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ORIENTING

D3.1

Data ontologies

Documentation of the ORIENTING LCSA ontology (ORIONT)

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TABLE OF CONTENTS

LIST OF TABLES AND FIGURES

Tables

Figures

Acronyms

BoM	Bill of Materials
BONT	BONSAI ontology
CF	Characterisation Factor
CTI	Circular Transition Indicators
eILCD	extended International Life Cycle Data format
EMMO	Elementary Multiperspective Material Ontology
ILCD	International Life Cycle Data system
IPCC	Intergovernmental Panel on Climate Change
ISO	International Organization for Standardization
LC	Life Cycle
LCA	Life Cycle Assessment
LCC	Life Cycle Costing
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LCSA	Life Cycle Sustainability Assessment
OM	Ontology of units of Measure
OOF	ORIENTING Output Format
ORIONT	ORIENTING LCSA ontology
OWL	Web Ontology Language
QUDT	Ontology for units of measure, QUantity kinds, dimensions and Data Types
RDFS	Resource Description Framework Schema
S-LCA	Social Life Cycle Assessment
XML	Extensible Markup Language

1. Executive summary

This report describes the LCSA ontology developed in the ORIENTING project: "ORIONT". The purpose of ORIONT is to structure the most important methodological and data elements (ontology classes) and their relationships. The elaboration of an ad hoc ontology helps in a) assuring conceptual consistency between the different sustainability topics to be integrated, b) facilitating interoperability between information resources, databases, and simulation software used for LCSA, and c) it can inform data format needs as discussed in ORIENTING deliverables D3.2 (ORIENTING, 2022b) and D3.3 (ORIENTING, 2022b).

ORIONT builds on previous ontology efforts in the sustainability field, in particular on the BONSAI ontology (BONT, Ghose et al., 2021) and on the eILCD data format (European Commission, 2022) developed within the LCA work of the European Commission, which has – as any data format – an ontology-like inherent structure. Thereby, ORIONT is aligned with existing ontologies and data formats. Furthermore, it is coherent with the methodological framework developed in ORIENTING. While being tailored to ORIENTING developments, ORIONT is kept general enough to be considered a general LCSA ontology.

The main role of ORIONT within ORIENTING is the content explication in order to align data structure and conceptually integrate data across sustainability topics. This is achieved by the ontology visualisation, which was discussed with topic experts within the project, and is described in this report.

2. Introduction

This report describes the LCSA ontology developed in the ORIENTING project: "ORIONT". The purpose of ORIONT is to structure the most important methodological and data elements (ontology classes) and their relationships. The elaboration of an ad hoc ontology helps in a) assuring conceptual consistency between the different sustainability topics to be integrated, b) facilitating interoperability between information resources, databases, and simulation software used for LCSA, and c) it can inform data format needs as discussed in deliverables D3.2 (ORIENTING, 2022b) and D3.3 (ORIENTING, 2022c).

ORIONT does not have to be created from scratch. Ontologies to structure data for sustainability assessments have already been proposed, for example, in Janowicz et al. (2015), Kuczenski et al. (2016), Pauliuk et al. (2019), and Ghose et al. (2021). Furthermore, existing data formats have a structure, which is ontology-like. In developing ORIONT, we have considered a) the latest "LCSA ontology" available, the BONSAI ontology (Ghose et al., 2021), which builds on the others mentioned above, and b) the eILCD data format, which was developed within the LCA work of the European Commission (European Commission, 2022). ORIONT is at the same time aligned with existing ontologies and data formats and coherent with the methodological framework developed in ORIENTING D2.3 (ORIENTING, 2022a) (see Figure 1 to see how these different elements were considered in the development of ORIONT). While being tailored to ORIENTING developments, ORIONT is kept general enough to be considered a general LCSA ontology.

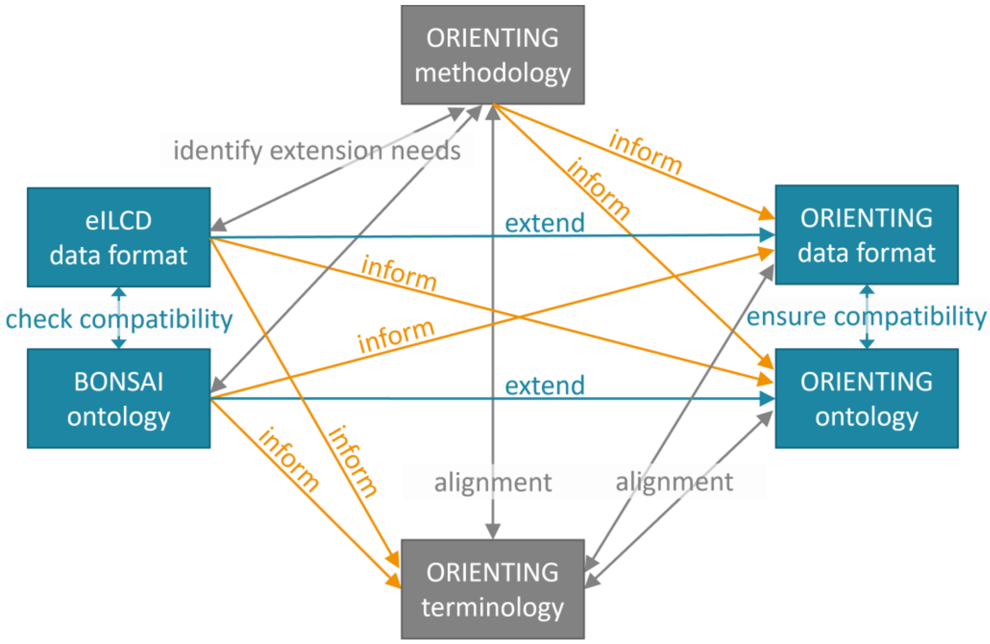

Figure 1. Material and workflow used to conceptualise the ORIENTING LCSA ontology (ORIONT) and data format.

This deliverable is structured as follows: First, this report gives a general introduction to ontologies in section 3. Then, the two main information sources, the BONSAI ontology and the eILCD format are compared in section 4. In section 5, the identified extension needs for an ORIENTING LCSA ontology are further discussed and ORIONT is documented in explained in more detail. Finally, section 6 provides the concluding remarks to this deliverable.

3. General introduction to ontologies

This section contains a general introduction to ontologies. The roles that ontologies can play in general are discussed. To conclude, their relationship to data format, especially in the ORIENTING LCSA context, is presented.

3.1. What is an ontology

An ontology is a description of concepts and their relationships (Gruber, 1995). Ontologies simplify the complexity of an application domain (for example LCSA in the ORIENTING case) and organize data into information and knowledge concepts (Wikipedia, 2022a). They allow keeping an easy and consistent communication among experts by providing the necessary structure to link one piece of information to other pieces of information and facilitate data linking and interpretation (Ontotext, 2022). Furthermore, because ontologies are used to specify common modelling representations of data from various systems, databases, and information sources, they enable interoperability of data sources, cross-database search, and smooth knowledge management. This is ensured by providing a controlled, formal vocabulary that consists of naming and defining categories in, properties of, and relations between the concepts, data and entities that substantiate one or several domains (Wikipedia, 2022a).

3.2. Ontology components

This section is based on Schrader (2020). Ontologies can be structured with the help of many different components. Which components are used is dependent on the domain for which the ontology is established. However, there are 3 main components that are essential for any ontology.

- Classes – types of things that exist in the data.
- Relationships – properties connecting two classes.
- Attributes – properties describing a class.

To make an example, data on books/publications might consist of the following classes:

- Books.
- Authors.
- Publishers.
- Locations.

Each of these classes will have several so-called “properties” specifying it. Some of these properties describe only the class Book, while others can represent a relationship to other classes. Each relationship should be defined as well.

- Book **has an** Author – Relationship.
- Book **has a** Publisher – Relationship.
- Book **is published on** Publication Date – own Attribute.
- Book **is followed by** Book (Sequel Publication) – Relationship.

3.3. Representing ontologies

This section is based on Schrader (2020). An ontology can be represented in a graph depicting the general concepts, classes, relationships, and attributes (see Figure 2).

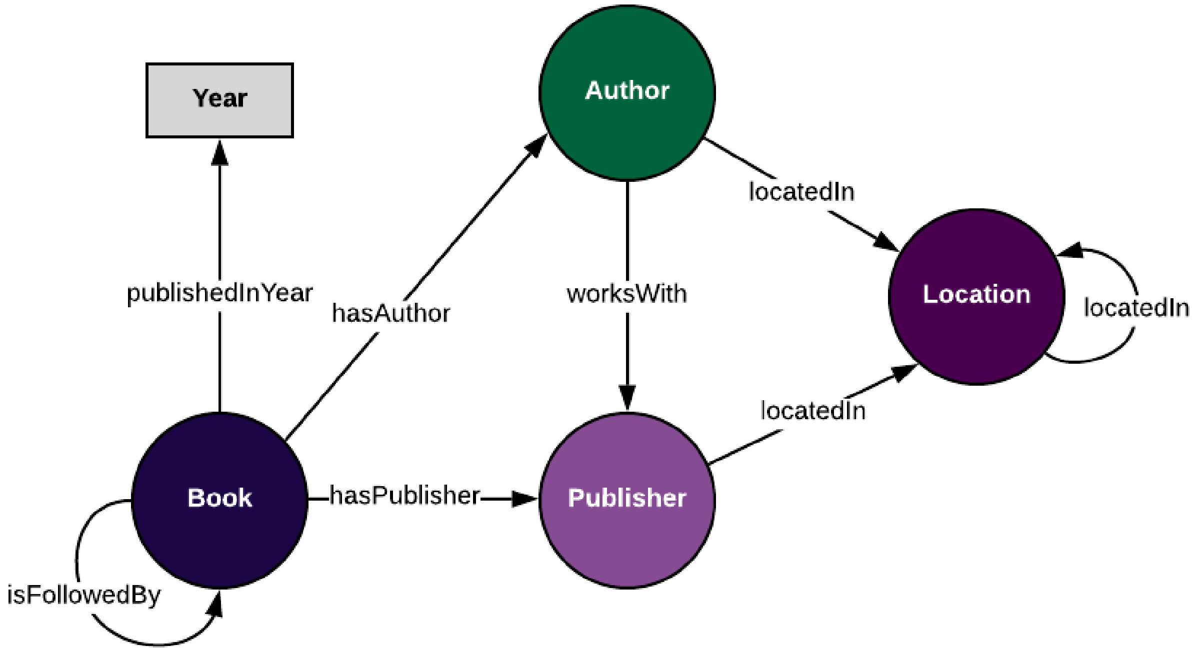

Figure 2. An ontology graph (taken from Schrader, 2020).

Once the general conceptualisation is related to specific data, a knowledge graph can be produced. A knowledge graph depicts the individual data points and their relationships based on the defined ontology (see Figure 3. In the following, we are only interested in the ontology).

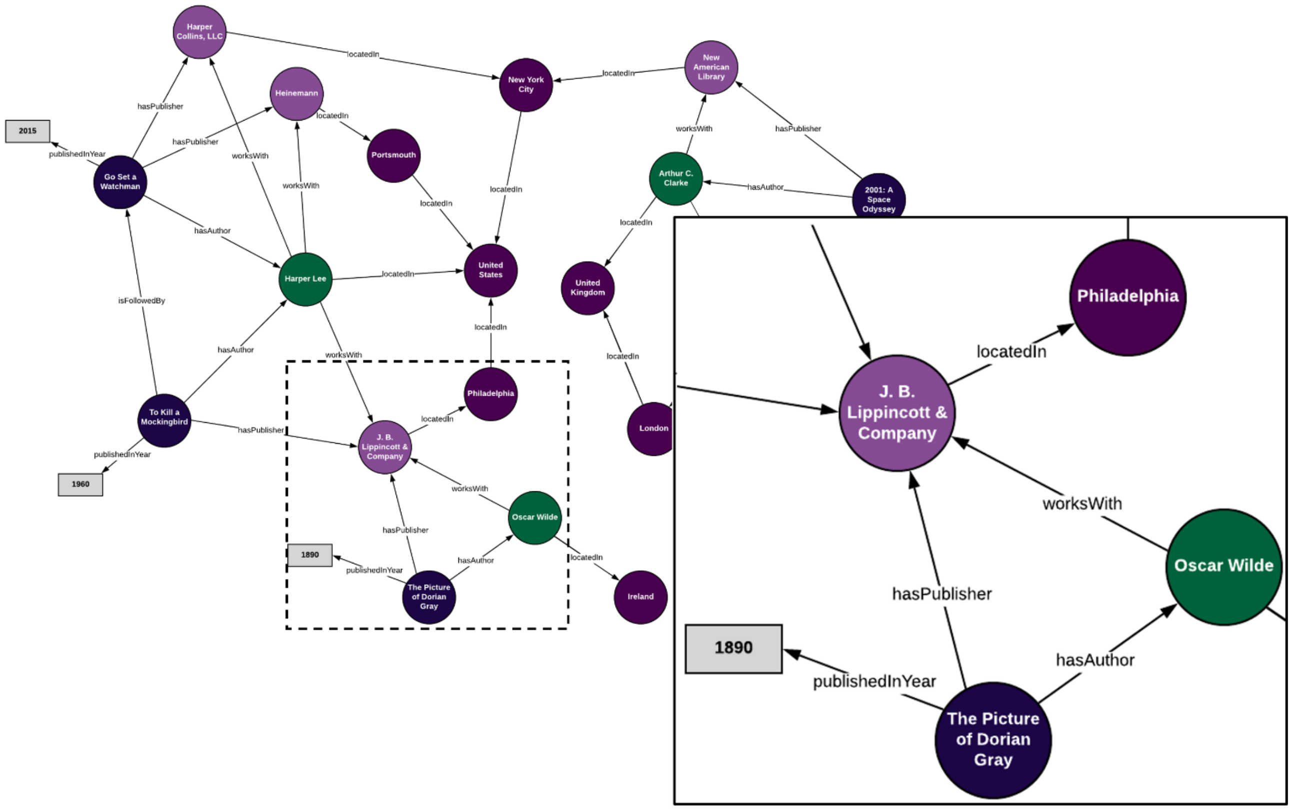

Figure 3. A Knowledge Graph using the ontology from Figure 2 as applied to 4 individual books (based on from Schrader, 2020).

3.4. Design criteria for ontologies

This section is based on Gruber (1995), according to whom the creation of an ontology is a design process. The design decisions must be guided by and evaluated against the purpose of the ontology. In other words, the design is judged by its utility for the domain of usage, people using the ontology and the purpose for which the ontology is defined. Ontologies do not aim to exhaustively describe and define all concepts within a domain, but rather to provide a consistent way of naming, defining, and interpreting a set of concepts relevant to the ontology's goal. There are several criteria that can help to design an ontology:

1. **Clarity:** An ontology should effectively communicate the intended meaning of defined terms. All concepts should have a definition in natural language. Definitions should be as objective and independent from other contexts as possible (for example, defining "ecosystem" in the context of the natural environment should not rely on the definition of ecosystem from the built environment). A complete definition should ideally include necessary and sufficient conditions to define a thing as belonging to the concept at hand.

2. **Coherence:** An ontology should be coherent. Inferences (deduced new information) based on the ontology representation must be consistent with the provided definitions and vocabulary.

3. **Extendibility:** An ontology should be designed so that one should be able to define new terms for special uses in a way that does not require revision of the existing definitions.

4. **Minimal encoding bias:** The concepts and their relationships should be specified based on knowledge rather than the ease of notating or representing the ontology.

5. **Minimal ontological commitment:** An ontology should make as few claims as possible about the world being represented. For example, an ontology can minimise the number of defined concepts to the ones essential to the knowledge domain and purpose of usage. This will allow most users to benefit from the ontology and allow for extendibility and specialization of the ontology.

3.5. Ontology tools

This section is based on Wikipedia (2022a). As ontologies are used across fields and disciplines, there are already tools available that facilitate creation and identification of relevant ontologies.

Languages

Ontologies can be created using a formally specified language that encodes the concepts and their relationships. Such language can then be automatically translated by other tools to create Ontology graphs or other representations of the ontology. An example of such a language is the Web Ontology Language (OWL; OWL, 2013).

Ontology Editors

Ontology Editors are software tools that enable easy creation and editing of ontologies. They also help with defining and visualising the ontology. Some of these tools are publicly available, while others might be a paid software. For OWL, there are, for example, the Protégé (Stanford University, 2020) or the OWLGrEd (IMCS UL, 2020) editors.

Libraries

With the growing number of available ontologies, services to collect and search existing ontologies emerged as well. For example, the BioPortal repository of biomedical ontologies approaches 1000 of available ontologies for biomedical sciences (Bioportal, 2022).

For ORIONT, the OWL language, the Owlready2 package for ontology-oriented programming in Python (Lamy, 2017), and the Protégé editor were used.

3.6. The roles of ontologies in data integration

The elaboration of an LCSA methodology includes the integration of different sustainability topics. Here, an ontology can be of help by ensuring conceptual consistency of information from these different topics. Generally, ontologies might play the following roles in data integration:

> *"Ontologies enable the unambiguous identification of entities in heterogeneous information systems and assertion of applicable named relationships that connect these entities together. Specifically, ontologies play the following roles:*
>
> ***Content Explication:*** *The ontology enables accurate interpretation of data from multiple sources through the explicit definition of terms and relationships in the ontology.*
>
> ***Query Model:*** *In some systems […], the query is formulated using the ontology as a global query schema.*
>
> ***Verification:*** *The ontology verifies the mappings used to integrate data from multiple sources. These mappings may either be user specified or generated by a system." (Wikipedia, 2022b)*

The main role of ORIONT within ORIENTING is the content explication in order to align data structure and conceptually integrate data across sustainability topics. However, it could be used, similar to the application shown in Ghose et al. (2021), for database integration and as a query model.

3.7. Ontology in ORIENTING

In the project proposal, ontology is described as follows:

> *"[…] a common structure and architecture – in terms of (1) Format, (2) Nomenclature and (3) Classification of activities and products, as well as regarding (4) Unit and (5) System construction – at the LCSA level."*

During the project and with learning about ontologies in information science, we have moved to a more formal understanding of ontology. **ORIONT aims at fulfilling the definition that "an ontology encompasses a representation, formal naming, and definition of the categories, properties, and relations between the concepts, data, and entities that substantiate one, many, or all domains of discourse" (Wikipedia, 2022a), the domain obviously being LCSA.**

4. Comparison of the BONSAI ontology (BONT) and the eILCD data format

Since the BONSAI ontology (BONT) and the eILCD data format build the basis for ORIONT (see Figure 1), they were compared for compatibility. In this section, first, the basic structure of BONT is introduced, subsequent, the eILCD data format, and finally, the two ontologies are compared.

In order to compare the BONSAI ontology and the eILCD data format, they need to be accessed. The BONSAI ontology is available from https://ontology.bonsai.uno/core/ontology_v0.2.ttl and can be accessed by means of the ontology editor Protégé, available from https://protege.stanford.edu/.[1] The eILCD data format is a collection of XML datasets. This list of datasets and what they contain can be best examined by having a look at the data format documentation here: https://eplca.jrc.ec.europa.eu/LCDN/developerILCDDataFormat.xhtml.

4.1. Ontologies in LCA/LCSA: the BONSAI ontology (BONT)

The BONSAI ontology (BONT) builds on previous ontologies suggested for sustainability assessment (Ghose et al., 2021). There are two main applications of this ontology: 1) data integration of two different publicly available databases, the EXIOBASE and the Yale Stock and Flow Database, and 2) querying the resulting integrated database (see roles of ontologies in data integration in section 3.6). BONT is displayed in Figure 4. Descriptions and examples for the different elements are provided in Table 1. Since BONT is rather generic/macro-level, it was deemed necessary to adapt it with the aim to be more specific and to cover all sustainability topics to arrive at an ORIENTING LCSA ontology (ORIONT) (see section 5).

[1] Please note that when trying to access the ontology online in October 2022 (via "Open from URL…" and putting https://ontology.bonsai.uno/core/ontology_v0.2.ttl), this did not work anymore. However, the ontology can still be downloaded from https://ontology.bonsai.uno/ and then opened in an editor.

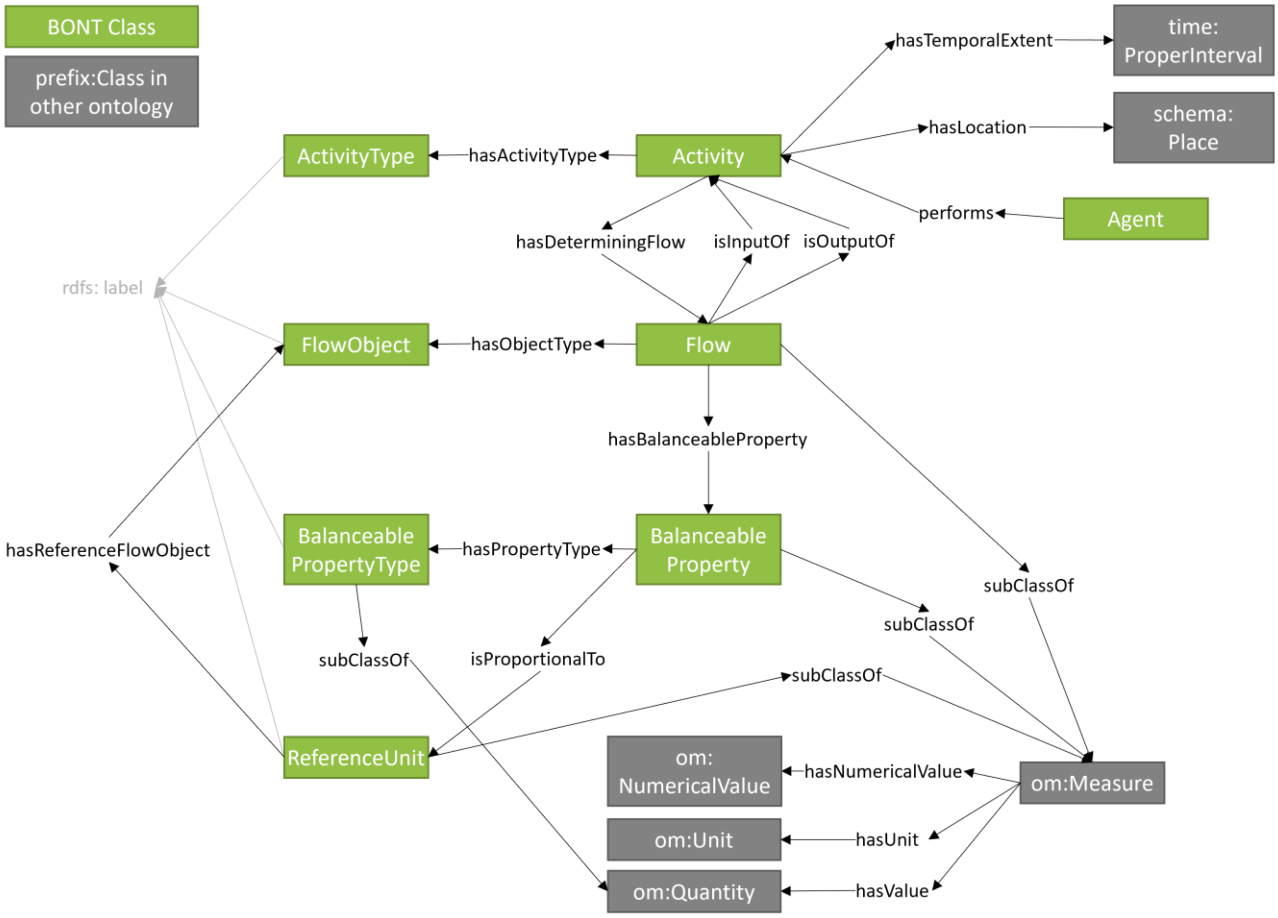

Figure 4. The BONSAI ontology (Ghose et al., 2021); rdfs: Resource Description Framework Schema; om: Ontology of units of Measure.

Table 1. Description of and examples for the different elements of the BONSAI ontology (Ghose et al., 2021) as shown in Figure 4.

Description	Example
Activity	
Making or doing something within a spatial and temporal delimitation.	"Cultivation of wheat" in Germany in the year 2020 or "Aluminium production" in China in the year 2020.
Activity Type	
This class includes the labels of activities.	"Cultivation of wheat" or "Aluminium production".
Agent	
An entity (person or thing) that performs an activity. An agent may have a location that may be different from the location of an Activity performed by it.	Within an activity, agents can perform different roles, for example, laborer, owner, purchaser, consumer.
Flow	
An input or output of an entity to or from an instance of an Activity or a directional exchange of an entity between two instances of Activity. A flow can be unidirectional, that is, a flow can be defined as an input or output of an activity without defining its origin or destination. The determining flow is a specific flow of an activity for which a change in demand or supply will affect the activity level.	Input of 2393 tonnes of "Aluminium and aluminium products" (FlowObject) to "Manufacture of motor vehicles" (ActivityType) in Germany in the year 2011.
Flow Object	
This class includes the labels of entities that are produced or consumed by an activity or added to or removed from a stock accumulation.	"Wheat" or "Aluminum and aluminium products".
Balanceable properties	
Properties of Flows.	Dry mass, wet mass, energy, elemental mass, monetary value (when measured in the same valuation) (non-balanceable properties: volume, number of units, Becquerel (unit to measure radioactivity).
Balanceable property type	
The property/"quantity" that is quantified.	mass
Reference unit	
A measure to which the numeric value representing the measure of a flow is expressed in proportion to, e.g. CO_2-emissions per kg-km transport covered. "Functional Units" are reference units, but not all reference units are "Functional Units."	Amount of CO_2 emitted from a transport activity may be expressed in proportion to the quantity of another flow of this activity (e.g., 1 km of distance covered) or to a time period (e.g., CO_2 emissions per year from transport).
Numerical value	
	1
Unit	
	kg
Quantity	
	mass

4.2. The eILCD data format

(This section is a short version of section 4 in ORIENTING (2022b)).

The eILCD data format – as its predecessor, the ILCD data format – is a collection of XML datasets (see introduction to section 4 for further details). These datasets have an implicit hierarchical structure as shown in Figure 5.

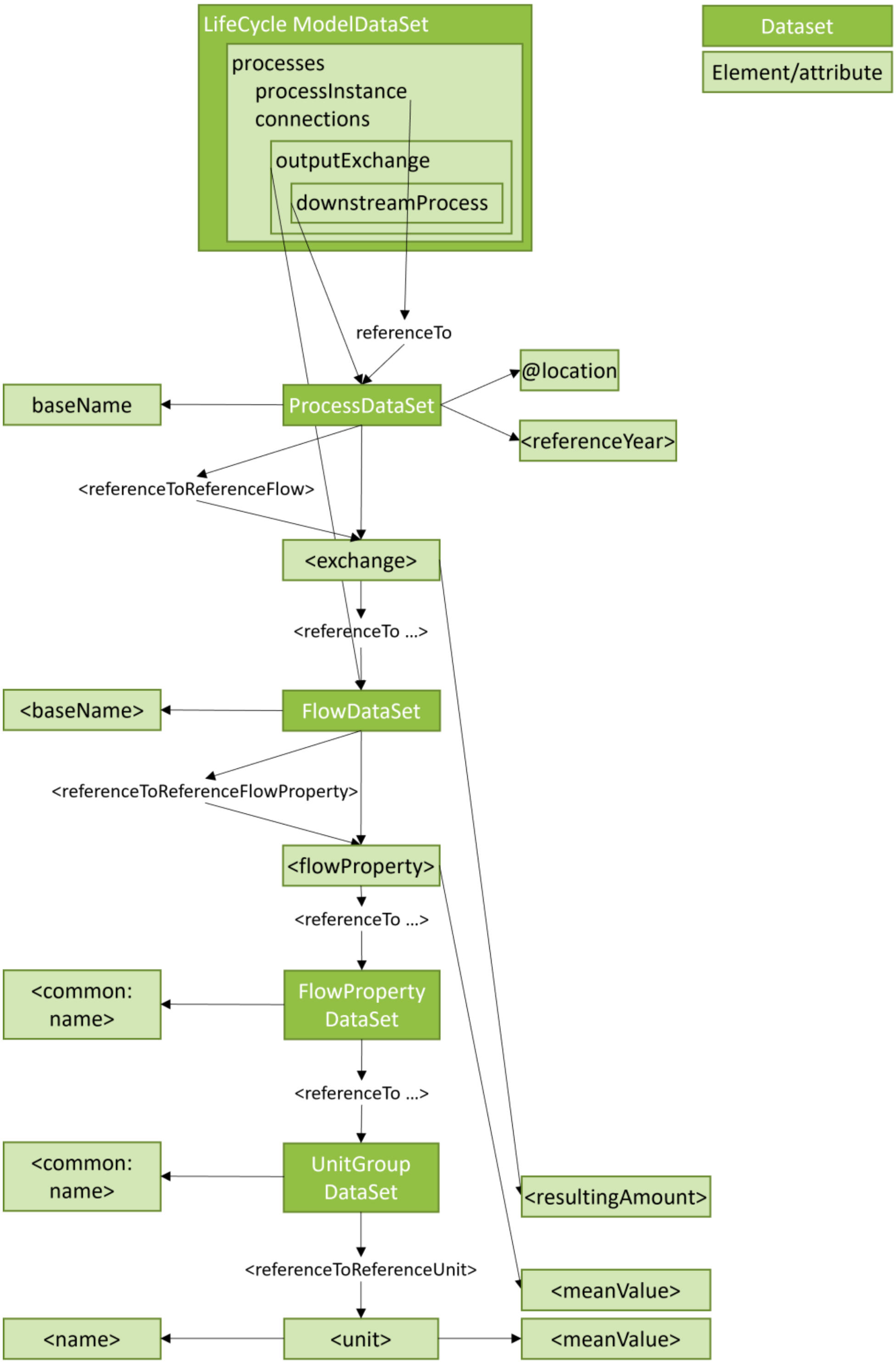

Figure 5. Basic hierarchical structure of the eILCD data format (European Commission, 2022).

The difference between the ILCD and the eILCD data format is the addition of the Life Cycle Model dataset (at the top in Figure 5). As the name states, it is a model that specifies processes included in a (foreground) product system as well as the connections between these processes. Furthermore, the model dataset format allows to specify parameter settings of processes and thereby assigning life cycle stages to processes. In a practical example: a Life Cycle Model dataset for “Packaging production” would specify how the process “Packaging production” is connected to several other processes through several flows (Figure 6). Furthermore, parameters in the transport dataset could be specified and life cycle stages could be assigned to the different processes, for example “Raw material acquisition” to “Plastic granulate production” and “Manufacturing” to “Packaging production”.

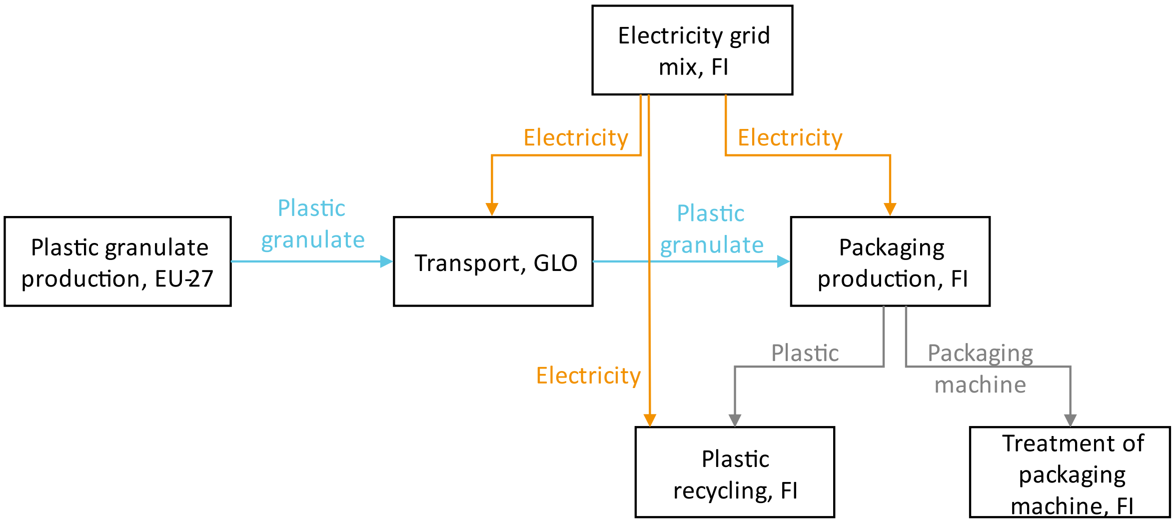

Figure 6. Example of an eILCD Life Cycle Model for “Packaging production, FI” (based on European Commission (2022)); FI: Finland; EU: European Union.

Processes are defined in dedicated datasets including the input and output flows. These flows are then again defined in dedicated datasets including relevant flow properties. Flow property datasets finally refer to unit group datasets, which contain the reference unit as well as other units that might be used for conversion (Figure 5). The connection between datasets follows the hierarchical structure. The connection is established with “referenceTo…” XML tags in the files, for example an input or output flow in a process dataset contains a reference to a flow dataset. Thereby, the reference flow, property, and unit to which the dataset refers and is scaled to is defined by “referenceToReferenceFlow”, “referenceToReferenceFlowProperty” and “referenceToReferenceUnit” tags in the single datasets.

Box 1. XML terminology

Tag: A tag begins with “<” and ends with “>”

Element: An element either begins with a start-tag and ends with a matching end-tag such as `<greeting>Hello, world!</greeting>`, or it consists only of an empty-element tag such as `<line-break/>`.

Attribute: An attribute is a name–value pair within a start-tag or empty-element tag such as `<img src="cat.jpg" alt="Cat" />`, where the names of the attributes are "src" and "alt", and their values are "cat.jpg" and "Cat" respectively.

Source: https://en.wikipedia.org/wiki/XML#Key_terminology

In the eILCD data format documentation (European Commission, 2022), attributes start with “@”. It is possible to include information as an element or as an attribute. The value of a flow, for example, could be included as an element (`<value>1</value>`) or as an attribute (`<flow value=”1”…>`)

4.3. Comparing the BONSAI ontology and the eILCD data format

The basic structure of the BONSAI ontology and the eILCD data format are similar, meaning that activities (or processes) have input and output flows, which have flow properties, which are measured in specific “quantities” (e.g. mass) and units. What is different in eILCD is the Life Cycle Model dataset, in that it allows modelling an activity/process as a system of several activities/processes connected through flows. The BONSAI ontology does not contain this part, but only “starts” from the activity/process level. Figure 7 and Figure 8 show an example of aluminium input into a car part manufacturing applied to the BONSAI ontology and the eILCD format, respectively, to showcase that they follow a similar logic and hence can contain the same information. The Life Cycle Model dataset could then be car manufacturing, which combines, for example, (metal) car part production and tire production as well as electricity production needed in car manufacturing.

The conclusion of the comparison between the BONSAI ontology and the eILCD data format is that the two are compatible from the activity/process level downwards. They can be taken and further developed in parallel to arrive at an ORIENTING LCSA ontology and data format.

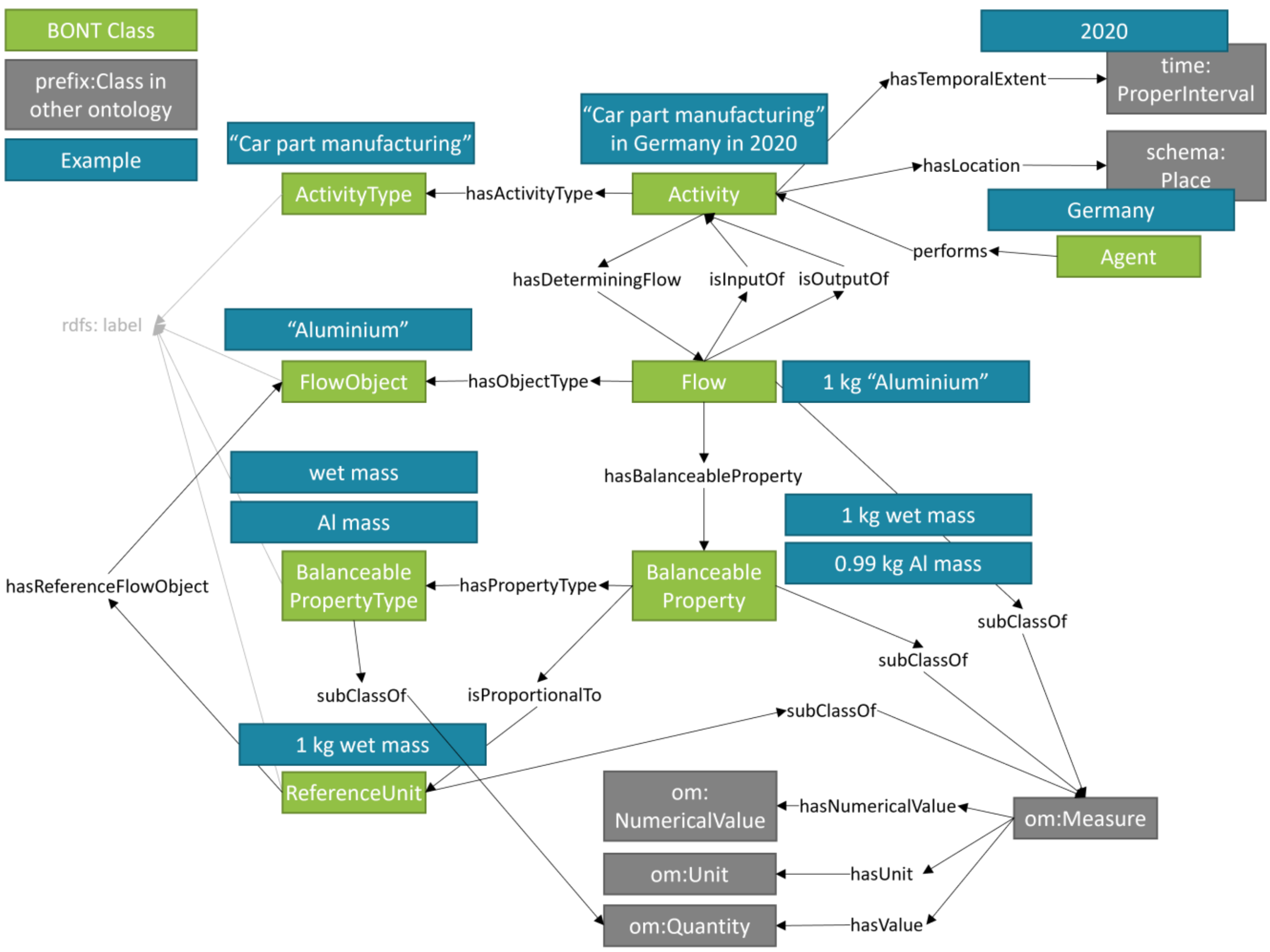

Figure 7. Aluminium in car manufacturing example applied to the BONSAI ontology (Ghose et al., 2021).

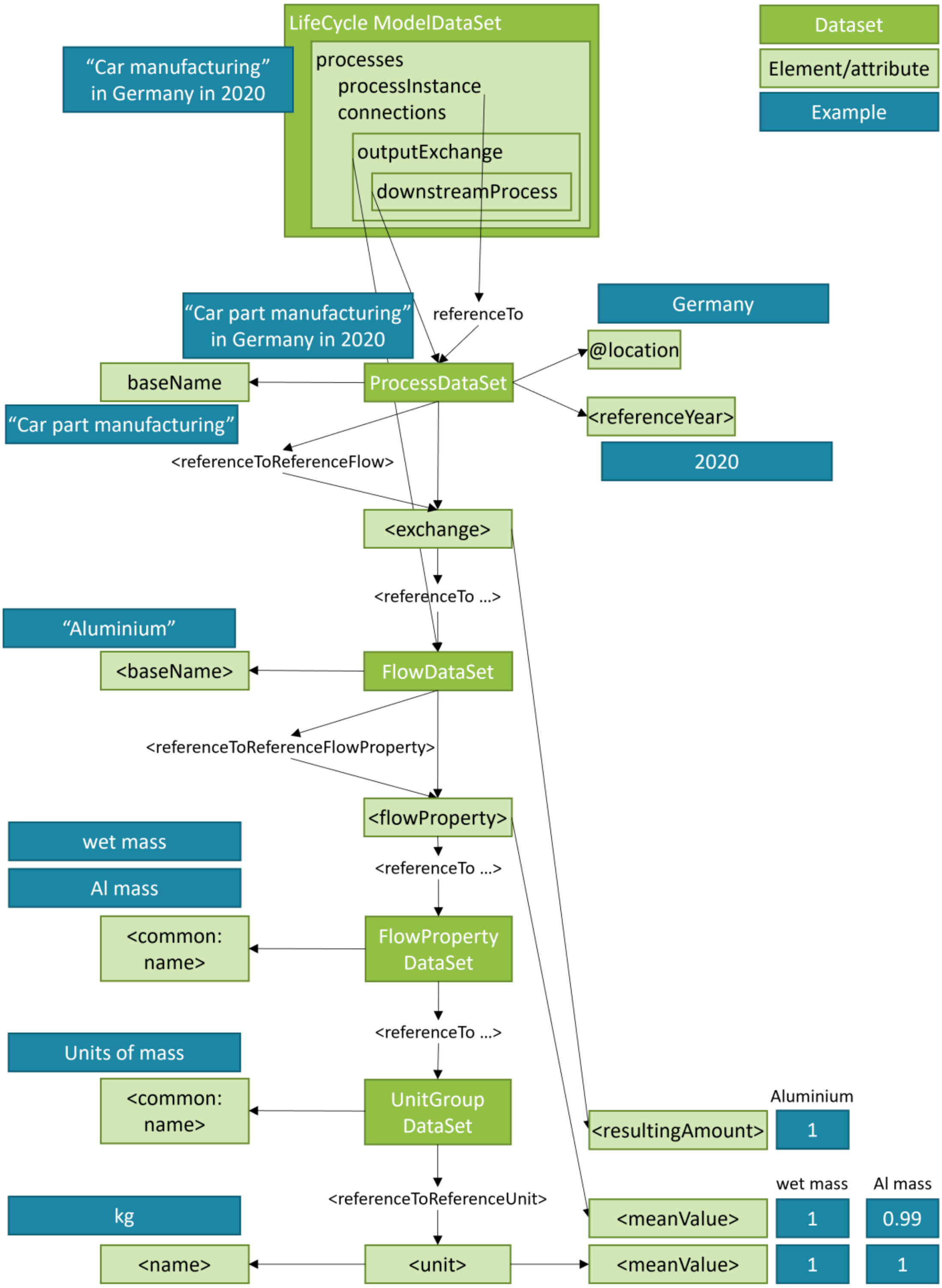

Figure 8. Aluminium in car manufacturing example applied to the eILCD data format (European Commission, 2022).

5. Creating an ORIENTING LCSA ontology: ORIONT

Both the BONSAI ontology (BONT) and the eILCD data format need further refinement and extensions to capture LCSA as defined in ORIENTING, including economic and social as well as material circularity and criticality assessments. Regarding the ontology, this means extending BONT with new classes, sub-classes, and ranges of instances to a) capture missing conceptual elements such as stakeholders; b) further distinguish existing elements such as flows, which can be sub-classified into different types of flows; and c) introduce LCIA.

A full visualization of the ontology can be found in Annex A. In this section, the elaborated ontology is divided into smaller parts (see sections 5.1 to 5.3). In addition, all ORIONT classes and properties are listed and described in section 5.4. The technical implementation is described in section 5.5.

(Since BONT was not accessible online anymore in October 2022 and hence no connection to this ontology could be established, BONT classes were re-introduced as ORIONT classes.)

5.1. Product system and BONT classes

Figure 9 shows the core part of the BONSAI ontology (BONT; BONT classes as used in ORIONT are displayed in bright green) and how they relate to the product system class (additional ORIONT classes are displayed in dark cyan). The ProductSystem (or life cycle model in eILCD terms) is the modelled foreground system containing foreground activities/processes and their connections (Flows) (see section 4.2). In the eILCD life cycle model dataset, foreground activities can be grouped into life cycle stages (LCStages), which then allows to have LCIA results (LCIAResult attached to Activity) per life cycle stage. The life cycle stages that are distinguished in the ORIENTING methodology are given in the ORIENTING Output Format (OOF, see ORIENTING (2022c)). What needed to be introduced additionally to “BalanceableProperties” in BONT are “OtherProperties”, which are needed for some of the assessments within ORIENTING LCSA. Product lifetime or recycled content, for example, are needed for the material circularity assessment.

By largely following eILCD, ORIONT treats temporal and spatial information differently from BONT. In eILCD, locations are given in a separate list, so the possibility of a connection to schema:Place as suggested in BONT would need to be further checked and probably would need some adaptations of the format. Another difference between ORIONT and BONT is that also flows have a location. The reason for this is that flows could have a different location than the activities they belong to because location information is not available at the same level: For example, an activity could theoretically have Europe as the location while the elementary flows are given for specific countries. However, in most cases, the flow should inherit the location of the activity. While the timespan for a process dataset is given in a similar structure as suggested by the connection in BONT to time:ProperInterval, we have introduced two classes following the eILCD format: ReferenceYear (start) and ValidityYear (end).

The connection to the OM ontology (Wageningen University, 2015) in order to deal with units as suggested in BONT seems possible. However, there would be other options for “unit” ontologies such as the QUDT ontology (QUDT, 2022) (as suggested by an ontology expert from the parallel project WISER (Leap, 2022)) or maybe also the latest version of EMMO (EMMC, 2022) as suggested to be consulted in the project proposal. All these ontologies offer similar things regarding units, and a more thorough assessment would be needed to decide which one fits best. Another issue with units are the units used in LCIA, which can be “special” such as "kg CO_2 equivalent" or "mol N equivalent". Existing ontologies could be extended by these special units, but for now, we introduced the class “IndicatorUnit” and specified the units used in ORIENTING impact assessment as the possible individuals (see section 5.4). Finally, we changed the direction of the relationship between om:Quantity and om:Measure following the original OM ontology.

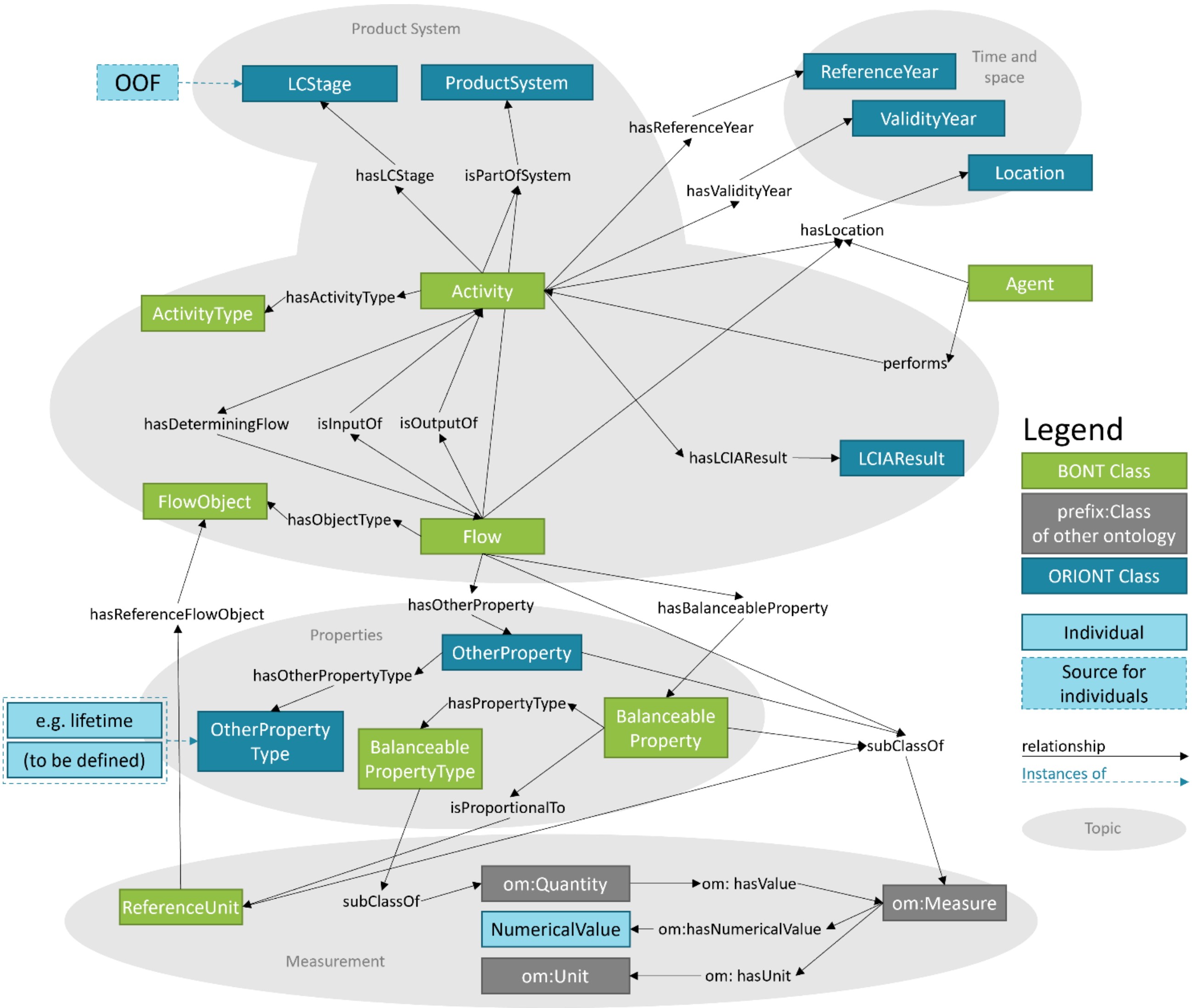

Figure 9. Part of ORIONT containing the product system and BONT classes.

5.2. Further classification of flows

Figure 10 shows the further classification of flows following the eILCD format. This is important because LCIA is introduced to the ontology (see section 5.3) and the connection between inventory (product system, see section 5.1) and LCIA is through elementary flows (for the LCA part and eventually for the criticality part). Furthermore, data points needed for material circularity might be introduced as other flows (see section 5.3 in ORIENTING (2022b)).

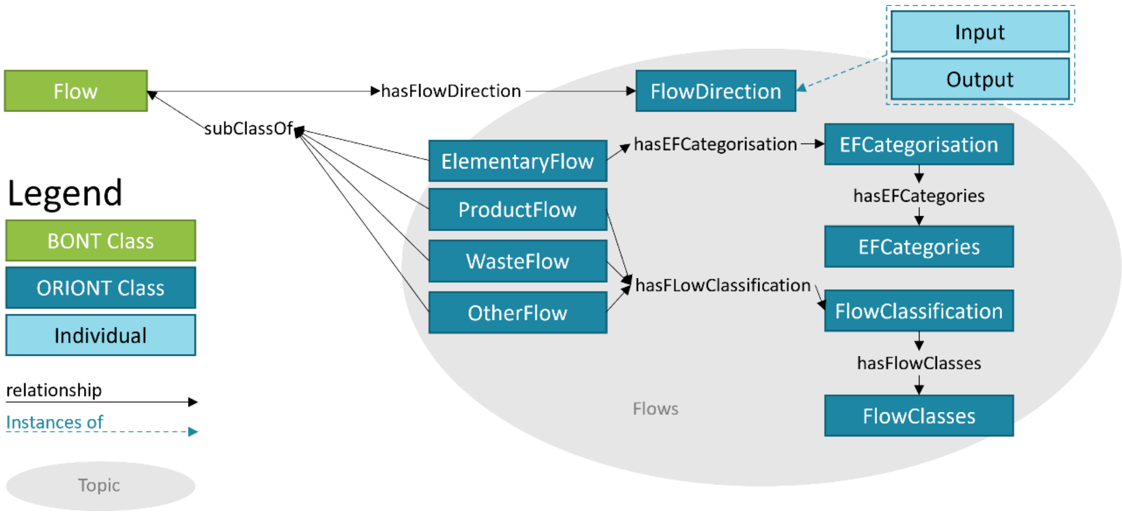

Figure 10. Part of ORIONT further classifying flows.

5.3. LCIA

Figure 11 shows the LCIA part of ORIONT. The central class is the “Method” class given that an LCIA method assesses a specific impact. To do so, a method uses a characterisation model to calculate characterization factors, which quantify impact indicators, which represent an impact category. This is what is included in a method. On the other hand, a method can be part of a methodology, which is a set of different methods that assess different impact categories. What is needed for an ORIENTING LCSA methodology is a set of different methodologies (and/or methods) that assess the different sustainability topics.

One method can calculate one or more impact category indicators: The IPCC method, for example, uses the IPCC model to calculate amounts of CO_2-equivalents for different greenhouse gases, quantifying indicators such as the global warming potential (GWP) for different time horizons (for example GWP_{20} or GWP_{100}). These indicators all assess the impact category “Climate change”. The same impact category can, as a matter of fact, be assessed with different methods having different indicators. However, in a given methodology, usually only one indicator according to one method is used to assess an impact category.

The above mainly describes the LCA approach. However, the ontology structure shall also cover the other sustainability topics. Table 2 shows examples of methodologies, methods, impact categories, indicators, and units used in the different ORIENTING sustainability topics.

Table 2. Examples for methodologies, methods, impact categories, indicators, and units used in the different ORIENTING sustainability topics.

Sustainability topic	Methodology (preliminary names)	Method (example)	(Impact category) indicator (example)	Unit (example)	Impact category (example)
LCA	EF v3.1	IPCC 2021	Global Warming Potential 100	kg CO_2 eq	Climate change
Material criticality	ORIENTING Criticality	EC-CA	EUCRM SR	-	Supply risk
Material circularity	ORIENTING Circularity	CTI 3.0	% Circularity	%	Material circularity
LCC	ORIENTING LCC	ORIENTING eLCC	Net Present Value	$€_{2020}$	Net Present Value
S-LCA	ORIENTING S-LCA	ORIENTING Social performance	Social performance	-	Child labour

The main differences between topics are in a) what is understood as an impact category and b) whether there are CFs as in LCA or what could be considered a CF, and to what these factors are applied. In LCA, an impact category describes a “class representing environmental issues of concern” (ISO, 2006). For the other topics, “environmental” might be replaced with “social” or “economic” for S-LCA and LCC, respectively. In S-LCA, the assessment does not necessarily only look at negative impacts, but the assessment of social performance includes positive and negative impacts (ORIENTING, 2022a). Accordingly, some prefer the term “social topic” over “impact category” and “social topic” is also used in the ORIENTING LCSA methodology (ORIENTING, 2022a). Therefore, “SocialTopic” is introduced as an equivalent class to “ImpactCategory” (no structural change in the ontology). In LCA, CFs are applied to elementary flows, meaning that the quantity of a given elementary flow in an LCI is multiplied by the value of the corresponding CF for calculating the impact result (x kg CO_2 * y [kg CO_2 eq / kg CO_2] = x*y kg CO_2 eq). For other sustainability topics, this may be slightly different (see Table 3). For material criticality, CFs might either be applied to elementary flows or to elemental amounts (which are balanceable properties) in a product (the bill of materials) (see Figure 11 and section 5.2 in ORIENTING (2022a)). For material circularity, the CF is already the calculated impact as the (impact category or) circularity indicator is calculated from different process and flow related properties of a product (see section 5.3 in ORIENTING (2022b)). It is therefore not a CF in its strict sense, but the structure given in the ontology is valid: the CTI model (WBCSD, 2022), for example, is used to calculate a numerical value for the CTI indicator “% Circularity”. In LCC, CF is not a regularly used term. One possibility, however, would be to interpret the discount factor (that is calculated based on the user-defined discount rate for each future year within the specified timeframe) as a CF in that it allows to make flows of money at different moments in time comparable[2]. The discount factors are applied to the different cost elements, which are considered flow properties (see section 5.4 in ORIENTING (2022b)). For S-LCA, the CF is equivalent to the social performance score, which is given on a scale from -2 to +2 (negative impact to positive impact). This value is not applied to any flow or flow property but is valid for an activity/process performed by a specific supplier/agent and thereby for the products/flows produced. However, S-LCA background databases do not have a product/country resolution but a sector-country/region resolution.

[2] When conducting the LCC from a more societal perspective, equity weighting might also be performed. In that case, the equity weights (accounting for different wealth/income levels and thus differences in the value of money across individuals/regions) can be regarded as CFs similar to discount factors (temporal dimension). Both would need to be applied. In the same spirit as discount factors, currency conversion factors, potentially even involving purchasing-power-parity adjustments, could also be interpreted as CFs in that they are applied to cost elements, allowing the user to define common base units and thus making values comparable. Somewhat similar to converting tonnes to kg, it needs to be noted that currency conversions are considered to be part of the LCI phase according to ORIENTING (2022a), noting that there is not only one way how to do this kind of unit conversion.

Hence, if social impacts are to be assessed by use of an S-LCA database, a connection needs to be made through attribution of activities and flows to sectors. See section 5.5 in ORIENTING (2022b) for more details about data for S-LCA.

Table 3. What characterization factors (CFs) quantify for the different ORIENTING sustainability topics.

Sustainability topic	**(Impact category) indicator (example)**	**What the CF quantifies**	**CF unit (example)**
LCA	Global Warming Potential 100	Impact per elementary flow	kg CO_2 equivalent / kg (elementary flow)
Material criticality	EUCRM SR	Impact per elementary flow or per content property (= amount in BoM)	score / kg (elementary flow/property)
Material circularity	% Circularity	Performance per product	% / product
LCC	Net Present Value	Discount factor: The value in a given base year relative to the time when costs or benefits accrue if a discount rate unequal to 0 is chosen.	unitless (per cost/benefit element/property)
S-LCA	Social performance	Performance per activity related to product	score / product

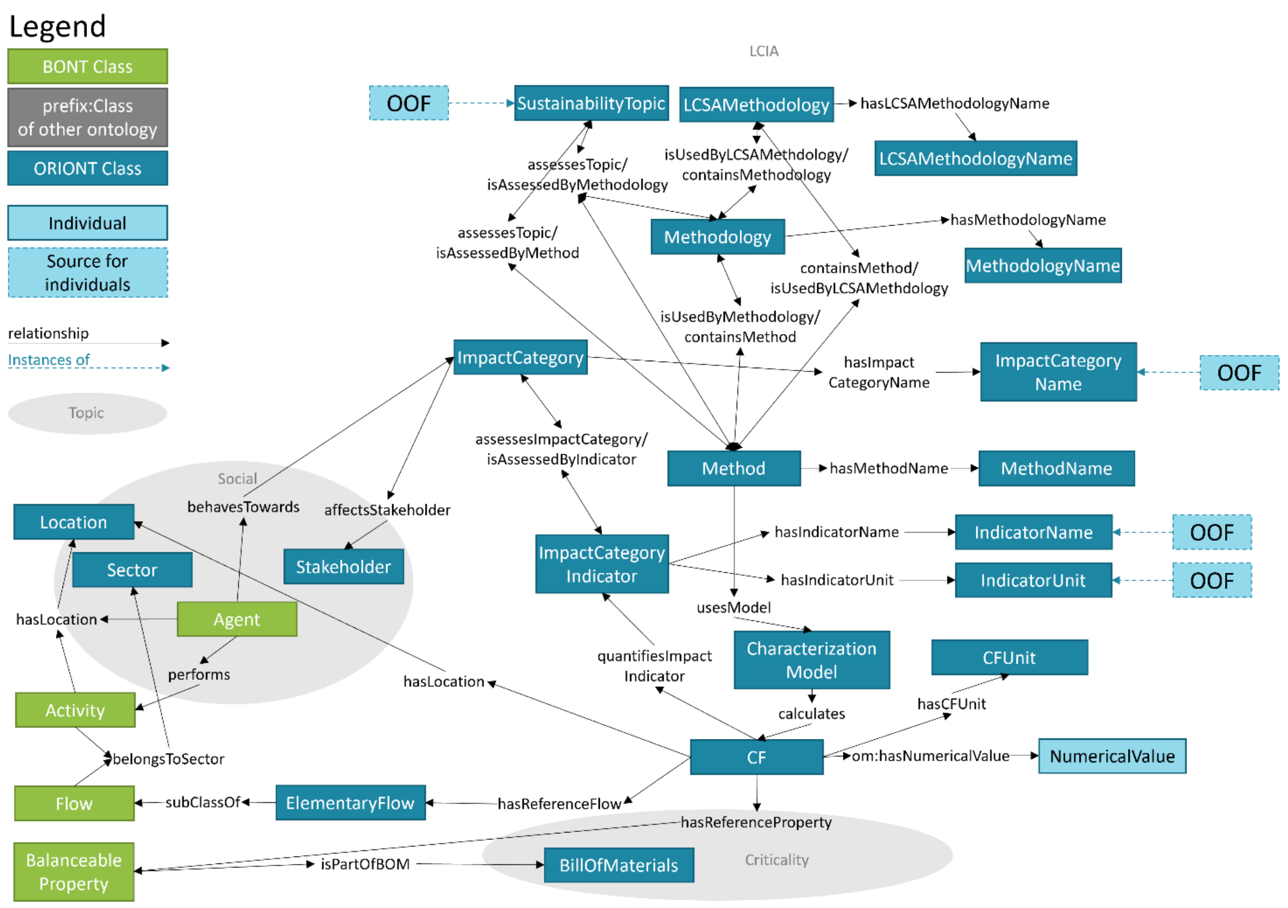

Figure 11. LCIA part of ORIONT.

Special attention needs to be paid to the “Agent” class, which is mainly relevant for S-LCA: “Differently from the other methodologies included in the LCSA framework, in S-LCA the data and the information collected in most of the cases are not directly related to the analysed product system but refer to company behaviour in relation to a defined social topic” (ORIENTING, 2022a). According to Ghose et al. (2021), an agent is “An entity (person or thing) that performs an activity”. This can mean different things and Ghose et al. (2021) specify that agents may play the roles of, for example, labourer, owner, purchaser, or consumer. In an earlier publication on which the BONSAI ontology builds, Janowicz et al. (2015) write that “Each activity is performed by at least one agent such as a coal power plant that performs the generation of electricity”. Related to defining what “Agent” involves is a discussion about locations. While Janowicz et al. (2015) wrote that “An activity is located via the location of the agent performing it”, Ghose et al. (2021) obviously changed this approach by stating that “An agent may have a location that may be different from the location of an Activity performed by it.” Considering the different roles an agent can play according to them, this makes sense. In the ORIENTING Output Format (OOF), the performing entity is called “supplier” (see ORIENTING (2022c)). Hence, while the “Agent” class can be used to include this “supplier”, it might not yet perfectly fit as it goes beyond one single role.

5.4. ORIONT classes and properties

In the coming section, the following tables are included: Table 4 with a list of ORIONT classes, Table 5 showing individuals or instances of classes, Table 6 with ORIONT object properties, and finally Table 7 presents ORIONT data properties.

Table 4. ORIONT classes. “ORIENTING” as a source refers to the working document of ORIENTING definitions and “ORIONT” as a source means that the term is only described here.

Class	Description
Activity	Activity is the act of making or doing something which is defined both spatially and temporally. This is one of the identifying dimensions of a datapoint. This class defines multiple properties on the type and direction of flows. ‘Process’ is a commonly used synonym in other LCA databases (Ghose et al. 2021).
ActivityType	The type of an activity, e.g, stock accumulation, steel production, etc. This class includes the labels of activities. Includes both human activities and environmental mechanisms (Ghose et al. 2021).
Agent	An entity (person or thing) that performs an activity, usually it has a specific location (Ghose et al. 2021).
BalanceableProperty	A quantity for which the sum for all input flows must equal the sum for all output flows. A quantity that follows a conservation law. Balanceable properties are particularly relevant for validating the completeness and consistency of an Activity description or a database of such activities (Ghose et al. 2021).
BalanceablePropertyType	Contains the labels of BalanceableProperty such as dry mass, wet mass, elemental mass, person-time, monetary value (Ghose et al. 2021).
BillOfMaterials	A bill of materials or product structure (sometimes bill of material, BoM or associated list) is a list of the raw materials, sub-assemblies, intermediate assemblies, sub-components, parts and the quantities of each needed to manufacture an end product (European Commission, 2018).
CF	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 (ISO 14040).
CFUnit	Units of characterisation factors are given in the unit of the indicator quantified divided by the unit of the reference flow or property (if any); otherwise it is equivalent to the indicator unit (ORIONT).
CharacterisationModel	A model underlying an LCIA method used to calculate characterization factors (ORIENTING)
EFCategories	Categories used in the elementary flow categorisation system (ORIONT).

EFCategorisation	Identifying category/compartment information exclusively used for elementary flows. E.g. "Emission to air", "Renewable resource", etc. (European Commission, 2022).
ElementaryFlow	(a) material or energy flow that has been drawn from the environment without previous human transformation and that enters the system being studied; or (b) material or energy flow that leaves the system being studied and is released into the environment without subsequent human transformation (ISO, 2006).
Flow	An input or output of an entity to or from an instance of an Activity or a directional exchange of an entity between two instances of Activity. This class contains the quantity of the entity (Flow Object) that is consumed as input or produced as output of an Activity (Ghose et al. 2021).
FlowClasses	Classes used in the flow classification system (ORIONT).
FlowClassification	Optional statistical or other classification of the data set. Typically, also used for structuring LCA databases (European Commission, 2022).
FlowDirection	Direction of Input or Output flow (European Commission, 2022).
FlowObject	This class includes the labels of entities that are produced or consumed by an activity or added to or removed from a stock accumulation (Ghose et al. 2021).
ImpactCategory	Class representing environmental issues of concern to which life cycle inventory analysis results may be assigned; for example, climate change or acidification (ISO, 2006).
ImpactCategoryIndicator	Quantifiable representation of an impact category (ISO, 2006).
ImpactCategoryName	Name of the impact category (ORIONT).
IndicatorName	Description of the meaning of the impact indicator (based on European Commission, 2022).
IndicatorUnit	Special units used for impact category indicators such as "kg CO_2 equivalent" or "mol N equivalent" (ORIONT).
LCIAResult	LCIA results provided for an activity (ORIONT).
LCSAMethodology	LCSA methodology is understood as a set of different methods to perform a life cycle sustainability assessment (ORIONT).
LCSAMethodologyName	Name of the LCSA methodology (ORIONT).
LCStage	Life Cycle Stage of a product system; the stages defined in ORIENTING are “Design - R&D”, “Raw material acquisition”, “Manufacturing”, “Installation/distribution/retail”, “Use”, “Maintenance, repair, refurbishment”, and “End-of-life”; “Design - R&D” and “Maintenance, repair, refurbishment” are additional to the minimum stages defined in the PEFCR guidance (ORIENTING).
Location	Location, country or region the data set represents (European Commission, 2022).
Method	Method refers to a procedure, e.g. evaluating the sustainability performance of products regarding an individual aspect (e.g. climate change, child labour, investment costs) under a life cycle perspective (ORIENTING).
MethodName	Name of the method. Composed as follows "LCIA methodology short name; Impact category/ies; midpoint/endpoint; Impact indicator; Source short name". Not applicable components are left out. Examples: "Impacts2007+; Climate change; midpoint; Global Warming Potential; IPCC 2001"; "ABC 2006; Acidification; endpoint; Species diversity loss; John Doe 2006"; "My-indicator2009; combined; endpoint; Ecopoints; various" (based on European Commission, 2022).
Methodology	Methodology is understood as a set of different methods (ORIENTING).
MethodologyName	Name of the LCIA methodology/ies the method belongs to, if any (based on European Commission, 2022).
OtherFlow	Exchange of a type other than elementary/product/waste, e.g. dummy or modelling support flows (based on European Commission, 2022).
OtherProperty	A quantity for which the sum for all input flows does not balance with the sum for all output flows (ORIONT).

OtherPropertyType	Contains the labels of UnbalanceableProperty such as product lifetime or recycled content (ORIONT).
ProductFlow	Products entering from or leaving to another product system (ISO, 2006).
ProductSystem	Product system: Collection of unit processes with elementary and product flows, performing one or more defined functions, and which models the life cycle of a product (ISO, 2006).
ReferenceUnit	Quantified performance of a product system to which LCSA data and impacts are referred (ORIENTING).
ReferenceYear	Start year of the time period for which the data set is valid (until ValidityYear). For data sets that combine data from different years, the most representative year is given regarding the overall environmental impact. In that case, the reference year is derived by expert judgement (European Commission, 2022).
Sector	Sector refers to economic/industry sectors as used in input-output models to consider transactions between these different sectors of a national economy or different regional economies (ORIENTING).
SocialTopic	A generic terminology used to describe more generically social issues of concern, both positive and negative. They can include social risks, or can be measured with reference to performances, or give rise to social impacts (ORIENTING).
SocialTopicName	Description of the meaning of the social topic (ORIONT).
Stakeholder	Person or organisation that can affect, be affected by, or perceive itself to be affected by a decision or activity" (ISO, 2020).
SustainabilityTopic	Sustainability topics in ORIENTING include the three classic sustainability domains or pillars (LCA, social LCA and Life Cycle Costing) as well as (material) Criticality and (material) Circularity (ORIENTING).
ValidityYear	End year of the time period for which the data set is still valid / sufficiently representative. This date also determines when a data set revision / remodelling is required or recommended due to expected relevant changes in environmentally or technically relevant inventory values, including in the background system (European Commission, 2022).
WasteFlow	Substances or objects which the holder intends or is required to dispose of (ISO 14040).
om:Measure	A measure combines a number to a unit of measure. For example, "3 m" is a measure (Wageningen University, 2015).
om:Quantity	A quantity is a representation of a quantifiable (standardised) aspect (such as length, mass, and time) of a phenomenon (e.g., a star, a molecule, or a food product). Quantities are classified according to similarity in their (implicit) metrological aspect, e.g. the length of my table and the length of my chair are both classified as length (Wageningen University, 2015).
om:Unit	A unit of measure is a definite magnitude of a quantity, defined and adopted by convention or by law. It is used as a standard for measurement of the same quantity, where any other value of the quantity can be expressed as a simple multiple of the unit. For example, length is a quantity; the metre is a unit of length that represents a definite predetermined length. When we say 10 metre (or 10 m), we actually mean 10 times the definite predetermined length called "metre" (Wageningen University, 2015).

Table 5. ORIONT individuals or instances of classes.

Class	Individual
FlowDirection	Input
FlowDirection	Output
ImpactCategoryName	Acidification
ImpactCategoryName	Climate change
ImpactCategoryName	Climate change: Biogenic
ImpactCategoryName	Climate change: Fossil
ImpactCategoryName	Climate change: Land use and land use change
ImpactCategoryName	Ecotoxicity, freshwater
ImpactCategoryName	Eutrophication, freshwater
ImpactCategoryName	Eutrophication, marine
ImpactCategoryName	Eutrophication, terrestrial
ImpactCategoryName	Human toxicity, cancer
ImpactCategoryName	Human toxicity, non-cancer
ImpactCategoryName	Ionising radiation, human health
ImpactCategoryName	Land use Biodiversity
ImpactCategoryName	Land use, Biotic resources
ImpactCategoryName	Land use, Soil Quality
ImpactCategoryName	Land use, total
ImpactCategoryName	Ozone depletion
ImpactCategoryName	Particulate Matter
ImpactCategoryName	Photochemical ozone formation - human health
ImpactCategoryName	Resource use, fossils
ImpactCategoryName	Resource use, minerals and metals
ImpactCategoryName	Water use
ImpactCategoryName	Supply risk
ImpactCategoryName	Economic Importance
ImpactCategoryName	Material criticality
ImpactCategoryName	Material circularity
ImpactCategoryName	Net Present Value
ImpactCategoryName	Present Costs
ImpactCategoryName	Total Undiscounted Costs
ImpactCategoryName	Total Undiscounted Value
IndicatorName	% Circularity
IndicatorName	EUCRM
IndicatorName	EUCRM EI
IndicatorName	EUCRM SR
IndicatorName	GeoPolRisk
IndicatorName	Material Circularity Indicator
IndicatorName	Net Present Value
IndicatorName	Present Costs
IndicatorName	Total Undiscounted Costs
IndicatorName	Total Undiscounted Value

IndicatorUnit	CTUe
IndicatorUnit	CTUh
IndicatorUnit	CTUh
IndicatorUnit	%
IndicatorUnit	kg CFC-11 eq
IndicatorUnit	kg CO_2 eq
IndicatorUnit	kg CO_2 eq
IndicatorUnit	kg CO_2 eq
IndicatorUnit	kg CO_2 eq
IndicatorUnit	kg NMVOC eq
IndicatorUnit	kg P eq
IndicatorUnit	kg P eq
IndicatorUnit	kg $PM_{2.5}$ eq
IndicatorUnit	kg Sb eq
IndicatorUnit	kg Sb eq
IndicatorUnit	kg U235 eq
IndicatorUnit	m3
IndicatorUnit	mol H+ eq
IndicatorUnit	mol N eq
IndicatorUnit	Pt
IndicatorUnit	Pt
IndicatorUnit	Pt
IndicatorUnit	Pt
LCStage	Design - R&D
LCStage	End-of-life
LCStage	Installation/distribution/retail
LCStage	Maintenance, repair, refurbishment
LCStage	Manufacturing
LCStage	Raw material acquisition
LCStage	Use
SocialTopic	Access to material, immaterial resources and cultural heritage
SocialTopic	Accessibility
SocialTopic	Affordability
SocialTopic	Child labour
SocialTopic	Community engagement
SocialTopic	Contribution to economic development (including local employment)
SocialTopic	Corruption
SocialTopic	Delocalization and migration
SocialTopic	Discrimination and equal opportunities
SocialTopic	Effectiveness and comfort
SocialTopic	End-of-life responsibility
SocialTopic	Ethical treatment of animals
SocialTopic	Fair competition
SocialTopic	Forced labour
SocialTopic	Freedom of association and collective bargaining

SocialTopic	Health and safety
SocialTopic	Prevention and mitigation of armed conflicts
SocialTopic	Privacy
SocialTopic	Promoting social responsibility and public commitments to sustainability issues
SocialTopic	Remuneration and social benefits
SocialTopic	Respect of indigenous rights and land rights
SocialTopic	Respect of intellectual property rights
SocialTopic	Responsible communication and feedback mechanisms
SocialTopic	Skill development and technology development
SocialTopic	Supplier relationships and fair trading
SocialTopic	Women’s empowerment
SocialTopic	Work life balance and working hours
Stakeholder	children
Stakeholder	Local community
Stakeholder	small scale entrepreneur
Stakeholder	society
Stakeholder	User/consumer
Stakeholder	value chain actor
Stakeholder	Worker
SustainabilityTopic	Material circularity
SustainabilityTopic	Material criticality
SustainabilityTopic	LCA
SustainabilityTopic	LCC
SustainabilityTopic	S-LCA

Table 6. ORIONT object properties.

ObjectProperty	Description
affectsStakeholder	Specifies the stakeholder that is affected by an impact category/social topic
assessesImpactCategory	Specifies the impact category that is assessed by an impact category indicator
assessesTopic	Specifies the sustainability topic that is assessed by a method or methodology
behavesTowards	Specifies the social topic/impact category towards which an agent behaves
belongsToSector	Specifies the sector to which an activity of flow belongs
calculates	Specifies the characterisation factor that is calculated by a characterisation model
containsMethod	Specifies the methods contained in a methodology
containsMethodology	Specifies the methodologies contained in an LCSA methodology
hasActivityType	Specifies the type of the Activity
hasBalanceableProperty	Specifies the Measure of a Flow when this Measure is a BalanceableProperty, that is, when it follows a conservation law
hasCFUnit	Specifies the unit of a characterisation factor
hasDeterminingFlow	Specifies a flow object produced or consumed by an activity for which a change in demand or supply will affect the activity level (such as its production volume or extent)
hasEFCategories	Specifies the categories of an elementary flow categorisation system

hasEFCategorisation	Specifies the categorisation of an elementary flow
hasFlowClasses	Specifies the classes of a flow classification
hasFlowClassification	Specifies the classification of a product, waste, or other flow
hasFlowDirection	Specifies the direction of a flow (input or output)
hasImpactCategoryName	Specifies the name of an impact category
hasIndicatorName	Specifies the name of an impact category indicator
hasIndicatorUnit	Specifies the unit of an impact category indicator
hasLCIAResult	Specifies the life cycle impact assessment results of an activity
hasLCSAMethodologyName	Specifies the name of an LCSA methodology
hasLCStage	Specifies the life cycle stage to which an activity belongs
hasLocation	Specifies the location of an Activity, Agent, Flow or Characterization Factor (CF)
hasMethodName	Specifies the name of a method
hasMethodologyName	Specifies the name of a methodology
hasObjectType	Specifies the Flow Object consumed or produced
hasOtherProperty	Specifies the Measure of a Flow when this Measure is a UnBalanceableProperty, that is, when it follows a conservation law
hasOtherPropertyType	Specifies the dimension (Quantity) of a Measure that is classified as a UnBalanceableProperty
hasPropertyType	Specifies the dimension (Quantity) of a Measure that is classified as a BalanceableProperty
hasReferenceFlow	Specifies the reference flow of a characterisation factor
hasReferenceFlowObject	Specifies a FlowObject that functions as the ReferenceUnit for a BalanceableProperty measure
hasReferenceProperty	Specifies the property that is assessed by a CF
isAssessedByIndicator	Specifies the impact category assessed by an impact category indicator
isAssessedByMethod	Specifies the sustainability topic assessed by a method
isAssessedByMethodology	Specifies the sustainability topic assessed by a methodology
isInputOf	Specifies the Activity that a Flow is an input to
isOutputOf	Specifies the Activity that a Flow is an output of
isPartOfBOM	Specifies the properties (elemental masses) that constitute the bill of materials
isPartOfSystem	Specifies the ProductSystem that an activity or flow belongs to
isProportionalTo	Specifies the reference unit that the amount of a BalanceableProperty of a Flow is proportional to
isUsedByLCSAMethodology	Specifies the methods and methodologies used by an LCSA methodology
isUsedByMethodology	Specifies the methods used by a methodology
performs	Specifies the Activity that an Agent performs
quantifiesImpactIndicator	Specifies the impact category indicator which is quantified by a CF
usesModel	Specifies the characterisation model used by a method to calculate characterisation factors
om:hasUnit	Specifies the unit of an om:Measure
om:hasValue	Specifies the value of an om:Quantity, which is a measure having a numerical value and a unit

Table 7. ORIONT data properties.

DataProperty	Description
hasReferenceYear	Specifies the reference year (start year) for which and activity dataset is valid
hasValidityYear	Specifies the last year for which and activity dataset is valid
om:hasNumericalValue	Specifies the numerical value of an om:Measure

5.5. Technical implementation

ORIONT was implemented using the Web Ontology Language (OWL; OWL, 2013), the Owlready2 package for ontology-oriented programming in Python (Lamy, 2017), and the Protégé editor (Stanford University, 2020). Excel tables containing terms (used as rdfs:label) and definitions (used as rdfs:comment) were extended to contain further information needed, for example, class and property names ("Impact category" written as "ImpactCategory"), superclasses, or code snippets needed for Owlready2. These tables were then fed into a Python code to which the generated code snippets were added. The code produces an owl file, which can be imported into Protégé, where the ontology can be reviewed and where further modifications can be made.

6. Conclusions

The main role of ORIONT within ORIENTING is the content explication in order to align data structure and conceptually integrate data across sustainability topics. This is achieved by the ontology visualisation, which was discussed with topic experts within the project, and is described in this report. ORIONT builds on BONT and is aligned with the ORIENTING methodology. This allows to come up with a controlled, formal vocabulary that consists of naming and defining categories in, properties of, and relations between the concepts, data and entities that substantiate the ORIENTING LCSA, but that also should be valid beyond ORIENTING. The technical implementation should be considered a draft suggestion as technical details might still be missing, and the ontology would need to be tested in applications. The connection to other ontologies (including BONT once it is available online again), would also need some testing. As discussed before, the connection to the OM ontology as suggested in BONT is possible, but there would be alternative ontologies that could fulfil the same purpose. Thereby, special attention needs to be paid to impact indicator units (and hence those of CFs) as they are special and might not (yet) be available. What for now has been organized in the "IndicatorUnit" class could also be integrated into one of the suggested ontologies containing units.

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8. Annexes

8.1. Annex A – Ontology file

The ORIONT ontology is available in the download section on the ORIENTING website in the following link: https://orienting.eu/wp-content/uploads/2022/10/ORIENTING_D3.1_Annex-A_ORIONT_V1.zip

The zip file contains the ORIENTING_D3.1_Annex-A_ORIONT_V1.owl file. A .owl file is best accessed with an ontology editor such as Protégé (Stanford University, 2020). For opening the file in Protégé, first the editor would need to be downloaded from the reference provided and then the file opened in the editor.

8.2. Annex B – Ontology visualisation