

Tools and Services Walkthrough Session - Ontology - a more detailed Guide

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... with ongoing engagement and collaboration within the **community**...



Part 1:

09:00 – 10:30 **Fundamentals of ontology development with reference to PMDco**

10:30 – 11:00 Break

Part 2:

11:00 – 12:00 **Example of describing material and process using PMDco**

12:00 – 13:00 Lunch Break (60min)

13:00 – 14:30 **Continuation**

14:30 – 15:00 Break

15:00 – 16:00 **Wrap-up & Feedback / Your modelling Q & our modelling A**
Share your modelling challenges



PMDco: Ontology Development

- Recap
- Consensus Building Process
- Ontology Development Process
 - the 15 steps
 - best practices
 - do's and don't and pitfalls
- How To Transform My Data



<https://miro.com/app/board/uXjVJnJwyj8=?moveToWidget=3458764676180921357&cot=14>



Recap

We already learned about:

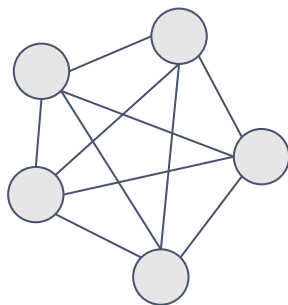
- Interoperability
- Ontology in philosophy and computer science
- RDF / OWL
- Triples and serialization
- Reasoning and triple stores
- Types of ontologies
- Protégé ontology editor
- BFO, RO & Co
- PMDco

Recap: Translation Problem

Solution 1:

- Between each dataset A and each dataset B a mapping is made

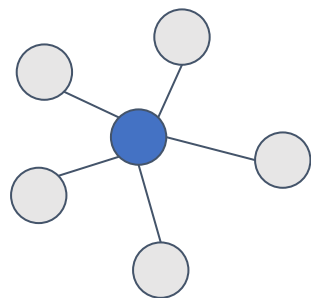
→ requires n^2 “translators”



Solution 2:

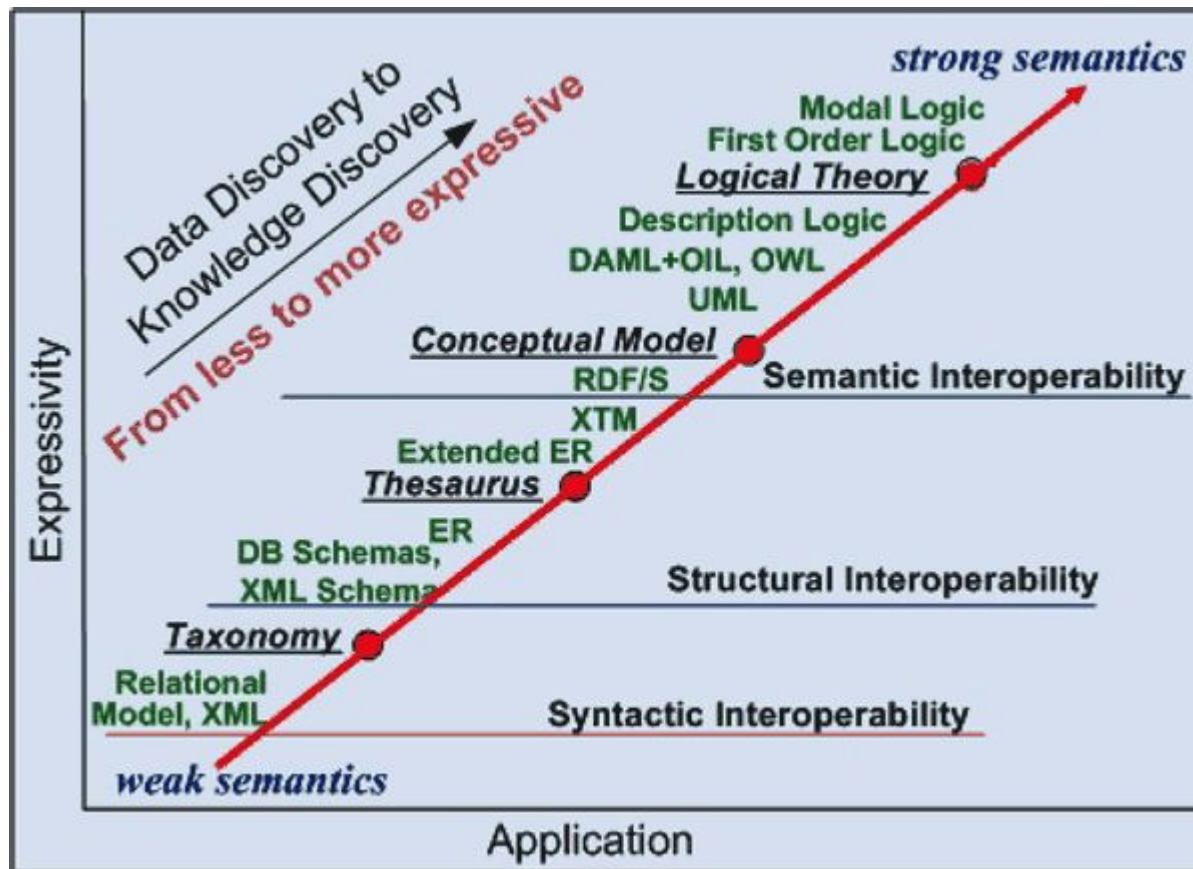
- Independent representation scheme (*Interlingua*)

→ requires n “translators”



Recap: The semantic ladder

- use a common language ...
- shared symbols and terms (**syntax**)
- agreement on their meaning (**semantics**)
- classification of terms (**taxonomy**)
- associations and connections between terms (**thesauri**)
- rules and knowledge about which connections are valid and meaningful (**ontologies**)



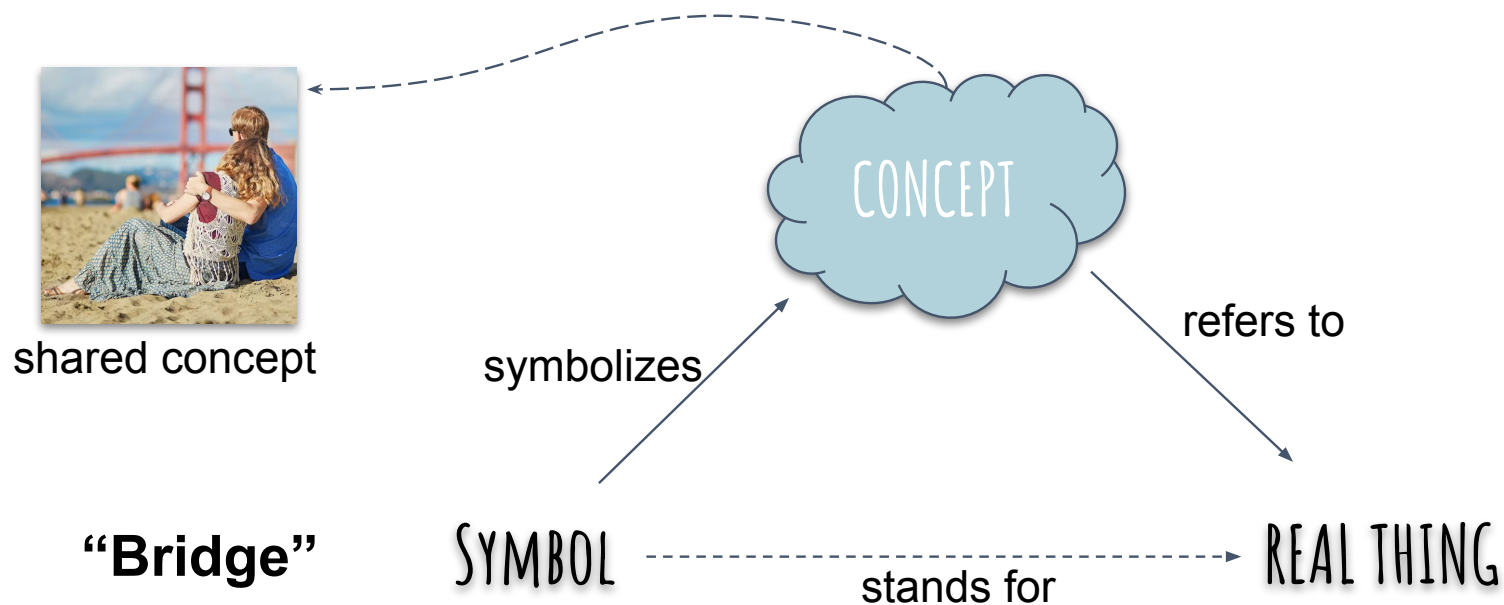
(Obrst, 2003)

An **ontology** is an **explicit, formal** specification of a **shared conceptualization**. The term is borrowed from philosophy, where an ontology is a systematic account of existence. For AI systems, what 'exists' is that which can be represented.

(Thomas R. Gruber, 1993)

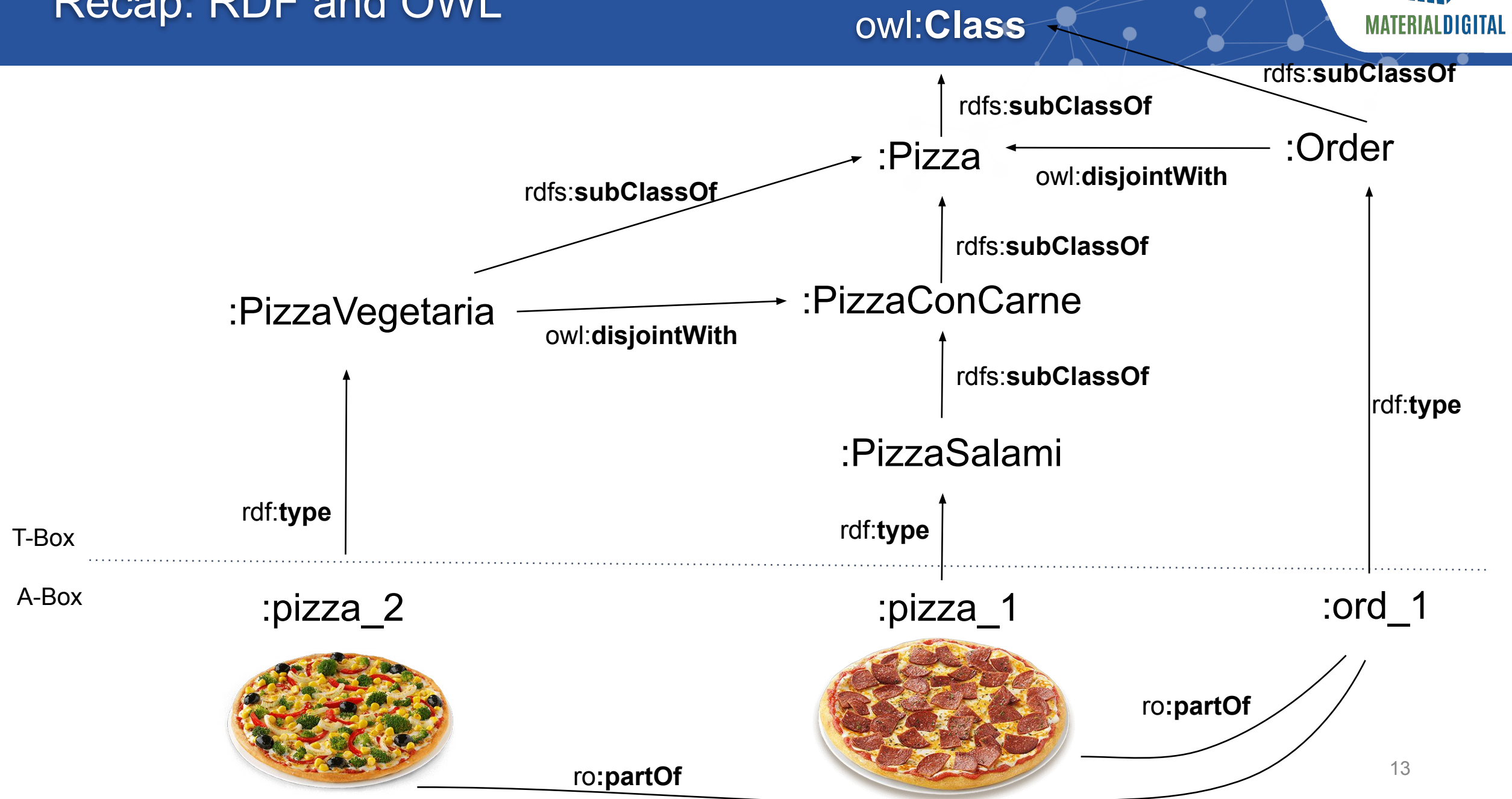
conceptualization:	abstract model (domain, relevant terms, relations)
explicit:	meaning of all terms is clearly and unambiguously defined
formal:	interpretable by machines
shared:	consensus

Recap: Conceptualization



Assignment of symbol (word) to object only possible indirectly, people assign objects to concepts that they name

Recap: RDF and OWL



Recap: Reasoning

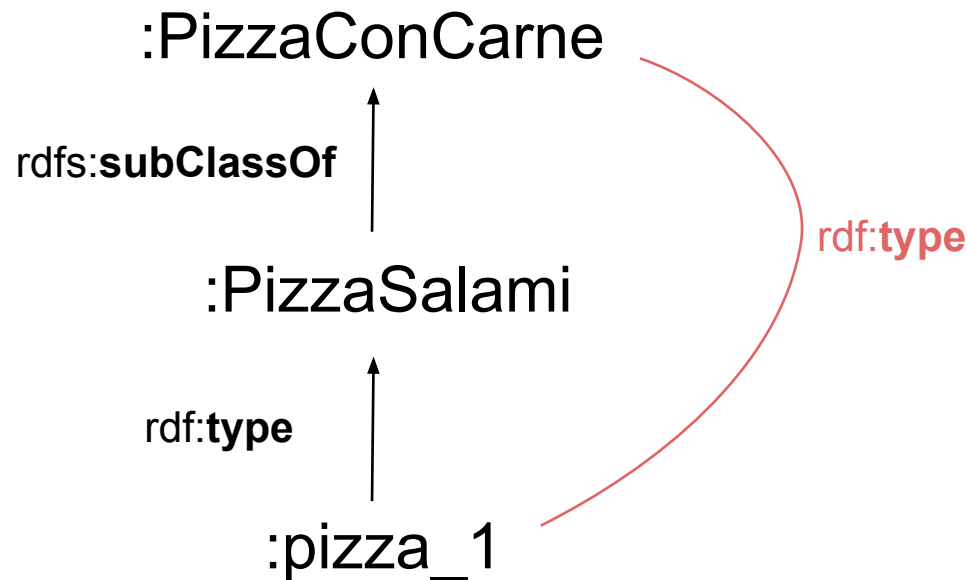
- Reasoner = (Theorem) Prover = Logical Inference Engine
- Can draw conclusions from logical axioms and statements
- Checks the consistency of ontologies
- Evaluates logical inference rules and thus generates information that is not explicitly contained in the ontology

RDFS Entailment Rules

Rule 9:

```
u rdfs:subClassOf x .  
v rdf:type u .
```

v rdf:type x .



:pizza_1
:PizzaSalami

rdf:type
rdfs:subClassOf

:PizzaSalami .
:PizzaConCarne .

:pizza_1

rdf:type

:PizzaConCarne .

PMDco: Ontology Development Process

Today

Consensus Building!

It is naive to think the ontology development process is just:

1. Gather domain knowledge from experts and texts
2. Translate concepts into RDF/OWL or formal logic
3. And all this fully automated

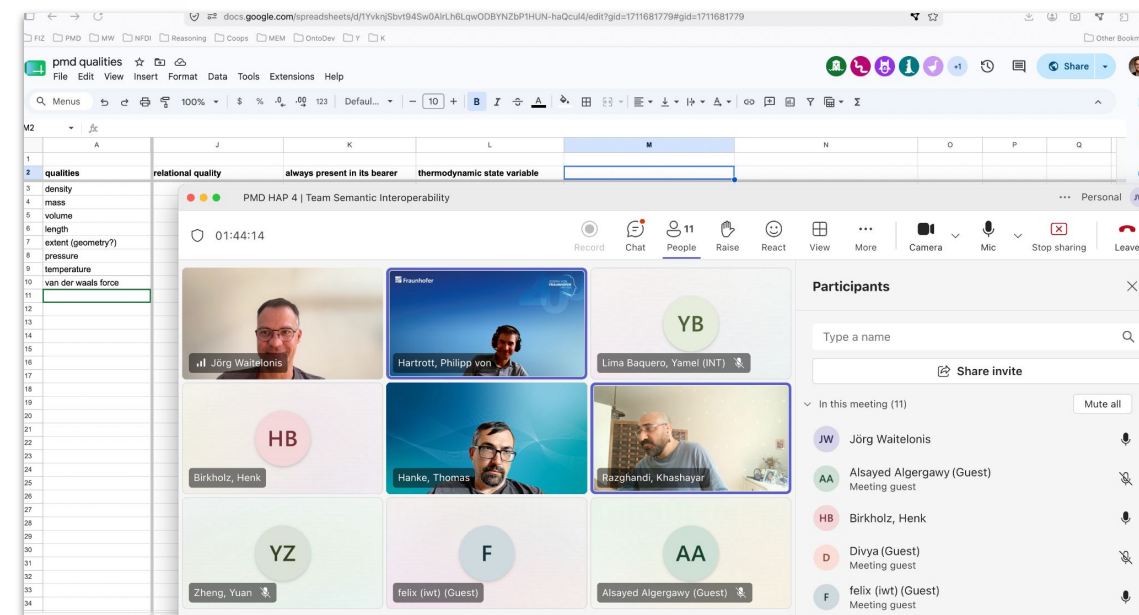
- Machines still have difficulties to process and "understand" natural language
- Also LLMs have their limits, because they mostly rely on text data, but not on emotions, facial-expressions, intention; and for real disambiguation we also need those, also in scientific or industrial contexts // use LLMs as inspiration, but don't expect that they can do the work
- Ontology development is more about **trust** and **transparency** and **reproducibility**
- Success depends on **adoption by a community**

- Ontologies define meanings of terms and relations
- **Consensus on meanings** reduces ambiguity
- Also experts often disagree on definitions and scope
- Differences emerge in **terminology** and **semantics**
- Even established sciences contain conceptual variation
- Example: multiple definitions of 'cell'
- Terms in an ontology need to be **unambiguously interpretable**
 - First by humans: **labels** and **textual definition**
 - By machines: **logical rules**

How to build consensus ??

Consensus building process (micro)

- Ontology experts and domain experts **together**
- **Domain experts:**
 - **provide** and **document** their **knowledge**
 - techniques: inclusive participatory discussions, notes, diagrams, etc.
- **Ontology expert:**
 - **moderate** and **mediate** the consensus building process
 - techniques: naive questions, paraphrasing, summarizing



PMDco core team; regular meetings on Tuesdays and Thursday

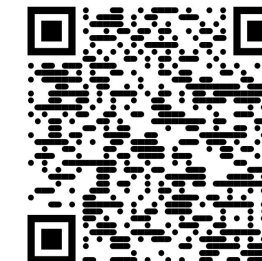
[1]

Meeting protocol: <https://docs.google.com/document/d/1f9WOIK18TZxJQDbQe0q1DYWtnDyLCuKICp2868pdGVE/edit?tab=t.0>

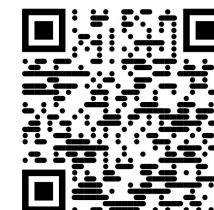
Consensus building process (macro)

- Encourage community-wide adoption
 - playgrounds
 - hackathons
 - conferences
- Open, extensible, and transparent ontology design
- Documentation and stakeholder engagement are essential
- Wider adoption increases interoperability value

Join our bi-weekly Fri. 1-2pm
public **Ontology
Playgrounds**



PMD Hackathon
October 2025 @ BAM

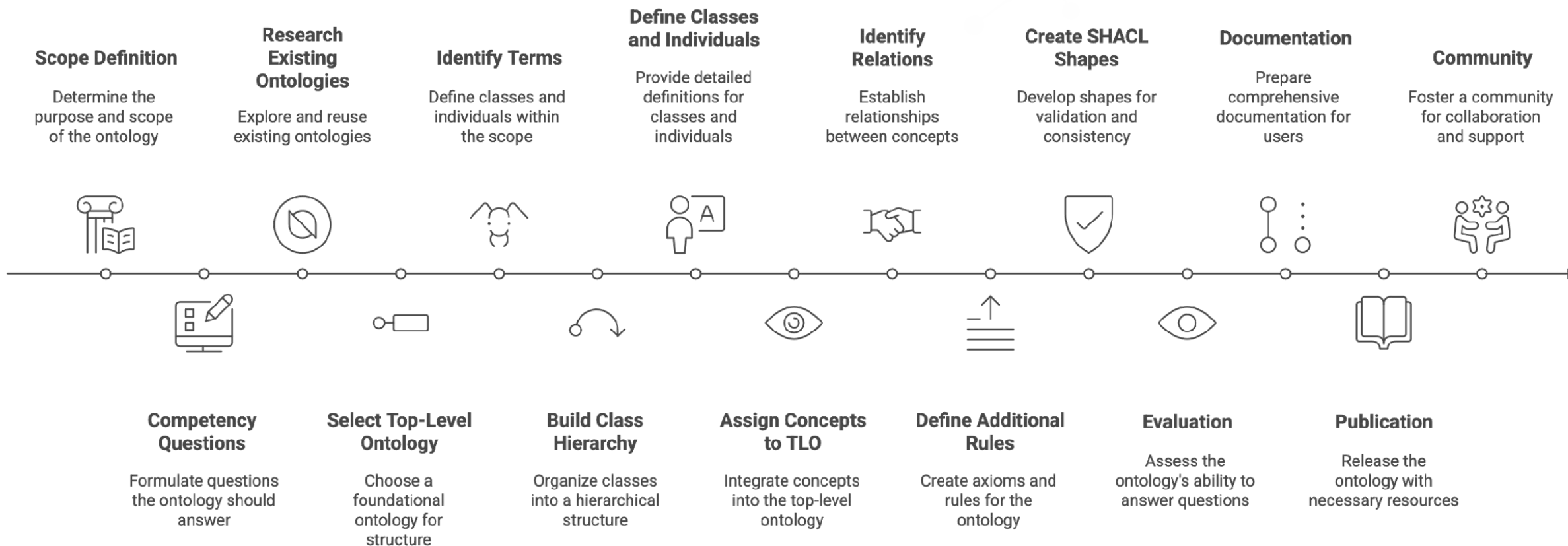


Check & Contribute to our
GitHub PMDco & Application Ontologies

[1]

- Many Design Methods
 - **Methontology** [2], **Ontology 101** [3], **Extreme Design** [4], **NeOn** [5] , etc.
- Problem:
 - many degrees of freedom → leads to different solutions
- Follow Principles:
 - Reuse; IRIs, definitions, naming conventions, annotations, design
 - e.g.: [OBO-Foundry principles](#)
- Follow Existing Patterns:
 - Reusable modeling solution to a recurrent ontology engineering problem.
- Use Standards: deployment, import management, versioning → [ODK](#)

Ontology Development Process



1. Scope Definition

- What is the purpose of the ontology?
- What is the concrete scope or the “subject matter” of the ontology?
- Which type of ontology is being targeted?
- If there are multiple “scopes,” should these perhaps become several ontologies/modules?
- Top-down vs. bottom-up?
- PMDco scope:
 - <https://materialdigital.github.io/core-ontology/docs/intro.html>

2. Competency Questions

Questions that the ontology should be able to “answer”.

- What is the expected answer?
- Check whether the desired answer can actually be derived from the data.

- Understanding the scope
- Validating the ontology
- Alignment and understanding the upper level / alignments
- Use cases

- Examples from PMDco:

<https://materialdigital.github.io/core-ontology/docs/intro.html#competency-questions>

3. Research of existing ontologies

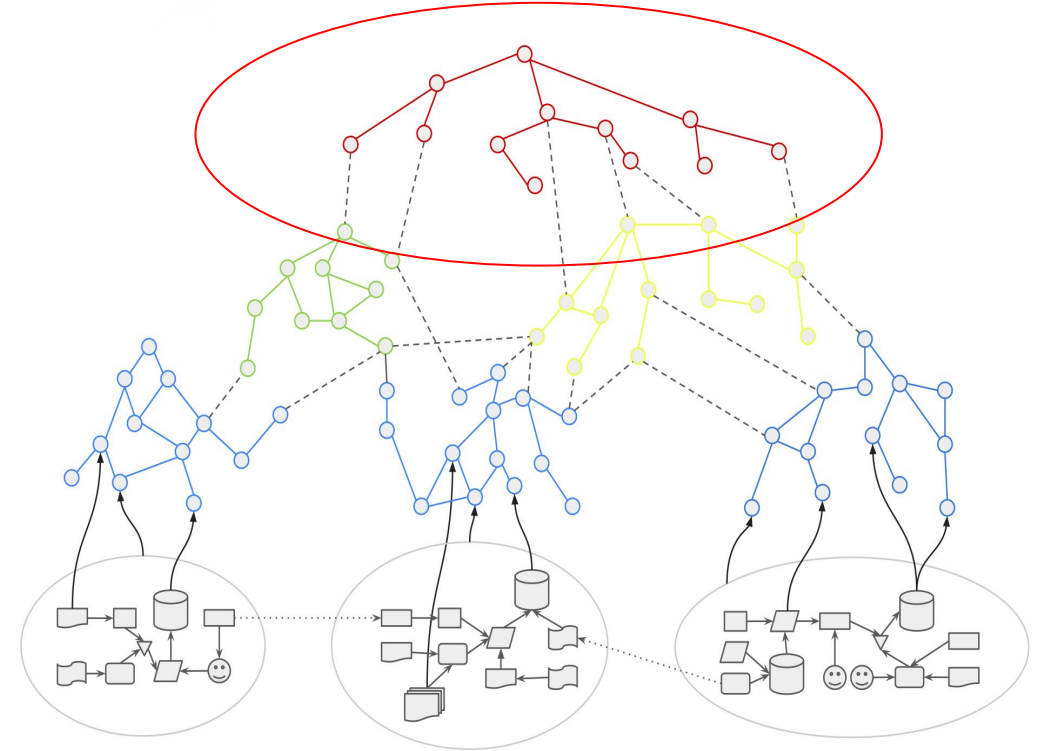
- **Re-use what already exists !!**
- Google
- Talk to people
- “Lookup” platforms and terminology services:
 - <https://bartoc.org/>
 - <https://ontobee.org/>
 - <https://www.ebi.ac.uk/ols4/index>
 - <https://lov.linkeddata.es/dataset/lov/>
 - <https://terminology.tib.eu/ts>
- Check suitability using the competency questions and scope(s).



Photo by [Compagnons](#) on [Unsplash](#)

4. Selection of a top-level ontology

- Provides structure,
- Promotes error prevention,
- Enables connection to other domains,
- Fosters reusability,
- Reduces uncontrolled growth,
- Increases acceptance,
- Supports community building,
- Decide also depending on what you can reuse
 - for PMDco we decided for BFO because we can easily reuse many parts from other ontologies, which we do not need to recreate



5. Identify terms: classes and individuals

- Discuss about their actual meaning
- Take **ambiguities** into account!
 - resolve them → consensus
- Even within a domain, there are many homonyms (same spelling + different meaning)
 - e.g. **phase**: thermodynamic phase, crystallographic phase, processing stage, project phase
- Think about different contexts and perspectives
- Be very precise
- Defined what level of granularity you would like to achieve
 - start with coarser grains
 - macro, meso, micro
- Sometimes it happens that you can't find a name for a meaning (to not get stuck on name finding: temporarily invent a “replacement” name for it “ the A thing”, “thing that relates to ...”)

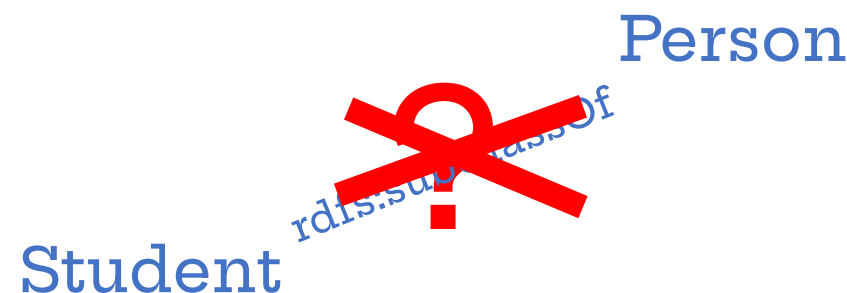
6. Build the class hierarchy

- Organize your classes in a hierarchy.
 - “A subclassOf B” means: **all** instance of **A** are also instances of **B** (at all times)
- → Frequent source of mistakes (or bad practices)
 - `:HeatedSteel subclassOf :Steel`
 - `:BrittleMaterial subclassOf :Ceramic .`
 - `:BrittleSteel subclassOf :BrittleMaterial .`
 - `:Alloy subclassOf :MetallicMaterial .`
 - `:MetallicMaterial subclassOf :Alloy .`

6. Build the class hierarchy: rigidity

Student vs. Person

- A person may be a member of the "Student" class **only for part of their life**.
- If "Student" is used as a superclass or central category in the ontology, reasoning about the individual's properties and identity can become inconsistent as **their status changes over time**. [6,9]
- Use a role pattern.

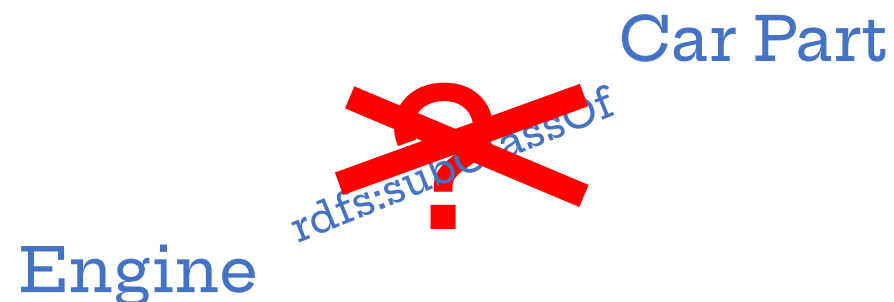


6. Build the class hierarchy: rigidity

Car Part vs. Engine

An "engine" is rigid (always an engine if it exists), but "car part" is non-rigid as an engine could cease being part of a car (e.g., moved to a boat).

If "car part" is modeled as a superclass for "engine," this creates a conflict because an engine can be an engine outside of being a car part. [7,9]



6. Build the class hierarchy: rigidity

→ Temporal Reasoning Burden

Non-rigid class membership is often time-dependent, requiring ontologies to track context or temporal attributes to preserve correct reasoning, significantly increasing modeling and inferencing complexity.



6. Build the class hierarchy: rigidity

Check the **rigidity** !!

If **i** is instance of **c**,

does this hold for **every time** and in **every situation** throughout the existence of **i**?

6. Build the class hierarchy: rigidity

Check the **identity** !!

If **p** is a subclass of **q**,

then **p** cannot define any new way of identifying its instances that **q** does not already define.

(e.g. Person identified by name vs. Student identified by matriculation number)

6. Build the class hierarchy: rigidity

Check the **unity** !!

For some classes, entities can be decomposed into instances of the same class → **anti-unity classes**

(e.g. group into two groups, portion of water into two portions of water)

Other classes only have “whole” instances → **unity classes**

For "whole" individuals, there is always a functional relation unambiguously relating a part to the whole

(e.g. person has some bodyparts, city has districts)

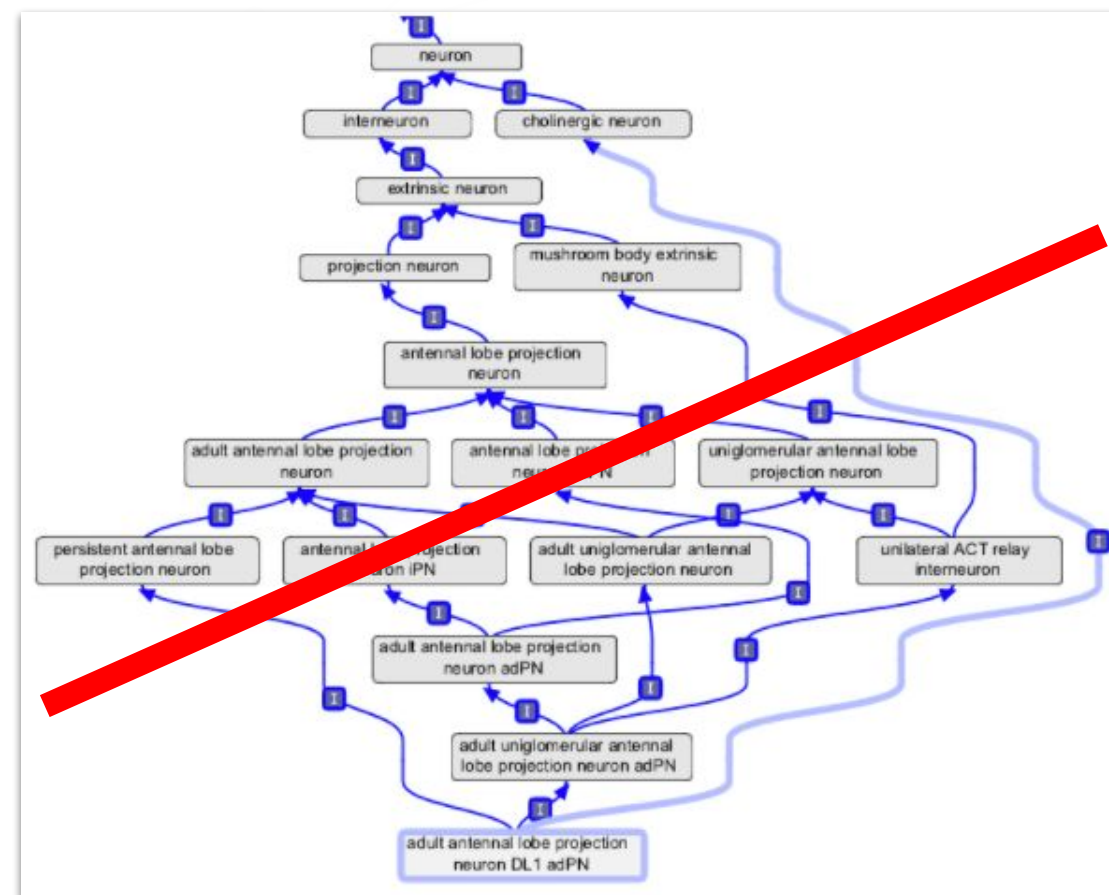
Unity classes may **only** have **unity classes** as their subclasses

Anti unity classes may only have **anti unity classes** as their subclasses

[9]

6. Build the class hierarchy

- Avoid poly-hierarchies!
- Very hard to maintain:
 - keeping track of multiple classification chains
 - avoid redundancy
- Keep a mono-hierarchy in the edit version and use the reasoner to infer the resulting polyhierarchy in release artefacts
- Rector normalization (e.g. via roles) [10]



[11]

7. Define classes and individuals

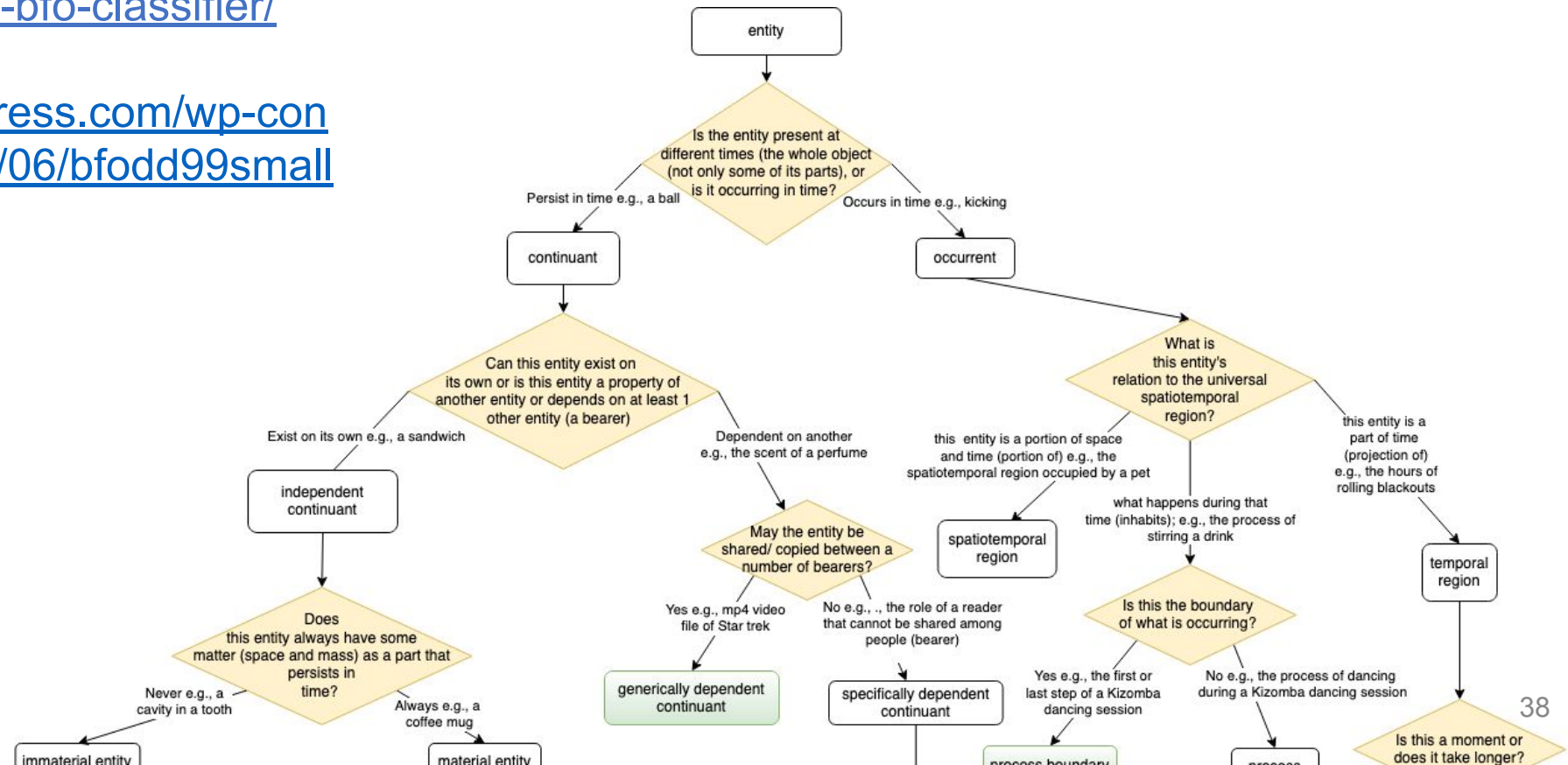
- A class without a definition is possible, but “meaningless”.
- What is a good definition?
- Aristotelian definition:
 - If A is a subclass of B, then the definition is:
 - $A := B + \Delta$
 - A is a B with the restriction that Δ
 - Example: *PizzaConCarne* is a *Pizza* that contains *Meat*.
 - Inconsistencies in the class hierarchy often become apparent here.

8. Assign concepts to the TLO

- If necessary, adapt and refine definitions again.

<https://keet.wordpress.com/2023/06/29/improved-the-bfo-classifier/>

<https://keet.wordpress.com/wp-content/uploads/2023/06/bfodd99small.png>



9. Identify relations between concepts

- If possible, (re)use relations from the top-level ontology.
 - avoid creating new ones; use classes to express relations
 - you cannot simply add additional info to properties (provenance: who, when, etc.)
 - except via formal reification (expensive) / rdf-star (not all tools support that)
- Special relations include: “part-whole” relationships, existential dependency, participation relationships, etc.
- Consider the temporal-spatial context of the relations (possibly define roles)
- Be very clear on use of “datatype property” vs. “object property”

10. Define additional rules (axioms)

- “If $\rightarrow$ Then,” e.g., using **SWRL rules**: <https://www.w3.org/submissions/SWRL/>
- **Property chains**:
 - owns **o** hasPart $\rightarrow$ owns
 - I own my car, my car hasPart engine $\rightarrow$ I own engine.
- SPARQL **construct queries** for expansion of shortcut relations [12]
 - defined by construct ([OMO_0002000](#))
- You can use this for mapping to external ontologies, without making an explicitly commitment

11. Create SHACL Shapes

- Shapes Constraint Language (SHACL)
- **For validation (consistency checking) of A-Box/T-Box**
- **Documentation (Patterns)**
 - Puzzle pieces to structure your data
- Ontology → describes what **IS**
- SHACL Shapes → describes what **SHOULD BE**



Photo by [Jonny Gios](#) on [Unsplash](#)

12. Evaluation

- Check whether the competency questions can be answered
- If not: return to step 1

13. Documentation

- Usage guide for users: how to reuse it?
- Provide example data
- Provide best practices and design guidelines for structuring concepts, relations, and axioms (ODPs).
- Formulate design principles and conventions (development guide)
- Prepare a concept for maintenance and further development

14. Publication of the ontology

- Namespace (e.g., via w3id.org or purl),
 - Prefix
 - Make sure you own it
- Dereferencing (can be implemented with GitHub)
 - the IRI should deliver information about the resource → Semantic Web
 - implement content negotiation: <https://www.w3.org/TR/cooluris/>
 - curl -L <https://w3id.org/pmd/co/3.0.0> → Website
 - curl -L -H "Accept: text/turtle" <https://w3id.org/pmd/co/3.0.0> → Turtle-File
- Publish a technical or research paper
- Registration with lookup portals and terminology services
- It is **not** enough to put an owl/ttl file to Github

15. Community

- Communication:
 - regular meetings; online and offline
- Form working groups; distribute responsibilities
- Provide development infrastructure, e.g., via GitHub, Miro, etc.
- Maintain and incentivize the community, e.g., academic publishing, funding opportunities, commercialization opportunities, recognition, and reputation
- Provide “playgrounds”, workshops, hackathons
- Governance
- Dissemination

- Ontology development is primarily a consensus-building activity, not just a technical one.
- The hardest part is agreeing on meanings, definitions, and scope, not writing OWL/RDF.
- Good ontologies emerge through discussion, negotiation, and reuse of existing standards.
- Reuse existing ontologies, standards, and design patterns whenever possible.
- Community adoption and governance are essential for success.
- It is normal to make mistakes:
 - ontology development is iterative, and continuous refinement is part of the process.

- [1] Neuhaus, Fabian & Hastings, Janna. (2022). Ontology Development is Consensus Creation, Not (Merely) Representation. 10.48550/arXiv.2210.12026.
- [2] Fernández-López, Mariano & Gomez-Perez, Asuncion & Juristo, Natalia. (1997). METHONTOLOGY: from ontological art towards ontological engineering. Engineering Workshop on Ontological Engineering (AAAI97).
- [3] Noy, N. & McGuinness, Deborah. (2001). Ontology Development 101: A Guide to Creating Your First Ontology. Knowledge Systems Laboratory. 32.
- [4] Valentina Presutti, Enrico Daga, Aldo Gangemi, and Eva Blomqvist. 2009. EXtreme design with content ontology design patterns. In Proceedings of the 2009 International Conference on Ontology Patterns - Volume 516 (WOP'09). CEUR-WS.org, Aachen, DEU, 83–97.
- [5] Suárez-Figueroa, Mari Carmen (2010). NeOn Methodology for Building Ontology Networks: Specification, Scheduling and Reuse. Thesis (Doctoral), Facultad de Informática (UPM) <https://doi.org/10.20868/UPM.thesis.3879>
- [6] <https://basic-formal-ontology.org/documents/seyed-shapiro-fois-2012.pdf>
- [7] <https://www.jarrar.info/courses/AAI/Jarrar.LectureNotes.AAI.2012S.OntologyModelingChallenges.pdf>
- [8] https://software-lab.org/publications/ontology_composition_gb.pdf
- [9] Guarino, Nicola and Chris Welty. 2002. Evaluating Ontological Decisions with OntoClean. Communications of the ACM. 45(2):61–65. New York:ACM Press
- [10] <https://douroucouli.wordpress.com/2019/06/29/ontotip-learn-the-rector-normalization-technique/>
- [11] <https://oboacademy.github.io/obook/explanation/intro-to-ontologies/>
- [12] C. Mungall, A. Ruttenberg, D. Osumi-Sutherland, Taking shortcuts with owl using safe macros, Nature Precedings (2010) 1–1. doi:<https://doi.org/10.1038/npre.2010.5292.1>.



PMDco: Data Transformation

How to transform my data?

1. Work out the patterns
2. Implement transformation method

Example: tensile-strength = 520 MPa

How to transform my data?

tensile-strength = 520MPa

- Find out what your data actually describes:
 - **when, how, who, what (thing, property, value), where**

when and where → **process** (occupies temporal region, occurs in location)

how → **plan specification** (e.g. document of a norm)

who → **agent** (persons, running software, or devices)

what thing → **object** or **information**

what property → **quality, disposition, or process-attribute**

what value → **value specification** and **datum** (setting/measurement)

tensile-strength = 520MPa

- Find out what your data actually describes:
 - Setting or Measurement? (“should be” or “is”)

What we know from the ontology:

- measured quality is a tensile strength
- a quality is inherent in some object (with role test piece)
- the quality has been measured
- the measurement has been carried out by a process
- the process has the object as a participant
- the measurement datum is the output of the process
- the measurement datum refers to a value specification, which describes the quality (tensile strength) and has value and unit

How to transform my data?

- the quality is a tensile strength
- a quality is inherent in some object (with role test piece)
- the quality has been measured
- the measurement has been carried out by a process
- the process has the object as a participant and realizes its test piece role
- the measurement datum refers to a value specification, which describes the quality (tensile strength) and has value and unit

```
ex:qual_1 rdf:type tensile_strength: .
```

```
ex:obj_1 has_quality: ex:qual_1 .
```

```
ex:obj_1 has_role: ex:role_1 .
```

```
ex:role_1 a :test_piece_role .
```

```
ex:datum_1 rdf:type measurement_datum: .
```

```
ex:datum_1 is_quality_measurement_of: ex:qual_1 .
```

```
ex:datum_1 specified_output_of: ex:proc_1 .
```

```
ex:proc_1 has_participant: ex:obj_1 .
```

```
ex:proc_1 realizes: ex:role_1 .
```

```
ex:datum_1 has_value_specification: ex:spec_1 .
```

```
ex:spec_1 specifies_value_of: ex:qual_1 .
```

```
ex:spec_1 has_specified_numeric_value: 520 .
```

```
ex:spec_1 has_measurement_unit_label: qudt:MegaPA .
```

How to transform my data?

RDF Triple

```
ex:qual_1 rdf:type tensile_strength: .
```

```
ex:obj_1 has_quality: ex:qual_1 .
```

```
ex:obj_1 has_role: ex:role_1 .
```

```
ex:role_1 a :test_piece_role .
```

```
ex:datum_1 rdf:type measurement_datum: .
```

```
ex:datum_1 is_quality_measurement_of: ex:qual_1 .
```

```
ex:datum_1 specified_output_of: ex:proc_1 .
```

```
ex:proc_1 has_participant: ex:obj_1 .
```

```
ex:proc_1 realizes: ex:role_1 .
```

```
ex:datum_1 has_value_specification: ex:spec_1 .
```

```
ex:spec_1 specifies_value_of: ex:qual_1 .
```

```
ex:spec_1 has_specified_numeric_value: 520 .
```

```
ex:spec_1 has_measurement_unit_label: qudt:MegaPA .
```

Prefixes

```
@prefix tensile_strength: <https://w3id.org/pmd/tto/TTO_0000053> .
```

```
@prefix has_quality: <http://purl.obolibrary.org/obo/RO_0000086> .
```

```
@prefix has_role: <http://purl.obolibrary.org/obo/RO_0000087> .
```

```
@prefix has_value_specification: <http://purl.obolibrary.org/obo/OBI_0001938> .
```

```
@prefix specifies_value_of: <http://purl.obolibrary.org/obo/OBI_0001927> .
```

```
@prefix has_participant: <http://purl.obolibrary.org/obo/RO_0000057> .
```

```
@prefix specified_output_of: <http://purl.obolibrary.org/obo/OBI_0000312> .
```

```
@prefix realizes: <http://purl.obolibrary.org/obo/BFO_0000055> .
```

```
@prefix has_specified_numeric_value: <http://purl.obolibrary.org/obo/OBI_0001937> .
```

```
@prefix has_measurement_unit_label: <http://purl.obolibrary.org/obo/IAO_0000039> .
```

```
@prefix measurement_datum: <http://purl.obolibrary.org/obo/IAO_0000109> .
```

How to transform my data?

Demo: <https://github.com/materialdigital/walkthrough-demos>

- Python tool with pattern replace
- Python tool with RDFlib: <https://rdflib.readthedocs.io/en/stable/>
- RML:
 - YARRRML mapping: <https://rml.io/yarrrml/>
 - (<https://github.com/Mat-O-Lab/RDFConverter>)
 - (<https://ontop-vkg.org/>)
- Robot Spreadsheet: <https://robot.obolibrary.org/template>
- OTTR template: <https://ottr.xyz/>

Anti-Patterns

- Don't **just change the structure** of your data.
- If you have “key” - “value” pairs in your data and you create properties “hasKey” and “hasValue”
 - `:data a :Entry .`
 - `:data hasKey "Tensile Strength" .`
 - `:data hasValue 520 .`
 - → you will not gain interoperability
- If you just transform you tabular data into CSVW
 - `ex:col2 a csvw:Column ;`
 - `csvw:name "tensile_strength_MPa" ;`
 - `csvw:value "520" .`
 - → you will not gain interoperability



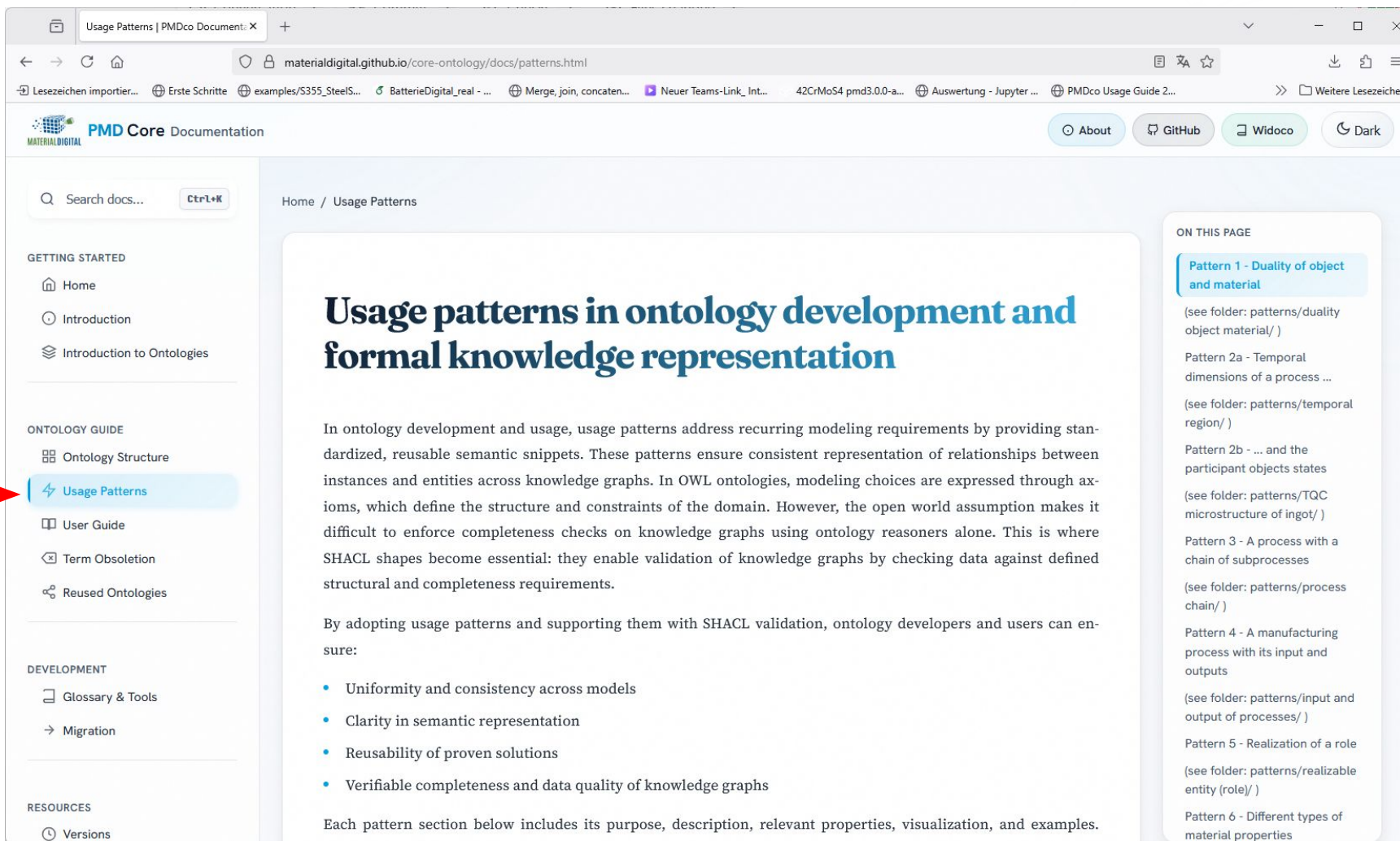
Thank you!!

PMDco: Ontology pattern and usage guide

Usage patterns:

- are a means of addressing recurring modelling situations
- allow for uniformity and consistency across different models
- provide clarity in semantic representation
- facilitate reusability of proven solutions
- give us a tool to verify completeness and data quality of knowledge graphs (to a certain extent)
- are usually expressed in the context of a “closed world” assumption
- can easily be expressed with the SHACL-language
- are **not** meant to replace the (OWL-) axioms that formulate classes and rely on the open world assumption

Lets learn to play piano by studying the piano score :)



The screenshot shows a web browser displaying the 'Usage Patterns' page of the PMD Core Documentation. The browser's address bar shows the URL materialdigital.github.io/core-ontology/docs/patterns.html. The page has a light blue header with the 'PMD Core Documentation' logo and navigation links for 'About', 'GitHub', 'Widoco', and 'Dark' mode. A search bar is located in the top left of the content area. The left sidebar contains a 'GETTING STARTED' section with links to 'Home', 'Introduction', and 'Introduction to Ontologies'. Below this is the 'ONTOLOGY GUIDE' section, where 'Usage Patterns' is highlighted with a blue bar and a red arrow points to it. Other links in this section include 'Ontology Structure', 'User Guide', 'Term Obsolescence', and 'Reused Ontologies'. The 'DEVELOPMENT' section has links to 'Glossary & Tools' and 'Migration'. The 'RESOURCES' section has a link to 'Versions'. The main content area features the title 'Usage patterns in ontology development and formal knowledge representation' in a large, bold, blue font. Below the title is a paragraph explaining that usage patterns address recurring modeling requirements by providing standardized, reusable semantic snippets. It mentions that in OWL ontologies, modeling choices are expressed through axioms, which define the structure and constraints of the domain. However, the open world assumption makes it difficult to enforce completeness checks on knowledge graphs using ontology reasoners alone. This is where SHACL shapes become essential: they enable validation of knowledge graphs by checking data against defined structural and completeness requirements. Below this paragraph is a list of four bullet points: 'Uniformity and consistency across models', 'Clarity in semantic representation', 'Reusability of proven solutions', and 'Verifiable completeness and data quality of knowledge graphs'. At the bottom of the main content area, a sentence states: 'Each pattern section below includes its purpose, description, relevant properties, visualization, and examples.' On the right side of the page, there is a 'ON THIS PAGE' section with a list of links to specific pattern sections: 'Pattern 1 - Duality of object and material', 'Pattern 2a - Temporal dimensions of a process ...', 'Pattern 2b - ... and the participant objects states', 'Pattern 3 - A process with a chain of subprocesses', 'Pattern 4 - A manufacturing process with its input and outputs', and 'Pattern 5 - Realization of a role'.

Usage Patterns | PMDco Document: X

materialdigital.github.io/core-ontology/docs/patterns.html

Leesezeichen importier... Erste Schritte examples/S355_SteelS... BatterieDigital_real - ... Merge, join, concaten... Neuer Teams-Link_Int... 42CrMoS4 pmd3.0.0-a... Auswertung - Jupyter ... PMDco Usage Guide 2... Weitere Leesezeichen

PMD Core Documentation

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Usage patterns in ontology development and formal knowledge representation

In ontology development and usage, usage patterns address recurring modeling requirements by providing standardized, reusable semantic snippets. These patterns ensure consistent representation of relationships between instances and entities across knowledge graphs. In OWL ontologies, modeling choices are expressed through axioms, which define the structure and constraints of the domain. However, the open world assumption makes it difficult to enforce completeness checks on knowledge graphs using ontology reasoners alone. This is where SHACL shapes become essential: they enable validation of knowledge graphs by checking data against defined structural and completeness requirements.

By adopting usage patterns and supporting them with SHACL validation, ontology developers and users can ensure:

- Uniformity and consistency across models
- Clarity in semantic representation
- Reusability of proven solutions
- Verifiable completeness and data quality of knowledge graphs

Each pattern section below includes its purpose, description, relevant properties, visualization, and examples.

ON THIS PAGE

- Pattern 1 - Duality of object and material
(see folder: patterns/duality object material/)
- Pattern 2a - Temporal dimensions of a process ...
(see folder: patterns/temporal region/)
- Pattern 2b - ... and the participant objects states
(see folder: patterns/TQC microstructure of ingot/)
- Pattern 3 - A process with a chain of subprocesses
(see folder: patterns/process chain/)
- Pattern 4 - A manufacturing process with its input and outputs
(see folder: patterns/input and output of processes/)
- Pattern 5 - Realization of a role
(see folder: patterns/realizable entity (role)/)
- Pattern 6 - Different types of material properties

<https://materialdigital.github.io/core-ontology/docs/patterns.html>

Reading the pattern: @PREFIX-trick

Typical usage:

```
@PREFIX schema: <https://schema.org/> .
```

```
<#philipp> a schema:person .
```

```
# ... is expanded to:
```

```
<#philipp> a <https://schema.org/person> .
```

Readability trick in pattern files:

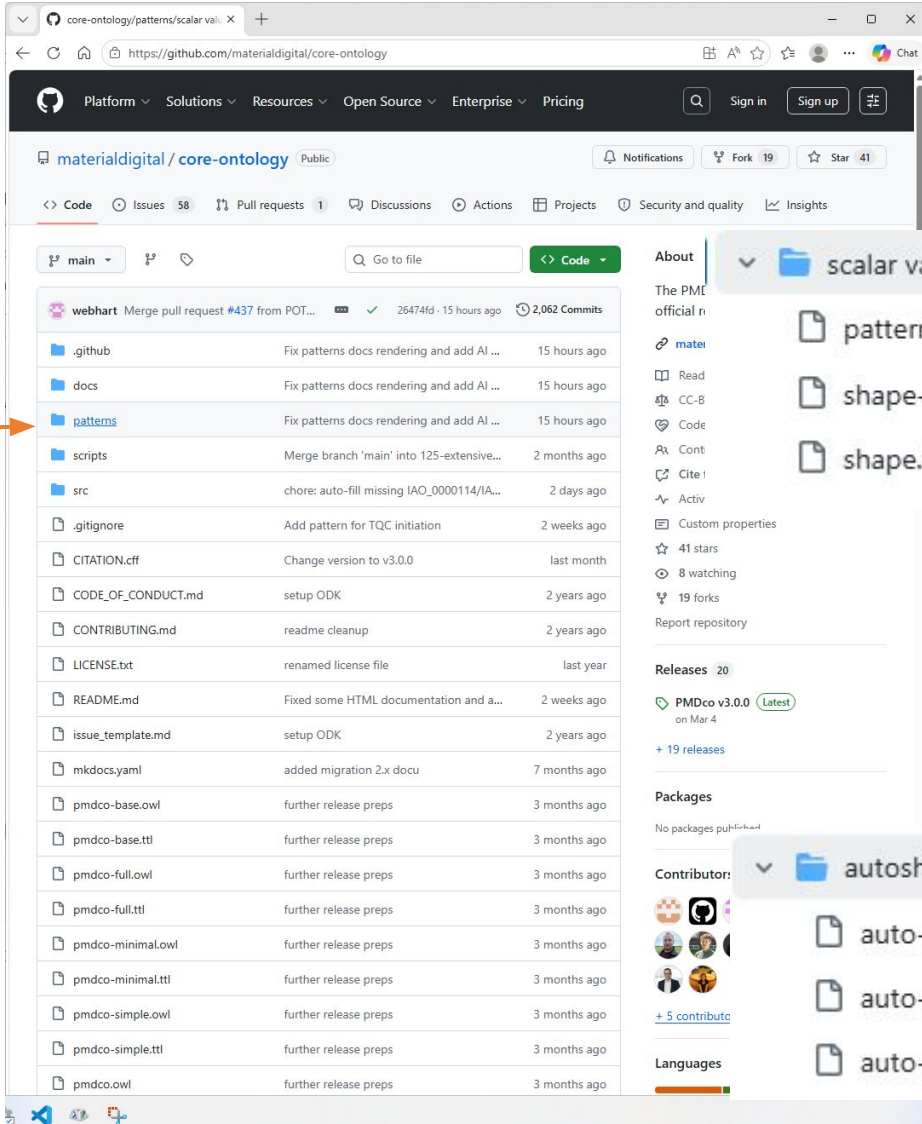
```
@PREFIX scalar_value_specification: <http://purl.obolibrary.org/obo/OBI\_0001931> .
```

```
<#mySVS> a scalar_value_specification: .
```

```
# ... is expanded to:
```

```
<#mySVS> a <http://purl.obolibrary.org/obo/OBI\_0001931> .
```

Organization of the pattern



pattern folder

specific pattern

scalar value specification

pattern.md

Introductory text

shape-data.ttl

Pattern application example

shape.ttl

SHACL shape

Shapes generated from OWL axioms, e.g. mandatory presence of SubClassOf axiom entities

autoshape

auto-shapes-closed.ttl

auto-shapes-open.ttl

auto-shapes-semi-closed.ttl

The **Platform MaterialDigital Core Ontology (PMDco)** is a mid-level semantic framework for Materials Science and Engineering (MSE). Aligning with the ISO/IEC 21838-2:2021 standard, PMDco is built on the *Basic Formal Ontology (BFO)* and reuses several BFO-aligned ontologies such as **RO**, **IAO**, and **OBI**. Its scope follows the fundamental paradigm of MSE — **processing, structure, and properties** — and provides general semantics for entities commonly required across MSE disciplines, such as devices, roles, functions, and plans.

Processes	Structure & State	Properties
MSE-related process chains, including materials manufacturing, characterization, and simulation processes.	Substances, engineered materials, their composition, and multiscale structural features.	Material properties and qualities, representing processing–structure–property dependences.

“Represent our knowledge of the MSE domain”

- **Pattern 1 - Duality of object and material**
- **Pattern 2 - Temporal dimensions of a process and the participant objects states**
- **Pattern 3 - A process with (a chain of) subprocesses**
- **Pattern 4 - A manufacturing process with its input and outputs**
- **Pattern 5 - Realization of a role (in a measurement)**

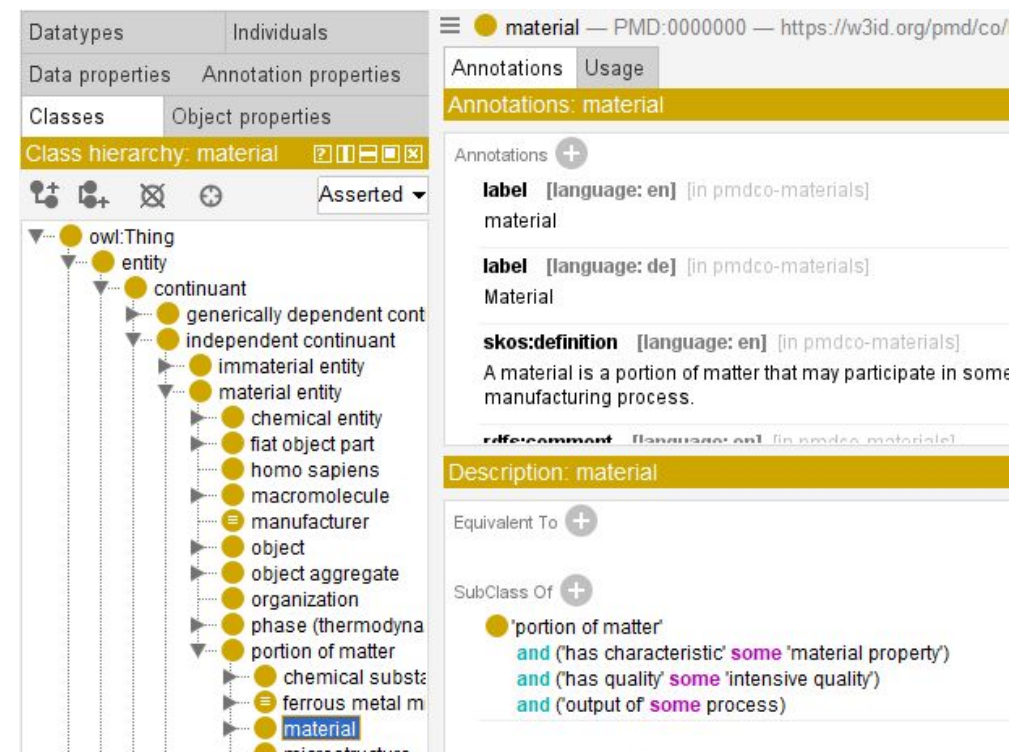


<https://www.lohmann-stahl.de/>

Two fundamental classes

portion of matter (pmd:PMD_0000001)
skos:definition “A material entity that is not demarcated by any physical discontinuities. At some finer level of granularity it is an object aggregate, at some coarser level of granularity it is a fiat object part, but at this level of granularity it is neither.”

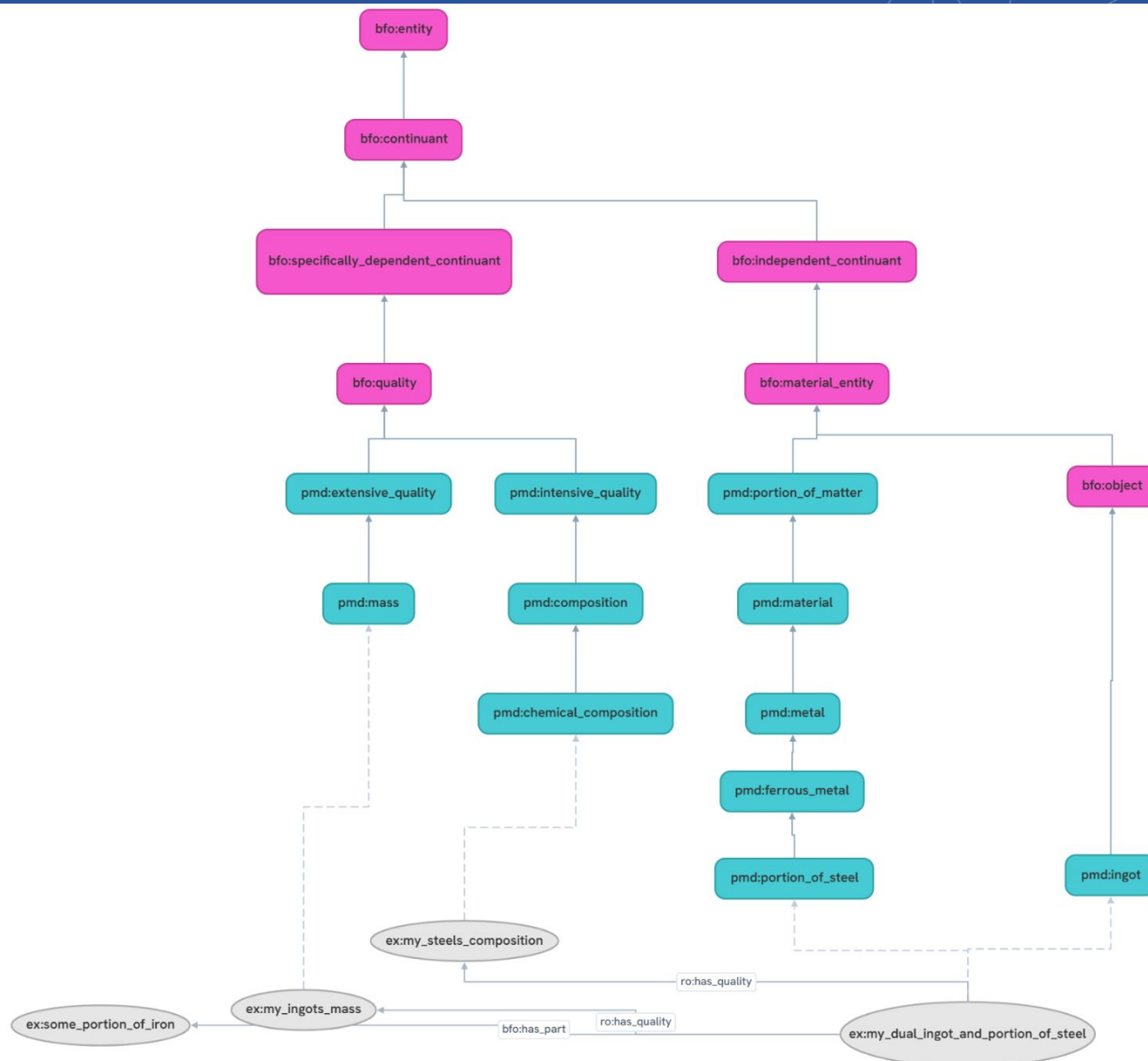
material (pmd:PMD_0000000)
skos:definition “A material is a portion of matter that may participate in some manufacturing process and whose shape is not relevant for its participation in the manufacturing process.”



The screenshot displays the PMD ontology editor interface. On the left, the 'Class hierarchy' panel shows a tree structure starting from 'owl:Thing', branching into 'entity', 'continuant', 'generically dependent cont', 'independent continuant', 'immaterial entity', 'material entity', 'chemical entity', 'fiat object part', 'homo sapiens', 'macromolecule', 'manufacturer', 'object', 'object aggregate', 'organization', 'phase (thermodyna', 'portion of matter', 'chemical subst', 'ferrous metal m', 'material', and 'microstructure'. The 'material' class is highlighted. On the right, the 'Annotations' panel for 'material' (PMD:0000000) is shown, including labels in English and German, a skos:definition in English, and a description. The 'Description' panel shows the class is equivalent to 'portion of matter' and is a subclass of 'portion of matter' with specific constraints.

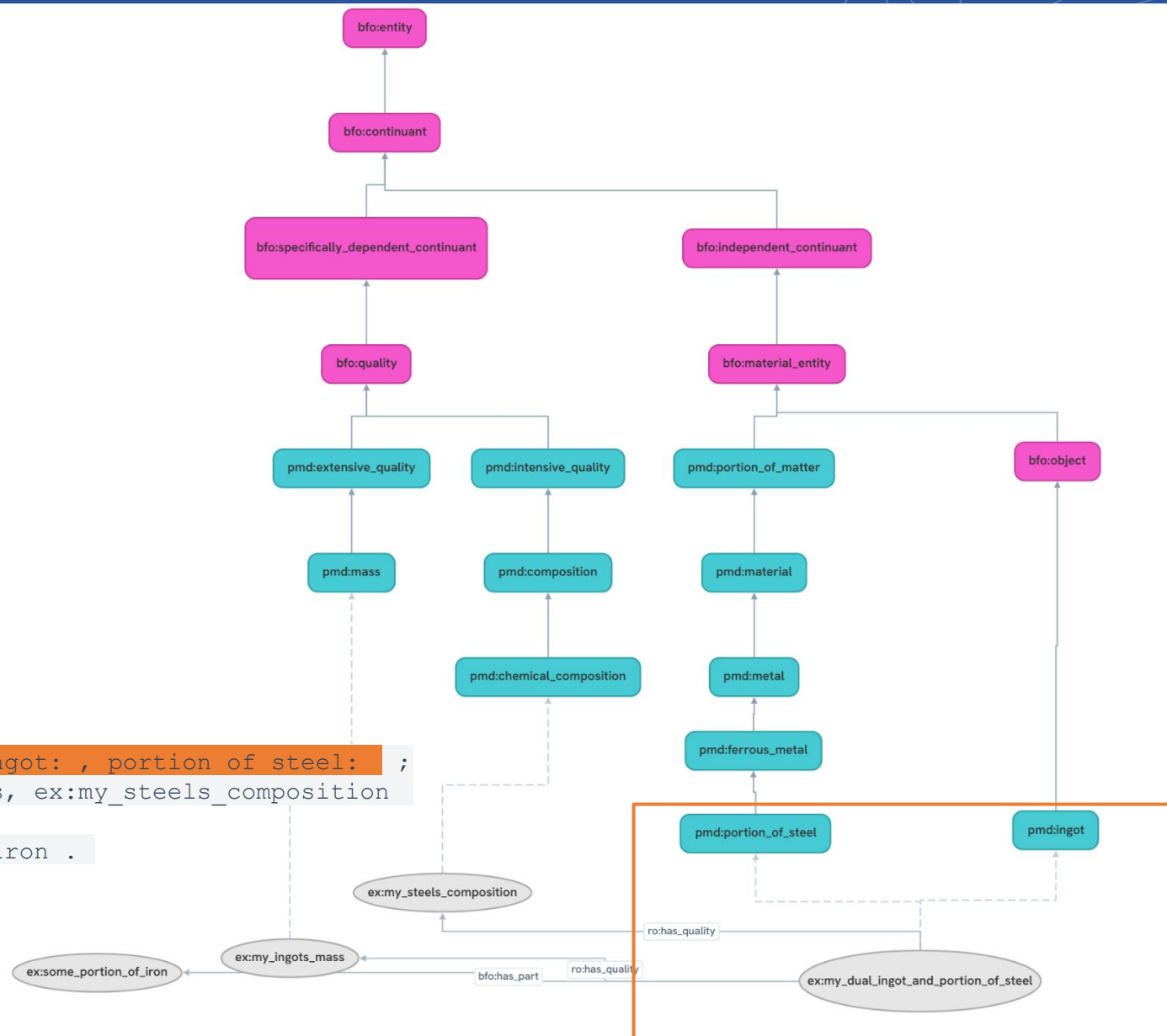
Pattern 1 - Duality of object and material

Purpose: Represents how objects and portions of matter are the same material entity, like a statue that is at the same time a portion of clay



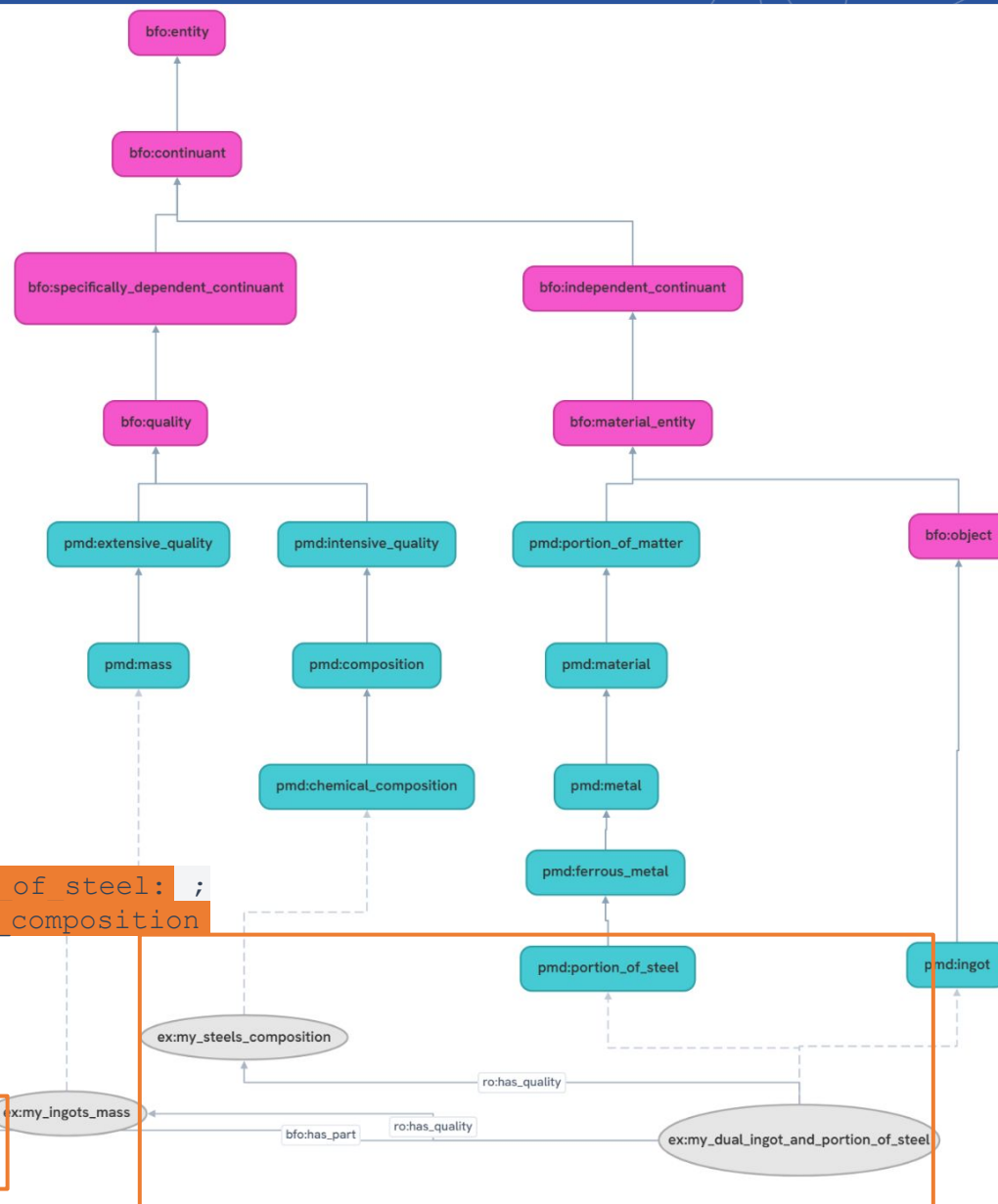
Pattern 1 - Duality of object and material

Purpose: Represents how objects and portions of matter are the same material entity, like a statue that is at the same time a portion of clay



Pattern 1 - Duality of object and material

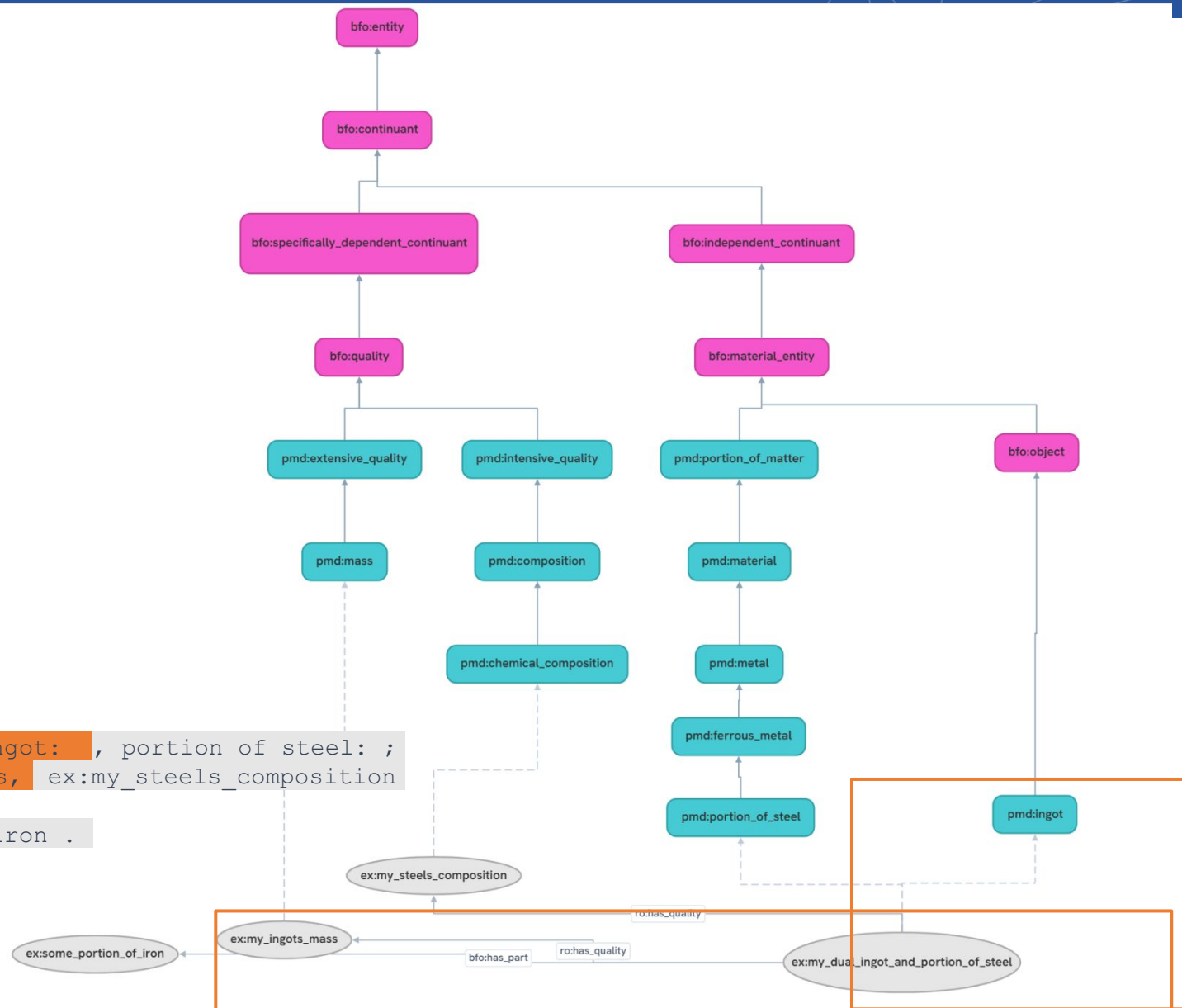
Purpose: Represents how objects and portions of matter are the same material entity, like a statue that is at the same time a portion of clay



```
ex:my dual ingot and portion of steel a ingot: , portion of steel: ;
;
has quality: ex:my_ingots_mass, ex:my_steels_composition
;
has part: ex:some_portion_of_iron .
```

Pattern 1 - Duality of object and material

Purpose: Represents how objects and portions of matter are the same material entity, like a statue that is at the same time a portion of clay



A large industrial facility, likely a nuclear reactor core, with a large circular structure in the foreground emitting a bright orange flame. A worker in a white protective suit is visible in the background.

The diagram illustrates a complex ontology structure with the following components and relationships:

- Entities and Processes (Pink rounded rectangles):**
 - `bfo:process`
 - `bfo:temporal_region`
 - `bfo:one-dimensional_temporal_region`
 - `bfo:temporal_interval`
 - `bfo:temporal_instant`
 - `bfo:zero-dimensional_temporal_region`
 - `bfo:continuant`
 - `bfo:independent_continuant`
 - `bfo:material_entity`
 - `bfo:object`
 - `bfo:entity`
- Examples (Gray ovals):**
 - `ex:annealing_start`
 - `ex:annealing_end`
 - `ex:temp_intvl_of_the_ingots_annealing`
 - `ex:the_ingots_annealing_process`
 - `ex:the_dual_ingot_and_portion_of_steel`
 - `ex:the_furnace`
- Material (Teal rounded rectangle):**
 - `pmd:ingot`
- Relationships (Solid and Dashed lines with labels):**
 - `bfo:has_first_instant` (from `ex:temp_intvl_of_the_ingots_annealing` to `ex:annealing_start`)
 - `bfo:has_last_instant` (from `ex:temp_intvl_of_the_ingots_annealing` to `ex:annealing_end`)
 - `bfo:occupies_temporal_region` (from `ex:the_ingots_annealing_process` to `ex:temp_intvl_of_the_ingots_annealing`)
 - `ro:participates_in` (from `ex:the_dual_ingot_and_portion_of_steel` to `ex:the_ingots_annealing_process`)
 - `ro:participates_in` (from `ex:the_furnace` to `ex:the_ingots_annealing_process`)
 - `pmd:participates_in` (from `ex:the_furnace` to `pmd:ingot`)
 - `bfo:participates_in` (from `ex:the_furnace` to `bfo:object`)
 - `bfo:participates_in` (from `pmd:ingot` to `bfo:object`)
 - `bfo:participates_in` (from `ex:the_dual_ingot_and_portion_of_steel` to `bfo:object`)
 - `bfo:participates_in` (from `ex:the_ingots_annealing_process` to `bfo:process`)
 - `bfo:participates_in` (from `ex:temp_intvl_of_the_ingots_annealing` to `bfo:temporal_region`)
 - `bfo:participates_in` (from `ex:annealing_start` to `bfo:temporal_instant`)
 - `bfo:participates_in` (from `ex:annealing_end` to `bfo:temporal_instant`)
 - `bfo:participates_in` (from `bfo:temporal_instant` to `bfo:zero-dimensional_temporal_region`)
 - `bfo:participates_in` (from `bfo:temporal_instant` to `bfo:continuant`)
 - `bfo:participates_in` (from `bfo:continuant` to `bfo:independent_continuant`)
 - `bfo:participates_in` (from `bfo:independent_continuant` to `bfo:material_entity`)
 - `bfo:participates_in` (from `bfo:material_entity` to `bfo:object`)
 - `bfo:participates_in` (from `bfo:object` to `bfo:entity`)
 - `bfo:participates_in` (from `bfo:process` to `bfo:entity`)
 - `bfo:participates_in` (from `bfo:temporal_region` to `bfo:entity`)

Pattern 2 - Temporal dimensions of a process and the participator objects states



Purpose: Specify the temporal extend and the temporal boundaries of a process on the time axis.

ex:the ingots annealing process a process: .

ex:temp intvl of the ingots_annealing a temporal_interval: .

ex:the furnace a object: .

ex:the dual ingot and portion of steel a ingot: .

ex:annealing start a temporal instant: .

ex:annealing_end a temporal_instant: .

ex:the ingots annealing process occupies_temporal_region:

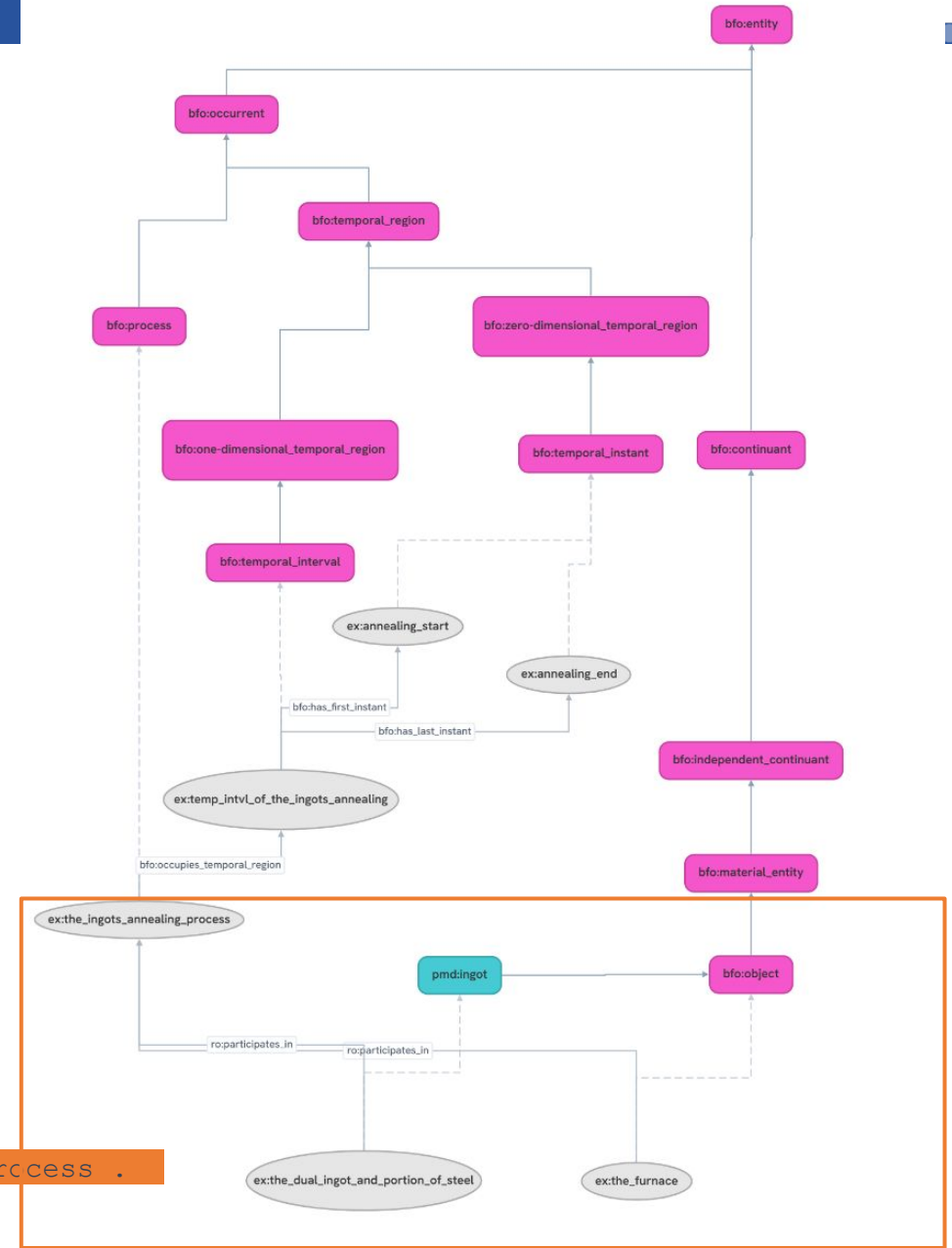
ex:temp intvl of the ingots annealing .

ex:temp intvl of the ingots annealing has first instant: ex:annealing start .

ex:temp intvl of the ingots annealing has last instant: ex:annealing_end .

ex:the furnace participates in: ex:the ingots annealing process .

ex:the dual ingot and portion of steel participates in: ex:the ingots annealing process .



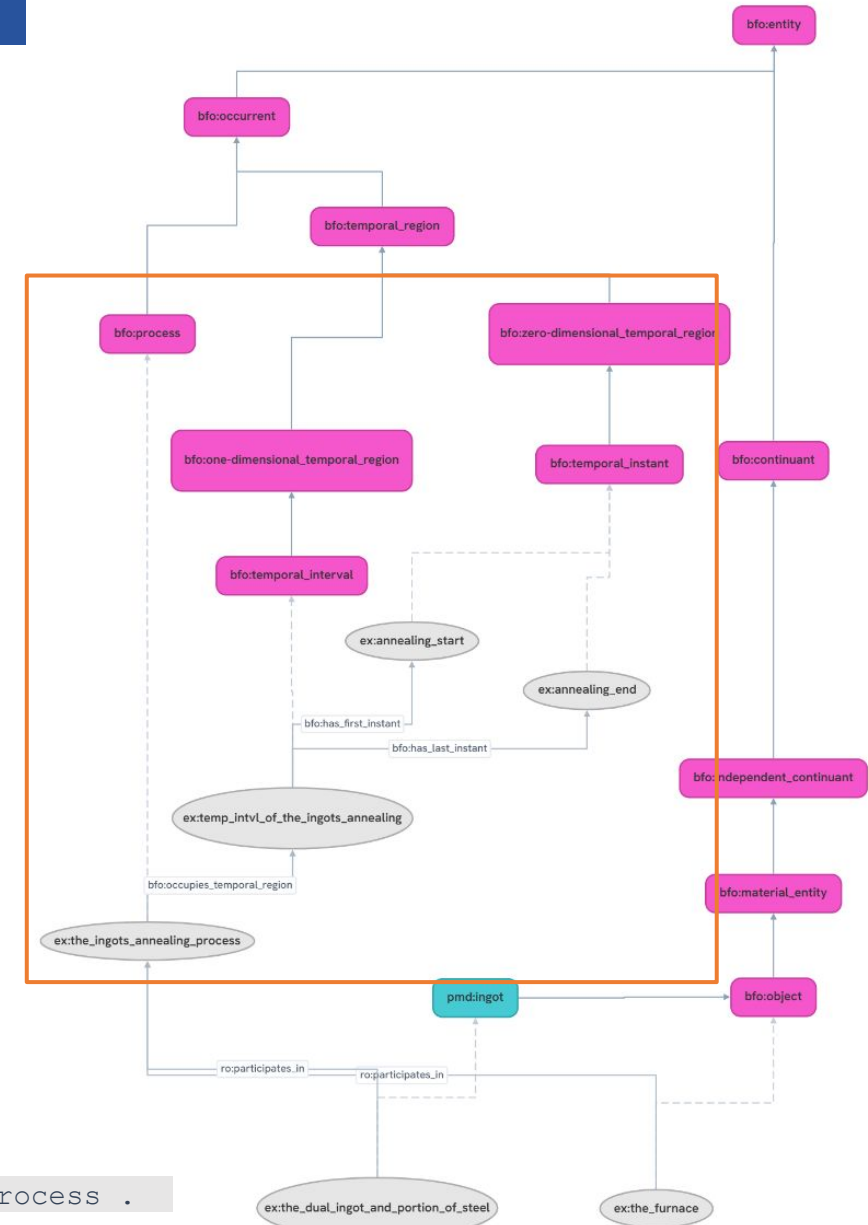
Pattern 2 - Temporal dimensions of a process and the participant objects states



Purpose: Specify the temporal extend and the temporal boundaries of a process on the time axis.

ex:the ingots annealing process a process: .
ex:temp intvl of the ingots annealing a temporal_interval: .
ex:the furnace a object: .
ex:the dual ingot and portion of steel a ingot: .
ex:annealing start a temporal instant: .
ex:annealing_end a temporal_instant: .

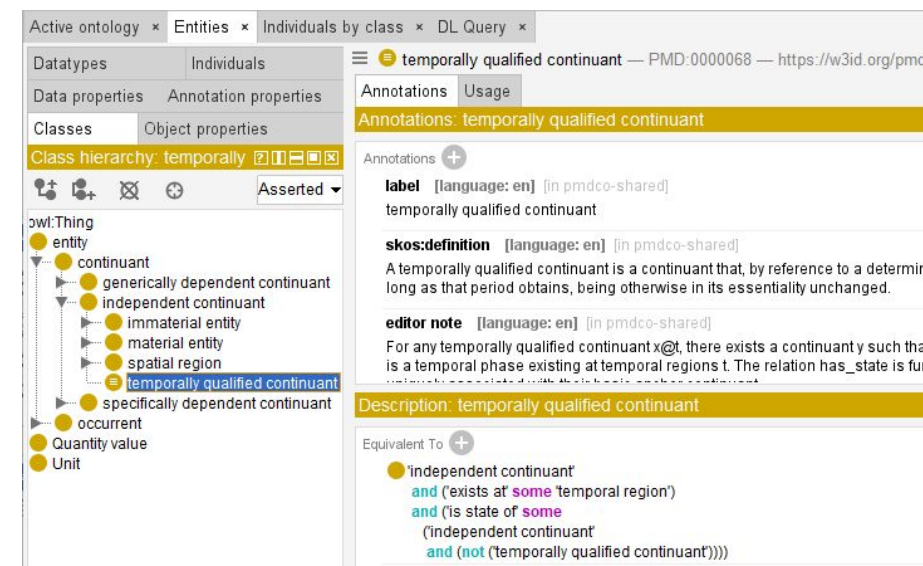
ex:the ingots annealing process occupies temporal region:
ex:temp intvl of the ingots annealing .
ex:temp intvl of the ingots annealing has first instant: ex:annealing start .
ex:temp intvl of the ingots annealing has last instant: ex:annealing_end .
ex:the furnace participates in: ex:the ingots annealing process .
ex:the_dual_ingot_and_portion_of_steel participates_in: ex:the_ingots_annealing_process .



temporally qualified continuant (pmd:PMD_0000068)
skos:definition “A temporally qualified continuant is a continuant that, by reference to a determinate temporal region, is such as to possess its properties only for so long as that period pertains, being otherwise in its *essentiality* unchanged.”

Side-note:

“**anchor**” === ('independent continuant'
and (not ('temporally qualified continuant')))



The screenshot shows the Protégé ontology editor interface. The left pane displays the class hierarchy under 'owl:Thing', with 'temporally qualified continuant' highlighted. The right pane shows the 'Annotations' tab for this class, including a label, a skos:definition, an editor note, and an 'Equivalent To' statement.

Active ontology x Entities x Individuals by class x DL Query x

Datatypes Individuals

Data properties Annotation properties

Classes Object properties

Class hierarchy temporally [?] [?] [?] [?] [?]

Asserted

owl:Thing

- entity
 - continuant
 - generically dependent continuant
 - independent continuant
 - immaterial entity
 - material entity
 - spatial region
 - temporally qualified continuant**
 - specifically dependent continuant
 - occurrent
 - Quantity value
 - Unit

Annotations temporally qualified continuant — PMD:0000068 — <https://w3id.org/pmdco>

Annotations Usage

Annotations: temporally qualified continuant

Annotations +

label [language: en] [in pmdco-shared]
temporally qualified continuant

skos:definition [language: en] [in pmdco-shared]
A temporally qualified continuant is a continuant that, by reference to a determinate temporal region, is such as to possess its properties only for so long as that period pertains, being otherwise in its essentiality unchanged.

editor note [language: en] [in pmdco-shared]
For any temporally qualified continuant $x@t$, there exists a continuant y such that y is a temporal phase existing at temporal regions t . The relation has_state is functional and associated with the has_state property.

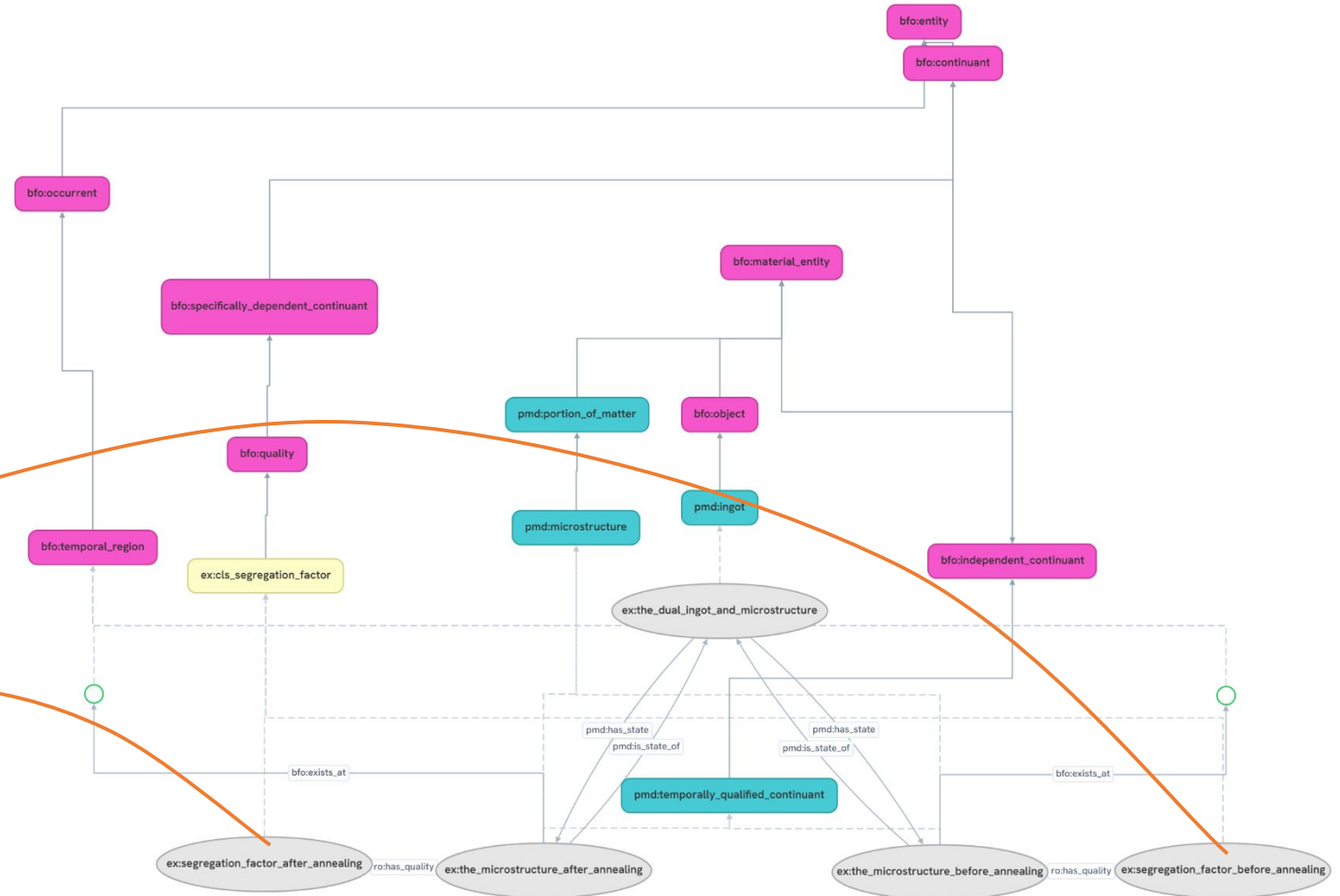
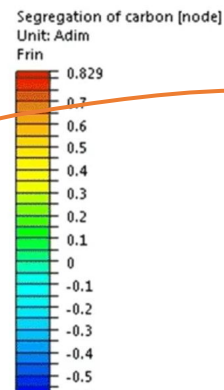
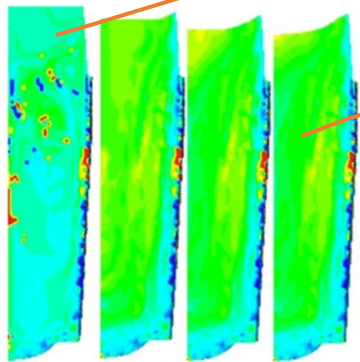
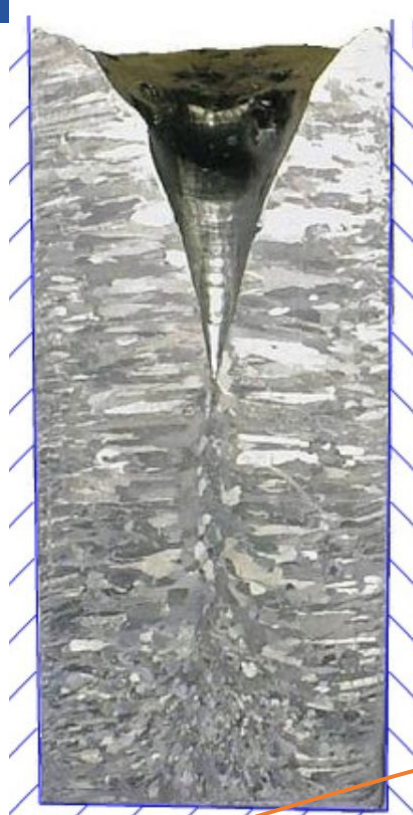
Description: temporally qualified continuant

Equivalent To +

- independent continuant
and ('exists at some temporal region')
and ('is state of some
(independent continuant
and (not ('temporally qualified continuant'))))

Pattern 2 - Temporal dimensions of a process and the participant objects states

<https://www.doi.poms.ac.uk/itlib/casting/microsegregation.php>



Pattern 2 - Temporal dimensions of a process and the participant objects states

```
# Define Object (Anchor)
```

```
ex:the dual ingot and microstructure a ingot: .
```

```
# ...and its variable states:
```

```
ex:the microstructure before annealing a microstructure: ,  
  temporally qualified continuant: .  
ex:the_microstructure_after_annealing a microstructure: ,  
  temporally qualified continuant: .
```

```
# Describe the states with their individual qualities
```

```
ex:segregation factor before annealing a ex:cls segregation factor .
```

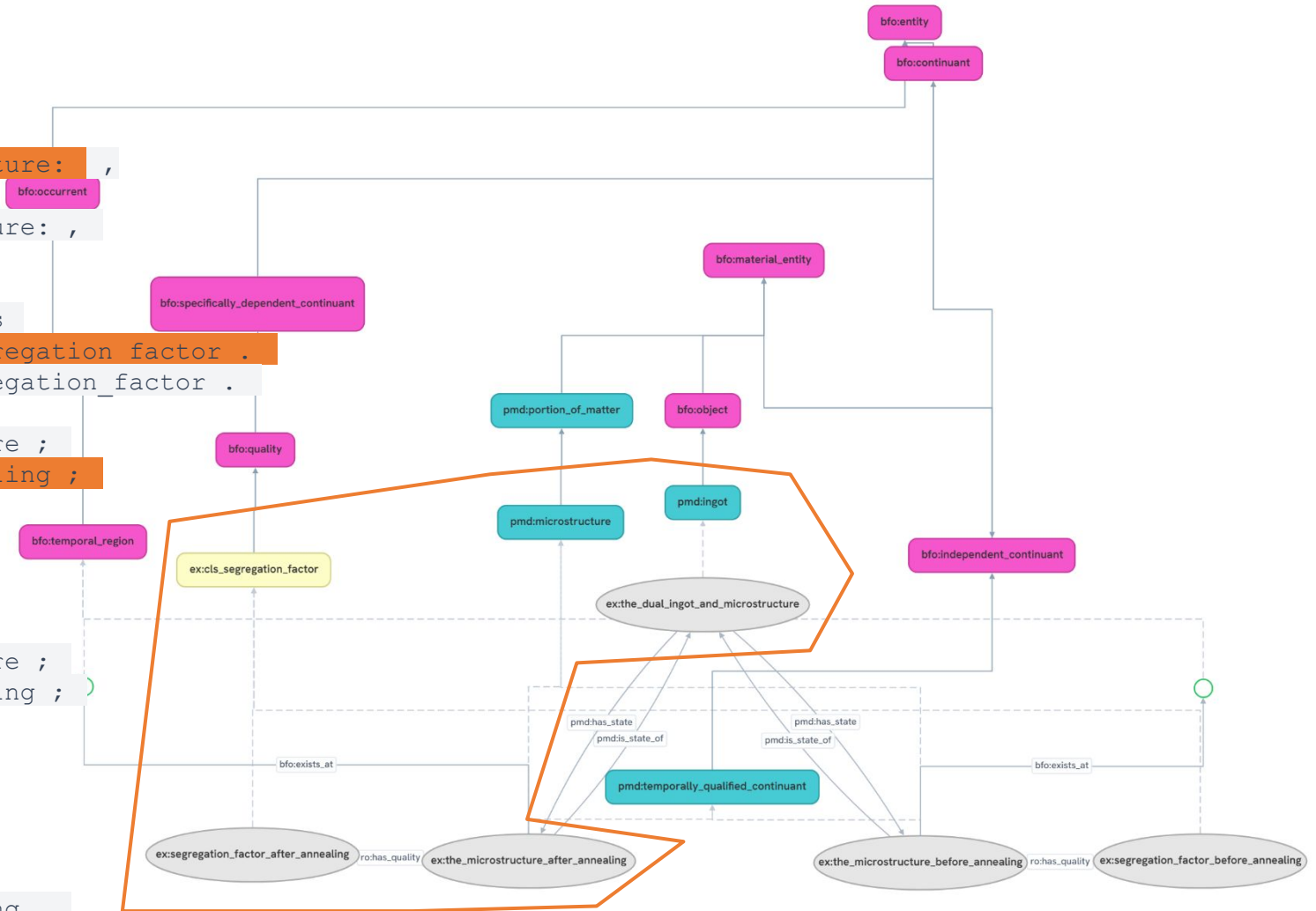
```
ex:segregation factor after annealing a ex:cls_segregation_factor .
```

```
ex:the microstructure before annealing  
  is state of: ex:the dual ingot and microstructure ;  
  has quality: ex:segregation_factor_before_annealing ;  
  exists at: [  
    a temporal_region:  
  ] .
```

```
ex:the microstructure after annealing  
  is state of: ex:the dual ingot and microstructure ;  
  has quality: ex:segregation_factor_after_annealing ;  
  exists at: [  
    a temporal_region:  
  ] .
```

```
# Link the states to their anchor and vice versa
```

```
ex:the dual ingot and microstructure  
  has state: ex:the microstructure before annealing ,  
            ex:the_microstructure_after_annealing .
```



Pattern 2 - Temporal dimensions of a process and the participant objects states

```
# Define Object (Anchor)
```

```
ex:the dual ingot and microstructure a ingot: .
```

```
# ...and its variable states:
```

```
ex:the microstructure before annealing a microstructure: ,  
  temporally qualified continuant: .
```

```
ex:the_microstructure_after_annealing a microstructure: ,  
  temporally qualified continuant: .
```

```
# Describe the states with their individual qualities
```

```
ex:segregation factor before annealing a ex:cls segregation factor .
```

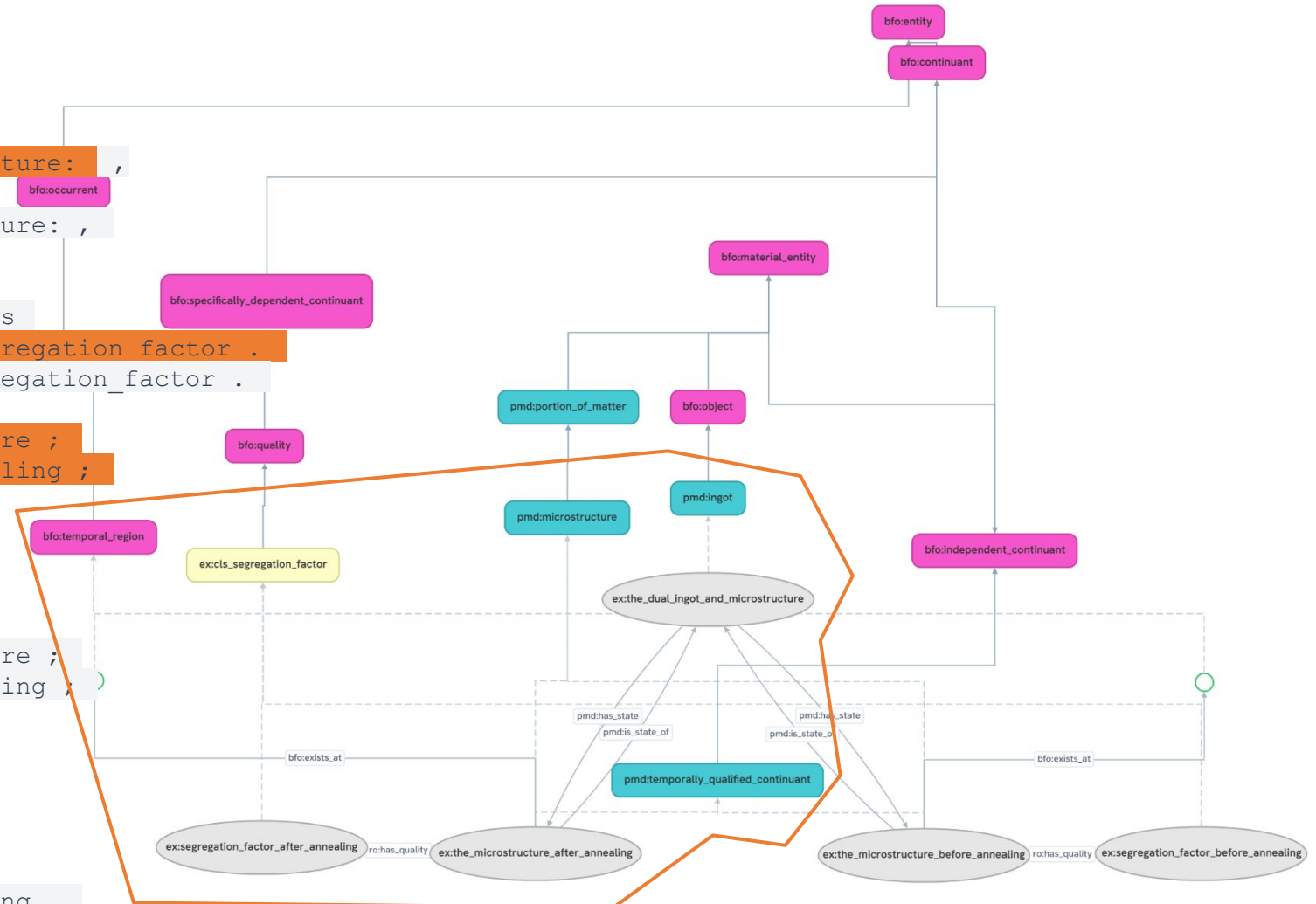
```
ex:segregation factor after annealing a ex:cls_segregation_factor .
```

```
ex:the microstructure before annealing  
  is state of: ex:the dual ingot and microstructure ;  
  has quality: ex:segregation_factor_before_annealing ;  
  exists at: [  
    a temporal_region:  
  ] .
```

```
ex:the microstructure after annealing  
  is state of: ex:the dual ingot and microstructure ;  
  has quality: ex:segregation_factor_after_annealing ;  
  exists at: [  
    a temporal_region:  
  ] .
```

```
# Link the states to their anchor and vice versa
```

```
ex:the dual ingot and microstructure  
  has state: ex:the microstructure before annealing ,  
            ex:the_microstructure_after_annealing .
```



Pattern 2 - Temporal dimensions of a process and the participant objects states

Define Object (Anchor)

ex:the dual ingot and microstructure a ingot: .

...and its variable states:

ex:the microstructure before annealing a microstructure: ,
temporally qualified continuant: .

ex:the microstructure after annealing a microstructure: ,
temporally qualified continuant: .

Describe the states with their individual qualities

ex:segregation factor before annealing a ex:cls segregation factor .

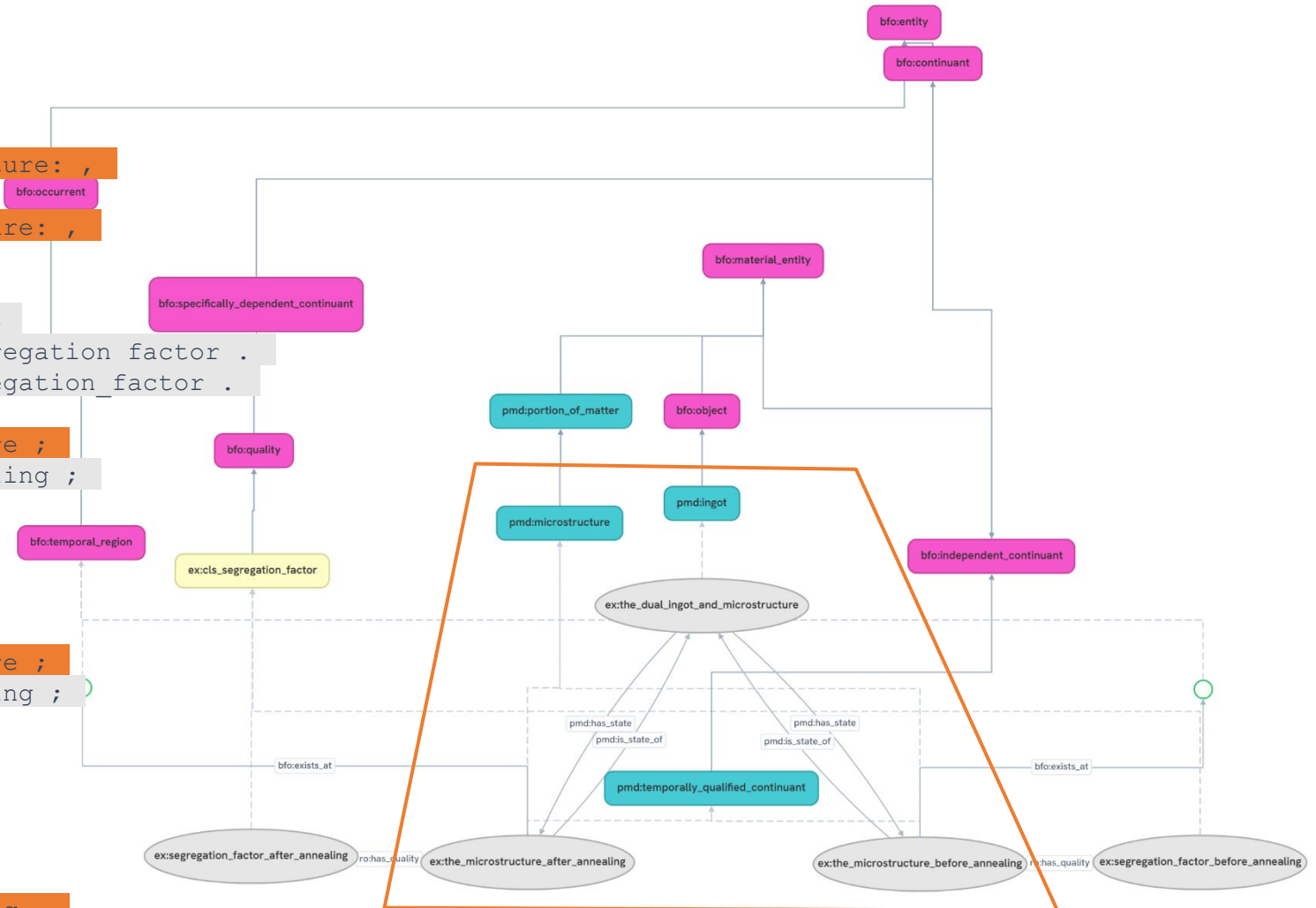
ex:segregation factor after annealing a ex:cls_segregation_factor .

ex:the microstructure before annealing
is state of: ex:the dual ingot and microstructure ;
has quality: ex:segregation_factor_before_annealing ;
exists at: [
a temporal_region:
] .

ex:the microstructure after annealing
is state of: ex:the dual ingot and microstructure ;
has quality: ex:segregation_factor_after_annealing ;
exists at: [
a temporal_region:
] .

Link the states to their anchor and vice versa

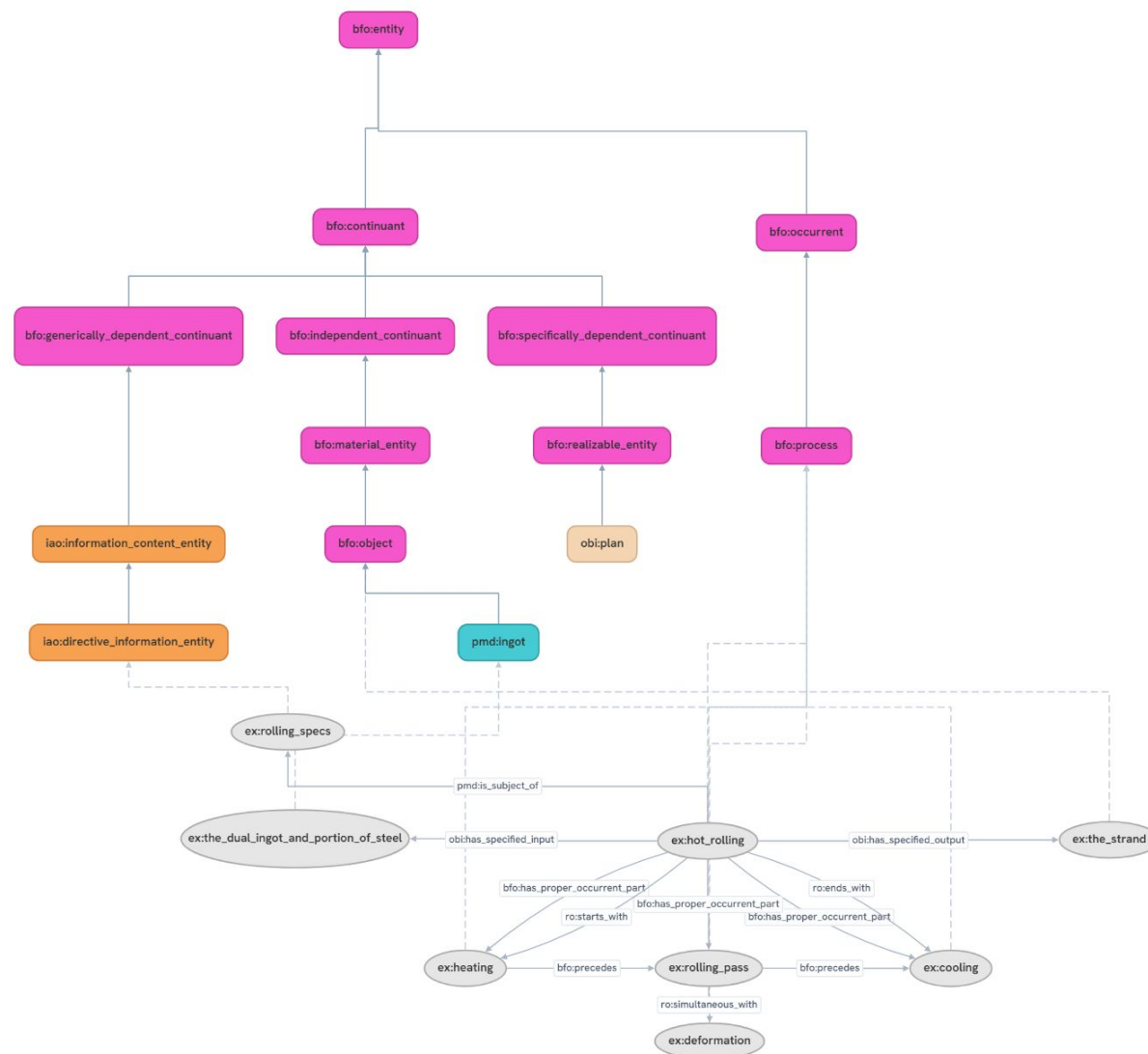
ex:the dual ingot and microstructure
has state: ex:the microstructure before annealing ,
ex:the microstructure after annealing .



Pattern 3 - A process with in/output and a chain of subprocesses



<https://www.wshampshire.com/industries/steel-aluminum/>



Pattern 3 - A process with in/output and a chain of subprocesses

```
ex:the dual ingot and portion_of_steel a ingot: .  
ex:the_strand a object: .
```

```
ex:hot_rolling a process: .  
ex:hot_rolling has specified input: ex:the dual ingot_and_portion_of_steel .  
ex:hot_rolling has specified output: ex:the_strand .
```

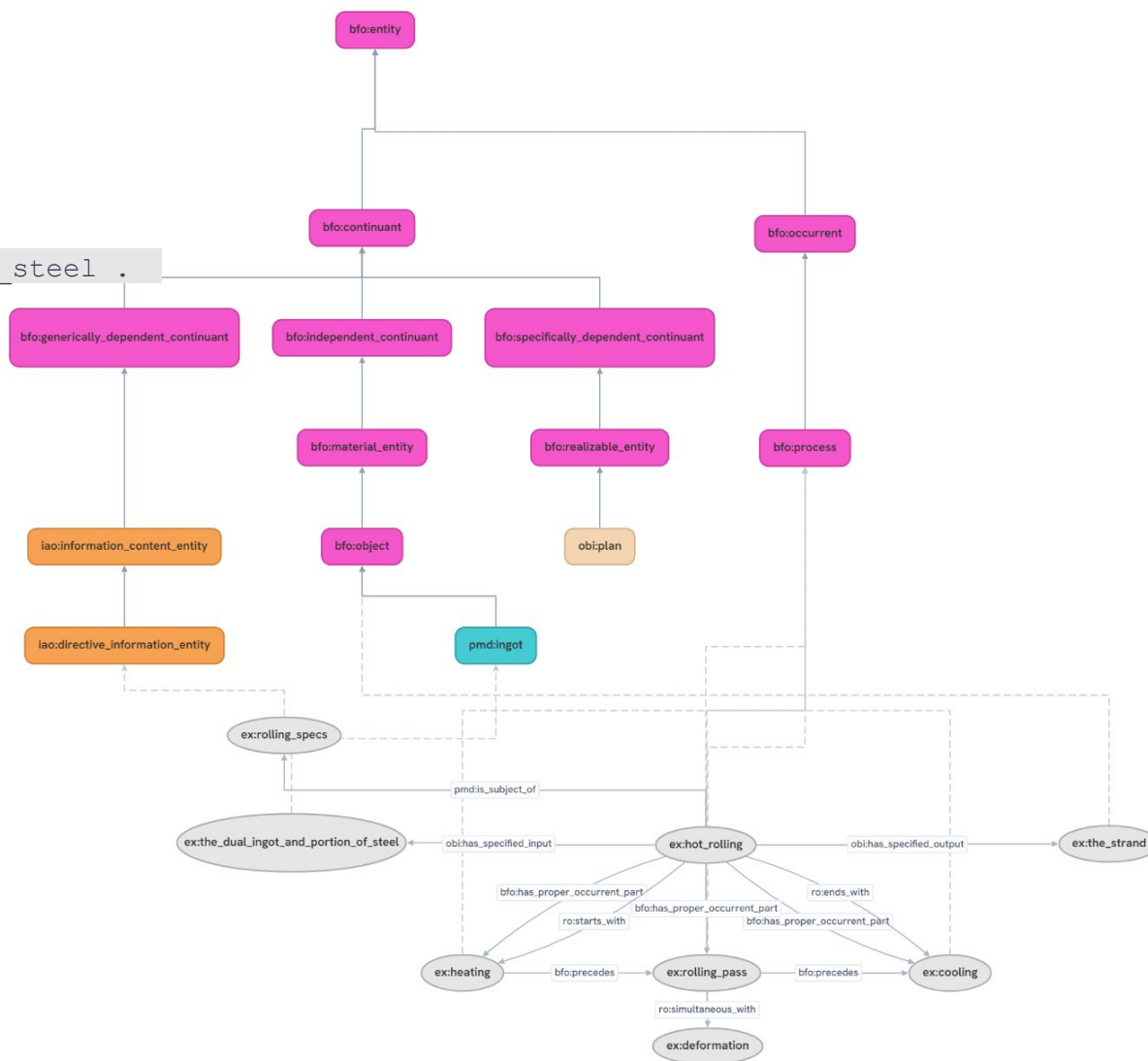
```
ex:heating a process: .  
ex:rolling_pass a process: .  
ex:deformation a process: .  
ex:cooling a process: .
```

```
ex:rolling_specs a directive_information_entity: .
```

```
ex:hot_rolling realizes: [  
    a plan: ;  
    concretizes: ex:rolling_specs  
] ;  
is_subject_of: ex:rolling_specs ;  
starts with: ex:heating ;  
ends with: ex:cooling ;  
has proper occurrent part: ex:heating,  
    ex:rolling_pass, ex:cooling .
```

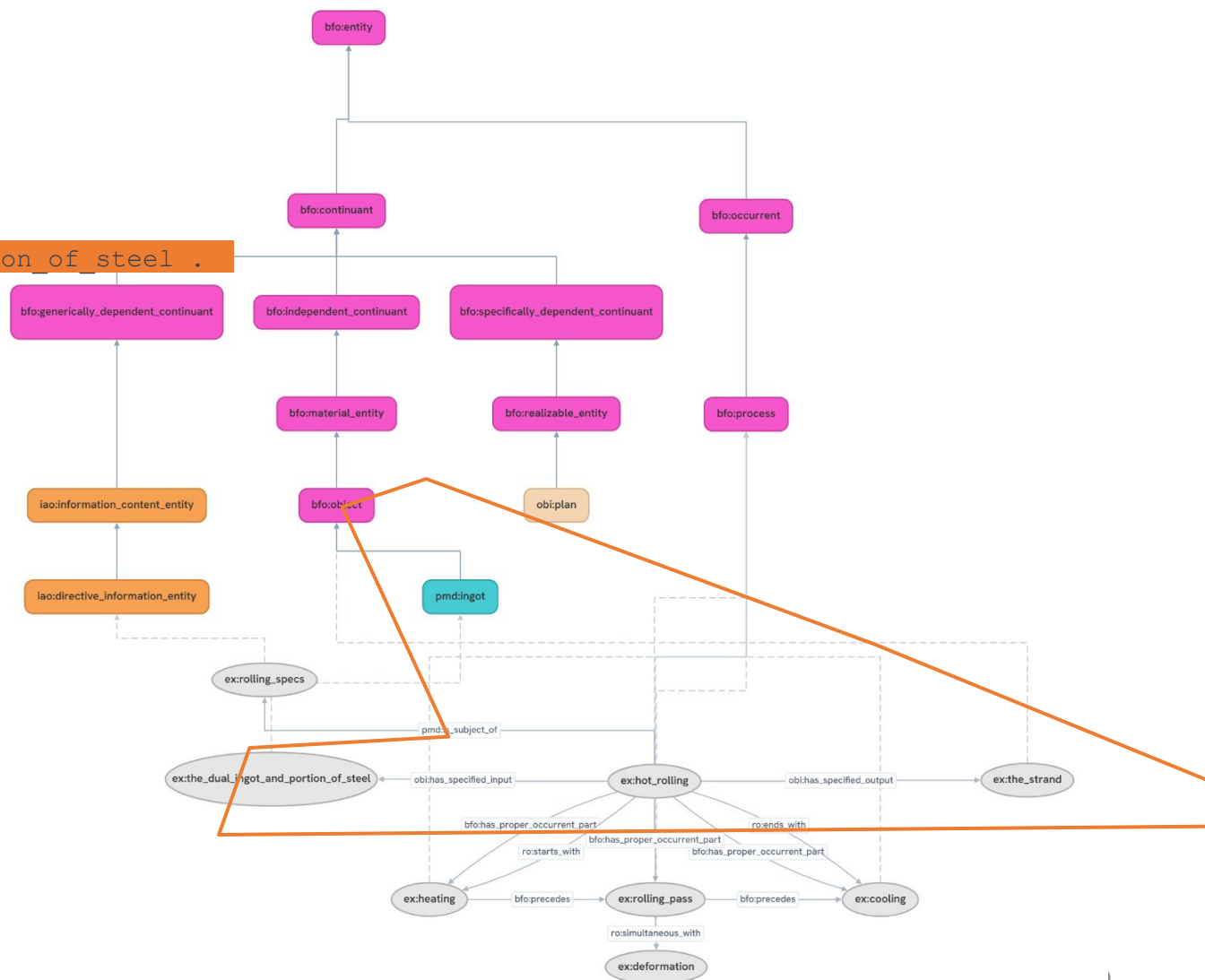
```
ex:heating precedes: ex:rolling_pass .  
ex:rolling_pass precedes: ex:cooling .
```

```
ex:rolling_pass simultaneous_with: ex:deformation .
```



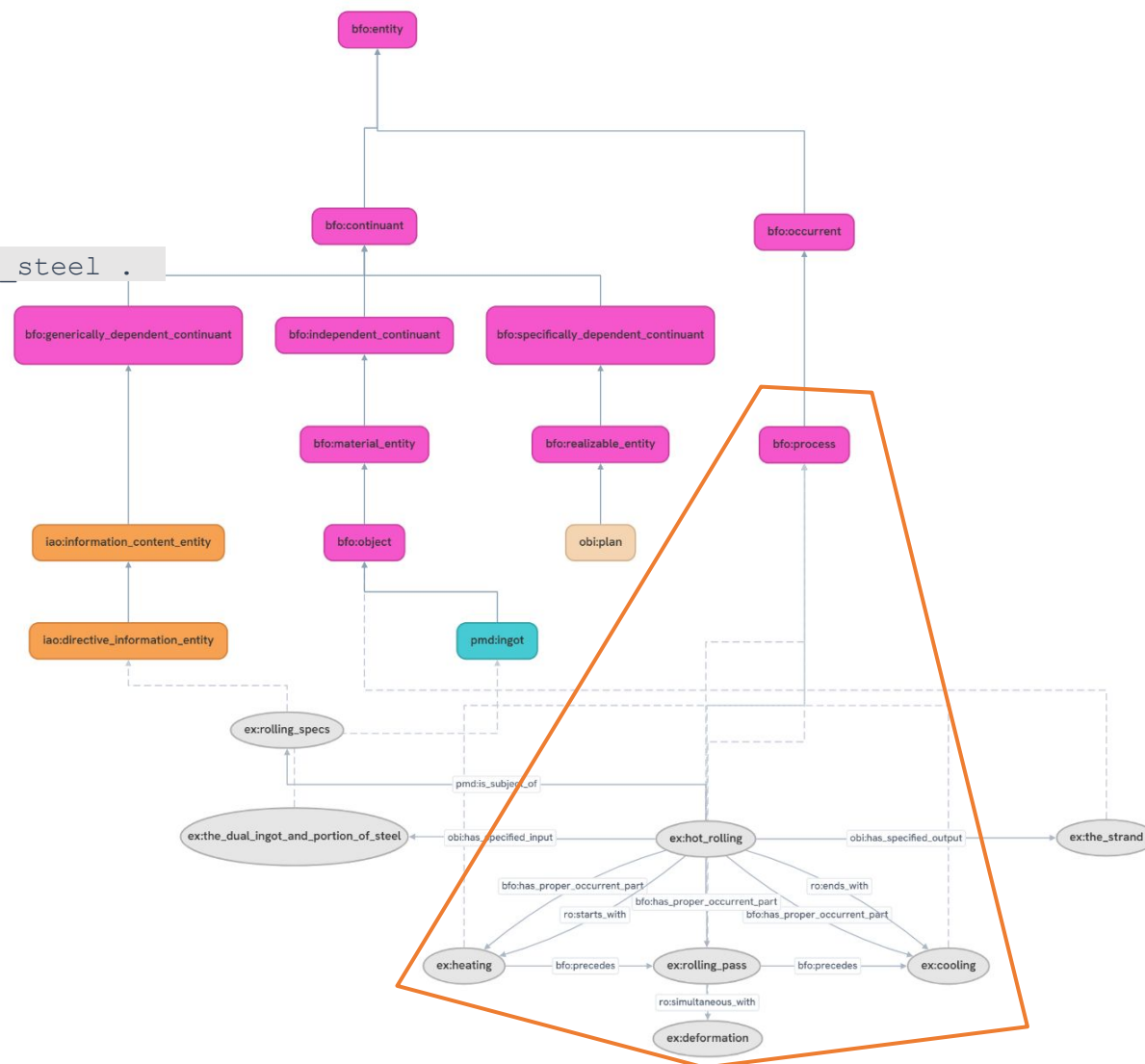
MATERIALDIGITAL

```
ex:rolling pass simultaneous with: ex:deformation .
```



MATERIALDIGITAL

```
ex:rolling pass simultaneous with: ex:deformation .
```



Pattern 3 - A process with in/output and a chain of subprocesses

```
ex:the_dual_ingot_and_portion_of_steel a ingot: .  
ex:the_strand a object: .
```

```
ex:hot_rolling a process: .  
ex:hot_rolling has_specified_input: ex:the_dual_ingot_and_portion_of_steel .  
ex:hot_rolling has_specified_output: ex:the_strand .
```

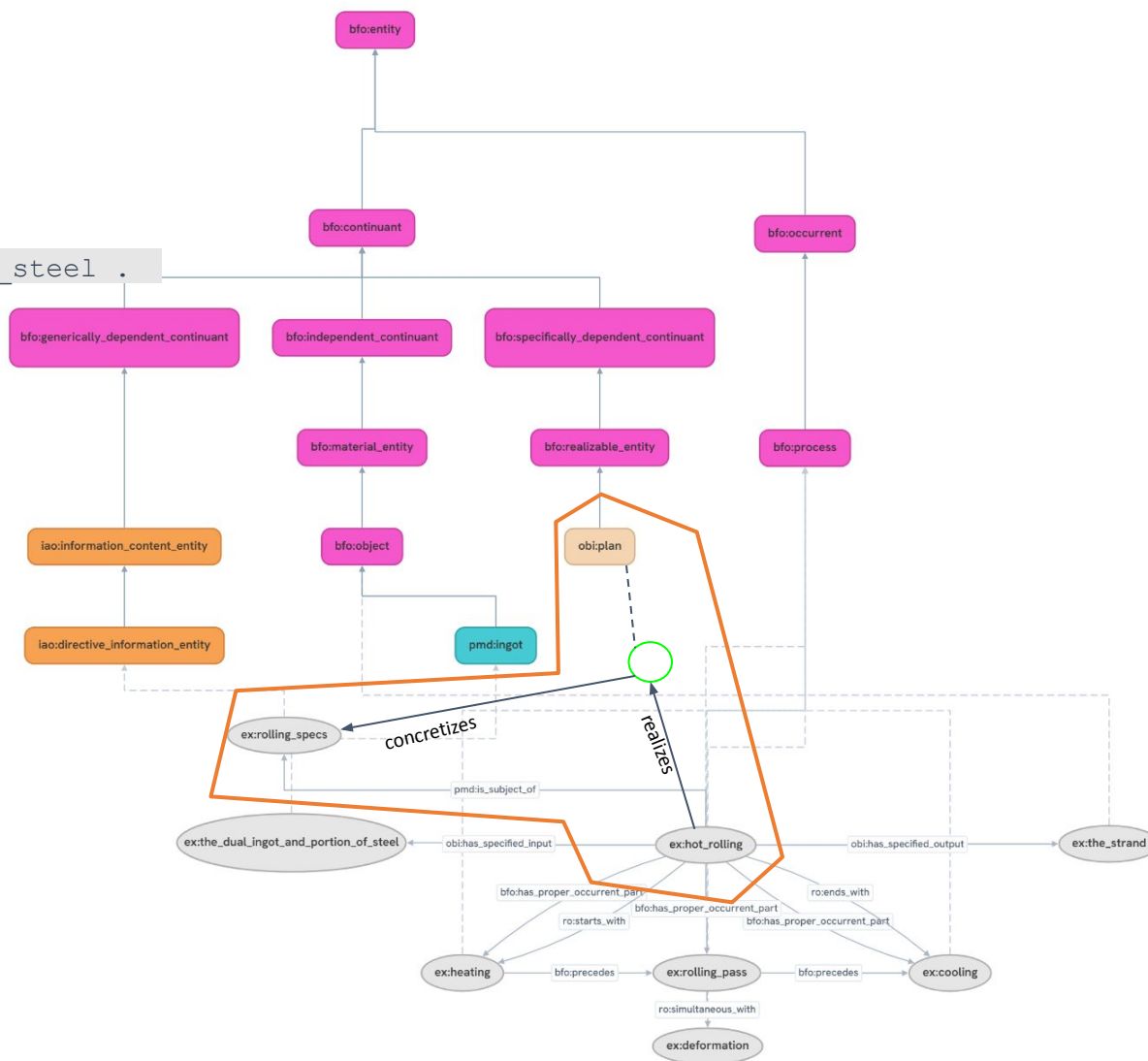
```
ex:heating a process: .  
ex:rolling_pass a process: .  
ex:deformation a process: .  
ex:cooling a process: .
```

```
ex:rolling_specs a directive_information_entity: .
```

```
ex:hot_rolling realizes: [  
    a plan: ;  
    concretizes: ex:rolling_specs  
] ;  
is_subject_of: ex:rolling_specs ;  
starts_with: ex:heating ;  
ends_with: ex:cooling ;  
has_proper_occurent_part: ex:heating,  
    ex:rolling_pass, ex:cooling .
```

```
ex:heating precedes: ex:rolling_pass .  
ex:rolling_pass precedes: ex:cooling .
```

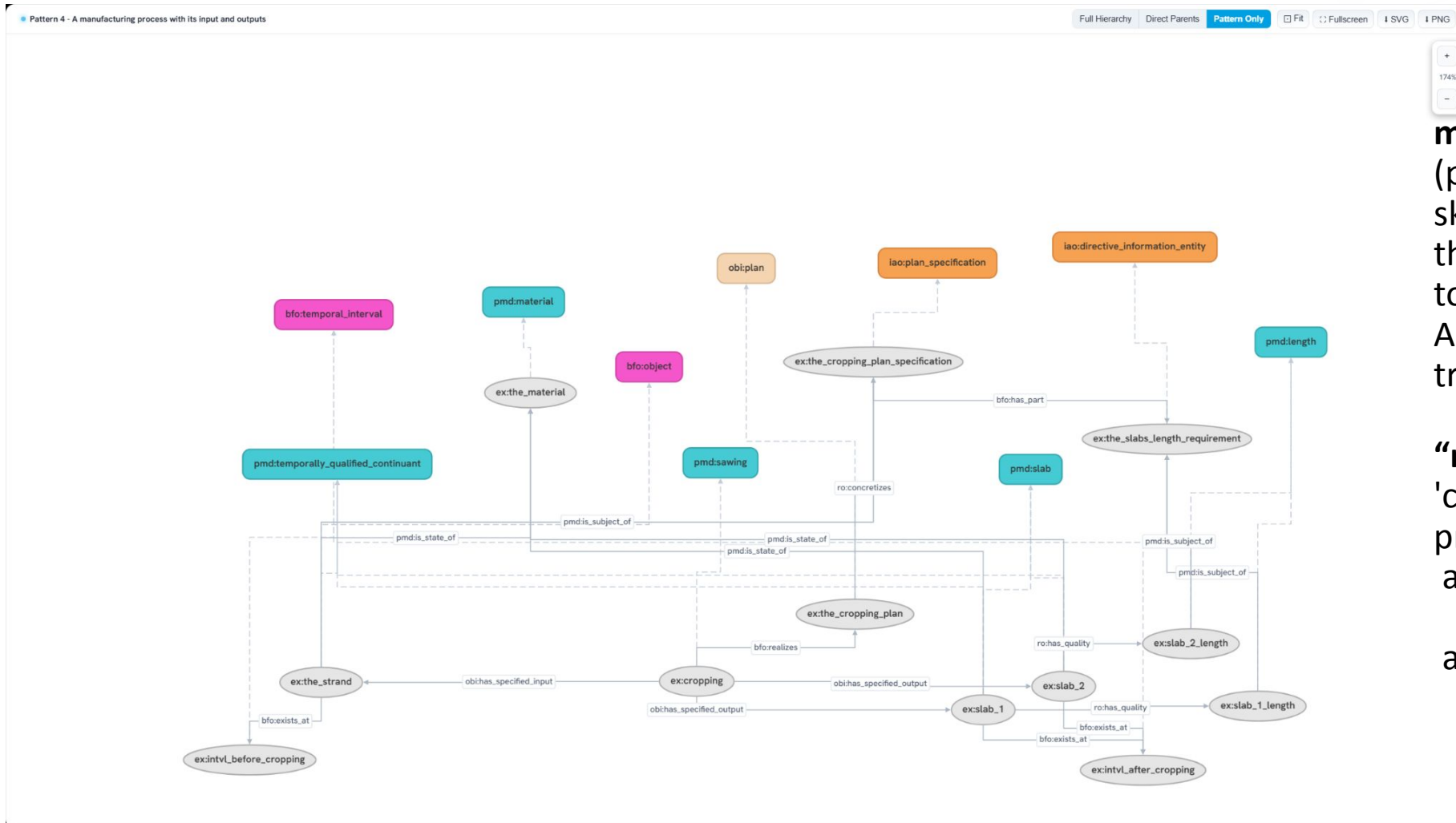
```
ex:rolling_pass simultaneous_with: ex:deformation .
```



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Pattern 4 - A manufacturing process with its input and outputs



manufacturing process

(pmd:PMD_0000833)

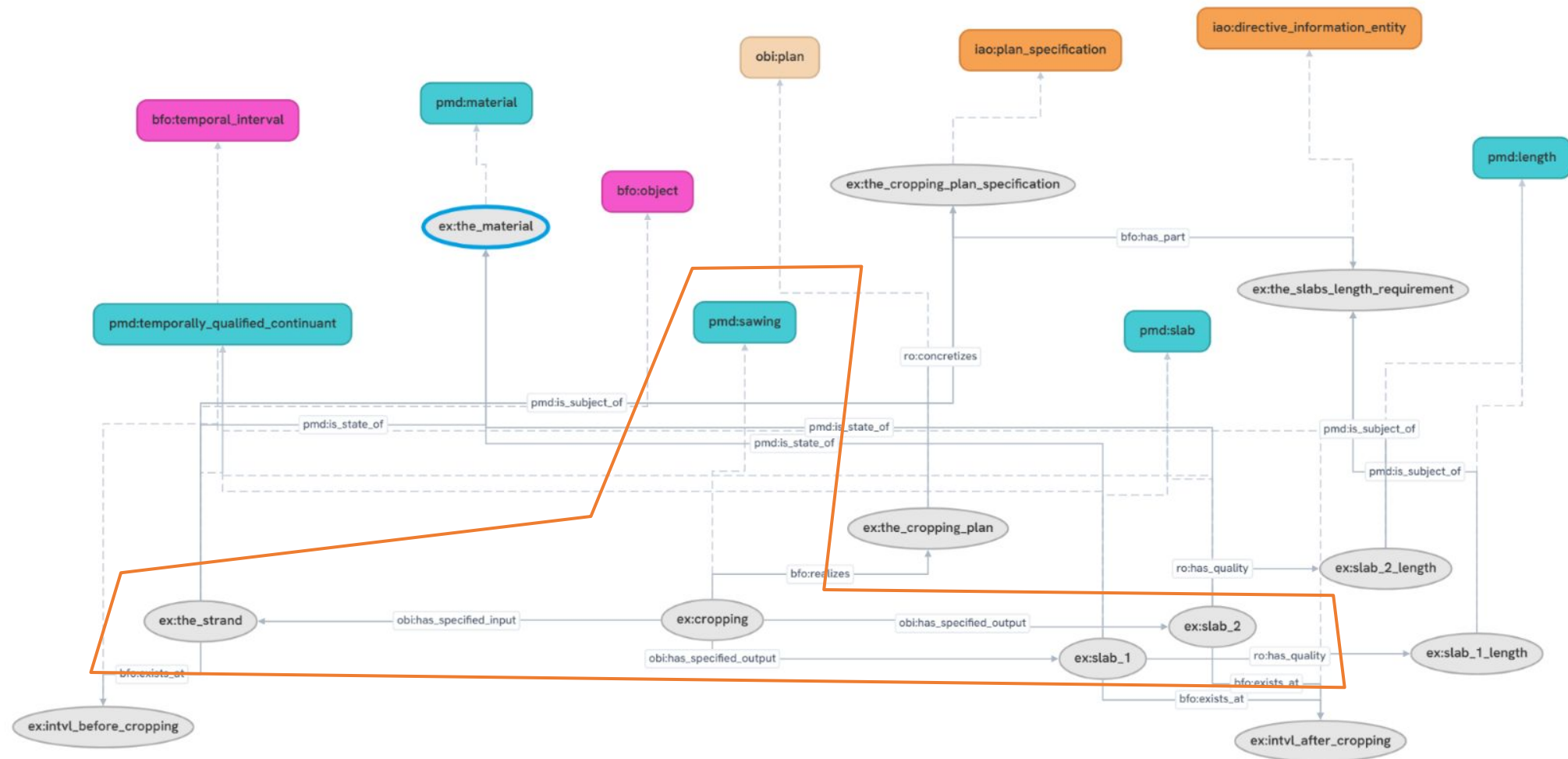
skos:definition "A planned process that is driven by the primary intent to transform objects

A manufacturing process is always a transformative process."

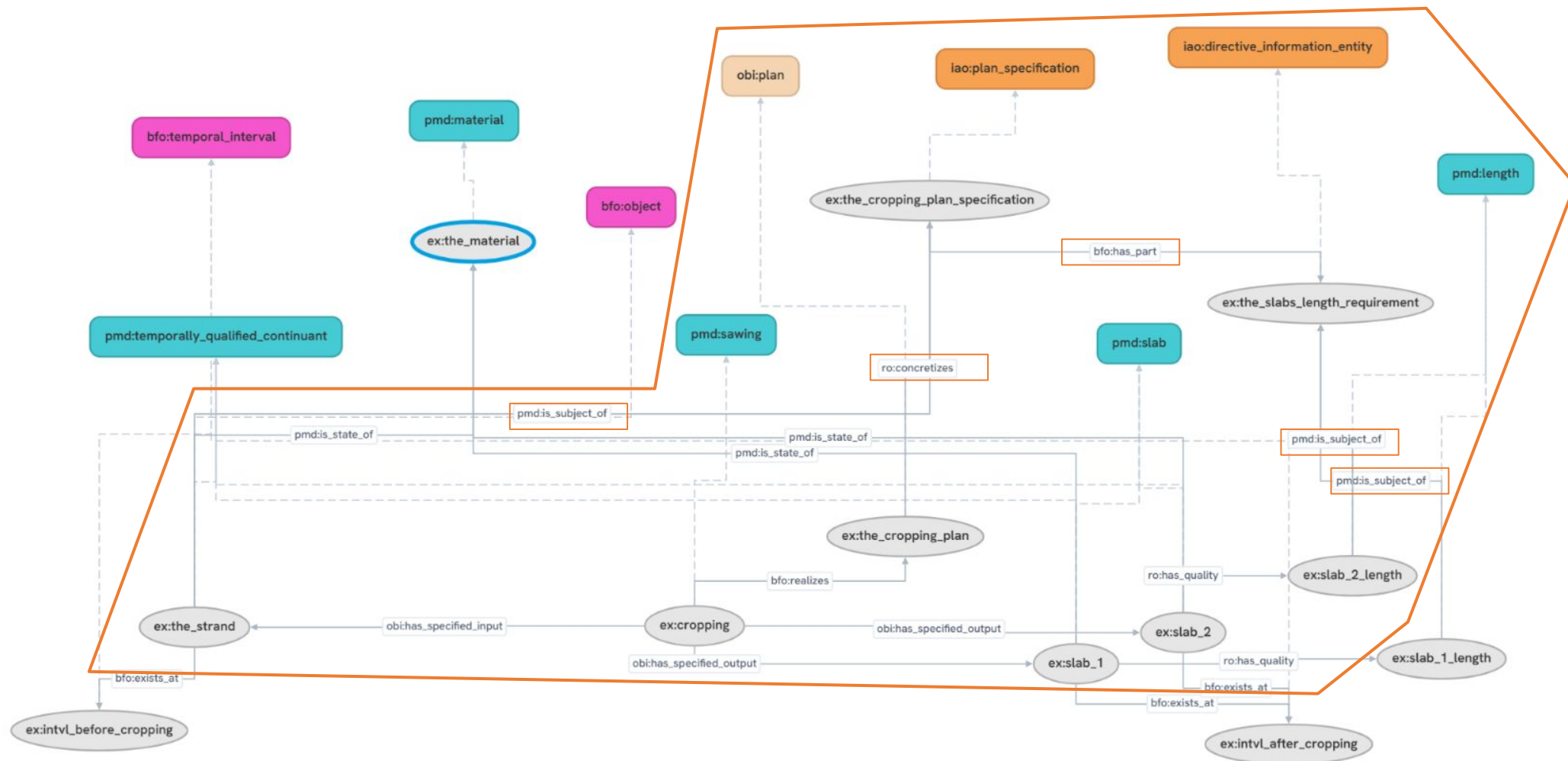
"manufacturing process" ===
'completely executed planned process'

and ('has specified input' some
('object aggregate' or object))
and ('has specified output' some
('object aggregate' or object))

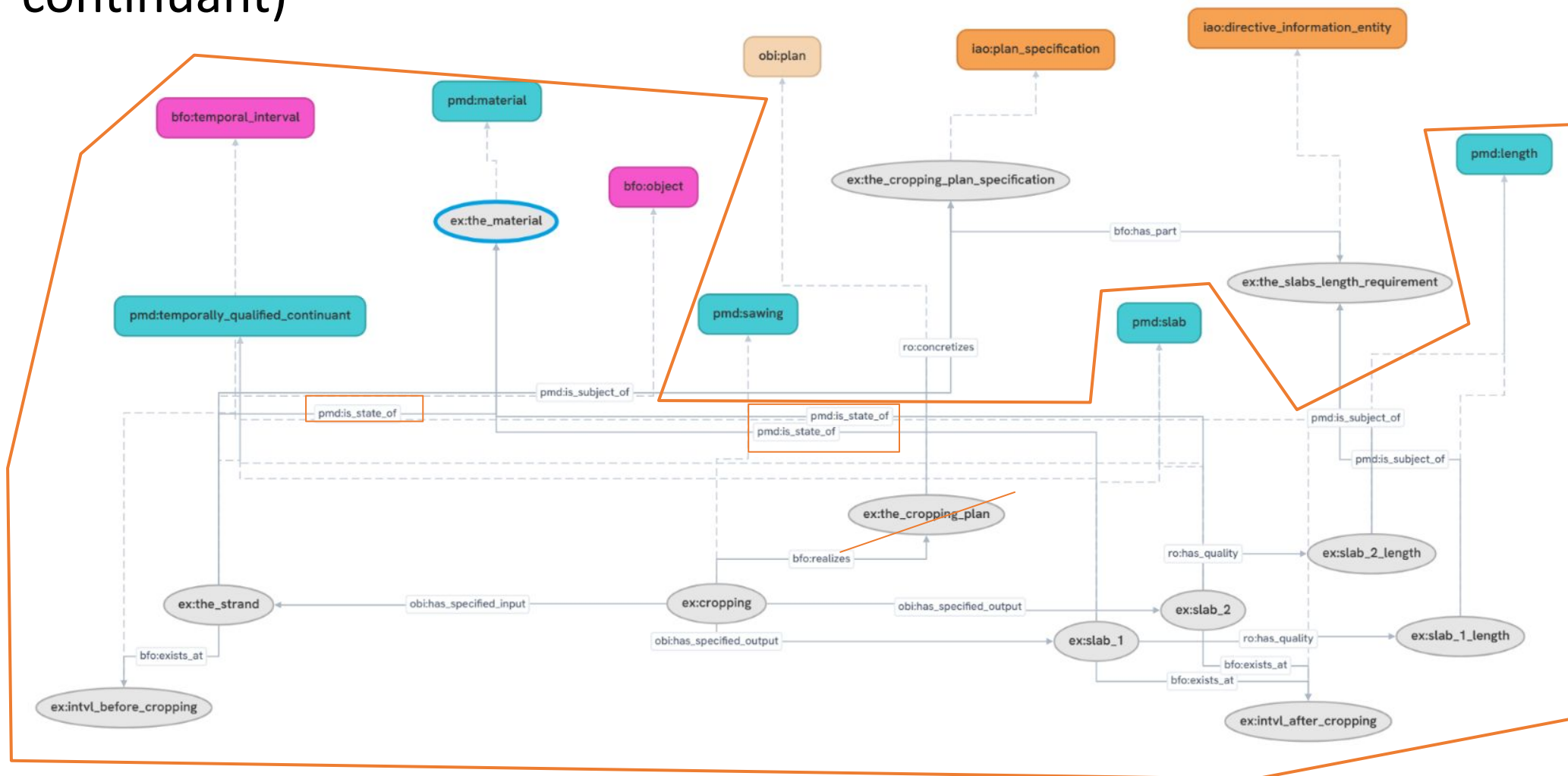
in- and output



the plan with its parts and aboutness



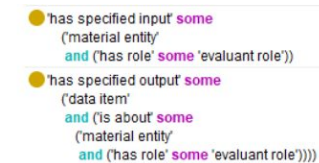
174%



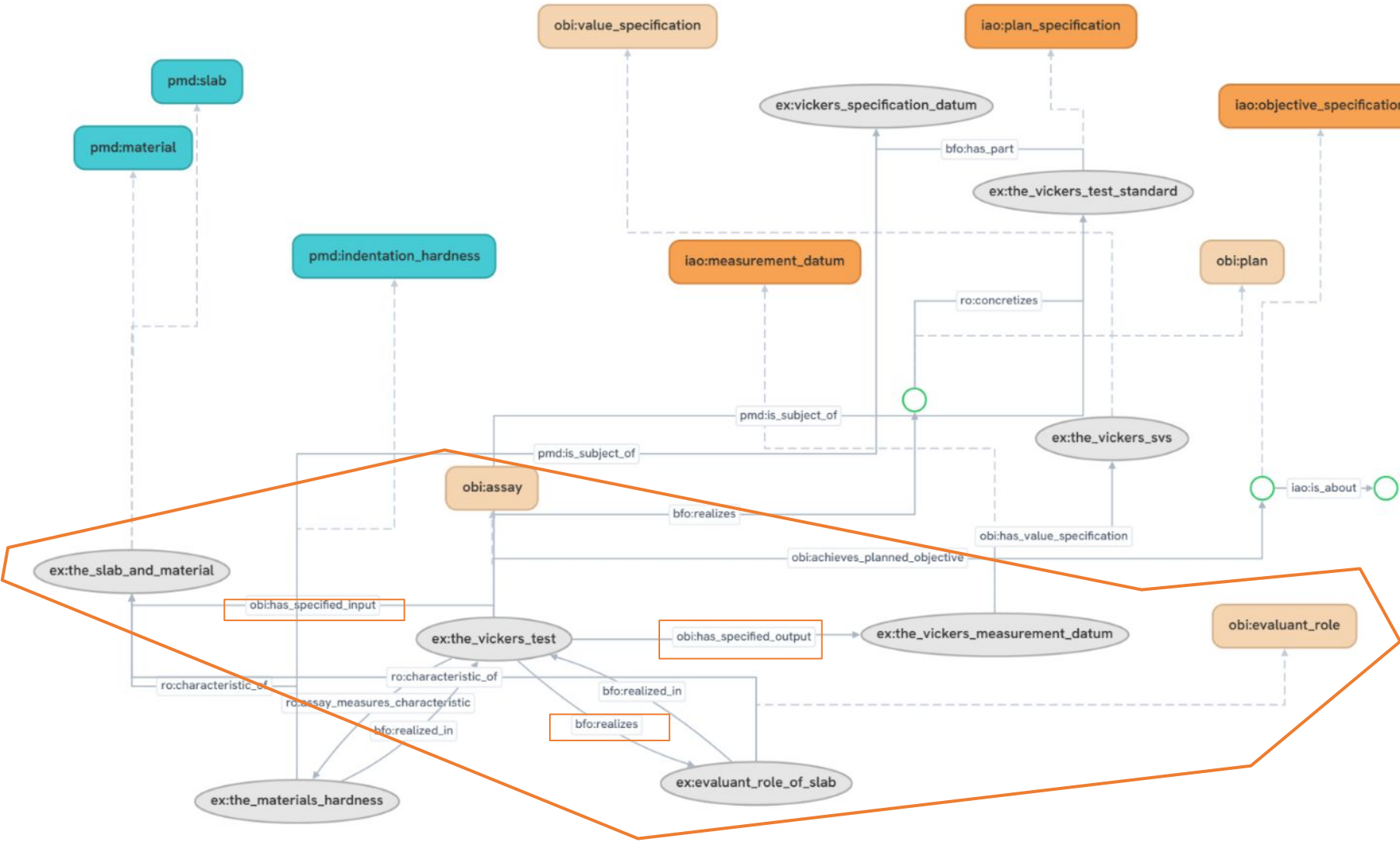
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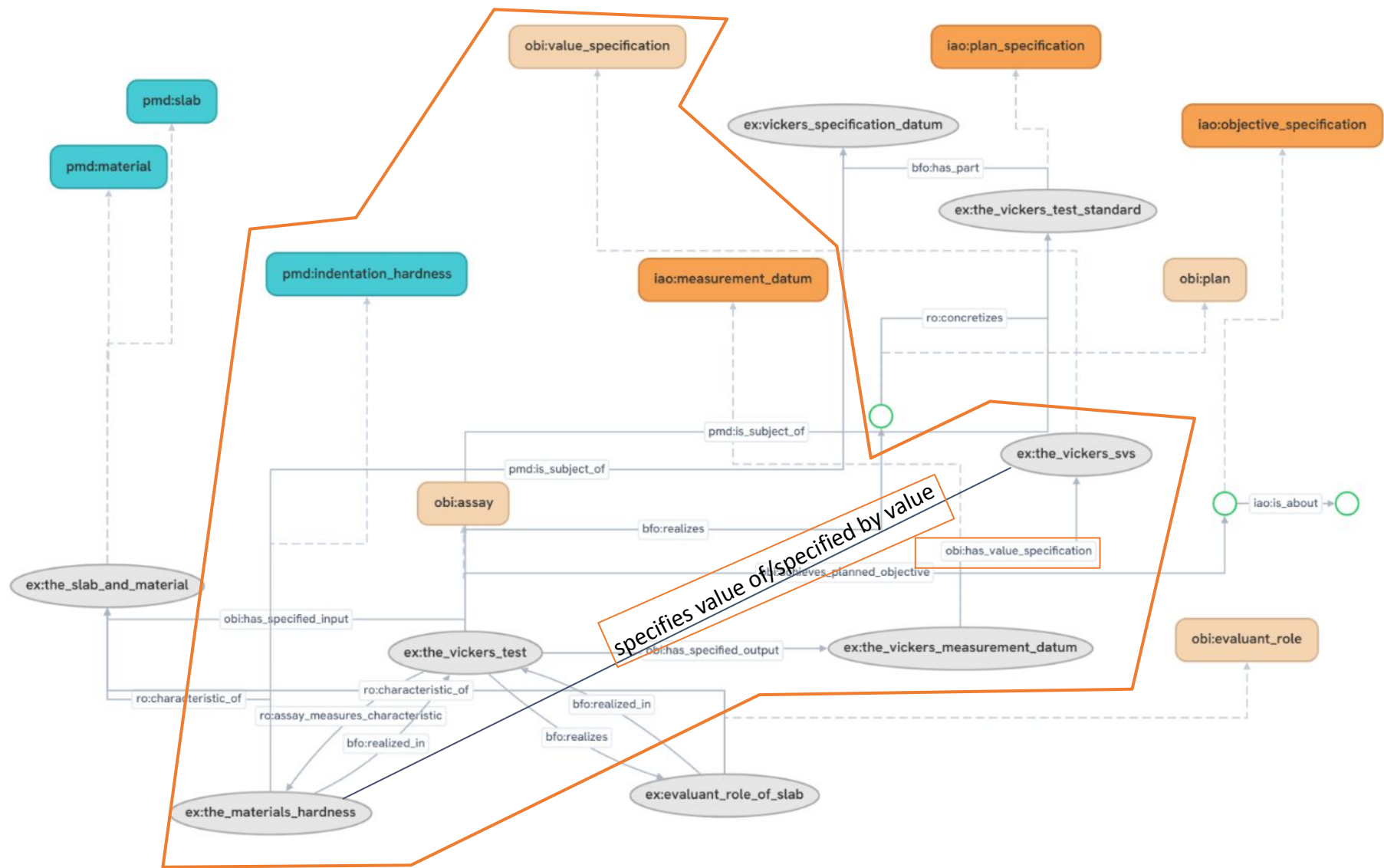
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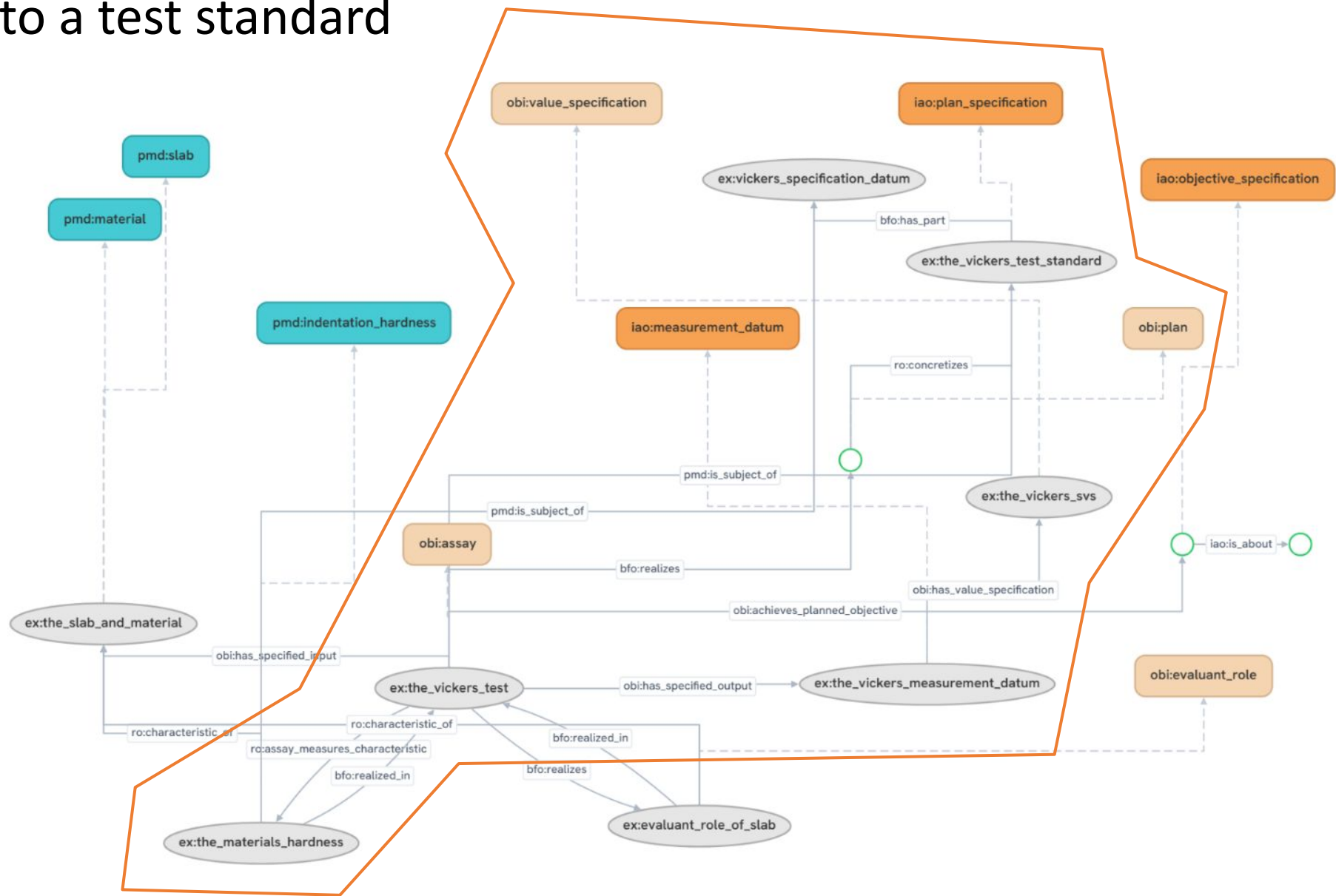
the assays input bearing an evaluant role and output data item



experimentally established value of a property



Reference to a test standard



These patterns are so frequent that they can be considered as “fixed shapes”

- Pattern 8a - Expressing a (scalar) value with "Scalar Value Specification"
- Pattern 6a - fundamental property
- Pattern 6c - relational property
- Pattern 7 - Measurement and setpoint

[Usage Patterns | PMDco Documentation](#)

Thank you!!



PMDco: AI outlook

- **Ontologies & Logic Programming** – Explicitly encode knowledge using formal logic rules and structured relationships to enable symbolic reasoning (e.g., OWL).
- **Rule-Based Expert Systems** – Apply hand-crafted IF-THEN rules to mimic human expertise and make decisions through logical inference.
- **Traditional Machine Learning** – Learn patterns from labeled data using explicit features and statistical methods like decision trees.
- **Deep Neural Networks** – Automatically learn hierarchical feature representations through many interconnected layers trained on large datasets
- **Transformers** – Learn complex patterns directly from raw data using self-attention mechanisms to capture relationships across entire sequences (e.g., GPT, BERT)

- Ontologies could be used as ground truth for LLMs
- LLMs could help to extract structured knowledge representations from ambiguous (natural language representations) and fill knowledge graphs
- LLMs can interact with ontologies via MCP ([GitHub - ai4curation/owl-mcp: MCP server for OWL applications · GitHub](#))