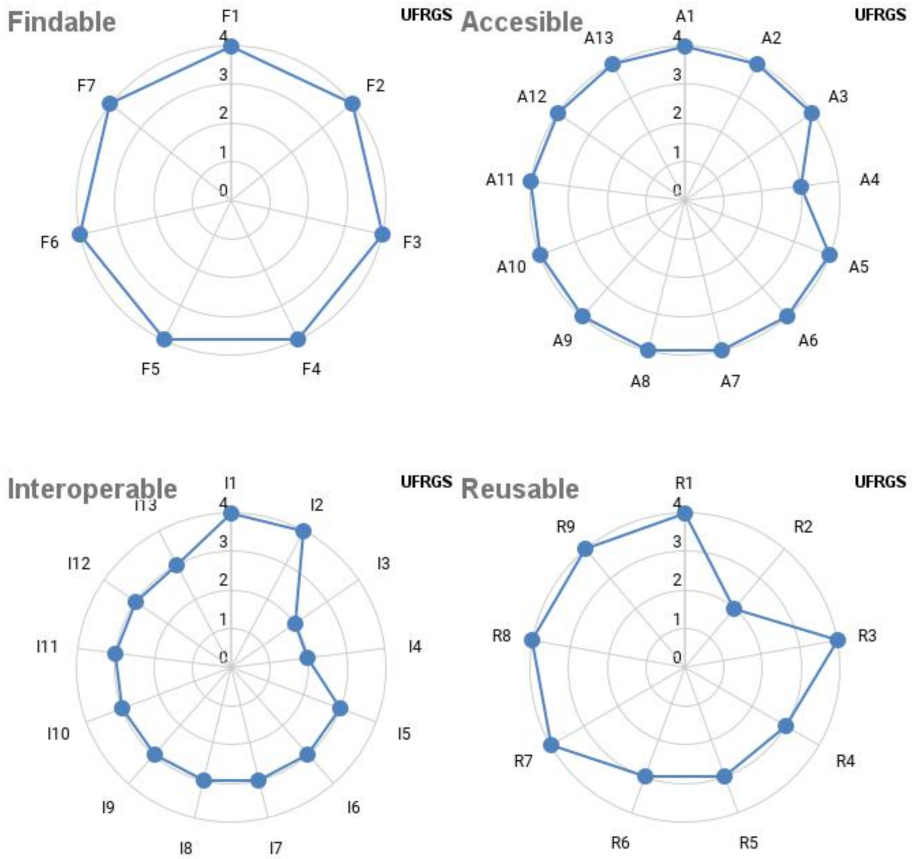
Ontologies considered:	• QU Ontology / developed by W3C Semantic Sensor Network Incubator Group. • SSU Ontology / developed by W3C Semantic Sensor Network Incubator Group. • IoT-Lite Ontology / developed by W3C Semantic Sensor Network Incubator Group. • POS Ontology / IEEE Std 1872-2015. • ROCO - Robotic Cloud Ontology / IEEE Std 1872-2015.
Primary purpose of ontology usage	Interoperability
Main challenges with the ontology usage and development:	Modelling large number of different type IoT devices
Tools adopted:	Protege OPC-UA Server MQTT Influx DB

Expected impact from OntoCommons

Semantic representation of heterogeneous IoT devices using unified IIoT ontology, based on well-established ontologies, in order to mitigate interoperability problems in industrial applications (data interoperability and interconnectivity).

Fairness Assessment

All FAIR principles have a quite high maturity where the entire Findable and Accessible dimensions are fully implemented or being implemented. The use case has no principles that is not being considered or not applicable, but still there is a marginal improvement room for Interoperable and Reusable dimensions.



3. Requirements

In this section we provide the initial set of requirements on ontologies (existing and new ones) and ontologies-tools, needed in the new 11 selected demonstration cases (Use Cases - UC, UC12 to UC22). The approach for the collection of the requirements from the demonstration cases included two main procedures:

- Using the template for the description of the use cases and the structured definition of requirements (see Section 2), the industrial partners involved in these new eleven cases, defined the requirements relevant for their demonstrators.
- In the scope of the several joint and bilateral meetings with the WP5 partners, the involved partners discussed and further extended the requirements.

The collected requirements have been analysed and harmonised. For example, a number of requirements in diverse use cases and those defined with the workshop were aggregated and put together. The following list includes harmonised requirements.

The requirements are structured in several groups and subgroups:

- General requirements including
  - Requirements concerning the use/application of ontologies
  - Requirements concerning standardisation
- Requirements on

- Development of Ontologies
- Maintenance/extension of ontologies
- Requirements on tools

The requirements are prioritised in three main groups: shall, should and may.

For each requirement the table includes references to the requirements defined by the specific use cases or within the different sessions carried out during the workshop.

The "UIDs" and the "Requirement Origin" IDs in the following tables, are defined in the following way:

- **CRQA_[CATEGORY]_[SERIAL NUMBER]**for all the harmonised demonstrator requirements

  where:

  CRQA = Common Requirement for Additional use cases,

  CATEGORY= **U** for use of ontologies, **D** for development, **S** for standardisation or **M** for maintenance

  SERIAL NUMBER = incremental identification number

e.g. CRQA_U_01

- **UC_x_RQ_[CATEGORY]_[SERIAL NUMBER]**for use-case-specific requirements,

where:
UC = Use Case
X = 12 to 22 for the identification number of the related use case.
RQ = Requirement
CATEGORY= **U** for use of ontologies, **D** for development, **S** for standardisation or **M** for maintenance

SERIAL NUMBER= incremental identification number
e.g. UC18_RQ_U_02

Please note that within the further work on the implementation of the new 11 demonstrators these requirements will be further elaborated and refined.

UID	Title	Description	Priority (Shall/ Should/ May)	Requirement Origin
Use/application of ontologies				
CRQA_U_01	Ontology for IT Systems	Ontology should allow for effective documentation and search of most common systems in any enterprise IT landscape (incl. edge devices).	Should	UC18_RQ_U_02 UC17_RQ_U_02
CRQA_U_02	Support rules	A set of rules will be created offline and will be running on top of the	Shall	UC15_RQ_U_02 UC15_RQ_U_03

	creation (offline) and have them supporting decision making and generation of alerts	semantic knowledge to generate alerts and support decision making. The ontologies should allow for easy adding/updating of application specific rules among the entities.		UC13_RQ_U_01 UC12_RQ_U_04
CRQA_U_03	Documentation of domain and topic-based metadata	Ontology shall allow for effective documentation of domain data and it shall be possible to assign metadata on document as well as topic level (so that users can find and access granular content)	Shall	UC17_RQ_U_04 UC13_RQ_U_02 UC21_RQ_U_02 UC14_RQ_U_02 UC20_RQ_U_02
CRQA_U_04	Support domain description	Ontologies to be used shall include the key aspects of domain terms and processes addressed in the use cases.	Shall	UC18_RQ_U_01 UC18_RQ_U_03 UC14_RQ_U_01 UC14_RQ_U_03 UC17_RQ_U_03
CRQA_U_05	Good alignment with corresponding domains	The ontology-based glossary shall be developed according to, and aligned with, top level ontologies to allow for interoperability.	May	UC18_RQ_U_04 UC14_RQ_S_02 UC19_RQ_U_02
CRQA_U_06	Real-time rule-based reasoning	Real-time rule-based reasoning will also be considered.	May	UC15_RQ_U_04
CRQA_U_07	Rules supporting indicators used for decision making across domains	The ontologies should enable horizontal cross-domain abstraction that is applicable for all actors in a supply chain when it comes to KPIs and other indicators required for collaborative supply chain improvement and optimization.	Should	UC12_RQ_U_01 UC12_RQ_U_02 UC12_RQ_U_03
CRQA_U_08	Ontologies re-use and modularisation	The ontologies should be possible to apply, as a whole or partly, in combination with other ontologies.	Shall	UC16_RQ_U_01 UC16_RQ_U_02 UC15_RQ_U_01 UC20_RQ_D_03
CRQA_U_09	Reasoning for traceability analysis	Ontology should allow engineers to analyse the traceability among different domain specific models.	Shall	UC14_RQ_U_04

Development of ontologies				
CRQA_D_01	Ontology and taxonomy scope	Ontology and/or taxonomy shall contain definitions to a range of entities and properties that are relevant to and provide agreeable coverage of the selected domain (e.g. IT system, data sources, images, digital twin, device data, etc)	Shall	UC18_RQ_D_01 UC18_RQ_D_02 UC18_RQ_D_03 UC18_RQ_D_04 UC18_RQ_D_05 UC18_RQ_D_06 UC18_RQ_D_07 UC18_RQ_D_08 UC15_RQ_D_01 UC13_RQ_D_01 UC21_RQ_D_01 UC14_RQ_D_01 UC14_RQ_D_02 UC14_RQ_D_03 UC20_RQ_D_01 UC22_RQ_D_01 UC22_RQ_D_02
CRQA_D_02	Ontology design	The design of the ontology will be as lightweight as possible.	Should	UC15_RQ_D_02 UC16_RQ_D_01
CRQA_D_03	Compliance to higher-level ontologies	Should allow to follow higher level ontology models (top or middle-level ontologies	Shall	UC20_RQ_D_02
CRQA_D_04	Methodology for ontology engineering	Methods/guidelines/tools should be provided for integration of different steps in the ontology engineering processes.	Shall	UC20_RQ_U_01 UC20_RQ_U_03
CRQA_D_05	Ontology documentation	The ontology will be sufficiently documented through respective annotation properties.	Should	UC15_RQ_D_03
CRQA_D_06	Ontology outcomes for changing inputs	Ontology should allow adaptations to new technologies of production processes.	Should	UC13_RQ_D_02
CRQA_D_07	Documentation for interoperability	The ontology documentation should define how the reuse and harmonisation of different ontologies could be achieved and ease the	Should	UC20_RQ_U_04

		transferability of the knowledge across different parties		
Maintaining/extension of ontologies				
CRQA_M_01	Easy maintenance of ontology	The ontology shall be easy to maintain (e.g. adding lower level terms, additional relations, etc.) from non-ontology experts (e.g. SW engineers).	Shall	UC18_RQ_M_01 UC15_RQ_M_01 UC13_RQ_M_01 UC14_RQ_M_01 UC16_RQ_M_01 UC20_RQ_M_01 UC22_RQ_M_01 UC21_RQ_M_01
CRQA_M_02	Usage instructions related to CRQA_U_08	For any ontology and taxonomy, instructions on where to download them, how to use them, how to query them shall be provided to the public.	Shall	UC18_RQ_M_02
CRQA_M_03	Allow/support different mechanisms to access data	The tools should support easy interaction with ontologies, for example, via REST APIs alongside SPARQL queries for retrieving data.	Shall	UC18_RQ_M_03 UC18_RQ_M_04 UC17_RQ_M_02 UC17_RQ_U_01 UC19_RQ_U_01
CRQA_M_04	Easy to use ontology results	The ontology shall be interpretable and applicable for different functions in a company.	Shall	UC13_RQ_M_02
CRQA_M_05	Possible extension of existing ontologies	The ontology shall be easily extendable with domain concepts. Wherever possible, existing resources will be reused and extended for the purposes of the use case.	Shall	UC17_RQ_M_01 UC15_RQ_S_02
CRQA_M_06	Link ontologies to existing SW	Ontologies shall be used to link different use case tools (and their output data)	Shall	UC21_RQ_M_02
Tools for ontology				
CRQA_T_01	Visualisation	The tools shall support visualisation of ontologies.	Shall	UC18_RQ_T_01 UC18_RQ_T_04 UC17_RQ_T_01 UC13_RQ_T_01

				UC21_RQ_T_01 UC14_RQ_T_01 UC14_RQ_T_03 UC14_RQ_T_04 UC14_RQ_T_05 UC16_RQ_T_03 UC20_RQ_T_01 UC15_RQ_T_04
CRQA_T_02	Collaboration of multiple stakeholders	The ontology development tool should allow different stakeholders to work simultaneously.	Shall	UC18_RQ_T_02 UC13_RQ_T_02 UC21_RQ_T_02 UC12_RQ_T_02 UC14_RQ_T_02 UC20_RQ_T_02
CRQA_T_03	Tool for ontology development	For the development of the ontology, we will rely on an established freely available ontology authoring environment.	May	UC15_RQ_T_01 UC12_RQ_T_01
CRQA_T_04	Ontology validation	The resulting ontology will be validated using appropriate freely available tools.	May	UC15_RQ_T_02
CRQA_T_05	Frontend assessment of taxonomy and ontology editing	Available visual tools for ontology and taxonomy development should be assessed and reflected according to use case requirements and organisational fit.	Should	UC18_RQ_U_05
CRQA_T_06	Tool for Knowledge Graph persistence	The storage of the Knowledge Graph will be undertaken by a freely available established triplestore solution.	Should	UC15_RQ_T_05
CRQA_T_07	Trust building	The ontology tool should allow for the interpretation of information based on trusted and validated inputs.	Should	UC13_RQ_T_03
CRQA_T_08	Tools to support selection and alignment of ontologies	Tools shall be provided to support establishment of relation of concepts from diverse ontologies.	Shall	UC12_RQ_T_03 UC16_RQ_T_02

CRQA_T_09	Use of existing commercial tools		May	UC16_RQ_D_02
CRQA_T_10	Version control of ontologies	Tools shall allow to support ontology development version control	shall	UC18_RQ_T_03
Standardisation				
CRQA_S_01	Conformance to standards	There shall be compliance to domain (i.e. IEEE), W3C, iiRDS standards (e.g. ISO) and reporting standards. The system should be built with existing, open and free standards to the greatest extent possible.	Shall	UC18_RQ_S_01 UC17_RQ_S_03 UC15_RQ_S_01 UC13_RQ_S_01 UC13_RQ_S_02 UC21_RQ_S_01 UC12_RQ_S_01 UC14_RQ_S_01 UC16_RQ_S_01 UC20_RQ_S_01 UC22_RQ_S_01 UC22_RQ_S_02
CRQA_S_02	EU legal framework for sustainability	Any EU requirements for reporting on sustainability shall be covered by taxonomies and ontologies developed in OntoCommons (e.g. Green deal, EU regulations for appliances (energy rating))	Shall	UC18_RQ_S_02
CRQA_S_03	Common data format	Use a common data format to deliver topic-level information so that customers can find information with high accuracy.	Shall	UC17_RQ_S_01
CRQA_S_04	Open for other stakeholders	Used data format should not be proprietary so that other stakeholders in the value chain can also provide information in the same format.	Shall	UC17_RQ_S_02
CRQA_S_05	customer specific extension	A customer-specific extension of the standard must be possible	Shall	UC17_RQ_S_04
Use case specific requirements				

CRQA_UCS_01	Define a universal structure of the Learning Digital Twin.	A learning digital twin needs to be developed in a manner that satisfies the criteria required for the project. The digital twin should be able to describe a complex product and its parts in all scales.	Shall	UC21_RQ_U_01
CRQA_UCS_02	Configuration of IIoT gateway.	The IIoT gateway shall be configured by the user using two ontology-based files (JSON and YAML files) and start the respective communication protocols servers and interoperability scripts.	Shall	UC22_RQ_U_01
CRQA_UCS_03	Simulation.	The use case interoperability shall be evaluated by running simulations with the IoT device's digital twins.	Shall	UC22_RQ_U_02
CRQA_UCS_04	Monitor real time data exchange.	All data exchanged between the devices can be monitored in real time by a SCADA system hosted by the IoT gateway.	Shall	UC22_RQ_U_03
CRQA_UCS_05	Data storage	The data exchanged by different IoT devices shall be stored in a database (influx DB) to be used as a dataset for future machine learning applications.	Shall	UC22_RQ_U_04
CRQA_UCS_06	Validation	The use case interoperability may be evaluated in a real industrial plant setup.	May	UC22_RQ_U_05
CRQA_UCS_07	Linguistic-driven generation of metadata	A linguistic engine must be able to analyze content and to add additional normalized metadata to documentation topics.	Shall	UC17_RQ_M_03
CRQA_UCS_08	Configuration of the linguistic engine	The linguistic engine must have a configuration to select und to program rules, to generate metadata for specific iiRDS classes.	Shall	UC17_RQ_M_04
CRQA_UCS_09	Semantic data integration	For the semantic data integration (i.e., ontology population), we will rely on novel tools developed by the CPSoSaware consortium.	Shall	UC15_RQ_T_03

CRQA_UCS_10	Automated remapping (alignment) of ontologies	The Dynaccurate AI will be used to examine and remap changes to the Knowledge Graph based on changes to the multiple ontologies in scope	Shall	UC16_RQ_T_01
CRQA_UCS_11	Semantic and integrated access	Provide semantic and integrated access to the OPTIMADE materials databases. We will provide a GraphQL and MDO-based interface to the OPTIMADE databases. It will allow queries using MDO terminology over multiple databases.	Shall	UC19_RQ_U_01

4. Conclusion and Future Work

In this deliverable, we presented the 11 newly acquired demonstrators. We reminded the selection criteria set for the demonstrator acquisition campaign that was active in the second half of 2021 and gave an overview of the demonstrators w.r.t. selection criteria. We observe that the selection criteria that were created with the expected impact and work description of the OntoCommons project in mind are fulfilled with the selected demonstrators to a great extent.

The selected demonstrators specified their use cases via a survey we prepared. The surveys were complemented with interviews to gain more insights about the use cases and initiate the engagement with the project. We compiled the main scenarios of the use cases, their challenges, expectations and their KPIs. Moreover, we created a baseline for the FAIRness of the newly acquired demonstrators.

The collected requirements from each use case have been consolidated to a set of requirements regarding ontology use and development as well as tools. Following requirements are observed to be dominant[25]:

- **Ontology and taxonomy scope:** Ontology and/or taxonomy shall contain definitions to a range of entities and properties that are relevant to and provide agreeable coverage of the selected domain (e.g. IT system, data sources, images, digital twin, device data, etc.)
- **Easy maintenance of ontology:** The ontology shall be easy to maintain (e.g. adding lower level terms, additional relations, etc.) from non-ontology experts (e.g. SW engineers).
- **Visualization:** The tools shall support visualisation of ontologies.
- **Collaboration of multiple stakeholders:** The ontology development tool should allow different stakeholders to work simultaneously.
- **Conformance to standards:** There shall be compliance to domain (i.e. IEEE), W3C, iiRDS standards (e.g. ISO) and reporting standards. The system should be built with existing, open and free standards to the greatest extent possible.

In the future work, we will coordinate our findings presented in this deliverable with the technical work packages of the project to guide their further development for the OntoCommons Ecosystem. We will continue to engage with the newly acquired demonstrators in order to finalize some of the FAIR assessments and monitor their progress. Moreover, we will examine agile ways to initiate the networking across all demonstrators and other project partners and find meaningful and efficient ways to bring their input to the project and present exploitable results to create impact in their use cases. Additionally, we will contribute to the preparation of focused global workshops to ensure that the demonstrators gain the optimal benefit from them. The upcoming deliverables will focuse on the monitoring and validation of the demonstrators.

[25] A dominant requirement is specified by 6 or more different demonstrators.

5. Appendix: Individual survey answers collected from the new demonstrators

5.1 UC12: Basajaun

Demonstrator general information

Demonstrator company name and contact person(s):

Paramountric, Andreas Rudenå, andreas@paramountric.com

Domain of application[26]

Value and supply chain for wooden building construction

Manufacturing

Processing

Materials development

Supply-chain (which covers multiple domains mentioned above)

Use case name:

Basajaun

Short Description:

Basajaun project builds two demo buildings and will be supported by a software platform. This platform would benefit from having a connection to an ontology layer and to related tools to cater for interoperability with and between supply chain domains and actors.

What are the major (expected) contributions of OntoCommons to the demonstrator?

This use case needs state of the art principles and the best possible strategy for horizontal ontology development and alignment between actors (and domains) across supply chains. Expected is a solution that fits in the best possible way into European international standards and that can be applicable to the most important supply chains in manufacturing that concerns sustainability measures for saving energy, waste and climate. Expected is a balanced approach between abstraction and implementability to ensure feasible industry adoption, yet being flexible enough to extend into any domain.

[26] industry where the ontology solution will be used, e.g. Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

Use Case requirements

Use case primary requirements				
UID	Title	Description	Priority (Shall/ Should/ May)	Comment
Use/application of ontologies				
UC12_RQ_U_01	Rules supporting standardized business processes in supply chains across actors	The ontologies should enable horizontal cross-domain abstraction that is applicable for all actors in a supply chain when it comes to business processes required for value chains.	Should	Refers to cross-domain interoperability
UC12_RQ_U_02	Rules supporting standard measures for life cycle analysis across domains	The ontologies should enable horizontal cross-domain abstraction that is applicable for all actors in a supply chain when it comes to LCA measures and indicators required for value chains.	Should	Refers to cross-domain interoperability
UC12_RQ_U_03	Rules supporting indicators used for decision making across domains	The ontologies should enable horizontal cross-domain abstraction that is applicable for all actors in a supply chain when it comes to KPIs and other indicators required for collaborative supply chain improvement and optimization.	Should	Refers to cross-domain interoperability
UC12_RQ_U_04	Rules supporting the decision making process considering stakeholder from different domains	The ontologies should enable horizontal cross-domain abstraction that is applicable for all actors in a supply chain when it comes to collaborative and reusable decision support processes.	Should	Refers to cross-domain interoperability
Tools for ontology				
UC12_RQ_T_01	Composition, alignment and extensions of ontologies in a value chain scope	The tools shall support a workflow for continuously assessing and updating the current selection of ontologies.	Shall	

UC12_RQ_T_02	Collaboration of multiple stakeholders	The ontology development tool shall allow different stakeholders to work simultaneously.	Shall	
UC12_RQ_T_03	Automated support on selection and alignment of ontologies	Prevent overwhelming selection of ontologies		
Standardisation				
UC12_RQ_S_01	Conformance to existing open and free standards	The system should be built with existing, open and free standards to the greatest extent possible. Ontologies should also be selected or developed with this conformance in mind.	Should	

Use Case specification

Please specify a scenario/goal for your use case.

Buildings are going to be planned and built or renovated using innovative wood based materials and components. This is very important considering the great share of energy used by buildings and the urgent need to tackle the energy and climate crisis. How can the different actors (architects, construction companies, building owners, forest owners, process industry actors, manufacturers) in the value chain estimate and collaborate around important information about supply and performance of relevant indicators during the process? How can they know what is really making a difference in the value chain if there is no transparency and shared knowledge about the important key indicators? Some main aspects of this concern the verification and traceability of sustainable efforts along the value chain such as certification and other sustainability measures.

What are the pre-conditions of your use case? In which state the system should be in before the scenario starts?

The system is in the state of partially real collected loosely semantic data, and partially loosely semantic synthetic data[27]. The system is accessible for the actor to start feeding data and data collection has already started to some extent. The only missing thing will be the system components and the schematic descriptions around the taxonomies/ontologies that are needed.

What are the post-conditions of your use case? What is the expected state of the system after the scenario is completed?

The actors perceive the solution used is sustainable in the sense that it's not forcing unnecessarily complex schemas or standards and can motivate further investments on digitalization that cater for interoperability through the value chain.

[27] Synthetic data is generated based on the previous observations when there is a lack of data from one source

Who are the actors (people or automated digital agents) involved in the scenario when in operation or needed during development?

Multiple digital twin systems or virtual subsystems acting as decentralised nodes and agents continuously supplying system state for a central broker and analysis platform. The central platform is hosted by Paramountric and several subsystems are hosted by Basajaun partners in cloud or on-premise. The actors from several subsystems are virtualized in the sense that they are represented in the system but the data supply is coming from a placeholder system that generated synthetic data. These virtual subsystems will likely be hosted in the cloud, but could also be simulated from desktop computers as representing actors that regularly disconnect from the Internet.

The actors represented is:

Forest owners, building owners, construction companies, architects, forestry operations, sawmilling, glulam factory and other parties for structural wooden elements, manufacturer of building materials and components, logistics.

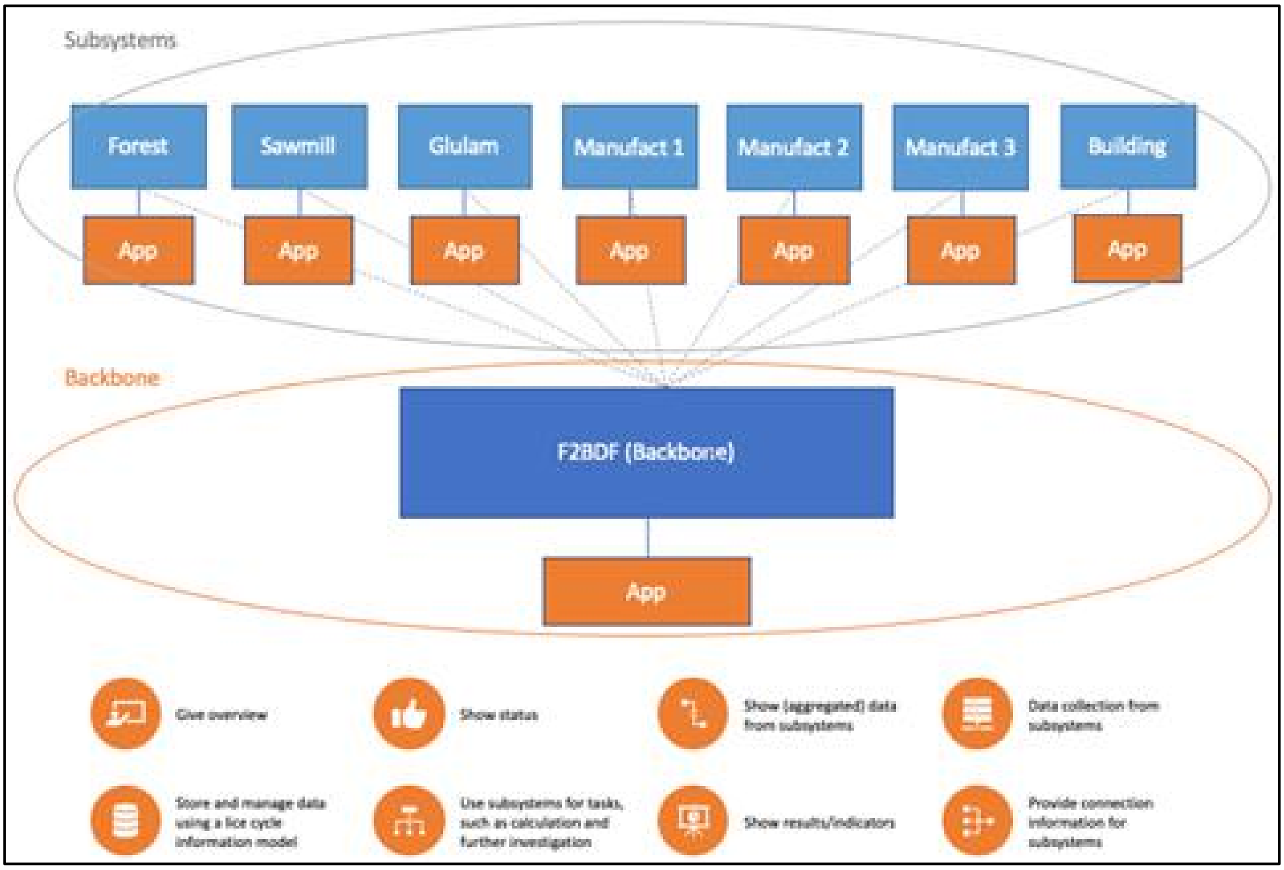
What are the steps of the main scenario?

Please add one row for each step in your scenario. If a step involves with an ontology or a tool, please specify its name and purpose at this step. If some of types of ontologies (Top Level Ontology, Mid-Level Ontology, Domain Ontology) are not used, explain why. Also include intentions for future development plans.

No	Description	TLO	MLO	DO	Tools
1	Identify actors in the supply chains and their domains	Note that the usage of ontologies is not known at this stage			Most, if not all tools used will be integrated in the existing platform (custom made or selected from already existing open source libraries).
2	Identify common KPIs and indicator framework that works across the supply chain and resonates with actors				
3	Identify processes that aligns between actor level and cross-actor level, and resonates with actors				
4	Map existing or other				

	available data sources that can be used to cross-over between actors and supply chain				
5	Collect data or generate synthetic data where data is missing				
6	Visualise the supply chain and alignment between actor domains with focus on the horizontal integration and common processes in a way that actors can draw conclusions on how to improve their own processes and communication with their neighbours				

Workflow



Which data sources are used? (Please cross-reference with the steps of the main scenario) Which is the domain of these data sources[28]?

GIS data for rural areas and forests. GeoJson is the main data format, but many OGC standards are supported.

Satellite data from the Copernicus project is used for forest analysis.

Harvesting data is covered by StanForD format, but the coverage is limited in Europe. This data comes from forest machines.

Transportation routes use mainly OpenStreeMaps.

Most factory and manufacturing data is completely proprietary and domain development is not prioritised in this use case but would be considered from case to case.

For most data collection NGSI-LD and linked data is used. JSON-LD principles will be used extensively.

Many of the data sources are synthetic which means that they are sampled from statistical analysis.

EPD (Environmental Product Declaration) is used as a data source.

Building life cycle is using IFC (Industry Foundation Classes) as data source from AEC industry.

Facility management will use a variety of sensor data sources which is still not decided.

Ontologies

Ontologies already used in the use case (consistent with the main scenario)

IfcOwl is used (in the building subsystem)

Primary purpose of ontology application in this use case

interoprability between different actors in the supply chain

Identified challenges in the use of ontologies in this use case

- finding the most suitable ontolofgy for a domain
- manual process of selecting ontologies or various part of ontologies.

(small) Examples of problems in ontology usage

- finidng relevant parts of ontologies for the being implemented system

[28] Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

Name the most important 20 terms for the domain of your use case. If available, please add any diagrams illustrating these terms (e.g UML diagram, ER diagram)

(note that the case is specifically about cross-domain problems)

Forestry and forest management

Process industry

Manufacturing

Materials

Circularity

Products

Value supply chain

Decision making

Construction industry

Building life cycle management

Life cycle analysis (LCA)

Collaboration between actors

Indicators and KPI

Sustainable measures

Wood quality

Tracing

Process operations

Predictions, Time

IoT, sensors and devices

Energy

Scenarios

National specifics such as language, code, regulations, governance, recommendations

Software tools to be used/developed

Systems that need to work/be integrated with ontologies

Custom ontology repository and potential integration with existing stable repositories

Inventory and search engine for selected ontologies

Integrated ontology alignment module

Visualisation tool for non-experts and users not accustomed to ontologies

Implementation Time Plan

Please provide a rough time plan for your implementation.

Particularly, list the scenario steps by when what will be developed.

Scenario steps	Expected finish time	Comments/Status
Scenario steps from Table above	09-2023	As for the ontology connection it's not possible to do a more detailed time plan at the moment

FAIR Survey

Please fill the survey at the link below in order to help us to understand the FAIR maturity level of your use case.

https://ec.europa.eu/eusurvey/runner/b64d2bc9-28da-3347-332b-0dc6970789d3

What are the future steps to improve FAIRness? What does the demonstrator want to improve? If there are no/little improvement made and/or foreseen, motivate why. If there is an interest to progress here, what are the roadblocks?

Technology Readiness Levels (TRL)

Using the standard definition[29], what is the current TRL of your use case?

Current: TRL2-TRL3

The ontology adoption of the Basajaun project may be implemented as a layer on top of existing layers. This means that the TRL for the overall platform might differ from the implementation that specifically targets the ontology functionality. It can be considered an extra feature of the system that enables actors to collaborate with existing schemas to quickly align or get started with new processes. The underlying system is expected to span between TRL5 and TRL7 depending on where in the supply chain the value proposition is fit to current market demands. The prioritisation will lie

[29] https://en.wikipedia.org/wiki/Technology_readiness_level

in the actors that invest in digitalization and integration with the system. When it comes to the ontology layer, it is expected to reach a slightly lower readiness level. As an example, integration between building construction and facility management could be a sub chain suitable for faster adoption using the existing digitalization in construction using BIM systems with IFC based ontologies and recent advances in smart building technology using BOT ontology as an example.

Key Performance Indicators (KPI)

Please add KPIs specific to your use case, particularly focusing on the KPIs related to evaluating ontology usage in you use case. You can take the generic KPIs below as example and extend table with your use cases specific ones.

KPI	Metric	Function	Range
TRL improvement	• TRL change	– 1/1+(TRL_end - TRL_start)	(0,1]
FAIR improvement	• average score in each FAIR dimension	– For each dimension, average based on final surveys	[0,4] for each dimension
Actor collaboration improvement	•	–	
Supply chain improvement	•	–	
Increase in transparent processes			
Tools improvement			
System interoperability improvement			

5.2 UC13: Life Cycle Sustainability Assessment of a Chemical Product

Demonstrator general information

Demonstrator company name and contact person(s):

BASF: peter.saling@basf.com

Other contacts within the ORIENTING project (https://orienting.eu):

- mauro.cordella@tecnalia.com (coordinator)

- marina.isasa@tecnalia.com
- carla.scagnetti@ibp.fraunhofer.de
- sonderegger@ecoinvent.org

Domain of application[30]

Chemical products manufacturing and sustainability assessment

Use case name:

Life Cycle Sustainability Assessment of a chemical product (to be revised by Ontocommons)

Short Description:

The use case will:

- Define the life cycle of the product, from extraction of raw materials to end of life fate and treatment (e.g., recycling, landfilling, incineration).
- Collect and analyse information about inputs and outputs associated with the life cycle of the product, such as consumption of resources, emissions, costs, information on social aspects.
- Calculate, integrate and interpret sustainability impacts through indicators addressing the environmental, economic and social performance of products, including also material criticality and circularity aspects.

What are the major (expected) contributions of OntoCommons to the demonstrator?

How to facilitate, as far as possible, automatization of calculations and sustainability assessments for chemicals.

Use Case requirements

Use case primary requirements				
UID	Title	Description	Priority (Shall/ Should/ May)	Comment
Use/application of ontologies				
UC13_RQ_U_01	Rules supporting reasoning and decision making	The ontologies **should** allow for easy adding/updating of application specific rules among the entities.	Should	
UC13_RQ_U_02	Documentation of domain (including	Ontology **shall** allow for effective documentation of	Shall	

30 industry where the ontology solution will be used, e.g. Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

	product functions and applications)	domain data, including sustainability aspects of materials in specific applications and related terms.		
Development of ontologies				
UC13_RQ_D_01	Ontology Scope	Ontology **shall** contain definitions to a range of entities that are relevant to and provide agreeable coverage of the selected domain.	**Shall**	
UC13_RQ_D_02	Ontology outcomes for changing inputs	Ontology **should** allow adaptations to new technologies of production processes.	**Should**	
Maintaining/extension of ontologies				
UC13_RQ_M_01	Easy maintenance of ontology	The ontology **shall** be easy to maintain (e.g. adding lower level terms, additional relations, etc.) from non-ontology experts (e.g. SW engineers).	**Shall**	
UC13_RQ_M_02	Easy to use ontology results	The ontology **shall** be interpretable and applicable for different functions in a company.	**Shall**	
Tools for ontology				
UC13_RQ_T_01	Visualisation	The tools **should** support visualisation of ontologies.	**Should**	
UC13_RQ_T_02	Collaboration of multiple stakeholders	The ontology development tool **should** allow different stakeholders to work simultaneously.	**Should**	
UC13_RQ_T_03	Trust building	The ontology tool **should** allow for the interpretation of information based on trusted and validated inputs.	**Should**	
Standardisation				
UC13_RQ_S_01	Conformance to technical standards	There **shall** be compliance to domain and W3C standards (e.g. ISO).	**Shall**	

UC13_RQ_S_02	Conformance to reporting standards	The ontology **should** be in-line with accepted reporting – standards.	Should	

Use Case specification

Please specify a scenario/goal for your use case.

Ontocommons should help Orienting in better defining possible solutions for the future mapping of LCSA information (input data across the life cycle of a products, output results from a software) in a harmonised way and the automatization of calculations in commercial databases and software. Ontocommons should help to treat a high number of information for a high number of applications.

What are the pre-conditions of your use case? In which state the system should be in before the scenario starts?

There are tools available for some specific topics of sustainability. In the field of LCA there is some harmonisation work on ontologies, as well as commercial software. However, no ontology nor software is addressing LCSA in a comprehensive way, nor it allows for calculation automatization. Orienting aims to make a first pragmatic step into that direction.

What are the post-conditions of your use case? What is the expected state of the system after the scenario is completed?

We expect that Ontocommons help Orienting better defining what should be the next steps to put mapping of information and automatization of calculations into practice. A challenge for the sustainability assessment of chemicals is that this implies linking and managing a large set of information (e.g., process and supply chain data, characterization factors for the quantification of KPIs, chemical properties and scenarios of use). Ontologies should help develop strategies for more sustainable and societally accepted industries.

Who are the actors (people or automated digital agents) involved in the scenario when in operation or needed during development?

BASF will collect and process LCSA data to calculate and interpret LCSA results. Other partners of Orienting will supervise and help as needed.

What are the steps of the main scenario?

Please add one row for each step in your scenario. If a step involves with an ontology or a tool, please specify its name and purpose at this step. If some of types of ontologies (Top Level Ontology, Mid-Level Ontology, Domain Ontology) are not used, explain why. Also include intentions for future development plans.

No	Description	TLO	MLO	DO	Tools
1	Data collection	x	x		Excel
2	Data processing	x	x		GaBi, Excel
3	Data implementation in software tool(s)		x	x	GaBi, Excel
4	Results calculation and interpretation			x	Excel, ppt

Workflow

See table above

Which data sources are used? (Please cross-reference with the steps of the main scenario) Which is the domain of these data sources[31]?

LCA software (GaBi)

Specific spreadsheets for Eco-Efficiency and SEEbalance methods

Databases (Gabi, …)

Ontologies

Ontologies already used in the use case (consistent with the main scenario)

- **If yes:**
  - **Top Level Ontologies used / Developed by:**
  - **Domain Ontologies Used / Developed by:**
  - **Other Ontologies / Taxonomies used or suggested to be used (developed by):**

Within ORIENTING, we will develop an LCSA ontology building from the BONSAI ontology (domain ontology) and the implicit ontology contained in the elLCD data format (see also figures below):

- https://ontology.bonsai.uno/core/ontology_v0.2.ttl;
- https://doi.org/10.1111/jiec.13220;
- https://eplca.jrc.ec.europa.eu/LCDN/developerILCDDataFormat.xhtml

Only for some cases ontologies are used in the context of sustainability assessments. The BONSAI ontology, for example, was applied for the database integration example further describe in Ghose et al. (2018) (https://doi.org/10.1111/jiec.13220), which is not a sustainability assessment. Within ORIENTING, the ontology might be used to facilitate the integration of non-LCSA data from non-

[31] Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

typical data sources such as non-LCA databases or reports. The EU taxonomy for sustainable activities can also be used for specific materials and technologies.

Primary purpose of ontology application in this use case

Sustainability assessment with multi-dimensions

Identified challenges in the use of ontologies in this use case

Data availability and data processing

(small) Examples of problems in ontology usage

Due to a lack of experience with applying ontologies, we cannot contribute here

Name the most important 20 terms for the domain of your use case. If available, please add any diagrams illustrating these terms (e.g UML diagram, ER diagram)

1. activity/process	set of interrelated or interacting activities that transforms inputs into outputs
2. flow/exchange	inputs and outputs of activities/processes
3. elementary flow/exchange	material or energy entering the system being studied that has been drawn from the environment without previous human transformation, or material or energy leaving the system being studied that is released into the environment without subsequent human transformation
4. intermediate flow/exchange	product, material, or energy flow occurring between activities/processes of the product system being studied
5. (flow) property	properties of flows such as mass, water content, elemental contents…
6. unit	unit of the flow property
7. functional unit	quantified performance of a product system for use as a reference unit, e.g. 1 kg chemical produced
8. reference unit	a measure to which the numeric value representing the measure of a flow is expressed in proportion to, e.g. CO2-emissions per kg chemical produced functional units are reference units, but not all reference units are functional units

9. reference flow	measure of the outputs from processes in a given product system required to fulfil the function expressed by the functional unit, e.g. chemical production
10. LCI result	Life Cycle Inventory (analysis) result: outcome of a life cycle inventory analysis that catalogues the elementary flows/exchanges related to an activity/process; provides the starting point for life cycle impact assessment
11. LCIA method	Life Cycle Impact Assessment methods are used to assess LCI results
12. impact category	class representing environmental issues of concern to which life cycle inventory analysis results may be assigned, e.g. climate change
13. impact indicator	an indicator that represents an impact, e.g. global warming potential 100
14. characterization factor	factor derived from a characterization model which is applied to convert an assigned life cycle inventory analysis result to the common unit of the category indicator, e.g. 1 kg CO2-equivalent / kg CO2 emission

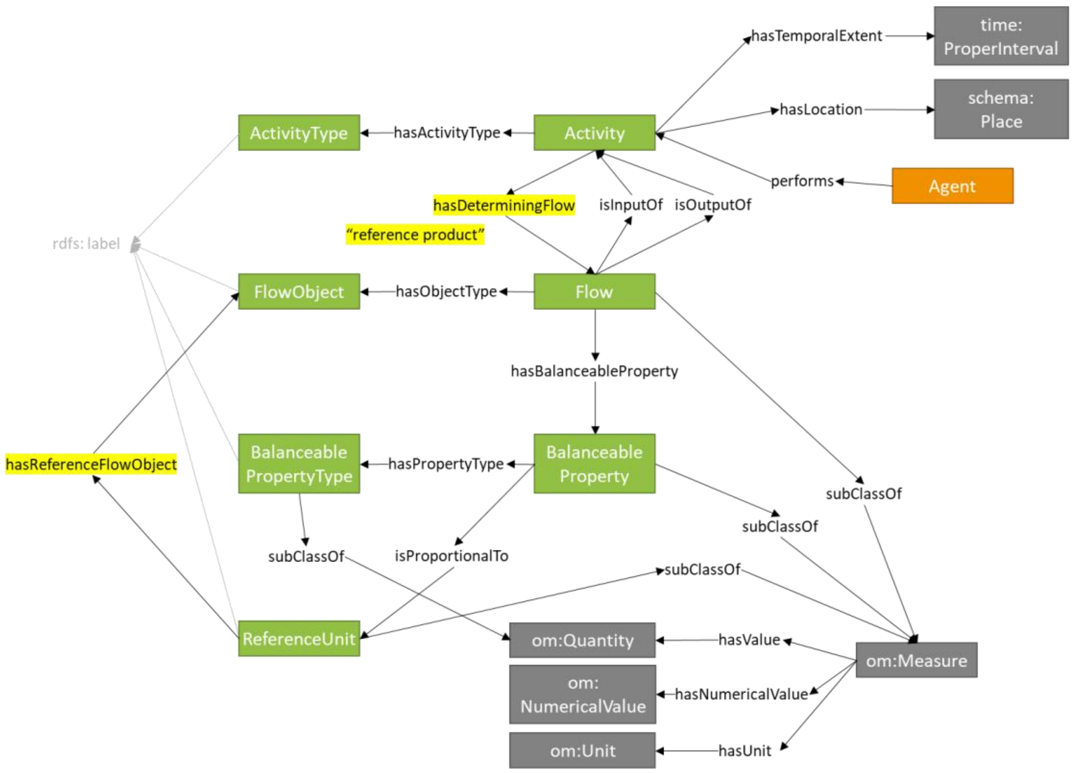


Figure 7 Structure of BONSAI ontology

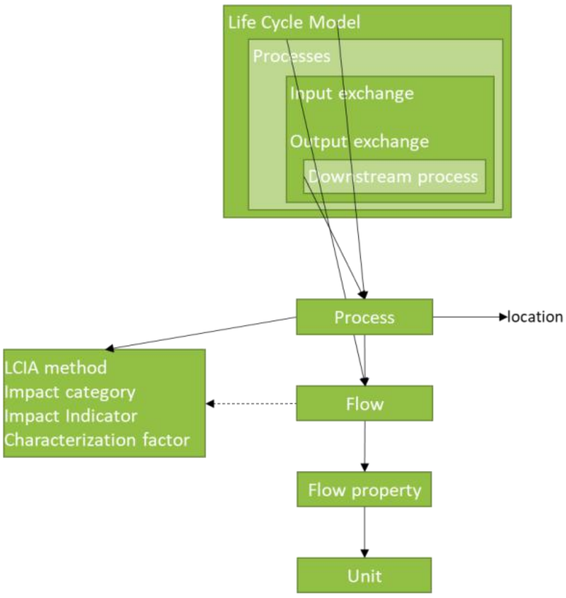


Figure 8 Structure of eILCD data format (https://eplca.jrc.ec.europa.eu/LCDN/developerILCDDataFormat.xhtml)

Software tools to be used/developed

Systems that need to work/be integrated with ontologies:

We aim to use commercial tools (see point above). Results addressing different domains of sustainability will be integrated in a html tool (to be developed).

To have a look at the BONSAI ontology, so far we have used the Protégé editor.

Implementation Time Plan

Please provide a rough time plan for your implementation.

Particularly, list the scenario steps by when what will be developed.

Scenario steps	Expected finish time	Comments/Status
Data collection	April to June 2022	
Data processing	June to September 2022	
Data implementation in software tool(s)	February to June 2023	
Results calculation and interpretation	February to August 2023	

FAIR Survey

Please fill the survey at the link below in order to help us to understand the FAIR maturity level of your use case.https://ec.europa.eu/eusurvey/runner/b64d2bc9-28da-3347-332b-0dc6970789d3

We aim to fill the questionnaire after Ontocommons check our answers, to know if some further detail is needed, and provide us with an official name/ID

What are the future steps to improve FAIRness? What does the demonstrator want to improve? If there are no/little improvement made and/or foreseen, motivate why. If there is an interest to progress here, what are the roadblocks?

Expectations reported in Section 3, to be linked with FAIRness once input to survey is provided.

Technology Readiness Levels (TRL)

Using the standard definition[32], what is the current TRL of your use case?

TRL 4

Key Performance Indicators (KPI)

Please add KPIs specific to your use case, particularly focusing on the KPIs related to evaluating ontology usage in you use case. You can take the generic KPIs below as example and extend table with your use cases specific ones.

KPI	Metric	Function	Range
TRL improvement	• TRL change	– 1/1+(TRL_end - TRL_start)	(0,1]
FAIR improvement	• average score in each FAIR dimension	– For each dimension, average based on final surveys	[0,4] for each dimension
Use case specific KPIs	•	–	

[32] https://en.wikipedia.org/wiki/Technology_readiness_level

5.3 UC14: Architecture design and ontology definition applied for Onboard Maintenance System of Aircraft

Demonstrator general information

Demonstrator company name and contact person(s):

Company name: COMAC BATR (Commercial Aircraft Corporation of China, Ltd.)

Contact person: Hao Wang (wanghao8@comac.cc)

Domain of application[33]

Aircraft and aerospace

Use case name:

Architecture design and ontology definition applied for Onboard Maintenance System of Aircraft

Short Description:

Onboard Maintenance System (OMS) is one of the important systems in aircraft, it is responsible for fault diagnosis and prediction, as well as data collection and transmission. However, due to its complexity, modelling OMS is recognized as a tough task for the avionics development in aircraft design. Although SysML/UML are helpful in some parts, but they are unable to express physical and electrical layers of the system. So here the KARMA (Kombination of ARchitecture Model specificAtion) language is proposed to support architecture design and process definition of OMS with a model-based systems engineering approach.

The multi-architecture modelling language KARMA is a semantic modelling language for a multi-architecture modelling approach. KARMA is expected to support descriptions and simulation of different architectural views of systems engineering. In our case, we plan to use KARMA to build OMS model though three perspectives: The reconfigurable process that helps for lifecycle process definition and analysis, the integrated modelling framework that covers Mission, scenario, function, logical and physical layer of the SOI, and apply them into OMS modelling; **GOPPRRE ontology** is used to construct knowledge graph models which are generated from KARMA models. Design structure matrix table is used to define the interrelationships among model elements and requirements. ReqIF is used to define the requirement items. The KARMA models, DSM tables, reqif requirement items are transformed to the ontology models which is defined based on BFO. Finally, some extra efforts will be made to interact with the existing SysML and Modelica models based on the ontology model for hybrid V&V consideration, which potentially will rebuild the ecosystem of M&S in MBSE area.

What are the major (expected) contributions of OntoCommons to the demonstrator?

Top level ontology to support aircraft design and manufacturing, particularly on model-based systems engineering and domain specific knowledge on fault detection.

33 industry where the ontology solution will be used, e.g. Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

Use Case requirements

Use case primary requirements				
UID	Title	Description	Priority (Shall/ Should/ May)	Comment
Use/application of ontologies				
UC14_RQ_U_01	Systems engineering formalism	The ontologies shall allow for easy defining the systems engineering perspective	Shall	
UC14_RQ_U_02	Documentation of aircraft domain	Ontology should allow for effective documentation of aircraft domain data including related terms.	Shall	
UC14_RQ_U_03	Domain Knowledge Graph for architecture model	Ontology should allow engineers to build Knowledge graph with fully structured and linked data to quickly build the digital prototype of an aircraft equipment.	Shall	
UC14_RQ_U_04	Reasoning for traceability analysis	Ontology should allow engineers to analyse the traceability among different domain specific models.	Shall	
Development of ontologies				
UC14_RQ_D_01	Ontology Scope	Ontology shall contain definitions to a range of entities that are relevant to and provide agreeable coverage of the selected domain	Shall	
UC14_RQ_D_02	Ontology for systems engineering	Ontology for defining systems engineering perspective	Shall	
UC14_RQ_D_03	Ontology for MBSE	Ontology for defining architecture modelling	Shall	
Maintaining/extension of ontologies				
UC14_RQ_M_01	Easy maintenance of ontology	The ontology shall be easy to maintain (e.g. adding lower level terms, additional relations, etc.) from non-	Shall	

		ontology experts (e.g. SW engineers).		
Tools for ontology				
UC14_RQ_T_01	Visualisation	The tools shall support visualisation of ontologies.	Shall	
UC14_RQ_T_02	Collaboration of multiple stakeholders	The ontology development tool should allow different stakeholders to work simultaneously.	Should	
UC14_RQ_T_03	Architecture design	The tools shall support visualisation of ontologies for architecture design.	Should	
UC14_RQ_T_04	Requirement definition	The tools shall support visualisation of ontologies for requirement definition.	Should	
UC14_RQ_T_05	DSM table design	The tools shall support visualisation of ontologies for requirement definition	Should	
Standardisation				
UC14_RQ_S_01	Conformance to standards	There shall be compliance to domain and W3C standards (e.g. ISO).	Shall	
UC14_RQ_S_02	BFO	There shall be compliance to domain and BFO.	Shall	

Use Case specification

Please specify a scenario/goal for your use case.

Develop architecture model for the onboard maintenance system of commercial aircraft and design the domain specific ontology for the PHM system.

What are the pre-conditions of your use case? In which state the system should be in before the scenario starts?

An architecture model for the onboard maintenance system, an ontology transformer is under development for generating ontology models from architecture models.

What are the post-conditions of your use case? What is the expected state of the system after the scenario is completed?

A formal ontology transformer should be developed based on some industrial standard.

Who are the actors (people or automated digital agents) involved in the scenario when in operation or needed during development?

EPFL, KARMA language and MetaGraph 2.0.

What are the steps of the main scenario?

Please add one row for each step in your scenario. If a step involves with an ontology or a tool, please specify its name and purpose at this step. If some of types of ontologies (Top Level Ontology, Mid-Level Ontology, Domain Ontology) are not used, explain why. Also include intentions for future development plans.

No	Description	TLO	MLO	DO	Tools
1	Architecture modelling for the aircraft PHM system			GOPPRRE ontology for architecture modeling	MetaGraph Purpose: architecture modelling and ontology generation
y					

Workflow

1. Develop an architecture model for the entire OMS including system artefacts and development process for OMS
2. Transform all these architecture models to ontology models
3. Develop a knowledge graph modelling platform the ontology models to manage such knowledge.

Which data sources are used? (Please cross-reference with the steps of the main scenario) Which is the domain of these data sources[34]?

Support aircraft OMS development

Ontologies

Ontologies already used in the use case (consistent with the main scenario)

- **If yes:**
  - **Top Level Ontologies used / Developed by:**
  - **Domain Ontologies Used / Developed by:** EPFL, GOPPRRE ontology for architecture modeling
  - **Other Ontologies / Taxonomies used or suggested to be used (developed by):**

[34] Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

Primary purpose of ontology application in this use case

Represent the architecture models using ontology.

Identified challenges in the use of ontologies in this use case

Interoperability among different modelling tools

(small) Examples of problems in ontology usage

Requirement diagram which is generated from ontology

Name the most important 20 terms for the domain of your use case. If available, please add any diagrams illustrating these terms (e.g UML diagram, ER diagram)

Graph

Object

Relationship

Point

Role

Property

Project

Language

Software tools to be used/developed

Systems that need to work/be integrated with ontologies

MetaGraph 2.0

Implementation Time Plan

Please provide a rough time plan for your implementation.

Particularly, list the scenario steps by when what will be developed.

Scenario steps	Expected finish time	Comments/Status
Scenario steps from table above	Month-Year	
	Month-Year	

	Month-Year	
	Month-Year	

FAIR Survey

Please fill the survey at the link below in order to help us to understand the FAIR maturity level of your use case.

https://ec.europa.eu/eusurvey/runner/b64d2bc9-28da-3347-332b-0dc6970789d3

What are the future steps to improve FAIRness? What does the demonstrator want to improve? If there are no/little improvement made and/or foreseen, motivate why. If there is an interest to progress here, what are the roadblocks?

More complex scenario will be used to evaluate the case study

Technology Readiness Levels (TRL)

Using the standard definition[35], what is the current TRL of your use case?

5 TRL

Key Performance Indicators (KPI)

Please add KPIs specific to your use case, particularly focusing on the KPIs related to evaluating ontology usage in you use case. You can take the generic KPIs below as example and extend table with your use cases specific ones.

KPI	Metric	Function	Range
TRL improvement	• TRL change	– 1/1+(TRL_end - TRL_start)	(0,1]
FAIR improvement	• average score in each FAIR dimension	– For each dimension, average based on final surveys	[0,4] for each dimension
Domain specific improvement	• completeness	– completeness of the domain specific knowledge	[0,4] for each dimension

[35] https://en.wikipedia.org/wiki/Technology_readiness_level

	• traceability	– traceability among different model elements	[0,4] for each dimension

5.4 UC15: Monitoring human operators' safety and well-being via semantic data integration in an automotive manufacturing setting

Demonstrator general information

Demonstrator company name and contact person(s):

CPSoSaware "*Computing technologies and engineering methods for cyber-physical systems of systems*", H2020 ICT-01-2019, https://cpsosaware.eu/

Contact person: Dr Efstratios (Stratos) Kontopoulos, Knowledge Scientist, Catalink Ltd, email: e.kontopoulos@catalink.eu

Domain of application[36]

Manufacturing

Assembly

Processing

Use case name:

Monitoring human operators' safety and well-being via semantic data integration in an automotive manufacturing setting

Short Description:

This demonstrator use case constitutes part of our work within the H2020 ICT-01-2019 project CPSoSaware "Computing technologies and engineering methods for cyber-physical systems of systems" and will take place within the context of Trail #2 of the project "Human – Robot Interaction in the Manufacturing Environment". Trail #2 takes place in a car assembly line involving collaborating robots that assemble car chassis (e.g., welding, bolting). The process is assisted by human operators that intervene in specific parts of the assembly line to perform operations that robots cannot make. Our aim in this use case is to develop a semantic data integration framework that will facilitate the monitoring of the human operators' safety and well-being as they are performing the requested operations.

[36] industry where the ontology solution will be used, e.g. Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

A set of IoT sensors send their measurements to respective analysis components: (a) wearables (inertial measurement units, i.e., accelerometers and gyroscopes) for motion analysis and body tracking; (b) footage from static cameras analysed by computer vision components for estimating the operator's posture. The analysis outputs are fed into an ontology-based semantic Knowledge Graph (KG) through CASPAR (https://catalink.eu/caspar), a flexible semantic data integration framework, which will be properly extended for the purposes of the use case. The aim is to perform an ergonomic analysis of the operator's estimated posture to assess their well-being, and, potentially, reconfigure the robots' position to avoid long-term musculoskeletal problems and other health and/or safety risks.

What are the major (expected) contributions of OntoCommons to the demonstrator?

We are looking forward to collaborating with OntoCommons experts in semantic technologies towards standardising the terminology and improving the cross-domain interoperability of our developed knowledge-based tools for scene analysis, posture recognition, and ergonomic assessment in a manufacturing environment. Our main expectation is to have a practical deployment of FAIR-compliant semantic knowledge representation and data integration in an industrial manufacturing setting. Testing the deployed solutions in additional industrial scenarios proposed by OntoCommons partners and/or affiliated stakeholders is also within our aims.

Use Case requirements

Use case primary requirements				
UID	Title	Description	Priority (Shall/ Should/ May)	Comment
Use/application of ontologies				
UC15_RQ_U_01	Input sources	Pose estimation algorithms from two different sources will provide instance data as input to the ontology: (a) static cameras, (b) IMUs.	**Shall**	
UC15_RQ_U_02	Rule-based decision support	A set of rules running on top of the semantic Knowledge Graph (i.e., ontology populated with instance data – see **UC_CPSoSaware_RQ_01**) will generate alerts and recommendations regarding the human operator's safety.	**Shall**	
UC15_RQ_U_03	Offline rule-based reasoning	Rule-based reasoning will be offline (i.e., not real-time).	**Shall**	

UC15_RQ_U_04	Real-time rule-based reasoning	Real-time rule-based reasoning will also be considered.	May	
Development of ontologies				
UC15_RQ_D_01	Ontology scope	The developed ontology will encompass all required concepts and properties for efficiently representing all aspects relevant to the use case.	Shall	
UC15_RQ_D_02	Ontology design	The design of the ontology will be as lightweight as possible.	Should	
UC15_RQ_D_03	Ontology documentation	The ontology will be sufficiently documented through respective annotation properties.	Should	
Maintaining/extension of ontologies				
UC15_RQ_M_01	Ontology maintenance	The design of the ontology will be such that it will facilitate ontology maintenance, i.e., updates and/or extensions to the ontology.	Should	
Tools for ontology				
UC15_RQ_T_01	Ontology development	For the development of the ontology, we will rely on an established freely available ontology authoring environment.	May	e.g., Protégé
UC15_RQ_T_02	Ontology validation	The resulting ontology will be validated using appropriate freely available tools.	May	e.g., OOPS!
UC15_RQ_T_03	Semantic data integration	For the semantic data integration (i.e., ontology population), we will rely on novel tools developed by the CPSoSaware consortium.	Shall	CASPAR framework

UC15_RQ_T_04	Knowledge Graph visualization	For the visualization of the resulting Knowledge Graph (i.e., ontology populated with instance data), we will rely on freely available ontology visualization tools.	May	e.g., OntoGraf, Graffoo
UC15_RQ_T_05	Knowledge Graph persistence	The storage of the Knowledge Graph will be undertaken by a freely available established triplestore solution.	Should	e.g., GraphDB, StarDog
Standardisation				
UC15_RQ_S_01	Conformance to standards	The developed ontology and rule-based reasoning will be based on W3C standards.	Shall	OWL, SPARQL
UC15_RQ_S_02	Reuse of existing resources	Wherever possible, existing resources will be reused and extended for the purposes of the use case.	May	E.g., standard ontologies, ODPs

Use Case specification

Please specify a scenario/goal for your use case.

Assess human operators' ergonomic safety and well-being.

What are the pre-conditions of your use case? In which state the system should be in before the scenario starts?

- IoT sensors (static cameras and wearables) are in place and operational.
- Actors (robotic arm and human operator) are in position.
- Analysis components are online and awaiting input from IoT sensors.
- Semantic data integration framework is online and awaiting input from analysis components.
- Triplestore is online and awaiting input from semantic data integration framework.

What are the post-conditions of your use case? What is the expected state of the system after the scenario is completed?

- Actors (robotic arm and human operator) have successfully performed the requested operations.
- Analysis components have submitted results to semantic data integration framework without errors.

- Semantic data integration framework has successfully completed ontology population without errors.
- Triplestore hosts a semantic Knowledge Graph (i.e., an ontology populated with instance data).
- A report on the human operators' ergonomic safety is generated based on the data stored in the KG.

Who are the actors (people or automated digital agents) involved in the scenario when in operation or needed during development?

- Human operator.
- Robotic arm.
- CPSoSaware platform (consisting of the IoT sensors, analysis components, semantic data integration framework, triplestore, and reports generator).

What are the steps of the main scenario?

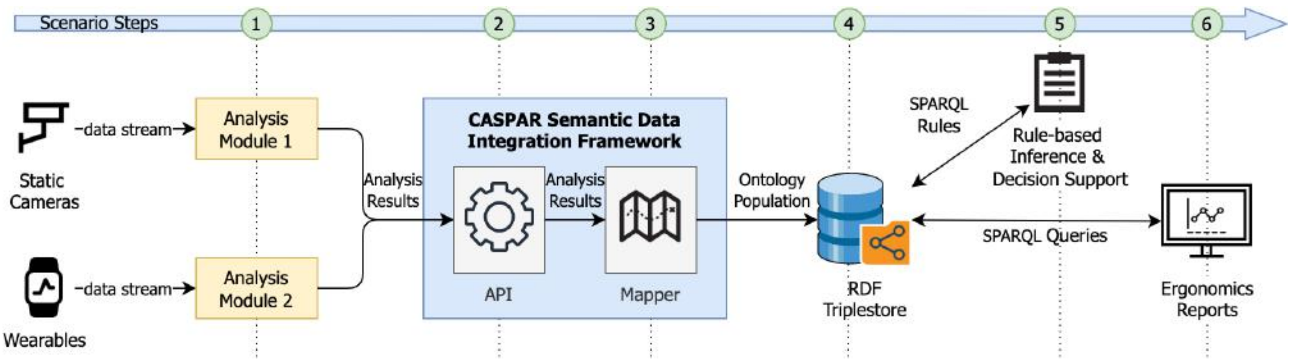
Please add one row for each step in your scenario. If a step involves with an ontology or a tool, please specify its name and purpose at this step. If some of types of ontologies (Top Level Ontology, Mid-Level Ontology, Domain Ontology) are not used, explain why. Also include intentions for future development plans.

No	Description	TLO	MLO	DO	Tools
1	Real-time analysis of inputs from IoT sensors (cameras & wearables)				CPSoSaware analysis components
2	Submission of analysis outputs to semantic data integration framework				CASPAR API (part of the CASPAR semantic data integration framework) Purpose: Ontology population
3	Ontology population		SSN/SOSA	CPSoSaware DO	CASPAR Mapper (part of the CASPAR semantic data integration framework) Purpose: Mapping of input fields to ontology constructs (classes/properties)

No	Description	TLO	MLO	DO	Tools
4	Semantic KG		SSN/SOSA	CPSoSaware DO	RDF triplestore Purpose: Hosting the populated ontology
5	Rule-based decision support		SSN/SOSA	CPSoSaware DO	SPARQL rules running on top of the semantic KG Purpose: Generate alerts and recommendations
6	Report generation		SSN/SOSA	CPSoSaware DO	SPARQL queries Purpose: Generate report about human operator's ergonomic safety

Workflow

The diagram below gives a diagrammatic overview of the steps described above – the foreseen technical architecture will be based on RabbitMQ for the exchange of messages between the various components.



Which data sources are used? (Please cross-reference with the steps of the main scenario) Which is the domain of these data sources[37]?

Data is dynamically (i.e., in real-time) generated by IoT devices (cameras and wearables) and is fed to the analysis components, which, in turn, process the data and generate their analysis results (i.e., observations). The latter are submitted to the CASPAR framework for semantic data integration.

The domains of the input data are: Manufacturing, Assembly, Processing.

[37] Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

Ontologies

Ontologies already used in the use case (consistent with the main scenario): In our preliminary experimentations towards developing the use case scenario, we have only relied on SSN/SOSA for representing analysis outputs as "observations" coming from the respective components, slightly extending it with domain-specific concepts for a more focused semantic representation.

Primary purpose of ontology application in this use case: The ontology serves as the uniform model for integrating inputs from heterogeneous sources.

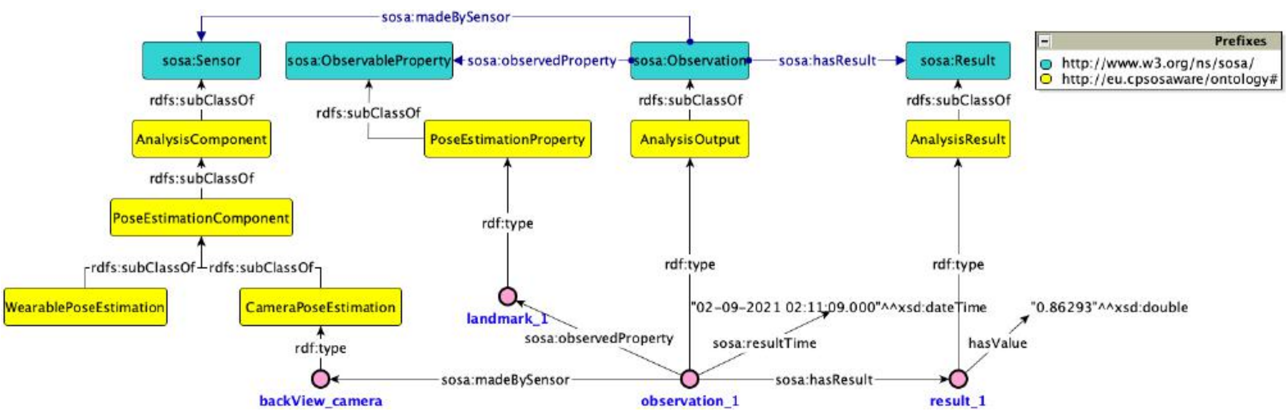
Identified challenges in the use of ontologies in this use case: It is not clear at this stage whether we will be facing scalability issues (in ontology population and rule-based reasoning) and whether we will be able to perform real-time (vs offline) semantic rule-based reasoning on top of the instance data stored in the semantic Knowledge Graph. The latter operation, however, is not a prerequisite for the use case (see also **UC_CPSoSaware_RQ_04**). There are not many domain-specific ontologies besides SOSA/SSN.

(small) Examples of problems in ontology usage: Poor performance in response times (during querying and rule-based reasoning).

Name the most important 20 terms for the domain of your use case. If available, please add any diagrams illustrating these terms (e.g UML diagram, ER diagram): At this early stage, we only have a few core concepts included in the semantic model:

- AnalysisComponent (and its specialisations) represents the components receiving the raw data measurements (e.g., camera feed and measurements from wearables), performing the respective analyses, and generating the results.
- AnalysisOutput represents the "observations", i.e., the outputs generated by the analysis components, accompanied by a respective timestamp.
- AnalysisResult represents the actual results from the analysis, i.e., values and units (if applicable).
- PoseEstimationProperty represents the observable property that is relevant to estimating the correctness or not of the human operator's pose.

A schematic diagram of the above, along with a sample instantiation, are illustrated in Graffoo[38] notation in the figure below:



[38] Graffoo specification: https://essepuntato.it/graffoo/specification/

Software tools to be used/developed

Systems that need to work/be integrated with ontologies: Our proprietary CASPAR framework serves as the semantic data integration "vehicle" towards this goal and needs to seamlessly feed the ontology with instance data. CASPAR will be extended accordingly, depending on the use case needs.

Implementation Time Plan

Please provide a rough time plan for your implementation.

Particularly, list the scenario steps by when what will be developed.

Scenario steps	Expected finish time	Comments/Status
Simulated environment		
Analysis of inputs from IoT sensors	April-2022	
Set-up RabbitMQ-based architecture	April-2022	Architecture for message exchange between the various components.
Submission of analysis outputs to semantic data integration framework	May-2022	Establish the message exchange format and operations.
Ontology population	June-2022	Create the CASPAR mappings for ontology population.
Semantic KG	June-2022	Set-up the triplestore for hosting the semantic KG. Establish interoperability with CASPAR.
Rule-based decision support	August-2022	Deploy set of SPARQL rules.
Report generation	August-2022	Deploy set of SPARQL queries.
Real-life environment		
Deployment in a real-life factory setting	November-2022	Test the above in the facilities of partner CRF (Fiat Research Centre).

FAIR Survey

Please fill the survey at the link below in order to help us to understand the FAIR maturity level of your use case.

https://ec.europa.eu/eusurvey/runner/b64d2bc9-28da-3347-332b-0dc6970789d3

Done

What are the future steps to improve FAIRness? What does the demonstrator want to improve? If there are no/little improvement made and/or foreseen, motivate why. If there is an interest to progress here, what are the roadblocks?

The developed ontology will be populated by instance data under various scenarios, resulting in multiple semantic KGs. The latter will be publicly available as outputs by the CPSoSaware project and, with help by our OntoCommons colleagues, we will ensure that they will be FAIR-compliant. To the best of our knowledge, no other such datasets exist containing higher-level analysis outputs from an industrial setting instead of plain raw IoT measurements. We do not foresee any roadblocks (e.g., permissions by project partners) to achieving this goal.

Technology Readiness Levels (TRL)

Using the standard definition[39], what is the current TRL of your use case?

Current TRL is at TRL3 and we are aiming for at least TRL6.

Key Performance Indicators (KPI)

Please add KPIs specific to your use case, particularly focusing on the KPIs related to evaluating ontology usage in you use case. You can take the generic KPIs below as example and extend table with your use cases specific ones.

KPI	Metric	Function	Range
TRL improvement	TRL change	1/1+(TRL_end - TRL_start)	(0,1]
Responsiveness	Response time (sec)	Time (in sec) between submission of query and retrieval of result-set	(0 sec, 1 sec]
Ontology validation	Evaluation report by OOPS!	Each detected pitfall belongs to one of the following categories (a) *Critical*, (b) *Important*, (c) *Minor*	We are aiming to have only *Minor* pitfalls, if any.
Adoption of standards	Count of adopted W3C-recommended standards	Use of imported concepts by ontology (via owl:imports)	Ontology is based on at least one W3C-recommended standard
Ontology documentation	Count of missing annotation properties	Use of annotation properties, indicatively: rdfs:label, rdfs:comment, skos:prefLabel, skos:definition	No core ontology concept should lack annotation properties

[39] https://en.wikipedia.org/wiki/Technology_readiness_level

5.5 UC16: Food Knowledge Graph

Demonstrator general information

Demonstrator company name and contact person(s):

Dermot Doyle, CEO, Dynaccurate SARL

Domain of application[40]

Biotechnology

Use case name:

Food Knowledge Graph

Short Description:

We would like to develop a proof-of-concept knowledge graph which is geared for additive or compound discovery in the sector of food processing or agri-science. An example could be using an Ontology to link databases available from the European Institutions (such as the Additive Database from DG Sante, the substance database from ECHA, the PubChem database from NIH etc.) with the objective of discovering substitute compounds to be used as additives, as well as potential usage limits etc. The main task of the use case is to keep ontologies in the knowledge graph consistent after updates and maintenance.

What are the major (expected) contributions of OntoCommons to the demonstrator?

We would very much like to network with members of the Ontocommons team or wider community in the biotech sector so that we can learn more about end-user needs, receive feedback and also receive guidance on particular approaches. We can provide demonstrator without this support, but obviously it will be more relevant if we can engage with others beforehand.

Use Case requirements

Use case primary requirements				
UID	Title	Description	Priority (Shall/ Should/ May)	Comment
Use/application of ontologies				
UC16_RQ_U_01	Reuse of existing ontologies	To provide semantic interoperability, our case study should be re-using ontologies as far as possible.	Shall	
UC16_RQ_U_02	A variety of different ontologies should be	Mapping existing ontologies provides wider	Shall	

40 industry where the ontology solution will be used, e.g. Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

	mapped	utility and proof of concept of the case study		
Development of ontologies				
UC16_RQ_D_01	Bespoke or tailored Ontology Development	We recognise that some ontology development may be necessary to create a coherent set of mappings. However, to promote efficiency and utility, ideally this will be minimised	**May**	
UC16_RQ_D_02	Use of existing commercial Knowledge Graphs	We will attempt to introduce an industry partner in the food science domain who can provide real-life Knowledge Graph requirements/contributions	**May**	
Maintaining/extension of ontologies				
UC16_RQ_M_01	Easy maintenance of ontology	This is a key objective of our project – the idea is that our mappings should be automatically updated based on top changes to existing ontologies / terminologies, to show how complex linkings can be managed in the long-term	**Shall**	
Tools for ontology				
UC16_RQ_T_01	Automated remapping (alignment) of ontologies	The Dynaccurate AI will be used to examine and remap changes to the Knowledge Graph based on changes to the multiple ontologies in scope	**Shall**	
UC16_RQ_T_02	Producing interoperable results	Tools for ontology development should produce interoperable results (i.e. following standards) that can be used by other tools in the workflow	**Shall**	

UC16_RQ_T_03	Visualisation	We will seek a collaboration with a KG application vendor for visualisation of the graph. This is not guaranteed but we have many contacts in the sector who may happy to collaborate with us to show tool utility	May	
Standardisation				
UC16_RQ_S_01	Conformance to standards	There shall be compliance to domain and W3C standards, especially in choice of interoperable file types conforming to semantic web norms.	Shall	

Use Case specification

Please specify a scenario/goal for your use case.

We will combine a number of food and substance related terminologies/ontologies/vocabularies into a single knowledge graph which can overlay multiple databases. The objective of the use case is to introduce changes into the mapped ontologies, which would normally then cause a ripple effect on the mappings (i.e. breaking the mappings). This is an extremely common occurrence in the life sciences, and is also very time consuming to rectify. The end-goal of our project is that our AI will identify the changes and remap accordingly, in a way which is hugely more time efficient.

What are the pre-conditions of your use case? In which state the system should be in before the scenario starts?

The ideal pre-conditions are that we have identified a range of different ontologies/terminologies/vocabularies which can be used. The 'FoodOn' Ontology in fact already has great potential as a starting point (https://bioportal.bioontology.org/ontologies/FOODON and www.foodon.org).

What are the post-conditions of your use case? What is the expected state of the system after the scenario is completed?

The post conditions are that all changes to the Ontologies have been identified automatically and queued for resolution by our AI, with automated changes proposed.

Who are the actors (people or automated digital agents) involved in the scenario when in operation or needed during development?

Actors: Data Scientist(s) and food and food science domain expert(s)

Digital Agents: DyLink (a mapping tool, potentially used), Dynaccurate AI (remapping tool, definitely used), Protégé (ontology editor, definitely used)

What are the steps of the main scenario?

See below steps. Please note, this is the main scenario, where we run our AI. Preparatory work would be carried out in Protégé and/or DyLink

No	Description	TLO	MLO	DO	Tools
1	Load an ontology or an ontology subset		e.g. FoodOn	FoodOn	Dynaccurate AI
2	Load counterparty ontology		Any of the mapped ontologies within FoodOn (see mappings on bioportal)	FoodOn	Dynaccurate AI
3	Load the mappings in a .csv file in SKOS format				Dynaccurate AI
4	Load an updated ontology or ontology subset, which will 'break' the mappings		e.g. FoodOn		Dynaccurate AI
5	Run a DIFF				Dynaccurate AI
6	Run a Remapping				Dynaccurate AI
7	Establish the changes and recommend actions				Dynaccurate AI

Workflow

Which data sources are used? (Please cross-reference with the steps of the main scenario) Which is the domain of these data sources[41]?

https://bioportal.bioontology.org/ontologies/FOODON and www.foodon.org

- This is a first potential ontology, it may be possible to incorporate others, however there are a lot of mappings already inside FoodOn.
- https://echa.europa.eu/web/guest
- Food additives[42]
- Biocides[43]
- Genetic information for organisms - such as probiotic cultures, yeasts etc.[44]
- Allergens[45]

Ontologies

Ontologies already used in the use case (consistent with the main scenario)

- If yes:
  - Top Level Ontologies used / Developed by:
  - Domain Ontologies Used / Developed by: https://bioportal.bioontology.org/ontologies/FOODON
  - Other Ontologies / Taxonomies used or suggested to be used (developed by): https://bioportal.bioontology.org/ontologies/FOODON

Primary purpose of ontology application in this use case

For FoodOn: Hsiao Lab initiated a search for a standardized food vocabulary in 2015 to support routine surveillance and outbreak analysis of foodborne pathogens, and quickly realized a new robust ontology needed to be developed for this purpose. Other curators within academia and the OBOFoundry.org community, having parallel needs for agriculture, nutritional analysis and food science research, quickly joined the consortium. (https://foodon.org/about/)

Identified challenges in the use of ontologies in this use case

[41] Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

[42] https://webgate.ec.europa.eu/foods_system/main/?event=substances.search&substances.pagination=1

[43] https://echa.europa.eu/information-on-chemicals/biocidal-products

[44] https://www.ncbi.nlm.nih.gov/genbank/samplerecord/#OrganismB

[45] http://www.allergenonline.org/databasebrowse.shtml

Generally speaking, any knowledge graph predicated on life sciences ontologies faces a major issue in management and remapping of those ontologies when the ontologies evolve to incorporate new terms etc. This is a generic problem in the life sciences.

(small) Examples of problems in ontology usage

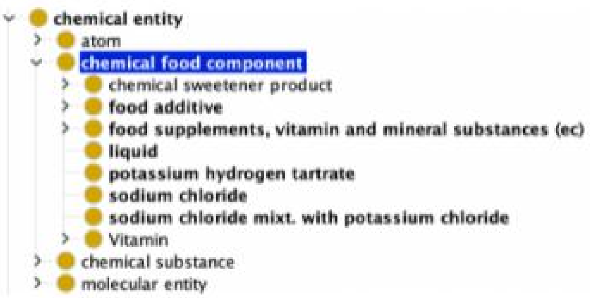
Subjective mappings: Conceptual heterogeneity of different ontologies in a domain

Name the most important 20 terms for the domain of your use case. If available, please add any diagrams illustrating these terms (e.g UML diagram, ER diagram)

Not yet selected, however, see the following as one example of structuring

Chemical food component

The "chemical food component" facet provides an overall branch for facets that cover carbohydrates, proteins, lipids, minerals, vitamins and secondary metabolite and additive classes. Much of this content ultimately yields CHEBI chemical entities, but organized from a food hierarchy perspective.



In 2021 FoodOn will be incorporating upcoming work from the Southern Cross University Crop Dietary Nutrition Ontology ontology for proteins, carbohydrates, lipids, minerals, etc. which will align with USDA Agricultural Research Service nutrient identifiers and FAO INFOODS nutrient measures.

Software tools to be used/developed

Systems that need to work/be integrated with ontologies

Protégé – open source editor

DyLink and Dynaccurate AI – proprietary tools of Dynaccurate SARL

Implementation Time Plan

Please provide a rough time plan for your implementation.

Particularly, list the scenario steps by when what will be developed.

Scenario steps	Expected finish time	Comments/Status
Scenario steps from table above	Month-Year	
	Month-Year	
	Month-Year	
	Month-Year	

FAIR Survey

Please fill the survey at the link below in order to help us to understand the FAIR maturity level of your use case.

https://ec.europa.eu/eusurvey/runner/b64d2bc9-28da-3347-332b-0dc6970789d3

What are the future steps to improve FAIRness? What does the demonstrator want to improve? If there are no/little improvement made and/or foreseen, motivate why. If there is an interest to progress here, what are the roadblocks?

Our contribution to FAIR is to establish how AI tools can overcome some of the biggest challenges in managing a knowledge at scale. Truthfully, it's actually impossible to manage large KG for the life sciences without some automation, because the cost of managing and remapping is prohibitively expensive when carried out manually. By utilising new technologies, more ambitious graphs can be created, with complete audit of the evolution, and zero loss of content due to ontology/terminology changes.

Technology Readiness Levels (TRL)

Using the standard definition[46], what is the current TRL of your use case?

TRL 5

[46] https://en.wikipedia.org/wiki/Technology_readiness_level

Key Performance Indicators (KPI)

Please add KPIs specific to your use case, particularly focusing on the KPIs related to evaluating ontology usage in you use case. You can take the generic KPIs below as example and extend table with your use cases specific ones.

KPI	Metric	Function	Range
TRL improvement	• TRL change	– 1/1+(TRL_end - TRL_start)	(0,1]
FAIR improvement	• average score in each FAIR dimension	– For each dimension, average based on final surveys	[0,4] for each dimension
Valid mapping of two ontologies by domain experts	•	–	
Drastic reduction on time spent on maintaining knowledge graphs in contrast to manual maintenance	•	–	

5.6 UC17: Using iiRDS in the industrial internet of things (IIoT) with Siemens Industrial Edge

Demonstrator general information

Demonstrator company name and contact person(s):

Siemens AG, Digital Industries

Domain of application[47]

Manufacturing, Technical Communication

Use case name:

Using iiRDS in the industrial internet of things (IIoT) with Siemens Industrial Edge

[47] industry where the ontology solution will be used, e.g. Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

Short Description:

Prototypical creation of iiRDS packages, evaluation of the customer view and content delivery

- Discuss with potential users
- Analyze and evaluate the customer benefits of an iiRDS delivery
- Estimate the effort, benefits and risks of generating and maintaining the data: for technical communicators and across teams
- Define requirements for a roll-out.

Create a productive application of the prototype for EDGE devices

What are the major (expected) contributions of OntoCommons to the demonstrator?

Ideas about general architecture / architectural framework

Place iiRDS in the general architectural framework

How to model terminologies as ontology > learn from other experiences/projects

Participation in webinars, exchange best practices

Use Case requirements

Scope:

- Edge enables data exchange between industry components and applications via APIs.
- The Edge technology provides a intermediate layer between industry components and the cloud. A typical Edge device is, for example, an industrial PC with apps for monitoring and controlling devices. The PC synchronizes data with the cloud, but may also work offline.
- Siemens wants to make technical documentation available in the Edge layer and use iiRDS for this.
- A central server shall provide information from the technical documentation (the platform product c-rex is used for this purpose).
- The technical documentation content is transformed and delivered to the Edge layer as iiRDS packages. Before delivering the content to c-rex, a linguistic tool is used to analyze the content and extract and assign metadata automatically, especially product metadata describing product features and product functions

Use case primary requirements				
UID	Title	Description	Priority (Shall/ Should/ May)	Comment
Format of ontological data of iiRDS and standardization				
UC17_RQ_S_01	Common data forma	Use a common data format to deliver topic-level information so that customers can find information with high	Shall	

		accuracy.		
UC17_RQ_S_02	Open for other suppliers	Do not use a proprietary data format so that other suppliers can also provide information in the same format.	Shall	
Use/application of ontologies				
UC17_RQ_U_01	Multifaceted search	As an Edge device user, I want to be able to filter information in the portal.	Shall	
UC17_RQ_U_02	Data retrieval	Edge device or smaller controls shall be able to retrieve data from the cloud.	Shall	
UC17_RQ_U_03	Event drives	Event shall be supported, in order to trigger output of information in the case of an event	Shall	
UC17_RQ_U_04	Topic-based metadata	It shall be possible to assign metadata on topic level (not just the document) so that users can find and access granular content	Shall	
Maintaining/extension of ontologies				
UC17_RQ_M_01	Extension of vocabulary	Siemens shall be able to extend the iiRDS vocabulary with own product metadata	Shall	
UC17_RQ_M_02	3rd party	Edge apps define their own use cases > 3rd party customers must be able to retrieve information specific to these use cases.	Shall	
UC17_RQ_M_03	Linguistic-driven generation of metadata	A linguistic engine must be able to analyze content and to add additional normalized metadata to documentation topics.	Shall	
UC17_RQ_M_04	Configuration of the linguistic engine	The linguistic engine must have a configuration to select und to program rules, to generate metadata for specific iiRDS classes.	Shall	

Tools for ontology				
UC17_RQ_T_01	Visualization	The tools shall support visualization of information based on ontologies.	**Shall**	
Standardisation				
UC17_RQ_S_03	Conformance to standards	There must be compliance to domain and iiRDS standards (e.g. ISO).	Shall	
UC17_RQ_S_04	customer specific extension	A customer-specific extension of the standard must be possible	**Shall**	

Use Case specification

Please specify a scenario/goal for your use case.

What are the pre-conditions of your use case? In which state the system should be in before the scenario starts?

- First version of the linguistic generator available
- iiRDS generator available
- Delivery portal available und configured
- iiRDS standard released

What are the post-conditions of your use case? What is the expected state of the system after the scenario is completed?

- Delivery of information to the Edge layer

Who are the actors (people or automated digital agents) involved in the scenario when in operation or needed during development?

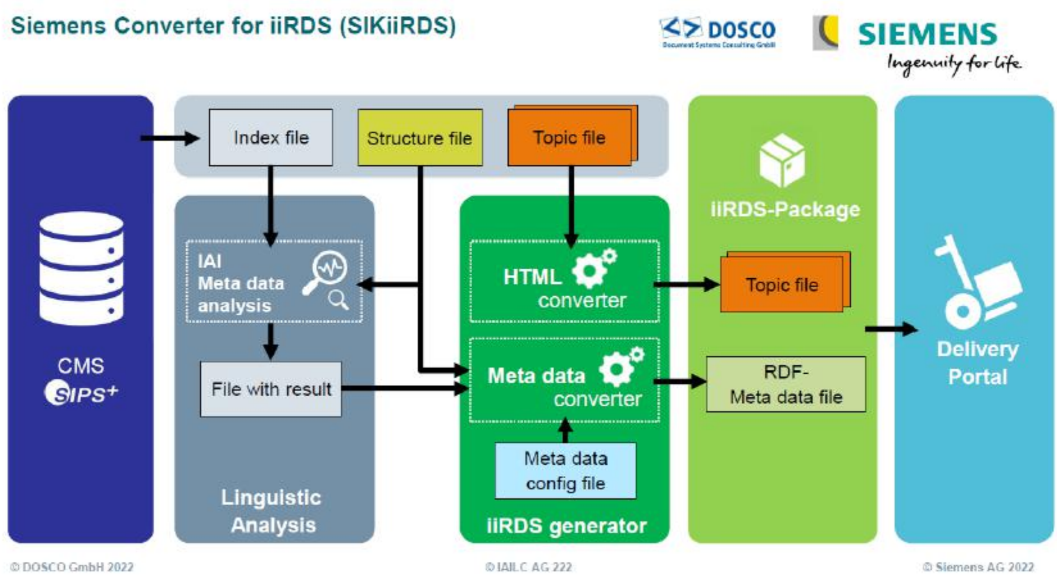
- Delivery portal supplier
- Linguistic Engine supplier
- iiRDS generator supplier
- Experts for the standard

What are the steps of the main scenario?

Please add one row for each step in your scenario. If a step involves with an ontology or a tool, please specify its name and purpose at this step. If some of types of ontologies (Top Level Ontology, Mid-Level Ontology, Domain Ontology) are not used, explain why. Also include intentions for future development plans.

No	Description	TLO	MLO	DO	Tools
1	Base content	n/a	iiRDS	Siemens extensions to iiRDS (industrial ontology)	Base set on metadata implemented in Siemens content management system SIPS+
2	Linguistic based addition of metadata	n/a	iiRDS	Siemens extensions to iiRDS (industrial ontology)	Linguistic engine from Congree
3	Generate an iiRDS package	n/a	iiRDS	Siemens extensions to iiRDS (industrial ontology)	Generator from DOSCO and Transformation Services from c-rex
4	Delivery		iiRDS classes		c-rex
5	Retrieval		iiRDS	Siemens extensions to iiRDS (industrial ontology)	Edge application from Siemens or 3rd party

Workflow



Which data sources are used? (Please cross-reference with the steps of the main scenario) Which is the domain of these data sources[48]?

Data sources:

- XML output from Siemens content management system SIPS+
- Markdown files from GitHub
- PDF files
- Word

Ontologies

Ontologies already used in the use case (consistent with the main scenario)

- **If yes:**
  - **Top Level Ontologies used / Developed by:**
  - **Domain Ontologies Used / Developed by:** iiRDS
  - **Other Ontologies / Taxonomies used or suggested to be used (developed by):** Siemens-specific extensions to iiRDS = metadata describing product features and product functions

Primary purpose of ontology application in this use case

- Use standardized vocabulary for enriching technical documentation content with metadata
- Enable semantic search and search facets in content delivery portal
- Enable targeted access and retrieval of content on Edge devices or from the Edge cloud based on use cases

Identified challenges in the use of ontologies in this use case

- How to assign the metadata automatically using a linguistic tool in multiple languages (around 22 languages planned)
- How to support 3rd party suppliers with their use cases

(small) Examples of problems in ontology usage

Name the most important 20 terms for the domain of your use case. If available, please add any diagrams illustrating these terms (e.g UML diagram, ER diagram)

- InformationUnit
- TopicType, e.g. Task, Concept, Reference
- DocumentType
- Component, e.g.
- ProductVariant
- InformationSubject, e.g. TechnicalOverview, genericCollection, restrictionOnUse
- Party
- ProductFeature
- PhaseOfProductLifeCycle, e.g. Deployment, Operation

[48] Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

Software tools to be used/developed

Systems that need to work/be integrated with ontologies

Content management system (SIPS+) (customized Cosima system)

iiRDS converter

Linguistic engine (CLAT, Congree)

Delivery and content integration platform: c-rex

Implementation Time Plan

Please provide a rough time plan for your implementation.

Particularly, list the scenario steps by when what will be developed.

Scenario steps	Expected finish time	Comments/Status
Scenario steps from table above	2022	
Technical concept completion for content delivery	12.2021	
UI concept completion for content delivery	12.2021	
Generation of iiRDS packages	12.2021- on giong	Test packages are created. More information, e. g. from 3rd party are planned.
First pilot of Industrial Edge portal	03.2022	Prototype of the content delivery.
Integration of the portal into the IT ecosystem	04.2022	Trying to integrate the portal into the IoT-Platform
Retrieval	~09.2022	Creation of Edge apps for intelligent information

FAIR Survey

Please fill the survey at the link below in order to help us to understand the FAIR maturity level of your use case.

Contribution ID: fca062a5-1952-48b9-bdea-9e7edbbc8f05

What are the future steps to improve FAIRness? What does the demonstrator want to improve? If there are no/little improvement made and/or foreseen, motivate why. If there is an interest to progress here, what are the roadblocks?

No future steps planned.

Technology Readiness Levels (TRL)

Using the standard definition[49], what is the current TRL of your use case?

TRL 6

Key Performance Indicators (KPI)

Please add KPIs specific to your use case, particularly focusing on the KPIs related to evaluating ontology usage in you use case. You can take the generic KPIs below as example and extend table with your use cases specific ones.

KPI	Metric	Function	Range
Percentage of topics with metadata created by linguistic tool	• *Percentage of topics with metadata generated by linguistic tool*	– Percentage of topics with auto-generated metadata related to total number topics	[70 %]
Number of languages for automatic assignment of metadata	• *Number of languages*	– Support for automatic assignment of metadata	At least 2

5.7 UC18: IKEA Knowledge Graph

Demonstrator general information

Demonstrator company name and contact person(s):

.. Inter IKEA Systems, Katariina Kari

Domain of application[50]

Home Furnishing

Materials modelling

Use case name:

IKEA Knowledge Graph

Short Description:

[49] https://en.wikipedia.org/wiki/Technology_readiness_level

[50] industry where the ontology solution will be used, e.g. Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

IKEA holds a lot of knowledge and understanding of people's lives at home, needs, wishes, dreams, and problems, as well as solutions to those. This knowledge is spread out and stored in data silos. In order to serve IKEA's digitalisation transformation efforts, the IKEA Knowledge Graph sets as its goal to connect the data and make it usable through out IKEA's services and systems.

What are the major (expected) contributions of OntoCommons to the demonstrator?

state of the art ontologies and solutions

technical know-how

Use Case requirements

I have listed below the use cases we are presenting in OntoCommons for the IKEA KG.

Use case primary requirements				
UID	Title	Description	Priority (Shall/ Should/ May)	Comment
Use/application of ontologies				
UC18_RQ_U_01	Generating RML/R2RML/TARQL mapping from describing data sources	A vocabulary for describing data sources (JSON, relational database, CSV) shall be defined or available. An open-source software project shall be available to generate mapping files instead of manually creating them.	Shall	
UC18_RQ_U_02	Ontology for IT Systems	Ontology should allow for effective documentation of most common systems in any enterprise IT landscape.	Should	
UC18_RQ_U_03	Health and Sustainable Living Ontology	We shall describe how activities at home and elsewhere impact sustainability and the planet.	May	Transparency on action and activities that contribute to a healthy and sustainable life.
UC18_RQ_U_04	General Object Taxonomy	For propping of pictures we may use a general object taxonomy that	May	

		includes a bowl of chips, an apple, a book etc.		
UC18_RQ_U_05	Frontend assessment of taxonomy and ontology editing	Available visual tools for ontology and taxonomy development should be assessed and reflected according to IKEA's requirements and organisational fit.	Should	
Development of ontologies				
UC18_RQ_D_01	Ontology Scope: IT Systems	How IT System interact with and relate to each other shall be covered in the range of properties. Classes shall reflect nature of different types of IT systems.	Shall	
UC18_RQ_D_02	Taxonomy Scope: IT Systems	Taxonomy should include vocabulary on vendors and usage of IT systems, e.g. Microsoft Word – text editing.	Should	
UC18_RQ_D_03	Ontology Scope: Data Sources	Classes and properties shall reflect the structure and makeup of data sources in general such as JSON, SQL database, and CSV.	Shall	
UC18_RQ_D_04	Taxonomy Scope: Data Sources	Vocabulary should reflect known data types and most common to IKEA cases of managing data, such as images, title, text etc.	Should	
UC18_RQ_D_05	Ontology Scope: Sustainable Living	Classes and properties shall reflect the variety of sustainability issues and considerations that have to do with waste, energy, water and how the activities of an individual can create an impact on them.	Shall	

UC18_RQ_D_06	Taxonomy Scope: Sustainable Living	Life at home vocabulary and sustainability topics shall be covered thoroughly.	**Shall**	
UC18_RQ_D_07	Ontology Scope: General Objects	How objects can be placed in space may be reflected by properties.	**May**	
UC18_RQ_D_08	Taxonomy Scope: General Objects	All possible objects found in a household shall be reflected in the vocabulary and paired with image data.	**Shall**	
Maintaining/extension of ontologies				
UC18_RQ_M_01	Easy maintenance of ontology	The ontology shall be easy to maintain (e.g. adding lower level terms, additional relations, etc.) from non-ontology experts (e.g. SW engineers).	**Shall**	
UC18_RQ_M_02	Usage instructions	For any ontology and taxonomy, instructions on where to download them, how to use them, how to query them shall be provided to the public.	**Shall**	
UC18_RQ_M_03	SPARQL endpoints	All ontologies and taxonomies shall be available via a secure SPARQL endpoint.	**Shall**	
UC18_RQ_M_04	Graph can be served via APIs	Custom made APIs built on top of the graph with SLAs fitting e-commerce shall be enabled	**Shall**	
Tools for ontology				
UC18_RQ_T_01	Visualisation	The tools shall support visualisation of ontologies according to IKEA's visual standards.	**Shall**	
UC18_RQ_T_02	Collaboration of multiple stakeholders	The ontology development tool shall allow different authorised and access controlled stakeholders to work simultaneously and allow	**Shall**	

		for comment threads for each node so that they can be discussed.		
UC18_RQ_T_03	Version control and 4-eye principle	Any authorised stakeholder shall be able to create a change to ontologies and taxonomies and submit that change for a review process before the change is accepted. The proposed version may be visualised and shall be tested against life systems before it is merged as part of the master definition (e.g. like code in a git pull request and staging environment for the PR's branch).	Shall	
UC18_RQ_T_04	Browsable ontologies and taxonomies and URIs as URLs	Anyone at IKEA may browse through the taxonomies and ontologies using a browser and the URIs of each concept resolve to a HTML page under a same-named URL.	May	
Standardisation				
UC18_RQ_S_01	Conformance to standards	There shall be compliance to domain and W3C standards (e.g. ISO).	Shall	
UC18_RQ_S_02	EU legal framework for sustainability	Any EU requirements for reporting on sustainability shall be covered by taxonomies and ontologies developed in OntoCommons.	Shall	e.g. Green deal, EU regulations for appliances (energy rating)

Use Case specification

Please specify a scenario/goal for your use case.

What are the pre-conditions of your use case? In which state the system should be in before the scenario starts?

An IKEA Knowledge Graph platform for authoring, storing, reviewing and serving the knowledge graph is set up and it is vendor agnostic, meaning one can switch which frontend to use for ontology authoring and which triple store to use for storing the knowledge graph data.

What are the post-conditions of your use case? What is the expected state of the system after the scenario is completed?

A performant and usable non-graph specific endpoint, such as an API, serves the respective use cases with whatever knowledge they need. The knowledge comes from the knowledge graph and no data silos exists to fuel the different use cases.

Who are the actors (people or automated digital agents) involved in the scenario when in operation or needed during development?

Stakeholders and subject-matter experts, stakeholder developers implementing the APIs, developers building the APIs, data and knowledge engineers building the IKG platform, knowledge modellers and ontologist modelling the IKG, and any supportive staff such as project manager, product owners, business owner.

Ontology editing frontend(s), governance review enabling process automation, data pipelines with mapping and transformations, deployment pipelines, triple store, open-to-the-internet API endpoints

What are the steps of the main scenario?

Please add one row for each step in your scenario. If a step involves with an ontology or a tool, please specify its name and purpose at this step. If some of types of ontologies (Top Level Ontology, Mid-Level Ontology, Domain Ontology) are not used, explain why. Also include intentions for future development plans.

No	Description	TLO	MLO	DO	Tools
SC-1	Semantic description of a data source, e.g. JSON			Represent a JSON object and connect it to concepts	Triple authoring
SC-2	Automated RML generation				Script for authoring a RML file from semantic description of a data source

SC-3	Annotate room and interior design images with the props used in them and change props.				Frontend tool for viewing images and switching around props in them.
SC-4	Semantic description of an IT System			System ontology	Triple authoring
SC-5	Conceptualise Sustainable Living DO and T				Workshopping to create a shared explicit conceptualisation together with SMEs
SC-6	Design Sustainable Living DO and T				Knowledge modelling, ontology definition and taxonomy work
SC-7	Develop Sustainable Living DO and T				Triple authoring
SC-8	Develop first use case powered by Sustainability Living DO and T				Product design and development work

Workflow

Please add here a picture that describes the best the aforementioned user story, in a compact way with discrete steps (e.g. as workflow).

Which data sources are used? (Please cross-reference with the steps of the main scenario) Which is the domain of these data sources51?

51 Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

Ontologies

Ontologies already used in the use case (consistent with the main scenario)

- If yes:
  - Top Level Ontologies used / Developed by:
  - Domain Ontologies Used / Developed by:
    - Used by stakeholders, developed by knowledge modelling team
  - Other Ontologies / Taxonomies used or suggested to be used (developed by):
    - Identified with the help from OntoCommons experts

Primary purpose of ontology application in this use case

In all use cases the ontology plays a central role in adding the IKEA Knowledge Graph and driving first identified use cases. Sometimes just to be able to maintain the vocabulary with proper governenace process beats the maintaining of this information in excel.

Identified challenges in the use of ontologies in this use case

Serving the ontologies via API endpoints requires a lot of software development work to setup a robust cloud-based platform for performantly storing and serving the knowledge graph and manage any deltas from stakeholder input or data sources.

(small) Examples of problems in ontology usage

Name the most important 20 terms for the domain of your use case. If available, please add any diagrams illustrating these terms (e.g UML diagram, ER diagram)

Software tools to be used/developed

Systems that need to work/be integrated with ontologies

Our use case requires us to build the systems for ontology authoring. The integration with other systems always happens via an API. Systems calling the APIs is out of scope for our use cases.

- Frontend for authoring and discussing modelling changes (classes, properties)
- Frontend for managing taxonomies
- Visualisation of IKG
- Visual editing
- Suggest changes and review changes in all above mentioned tooling to enable governance

Implementation Time Plan

Please provide a rough time plan for your implementation.

Particularly, list the scenario steps by when what will be developed.

Scenario steps	Expected finish time	Comments/Status
SC-1	May-2022	
SC-2	June-2022	
SC-3	May-2023	
SC-4	January 2023	
SC-5	June-2022	
SC-6	July-2022	
SC-7	September-2022	
SC-8	October-2022	

FAIR Survey

Please fill the survey at the link below in order to help us to understand the FAIR maturity level of your use case.

https://ec.europa.eu/eusurvey/runner/b64d2bc9-28da-3347-332b-0dc6970789d3

26a6614e-2a8c-4d57-a462-46d19e318861

What are the future steps to improve FAIRness? What does the demonstrator want to improve? If there are no/little improvement made and/or foreseen, motivate why. If there is an interest to progress here, what are the roadblocks?

It is not clear yo me what the definition of metadata vs data is. The way I see it is that our use cases provide metadata most and foremost attached to some little amount of data or according to requests referring to data identifiers returns appropriate metadata. In order to advance FAIRness we need to get to the implementation phase. We will also not work on R on a public scale yet, are however to work on that at some point, as well.

The problem with FAIRness is that is does not conisider the Enterprise setting of Reusability internally (inner-source) and publically (outer-source). It also assumes that the only way to share knowledge in an enterprise is by sharing RDF data, which is incorrect, since an enterprise may also choose the have Knowledge as a Service.

Technology Readiness Levels (TRL)

Using the standard definition52, what is the current TRL of your use case?

TRL 4

Key Performance Indicators (KPI)

Please add KPIs specific to your use case, particularly focusing on the KPIs related to evaluating ontology usage in you use case. You can take the generic KPIs below as example and extend table with your use cases specific ones.

KPI	Metric	Function	Range
TRL improvement	• TRL change	– 1/1+(TRL_end - TRL_start)	(0,1]
FAIR improvement	• average score in each FAIR dimension	– For each dimension, average based on final surveys	[0,4] for each dimension
Amount of consumers for knowledge in the IKG	• Human access • API access • SPARQL endpoint users	–	
….	•	–	

5.8 UC19: Materials Databases Integration using the Materials Design Ontology

Note: The survey is tentatively filled.

1. General description of the use case	
Use Case ID / Demonstrator Name	Materials Databases Integration using the Materials Design Ontology
Main point of use case scope (please choose between or provide your	Data integration

52 https://en.wikipedia.org/wiki/Technology_readiness_level

own: Decision System Innovation Project Workflow QA/QC Guided AI Data Parsing Data Integration Interoperability)	Interoperability
Use Case Company Name	Linköping University
OntoCommons Participant Responsible for Demonstrator Contact - Affiliation	Patrick Lambrix, Linköping University, Sweden
Domain of Application (industry where the ontology solution will be used, e.g. Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety)	Materials development
Domain of Data Used (if it different from the previous, otherwise leave empty)	Materials databases via OPTIMADE
Actor Roles of the use case (e.g., knowledge scientist/engineer, material scientist)	Knowledge engineer Material Scientist

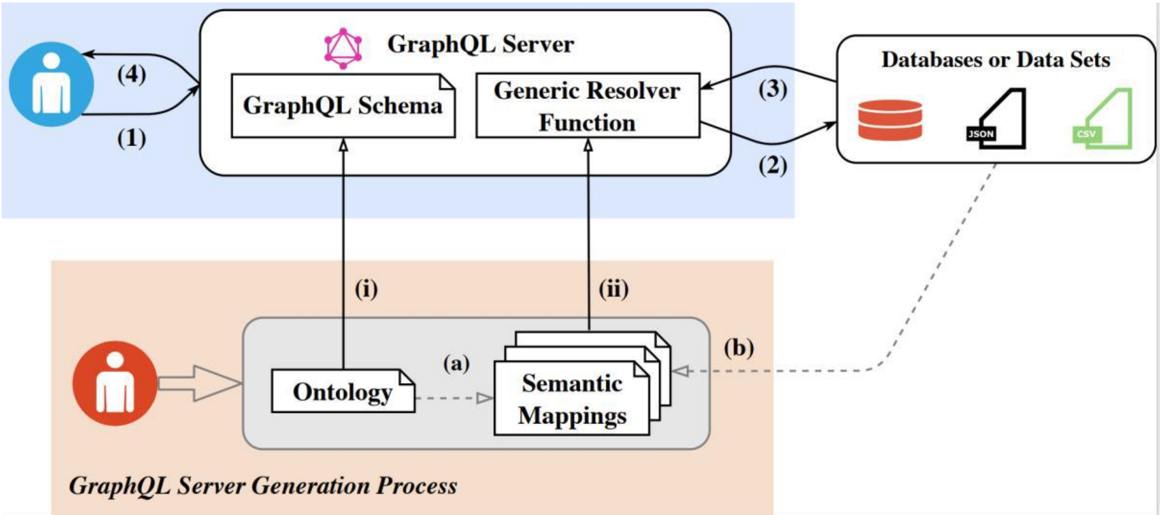
2. Ontology use in the use case	
Ontologies already used in the use case (if No please answer the following fields with the ontologies/vocabularies that you are planning to use within your demonstrator)	Materials Design Ontology (MDO) / Linköping University

Top Level Ontologies used / Developed by	
Domain Ontologies Used / Developed by	
Other Ontologies / Taxonomies used or suggested to be used (developed by)	We will investigate connections to top level ontologies such as EMMO. Initial connections to EMMO, Prov-O, CheBI, QUDT
Actor Roles of the ontologies used or those to be developed (e.g. who can develop them within the use case company, or who can maintain them)	
Primary purpose of ontology application in this use case (What would fit at most for the intended use of ontologies within this use case. Please choose one of the following: Data model / data structuring Data sharing Overview and visualisation Context bridging in digital communication Software customisation Artificial Intelligence Service extension Business planning / communication)	Data Integration Data model / data structuring Data sharing
Secondary purpose of ontology application (as in the previous point, if more than one, please add them in rows with enter, based on their priority)	
Identified challenges in the use of ontologies in this use case (e.g. not enough data available for the population of the ontology, data format too diverse)	• compatibility of MDO and top level ontologies, with EMMO as first candidate, regarding ontological commitment.

Data Sources (software and/or hardware based) to be accessed/used with the ontologies for this use case	• Databases in the OPTIMADE consortium • https://www.optimade.org/
(small) Examples of problems in ontology usage	

3. Use case primary requirements				
UID	Title	Description	Priority (Shall/Should/May)	Comment
Use/application of ontologies				
UC19_RQ_U_01	Semantic and integrated access	Provide semantic and integrated access to the OPTIMADE materials databases. We will provide a GraphQL and MDO-based interface to the OPTIMADE databases. It will allow queries using MDO terminology over multiple databases.	Shall	
UC19_RQ_U_02	compatibility of MDO and top level ontologies	Investigating the compatibility of MDO and top level ontologies, with EMMO as first candidate, regarding ontological commitment. Based on the outcome of this investigation we will align MDO and EMMO/a top level ontology as much as possible. If this alignment is not desired, we will report on the reasons why such an alignment is difficult.	Should	

4. User-story short description
The Materials Design Ontology is used for semantic and integrated access to the computational

materials databases in the OPTIMADE consortium, dealing with the heterogeneity of the databases in terms of underlying data models and use of terminology.	
Workflow	
	
Important points to be considered in the use case for better understanding	
Actor	
Associated Requirements	
Triggers	
Preconditions	

6. Purpose of ontology application in the use case (mark the primary with orange colour)

	UC
Data model / data structuring	X
Data sharing	X
Overview and visualisation	
Context bridging in digital communication	

Software customisation	
Artificial Intelligence	
Service extension	
Business planning / communication	
Decision System	
Innovation Project	
Workflow	
QA/QC	
Guided AI	
Data Parsing	
Data Integration	
Interoperability	
Other:_____	

7. FAIR data maturity level

Currently MDO is available online.

8. Technology readiness level assessment

Current TRL 3, Targeted TRL 6

5.9 UC20: Materials Characterisation Ontology

Demonstrator general information

Demonstrator company name and contact person(s):

Goldbeck Consulting Ltd / Gerhard Goldbeck, Pierluigi Del Nostro

Domain of application[53]

[53] industry where the ontology solution will be used, e.g. Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

Materials characterisation

Use case name:

Materials Characterisation Ontology (CHADA Ontology)

Short Description:

In the NanoMECommons project, we are ontologising characterisation to capture potentially any type of materials characterisation method and enable harmonisation. The starting point is a human readable metadata called CHADA and the work is to provide an EMMO compliant ontology. Current status is a scope and mapping to EMMO.

What are the major (expected) contributions of OntoCommons to the demonstrator?

We would like to utilise OntoCommons recommendations for ontology development and implementation and ensure TLO/MLO compliance.

Use Case requirements

Use case primary requirements				
UID	**Title**	**Description**	**Priority (Shall/ Should/ May)**	**Comment**
Use/application of ontologies				
UC20_RQ_U_01	Method specific ontology development	The CHADA ontology shall allow for the development of method specific ontologies.	**Shall**	
UC20_RQ_U_02	Documentation of domain	The CHADA ontology should allow for effective documentation of domain concepts and properties, including related terms.	**Should**	
UC20_RQ_U_03	Support procedure harmonization	The CHADA ontology should support the harmonization of different characterisation procedure	**Should**	
UC20_RQ_U_04	Knowledge transferability	As a common framework for the documentation of characterisation methods, the CHADA ontology may ease the transferability of the knowledge on characterisation procedures across different parties.	**May**	
Development of ontologies				
UC20_RQ_D_01	Ontology Scope	Ontology shall contain definitions to a range of	**Shall**	

		entities that are relevant to and provide agreeable coverage of the selected domain. The CHADA ontology is not meant to store the measurements' fine grained data.		
UC20_RQ_D_02	Compliance with EMMO	The CHADA ontology shall be compliant with the EMMO TLO and MLO.	**Shall**	
UC20_RQ_D_03	Integration with taxonomies	The CHADA ontology should be integrated with taxonomies for the specialization of the different concepts in CHADA	**Should**	
Maintaining/extension of ontologies				
UC20_RQ_M_01	Easy maintenance of ontology	The ontology shall be easy to maintain (e.g. adding lower level terms, additional relations, etc.) from non-ontology experts (e.g. SW engineers).	**Shall**	
Tools for ontology				
UC20_RQ_T_01	Visualisation	The tools shall support visualisation of ontologies.	**Shall**	
UC20_RQ_T_02	Collaboration of multiple stakeholders	The ontology development tool should allow different stakeholders to work collaboratively.	**Should**	
Standardisation				
UC20_RQ_S_01	Conformance to standards	There shall be compliance to domain and W3C standards (e.g. ISO).	**Shall**	

Use Case specification

Please specify a scenario/goal for your use case.

The goal is to develop an OWL-DL CHADA ontology based on the human readable documentation template for the characterisation data called CHADA. The ontology should in principle support a range of queries regarding the characterisation methodology and protocol.

What are the pre-conditions of your use case? In which state the system should be in before the scenario starts?

- The CHADA document template.
- CHADA filled by industrial partners.
- Answers by industrial partners to competency questions regarding materials characterisation

What are the post-conditions of your use case? What is the expected state of the system after the scenario is completed?

- A publicly available OWL-DL implementation of the CHADA ontology.

Who are the actors (people or automated digital agents) involved in the scenario when in operation or needed during development?

- Industrial partners.
- Characterisation Methods Experts (method developers and academic expert users)
- Ontology developers.

What are the steps of the main scenario?

Please add one row for each step in your scenario. If a step involves with an ontology or a tool, please specify its name and purpose at this step. If some of types of ontologies (Top Level Ontology, Mid-Level Ontology, Domain Ontology) are not used, explain why. Also include intentions for future development plans.

No	Description	TLO	MLO	DO	Tools
1	Identification of the main concepts, attributes and properties from the CHADA documents and the competency questions filled by the industrial partners.				Tables
2	Design of the CHADA ontology	EMMO	EMMO		Miro board
3	Mapping with EMMO	EMMO	EMMO		Protégé

4	Mapping with DO			Materials ontology; Manufacturing ontology, To capture different types of materials and the way they are made. Software, models To integrate with models used to determine properties	Protégé
5	Implementation in OWL-DL	EMMO	EMMO		Protégé
6	Identify and review other taxonomies to be linked to the CHADA ontology				Protégé

Note that EMMO is used as TLO to ensure interoperability with related developments in materials modelling.

Workflow

Clarify meaning of CHADA terms/fields, attributes and properties

↓

Compile and review competency questions

↓

First design of the CHADA ontology

↓

Map/align with EMMO MLO

↓

Mapping with DO

↓

Implementation in OWL-DL

↓

Identify and review other taxonomies to be linked to the CHADA ontology

Which data sources are used? (Please cross-reference with the steps of the main scenario) Which is the domain of these data sources[54]?

Materials Characterisation experiments carried out by project partners.

Ontologies

Ontologies already used in the use case (consistent with the main scenario)

- If yes:
  - Top Level and Mid-level Ontologies used / Developed by:
    - EMMO / EMMO developers, see https://github.com/emmo-repo/EMMO
  - Domain Ontologies Used / Developed by:
    - Materials
    - Manufacturing
    - Software
    - Mechanical Testing Ontology
      Developed by related projects (MarketPlace, OYSTER), see also https://github.com/emmo-repo/OIE-Ontologies https://github.com/emmo-repo/domain-mechanical-testing
  - Other Ontologies / Taxonomies used or suggested to be used (developed by):
    - See https://github.com/emmo-repo/domain-characterisation-methodology/blob/main/resources.md

Primary purpose of ontology application in this use case

Harmonize the documentation of characterisation procedures in a machine-readable way, exploiting structured information through taxonomies, overcoming the limitations of free text documentation and heterogeneous terminology.

Identified challenges in the use of ontologies in this use case

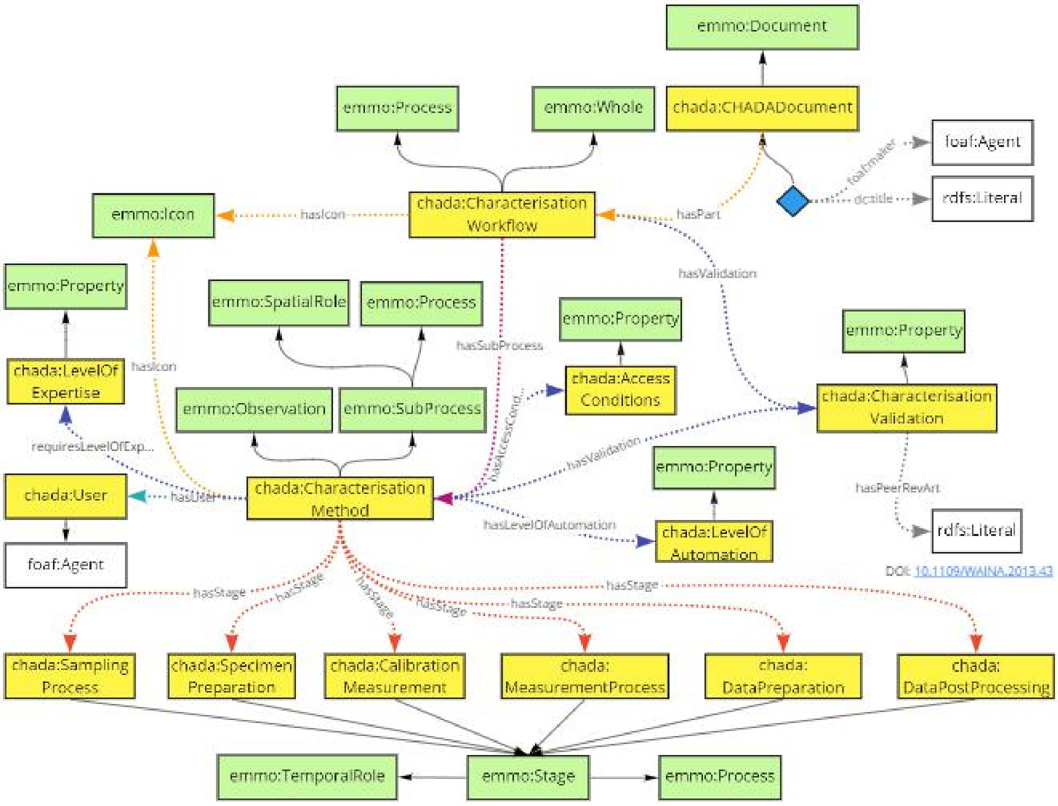
(small) Examples of problems in ontology usage

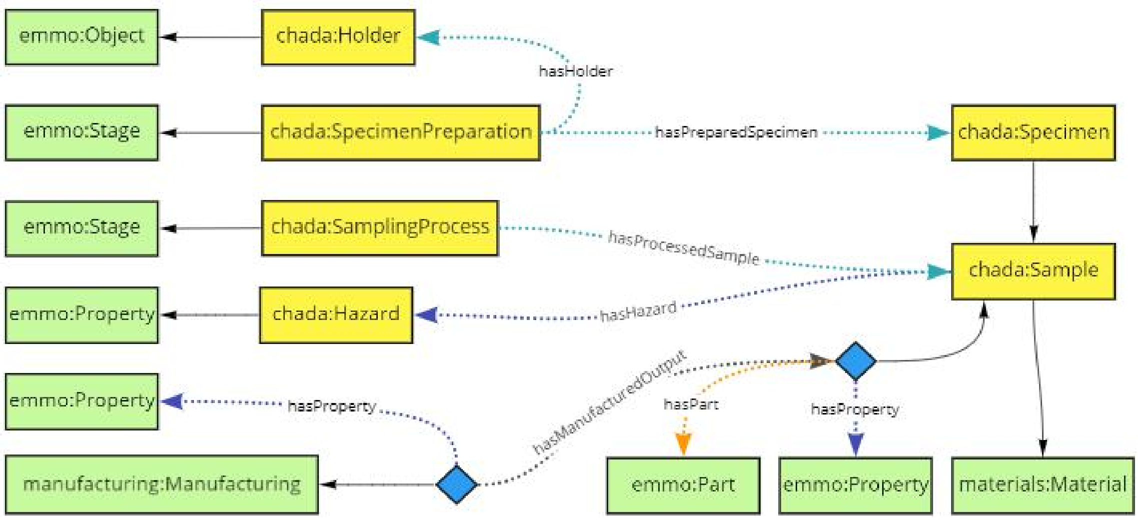
Name the most important 20 terms for the domain of your use case. If available, please add any diagrams illustrating these terms (e.g UML diagram, ER diagram)

1. Material
2. Sample
3. Specimen
4. Characterisation Workflow
5. Characterisation Method
6. Sampling Process

[54] Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

7. Specimen Preparation
8. Calibration Measurement
9. Measurement Process
10. Measurement Parameter
11. Characterisation Environment
12. Data Preparation
13. Data Post Processing
14. Characterisation System
15. Characterisation Machine
16. Probe
17. Detector
18. Raw Data
19. Calibration Data
20. Characterisation Property

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chada:Specimen
emmo:Stage
chada:SamplingProcess
hasProcessedSample
chada:Sample
emmo:Property
chada:Hazard
hasHazard
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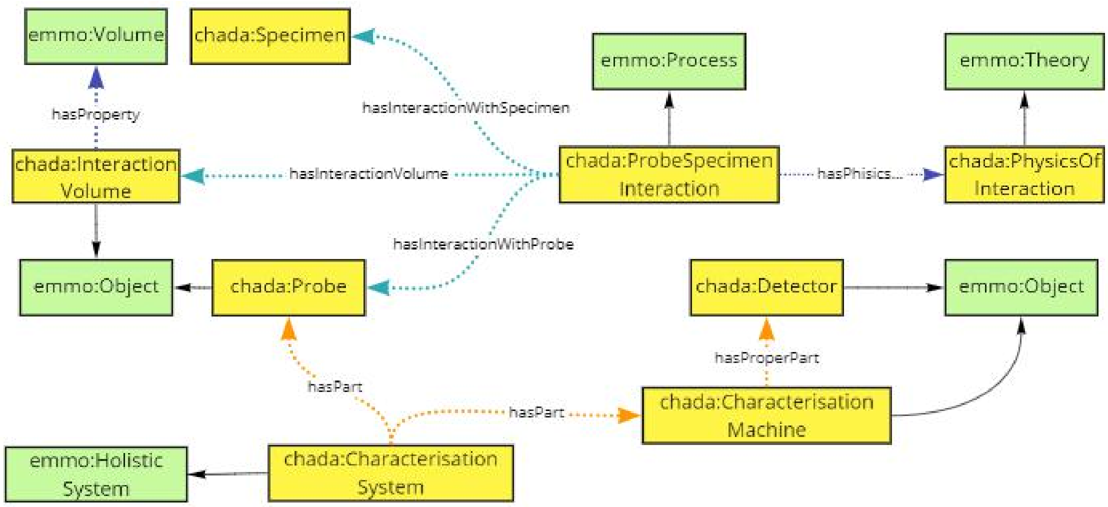
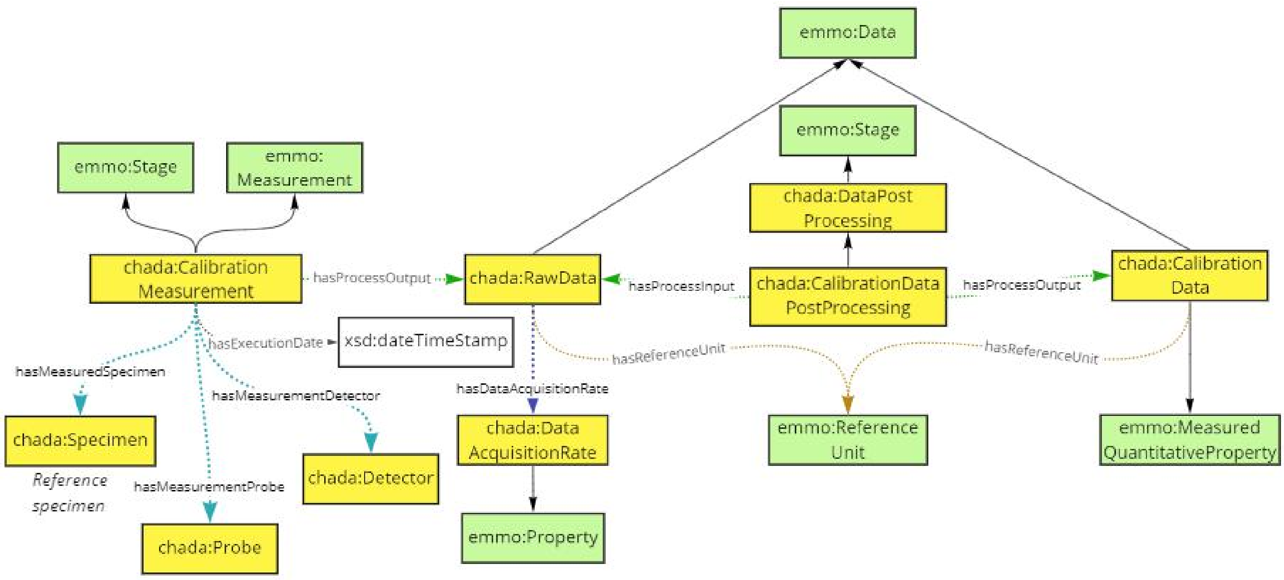
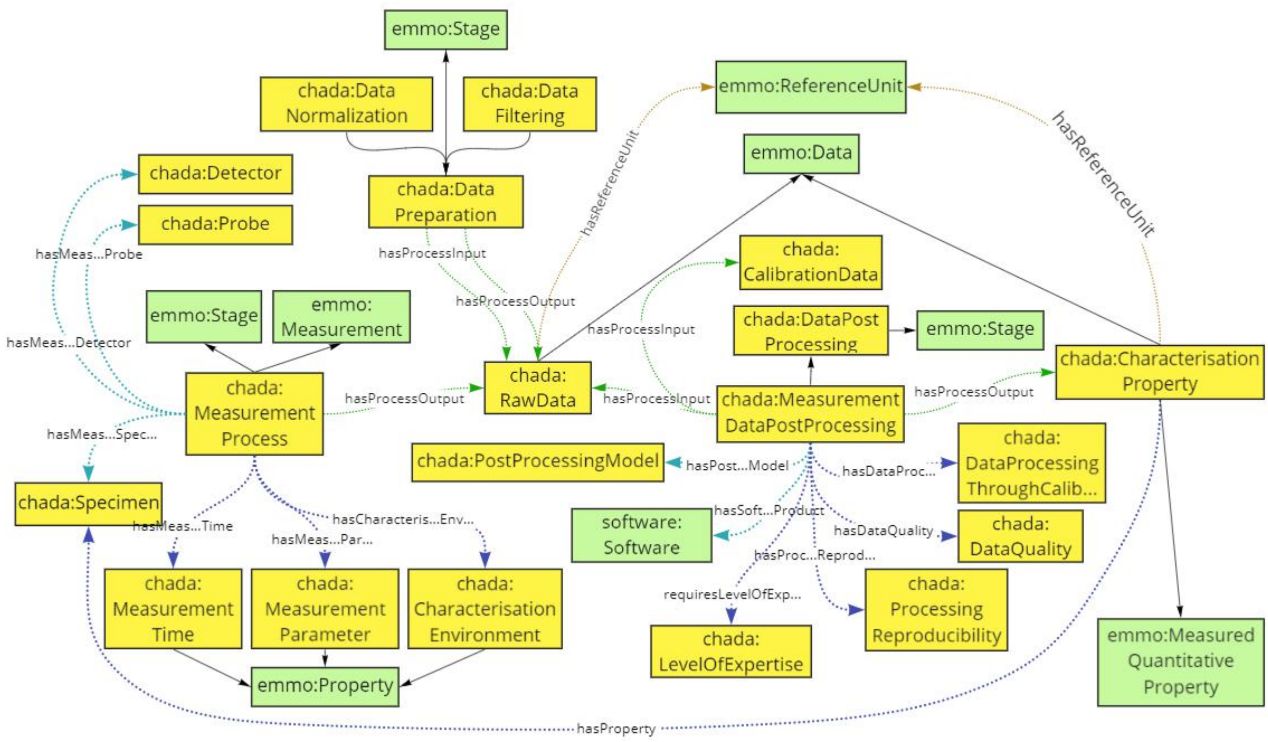
hasProperty
hasManufacturedOutput
hasPart
hasProperty
manufacturing:Manufacturing
emmo:Part
emmo:Property
materials:Material


emmo:Volume
chada:Specimen
emmo:Process
emmo:Theory
hasProperty
hasInteractionWithSpecimen
chada:Interaction Volume
hasInteractionVolume
chada:ProbeSpecimen Interaction
hasPhisics...
chada:PhysicsOf Interaction
hasInteractionWithProbe
emmo:Object
chada:Probe
chada:Detector
emmo:Object
hasProperPart
hasPart
hasPart
chada:Characterisation Machine
emmo:Holistic System
chada:Characterisation System


emmo:Data
emmo:Stage
emmo:Stage
emmo: Measurement
chada:DataPost Processing
chada:Calibration Measurement
hasProcessOutput
chada:RawData
hasProcessInput
chada:CalibrationData PostProcessing
hasProcessOutput
chada:Calibration Data
hasExecutionDate
xsd:dateTimeStamp
hasReferenceUnit
hasReferenceUnit
hasMeasuredSpecimen
hasMeasurementDetector
hasDataAcquisitionRate
chada:Specimen
Reference specimen
hasMeasurementProbe
chada:Detector
chada:Data AcquisitionRate
emmo:Reference Unit
emmo:Measured QuantitativeProperty
chada:Probe
emmo:Property



Software tools to be used/developed

Systems that need to work/be integrated with ontologies

Open Innovation Environment based on https://github.com/simphony/osp-core

Implementation Time Plan

Please provide a rough time plan for your implementation.

Particularly, list the scenario steps by when what will be developed.

Scenario steps	Expected finish time	Comments/Status
Identification of the main concepts, attributes and properties from the CHADA documents and the competency questions filled by the industrial partners.	09-2021	
Design of the CHADA ontology	10-2021	

Mapping with EMMO		
Mapping with DO		
Implementation in OWL-DL	03-2022	
Identify and review other taxonomies to be linked to the CHADA ontology	07-2022	

FAIR Survey

Please fill the survey at the link below in order to help us to understand the FAIR maturity level of your use case.

https://ec.europa.eu/eusurvey/runner/b64d2bc9-28da-3347-332b-0dc6970789d3

What are the future steps to improve FAIRness? What does the demonstrator want to improve? If there are no/little improvement made and/or foreseen, motivate why. If there is an interest to progress here, what are the roadblocks?

Technology Readiness Levels (TRL)

Using the standard definition[55], what is the current TRL of your use case?

TRL3

Key Performance Indicators (KPI)

Please add KPIs specific to your use case, particularly focusing on the KPIs related to evaluating ontology usage in you use case. You can take the generic KPIs below as example and extend table with your use cases specific ones.

KPI	Metric	Function	Range
TRL improvement	• TRL change	– 1/1+(TRL_end - TRL_start)	(0,1]
FAIR improvement	• average score in each FAIR dimension	– For each dimension, average based on final surveys	[0,4] for each dimension
Expressiveness	• Percentage of Competency	– Answer CQ/Total CQ	[0,1]

[55] https://en.wikipedia.org/wiki/Technology_readiness_level

	Questions (CQ) that the ontology can answer through SPARQL		

5.10 UC21: Lubricant Designer

Demonstrator general information

Demonstrator company name and contact person(s):

.Scienomics SAS, Xenophon Krokidis, Andreas Bick

Domain of application[56]

Materials Development, Processing, Life Cycle assessment,

Use case name:

Lubricant Designer

Short Description:

SCIENOMICS is developing a platform of virtual experiments for sustainable materials and product development. These virtual experiments integrate materials and process simulation technology.

Interoperability is a limitation factor and therefore SCIENOMICS is seeking to adopt the relevant ontologies that would allow the communication between different simulation engines which are involved in a virtual experiment.

In this demonstration case we will develop and demonstrate (a) the technology of our platform and how it is possible to easily create user interfaces and (b) using domain ontologies it is possible to develop value-adding workflows. The demonstration case will show, on a practical level, how to develop a Designer for lubricants that fulfil both materials and use constraints.

What are the major (expected) contributions of OntoCommons to the demonstrator?

Scienomics expects access to the standards provided by the OntoCommons project. Scienomics also expects this case to benefit from the wide networking opportunity of the project and the ontology expertise available.

[56] industry where the ontology solution will be used, e.g. Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

Use Case requirements

Use case primary requirements				
UID	Title	Description	Priority (Shall/ Should/ May)	Comment
Use/application of ontologies				
UC21_RQ_U_01	Define a universal structure of the Learning Digital Twin.	A learning digital twin needs to be developed in a manner that satisfies the criteria required for the project. The digital twin should be able to describe a complex product and its parts in all scales.	Shall	
UC21_RQ_U_02	Documentation of domain	Ontology should allow for effective documentation of domain data including related terms.		
Development of ontologies				
UC21_RQ_D_01	Ontology Scope: Develop domain ontology to describe system and communicate with digital twin	Develop a domain ontology that can provide the data model for the digital twin of the system/product studied. The ontologies should enable communication and transition between the different level of scales.	Shall	
Maintaining/extension of ontologies				
UC21_RQ_M_01	Explore existing ontologies e.g., MDO and necessary extensions in order to cover the needs for modeling systems of interest such as formulations	The ontology shall be easy to maintain (e.g. adding lower level terms, additional relations, etc.) from non-ontology experts (e.g. SW engineers).	Shall	
UC21_RQ_M_02	Link ontologies of digital twin and engines.	Ultimately all input for the engines should be gathered from the digital twin and output from the engines	Shall	

		should be entered into the digital twin at the appropriate scale (learning). Ontologies are needed to achieve this goal.		
Tools for ontology				
UC21_RQ_T_01	Visualisation	The tools shall support visualisation of ontologies.	Shall	
UC21_RQ_T_02	Collaboration of multiple stakeholders	The ontology development tool should allow different stakeholders to work simultaneously.	Shall	
Standardisation				
UC21_RQ_S_01	Conformance to standards	Evolve ontologies. It will be important that SIMAGORA is ontology agnostic. Therefore, ontologies need to be evolved, so that SIMAGORA does not depend on only one ontology. There should also be a mechanism to automatically query the web for new developments in the field of ontology (publications, GitHub, etc.)	Shall	

Use Case specification

Please specify a scenario/goal for your use case.

SCIENOMICS SAS, a company specialized in materials simulations, has identified a need for the development of a new environment capable to provide seamless simulation technology for product design and development, where both materials and process simulations involved are considered concurrently. These are implemented in **virtual experiments**. In addition, SCIENOMICS considers the democratization of product design technology essential and therefore it is important to develop an expert system, using artificial intelligence, capable to support decision making processes and consequently make the use of product design techniques by companies of any size possible. Considering the range of all simulation technologies needed in product design and development, it is deduced that a **crowdsourced environment,** which will operate as a **marketplace,** is needed. In this marketplace individual scientists, and engineers along with software companies will offer their integrated virtual experiments technology to address specific product design questions.

Currently SCIEMOMICS has developed a prototype of this marketplace. The protype is aimed to identify critical issues and determine solutions for these issues. The constrains of the project which are related to (a) navigating through the different product scales and aspects; (b) bringing together a diverse audience, **SimTech Providers**[57] and **SimTech Users**[58]; (c) combining different domains of expertise, materials and process simulations and (c) the underlying interoperability impose the use of robust and expandable standardized ontologies.

This document is a storyline for defining the project which will aim to explore alternatives and develop an implementation plan of the ontological framework of SIMAGORA. It will ensure the interconnectivity between the digital representation of the system/product studied and the simulation engines used

What are the pre-conditions of your use case? In which state the system should be in before the scenario starts?

Currently, SCIENOMICS has completed the pilot project **SIMAGORA 0.1** which was aimed to demonstrate the concepts and develop a prototype of the platform which implements several key technologies needed for an open-crowdsourced platform of virtual experiments. In addition, three virtual experiments address specific product design aspects. Working with virtual experiments in SIMAGORA involve three steps.

The first step consists in **defining** the object to be studied. By object we mean the physical product of interest, e.g., a lubricant or a washing powder or even a more complex system such as a recipient (a formulated material product) and its content (a formulated mixture).

The object can be defined using features such as its commercial name, composition and properties that are needed to uniquely identify this object. This step serves also in creating the **Learning Digital Twin (LDT)**[59] of this object, i.e., the digital replica of the object or a component in the form of an entry in a database. The chemicals composing the object are stored in a separate database that contains validated information that can be used by other as source of information.

In this first step the user also defines **the criteria of success**. For instance, the request could be "the optimization of a lubricant". In the final form of the platform an Artificial Intelligence based engine, the **DECISION HUB**, should first identify the expectations. i.e., "optimize", the variables of the problem, e.g., composition or quantities of each component and the criteria of success, e.g., "increased lubrication" or "elimination of a toxic component while keeping all other aspects the

[57] **SimTech Provider** designates a scientist a specialist in simulations who develops virtual experiments in SIMAGORA.

[58] **SimTech User** is an individual who wants to use an existing virtual experiment (either build by her-/himself of by someone else).

[59] Learning Digital Twin should be understood as an evolving entry in a database where knowledge about properties and other aspects of the object under scrutiny is gained and stored in a standardized and retrievable manner. This knowledge is structured following a domain specific ontology.

same". The DECISION HUB would also identify the appropriate virtual experiments for this request with regards to their performance, reliability, costs, etc.

In a second step, the relevant properties of the product of interest are calculated by appropriate simulation engines, e.g., chemical engineering engines, which in return require input related to the properties of the materials that constitute the object studied. These materials should have their own learning digital twin, stored in a separate database containing all validated information which can be either shared or private (altogether or segments of it). For known chemicals reliable external databases can be used or data produced earlier. In the case of new chemicals or when information in databases is not available, materials simulations techniques, including machine learning based models, can be used. Specific requirements for Machine Learning Models are defined in a separate document

The third step finally involves the execution of the virtual experiment(s) and the updates of the information associated to the learning digital twin of the product.

What are the post-conditions of your use case? What is the expected state of the system after the scenario is completed?

Currently, the learning digital twin data structure (properties and their relations) are "hard-coded". This approach has several limitations, and it is understood that it is not sustainable, especially when the final version of the platform will be open to a large and diverse community with an increased number of expectations. Therefore, step involves the execution of the virtual experiment(s) and the updates of the information associated to the learning digital twin of the product.

Each level of information can be characterized by a learning digital twin ID, a scale ID (e.g., macroscale), and a sub-ID for each scale (since there can be many parts/segments of the same one object). Every additional information gained by operating any node in a virtual experiment should be transferred back to the digital twin and enrich its knowledge. By operating this way, a dynamic ontology is created.

Another advantage of such a design is the fact that no adapters will be required between the nodes of a virtual experiment, since the knowledge graph connects all engines with the learning digital twin, from where all model related information can be obtained by the relevant engines.

Who are the actors (people or automated digital agents) involved in the scenario when in operation or needed during development?

SimTech Providers and **SimTech Users** as explained in the above outline of the project, combining different domains of expertise, materials and process simulations The underlying interoperability imposes the use of robust and expandable standardized ontologies and use of artificial intelligence to facilitate the dialogue and execution of the tasks.

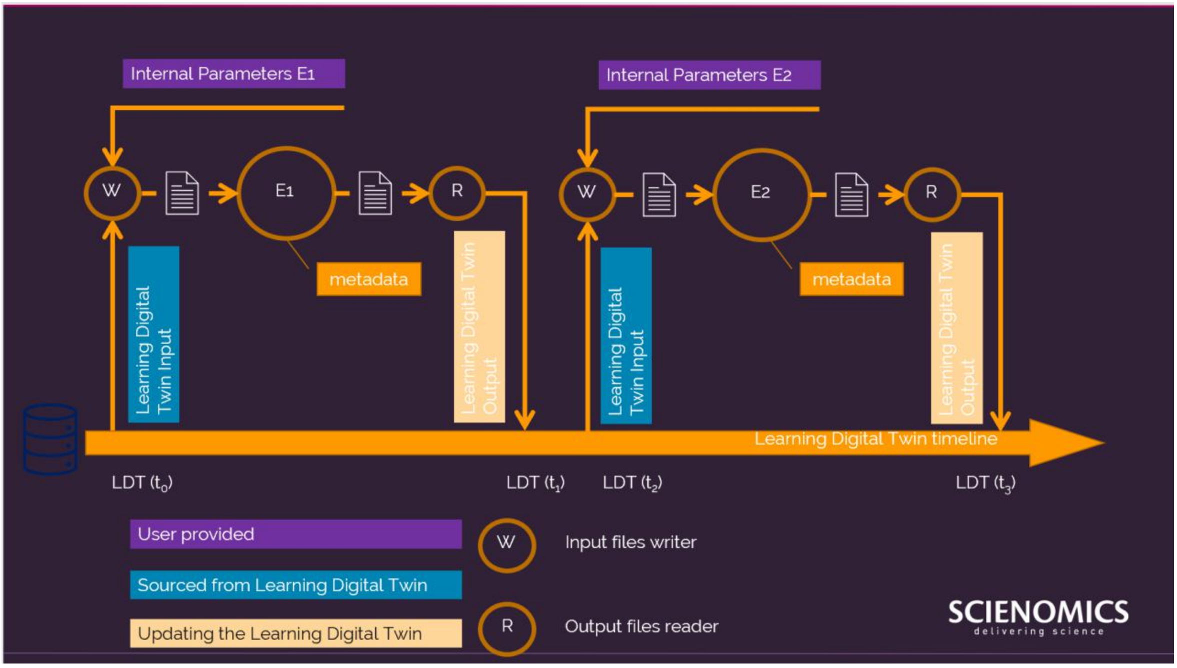
What are the steps of the main scenario?

Please add one row for each step in your scenario. If a step involves with an ontology or a tool, please specify its name and purpose at this step. If some of types of ontologies (Top Level Ontology, Mid-Level Ontology, Domain Ontology) are not used, explain why. Also include intentions for future development plans.

No	Description	TLO	MLO	DO	Tools
X1	Define a universal structure of the Learning Digital Twin.			Create underlying infrastructure for all ontologies to communicate with.	OWL
Y2	Develop a domain ontology that can provide the data model for the digital twin of the system /product studied.	Yet to be identified	MDO and necessary extensions in order to cover the needs for modeling systems and processes of interest	Domain ontology for engines, domain ontology for products, domain ontology for processes	OWL

Workflow

Please add here a picture that describes the best the aforementioned user story, in a compact way with discrete steps (e.g. as workflow).



Which data sources are used? (Please cross-reference with the steps of the main scenario) Which is the domain of these data sources[60]?

Data will be used to describe the systems to be treated, the processes to be described and the engines to be integrated. Engine data will be provided by the SimTech providers.

End users will provide systems and process data on a non-proprietary basis. Additional data sources are publicly available databases, for example DIPPR.

Ontologies

Ontologies already used in the use case (consistent with the main scenario)

- If yes:
  - Top Level Ontologies used / Developed by:
  - Domain Ontologies Used / Developed by:
  - Other Ontologies / Taxonomies used or suggested to be used (developed by):

Primary purpose of ontology application in this use case

Interoperability

Identified challenges in the use of ontologies in this use case

Existing Ontologies will not cover all needs of the project, extensions will be needed for all scenarios

(small) Examples of problems in ontology usage

Name the most important 20 terms for the domain of your use case. If available, please add any diagrams illustrating these terms (e.g UML diagram, ER diagram)

Work in progress

Software tools to be used/developed

Neo4j, Protege, Java, GraphQL

Implementation Time Plan

Please provide a rough time plan for your implementation.

Particularly, list the scenario steps by when what will be developed.

Scenario steps	Expected finish time	Comments/Status
UC1 WP 1 -4	06.2022r	
UC1 WP 5	12.2022	

[60] Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

	Month-Year	
	Month-Year	

FAIR Survey

Please fill the survey at the link below in order to help us to understand the FAIR maturity level of your use case.

https://ec.europa.eu/eusurvey/runner/b64d2bc9-28da-3347-332b-0dc6970789d3

What are the future steps to improve FAIRness? What does the demonstrator want to improve? If there are no/little improvement made and/or foreseen, motivate why. If there is an interest to progress here, what are the roadblocks?

Technology Readiness Levels (TRL)

Using the standard definition[61], what is the current TRL of your use case?

We are currently at TRL4, with the aim to reach TRL 6

Key Performance Indicators (KPI)

Please add KPIs specific to your use case, particularly focusing on the KPIs related to evaluating ontology usage in you use case. You can take the generic KPIs below as example and extend table with your use cases specific ones.

KPI	**Metric**	**Function**	**Range**
TRL improvement	• TRL change	Improve project from TRL 4 to TRL 6	4,6
FAIR improvement	• average score in each FAIR dimension	– For each dimension, average based on final surveys	[0,4] for each dimension

[61] https://en.wikipedia.org/wiki/Technology_readiness_level

Use case specific KPI - 1	•	–	
.	•	–	

5.11 UC22: Automated production of a nutrient solution for soil-less culture application.

Demonstrator general information

Demonstrator company name and contact person(s):

UFRGS - Edison Pignaton de Freitas (edison.pignaton@ufrgs.br)
Pedro H Morgan Pereira (phmorganpereira@gmail.com)

Domain of application[62]

Agriculture, Industry, IoT.

Use case name:

Automated production of a nutrient solution for soilless culture application.

Short Description:

Automated production of a nutrient solution is of paramount importance for soilless culture applications, e.g., hydroponics agriculture techniques. This can be accomplished by monitoring the environment and remote controlling a sequence of processes. The use of heterogeneous IIoT devices equipped with different sensors and actuators allows this to happen. These devices can use distinct communication protocols and data structuring, which increases interoperability problems. An industry 4.0 oriented ontology, based on the IEEE 1872 international standard, is in development to mitigate these problems.

What are the major (expected) contributions of OntoCommons to the demonstrator?

Semantic representation of heterogeneous IoT devices using unified IIoT ontology, based on well-established ontologies, in order to mitigate interoperability problems in industrial applications (data interoperability and interconnectivity).

[62] industry where the ontology solution will be used, e.g. Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

Use Case requirements

Use case primary requirements				
UID	Title	Description	Priority (Shall/ Should/ May)	Comment
Use/application of ontologies				
UC22_RQ_U_01	Configuration of IIoT gateway.	The IIoT gateway shall be configured by the user using two ontology-based files (JSON and YAML files) and start the respective communication protocols servers and interoperability scripts.	Shall	
UC22_RQ_U_02	Simulation.	The use case interoperability shall be evaluated by running simulations with the IoT device's digital twins.	Shall	
UC22_RQ_U_03	Monitor real time data exchange.	All data exchanged between the devices can be monitored in real time by a SCADA system hosted by the IoT gateway.	Shall	
UC22_RQ_U_04	Data storage	The data exchanged by different IoT devices shall be stored in a database (influx DB) to be used as a dataset for future machine learning applications.	Shall	
UC22_RQ_U_05	Validation	The use case interoperability may be evaluated in a real industrial plant setup.	May	
Development of ontologies				
UC22_RQ_D_01	Description of communication protocols	The ontology shall describe all communication protocols present in the use case, as well as, all its configuration information (such as, MQTT url, port, and topics).	Shall	
UC22_RQ_D_02	Description of device data	The ontology shall describe the type of data exchanged by IoT devices and present the dependency data for each node.	Shall	
Maintaining/extension of ontologies				
UC22_RQ_M_01	Easy maintenance of ontology	The ontology shall be easy to maintain (e.g. adding lower level	Shall	

		terms, additional relations, etc.) from non-ontology experts (e.g. SW engineers).		
Standardisation				
UC22_RQ_S_01	Conformance to standards	There shall be compliance to domain and W3C standards (e.g. ISO).	Shall	
UC22_RQ_S_02	Conformance to standards	There should be compliance to other relevant domain standards (e.g. IEEE)	Should	

Use Case specification

Please specify a scenario/goal for your use case.

An industrial environment is monitored and controlled by heterogeneous IoT devices equipped with several sensors and actuators. These devices must communicate and understand each other to reach a common goal even using divergent communication protocols and data structures.

What are the pre-conditions of your use case? In which state the system should be in before the scenario starts?

Before the application starts a researcher/engineer must describe all assets, gateway, IoT nodes, sensors, and actuators. After correctly describing and configuring the gateway, the application will start when prompted and run autonomously until it's prompted to stop.

What are the post-conditions of your use case? What is the expected state of the system after the scenario is completed?

After the application is finished it can be restarted without any change if all devices are the same. Otherwise, if a new device is included in the application or a new sensor is connected to a node the ontology must be adjusted. If not, the gateway's configuration file will lead to communication and syntactical errors.

Who are the actors (people or automated digital agents) involved in the scenario when in operation or needed during development?

During the development, at least one person is needed for describing the use case, since it will be used to create two configuration files. One of these files will describe the different communication protocols used by the IoT nodes in order to configure the communication protocol translator scripts used by the gateway correctly. And the other one will identify the type of sensors and actuators used and their respective dependencies. On the other hand, during the application, the process will be carried out automatically by the gateway and the IoT nodes.

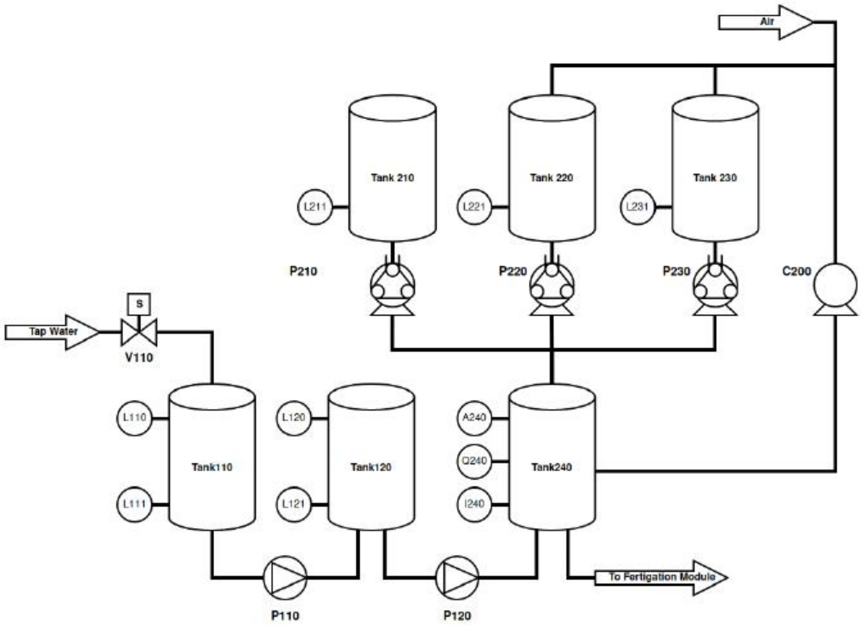
What are the steps of the main scenario?

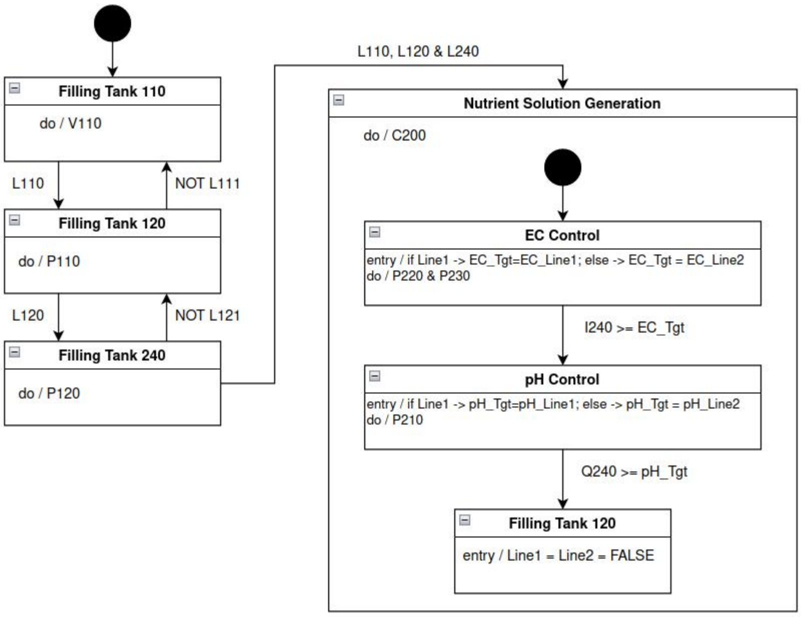
Please add one row for each step in your scenario. If a step involves an ontology or a tool, please specify its name and purpose at this step. If some types of ontologies (Top Level Ontology, Mid-Level Ontology, Domain Ontology) are not used, explain why. Also include intentions for future development plans.

No	Description	TLO	MLO	DO	Tools
1	Initial IIoT ontology based on IEEE Std 1872-2015.			Literature search for international standards	Open source ontology editor and framework Protégé.
2	Well established sensor and IoT based ontology			Literature search for sensor related standardised ontologies	Open source ontology editor and framework Protégé.
3	Use case described in the developed IIoT based ontology.			Description of sensors, actuators, IoT devices and gateways based on the developed ontology.	Open source ontology editor and framework Protégé.
4	Gateway configuration files.			Creation of two gateway configuration files based on the information used on the developed ontology.	YAML and JSON files.
5	Gateway configuration and bridging scripts.			Gateway configuration using both ontology related files. Creation of bridging scripts for MQTT, DDS and OPC-UA	The Robot Operating System (ROS) 2 Galactic.

				communication protocols using python scripts.	
6	Digital Twin Scripts.			Creation of each IoT device digital twin script for simulating the use case on a non physical (pandemic) scenario.	The Robot Operating System (ROS) 2 Galactic.
7	SCADA			Development of and scada system for monitoring sensors and actuators data on real time.	Node-RED programming tool.
8	Use case simulation			Use case simulation using the communication bridging script. Monitoring data through the SCADA system and simulating three devices using three different digital twin scripts.	
9	Database			Database creation for storing simulation data	Influx DB
10	Final simulations, dataset			will be carried out several simulations in which data will be stored in database buckets for creating datasets for machine learning applications.	

Workflow





Which data sources are used? (Please cross-reference with the steps of the main scenario) Which is the domain of these data sources[63]?

In this use case, the main data sources are the sensors (temperature, pH, and Ec) and the actuators (valves and pumps). Each IoT device shares its data through a robust IoT gateway regardless of the communication protocol or data structure. Still, it is possible to carry out simulations of this application using digital twins of the devices, and consequently, their

[63] Manufacturing, Processing, LCA, Materials development, Materials Modelling, Materials Characterisation, Nano-safety

sensors and actuators. In this case, the data will be generated synthetically by some programming script to certify interoperability within the use case.

Ontologies

Ontologies already used in the use case (consistent with the main scenario)

- If yes:
    - **Top Level Ontologies used / Developed by:**
      Sumo / Developed by the Teknowledge Corporation
    - **Domain Ontologies Used / Developed by:**
    - **Other Ontologies / Taxonomies used or suggested to be used (developed by):**

      QU Ontology / developed by W3C Semantic Sensor Network Incubator Group.

      SSU Ontology / developed by W3C Semantic Sensor Network Incubator Group.

      IoT-Lite Ontology / developed by W3C Semantic Sensor Network Incubator Group.

      POS Ontology / IEEE Std 1872-2015.

      ROCO - Robotic Cloud Ontology / IEEE Std 1872-2015.

Primary purpose of ontology application in this use case

Help to mitigate interoperability problems in industrial applications (data interoperability and interconnectivity) by using and standardised data structure based on the IIoT nodes communication protocols and data specified in the developed ontology.

Identified challenges in the use of ontologies in this use case

The big challenge regarding the use of ontologies in this use case is to create the description of a high number of IoT devices. The main characteristics of the devices must be presented, as its communication protocol. Furthermore, each IoT node can have several sensors and actuators, for each one, its main characteristics such as scale, type, and unit must be described. The large quantity of devices leads to a high development time.

(small) Examples of problems in ontology usage

When creating the ontology, the device characteristics and its sensors and actuators must be correct. Otherwise, a single error in the definition of the device's communication protocol or the type of the sensor will lead to more interoperability problems, preventing communication/ data understanding between the IIoT nodes.

Name the most important 20 terms for the domain of your use case. If available, please add any diagrams illustrating these terms (e.g UML diagram, ER diagram)

Interoperability, IIoT, Devices, Gateway, Sensors, Actuators, Communication protocols, Asset, AAS, Scada, Database, Digital Twin, Automation, Nutrient Solution, pH, Ec.

Software tools to be used/developed

First, it describes the use case ontology in the software Protégé. Using the ontology specification, it is generated two configuration files (JSON and YAML files). One of these files describes the IoT devices, such as their communication protocol, sensors, actuators, and data dependencies. The second file specifies the communication protocols information, such as credentials, security certificates, servers, and brokers' URLs.

Second, both ontology-based files are used to configure the gateway. After the configuration, both the OPC-UA server and the MQTT broker must start, sequentially, the database (influx DB) and the bridging scripts (python). To monitor the sensors and actuator's status the Node-Red dashboard is used in which it is also possible to start the simulation by running the digital twin scripts (python) for all devices.

Implementation Time Plan

Please provide a rough time plan for your implementation.

Particularly, list the scenario steps by when what will be developed.

Scenario steps	Expected finish time	Comments/Status
1 to 3	April-2021	Concluded
4 and 5	Jul-2021	Concluded
6	Sep-2021	Concluded
7	Oct-2021	Concluded
8	Dec-2021	Concluded
9	Feb-2022	On going
10	March-2022	After scenario step 9 is over.

FAIR Survey

Please fill the survey at the link below in order to help us to understand the FAIR maturity level of your use case.

https://ec.europa.eu/eusurvey/runner/b64d2bc9-28da-3347-332b-0dc6970789d3

What are the future steps to improve FAIRness? What does the demonstrator want to improve? If there are no/little improvements made and/or foreseen, motivate why. If there is an interest to progress here, what are the roadblocks?

The future steps would be targeting the deployment in a real industrial plant to check validity.

The demonstrator wants to improve interoperability between different devices.

Technology Readiness Levels (TRL)

Using the standard definition[64], what is the current TRL of your use case?

TRL 5

Key Performance Indicators (KPI)

Please add KPIs specific to your use case, particularly focusing on the KPIs related to evaluating ontology usage in your use case. You can take the generic KPIs below as example and extend table with your use cases specific ones.

KPI	Metric	Function	Range
Number of gateways	• quantity of gateways used for the specific application	– Add more gateways to the application depending on the number of devices and the physical area of the use case.	(0,QTD*gateways*]
Number of communication protocols	• quantity of communication protocols supported by the platform	– For each new communication protocol a new bridging script must be developed.	[0,QTD*CommProtocols*]

[64] https://en.wikipedia.org/wiki/Technology_readiness_level

		– Nbscripts = QTD*CommProtocols*	
Saving time for new devices integration	• Required time to insert a new device into the system	– Add new devices to the system	(0, elapsed_time_to_insert_device)
	•	–	