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Emanuele:
How can we understand materials and each other?

Our perspectives

Tackling Materials and Manufacturing Innovation Challenges with Digitalised Translation – from conceptualisation to ontology

Michael:
How can we accomplish innovation in manufacturing?

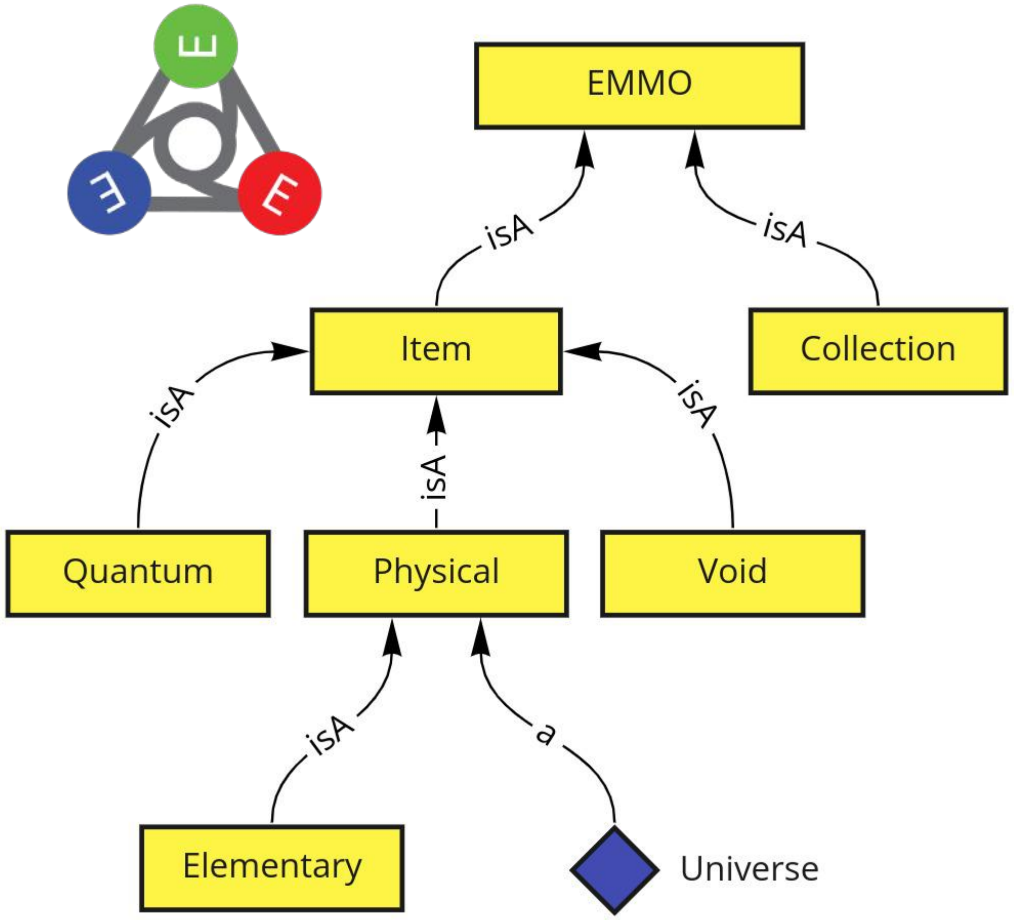
Emanuele:
How can we understand materials and each other?

Jesper:
How can we communicate and share materials data?

EMMO Motivations

As EMMC we faced to need for an ontology able to express the concepts and the constraints coming from the field of materials modelling, and more in general of applied sciences.

For this reason in the 2017 we started the development of the European Materials Modelling Ontology now the Elementary Multiperspective Material Ontology (EMMO) to define a fundamental set of classes and relations based on an applied science philosophical commitment, to facilitate the representation of our domains of interest.



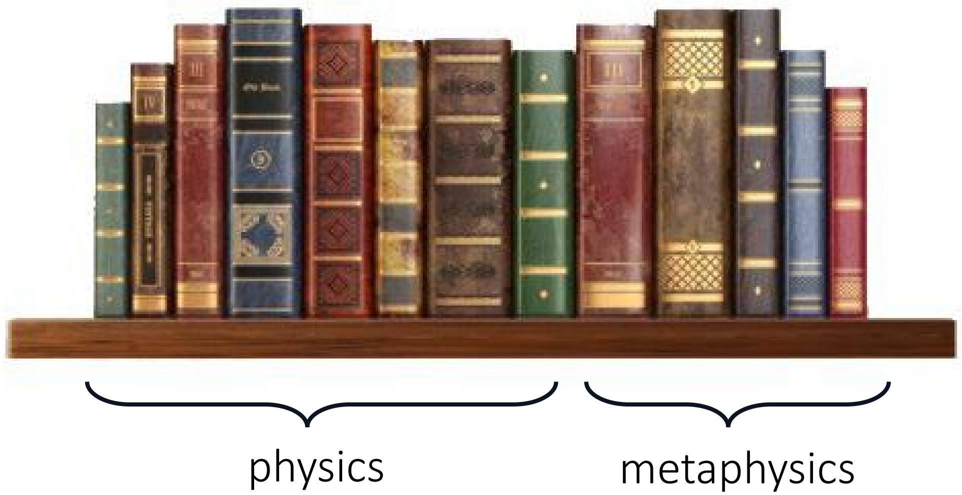
A look at Aristotle's Bookshelf

To understand what **Ontology** means we need to check a very old bookshelf.

Aristotle was the first philosopher to formalize the study of what he called **First Philosophy**, called only after his death as **Metaphysics**, which can be defined as the science that deals with *being as such*, or with the *first causes of things*, or with the *things that do not change*.

More specifically, it deals with:

- the **existence** of things (necessity vs contingency)
- the **properties** of things (essential vs accidental)



μετά φυσικά

meta (after) – physica (physics)

"Being is; not-being is not", Parmenides

"Essence precedes existence", Avicenna

"Existence in reality is greater than existence in the understanding alone", St Anselm

"Existence is a perfection", Descartes

"Being is the most barren and abstract of all categories", Hegel

"Affirmation of existence is in fact nothing but denial of the number zero", Frege

"Universals do not exist but rather subsist or have being", Russell

"To be is to be the value of a bound variable", Quine

https://plato.stanford.edu/entries/metaphysics/

A new-old tool for the information revolution

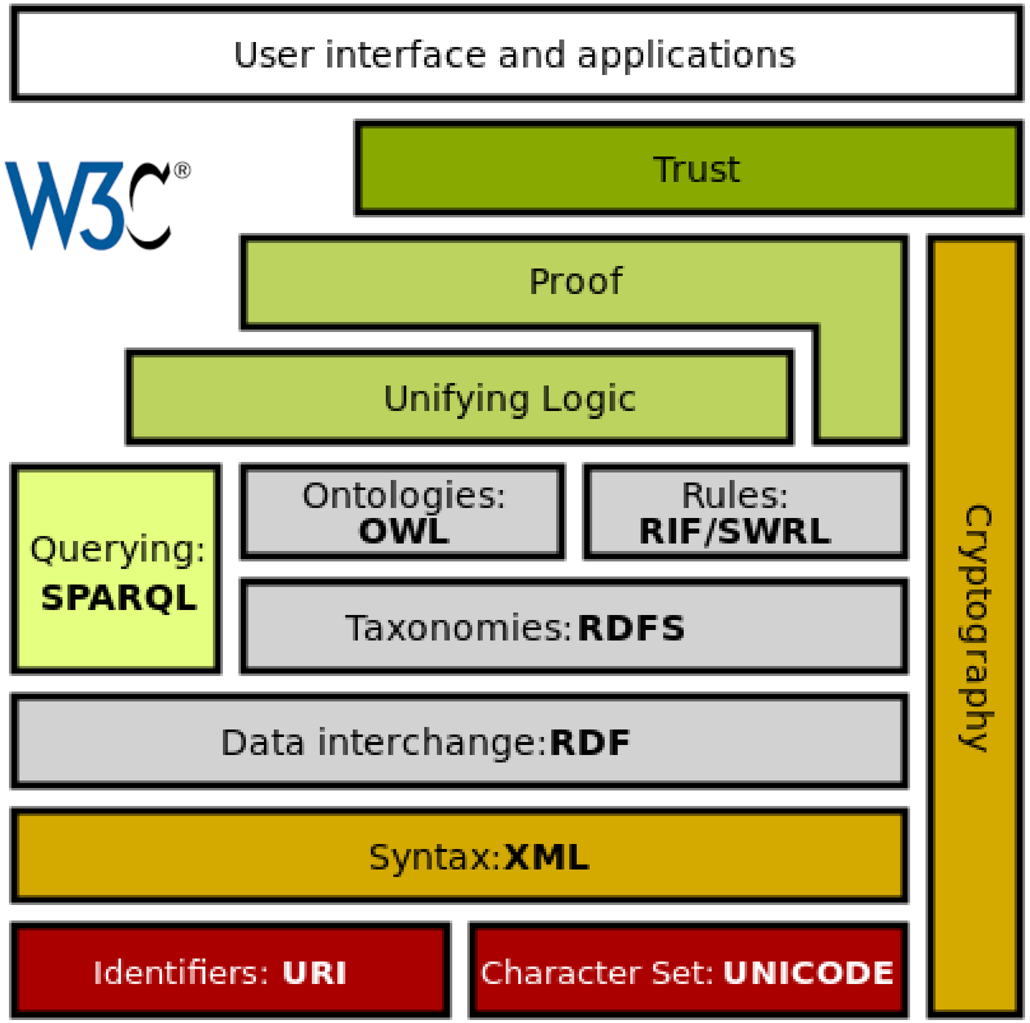
A great boost towards the use of formal ontologies in practice came in the ‘90 from the Semantic Web extension of the World Wide Web, thanks to the W3C standardization activities.

The objective Semantic Web is to make Internet data machine-readable.

Ontologies (in particular formal ontologies) play an important role in the Semantic Web and are placed in the higher levels of the architecture of languages.

However, the scope and ambition of such ontologies differ substantially from the ones coming from the philosophical community.

But an important concept as been introduces: the need for practical applications!



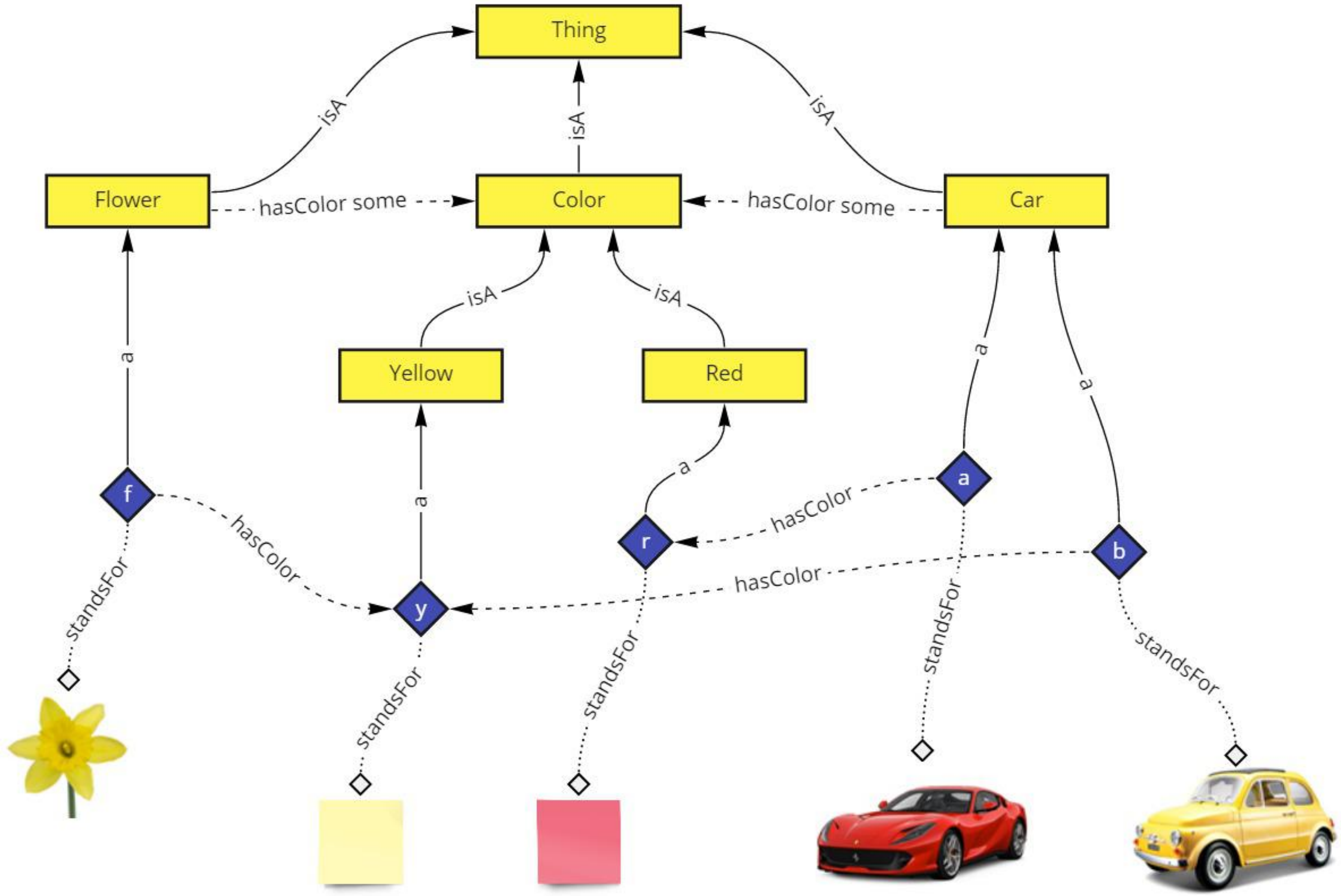
OWL 2 Ontology Example

Ontology Entities

class relation individual

Example of axioms:

```
ClassAssertion( :a :Car)
ClassAssertion( :r :Color)
ObjectPropertyAssertion( :hasColor :a :r )
```

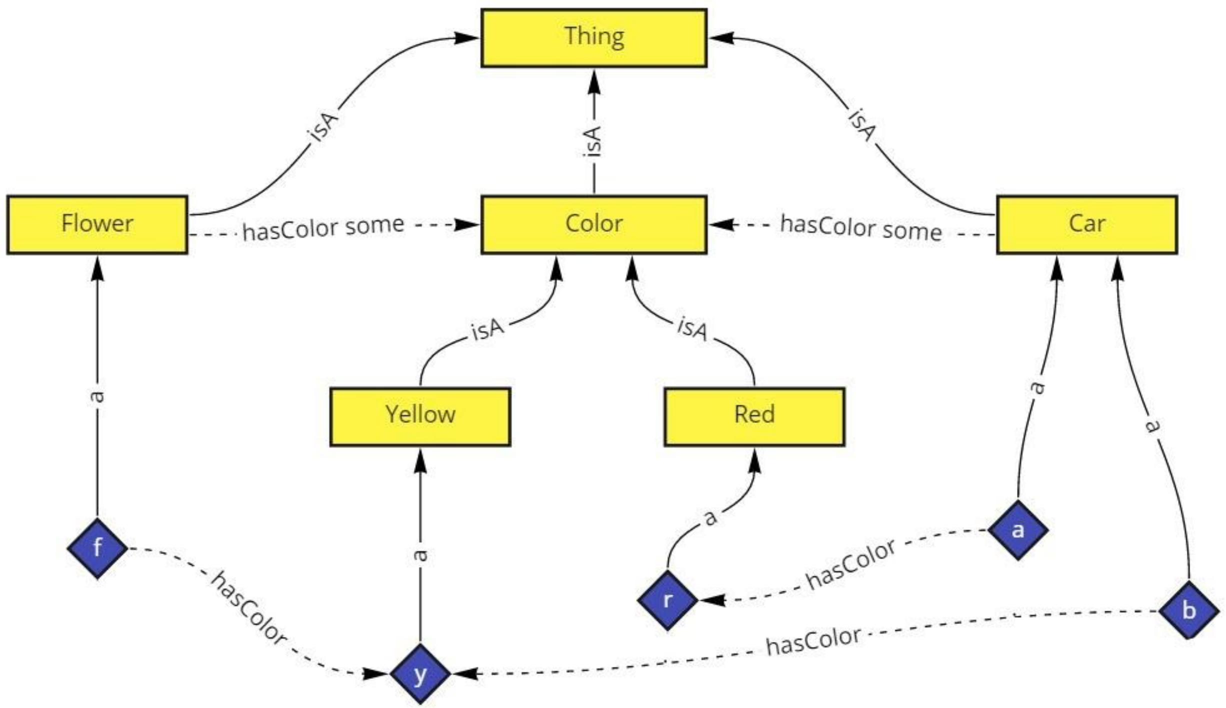


Real-world objects

No specific ontological commitment about the meaning of ‘real’ and ‘object’ in OWL 2. Relying on common sense.

OWL 2 Ontology in Flesh & Bones

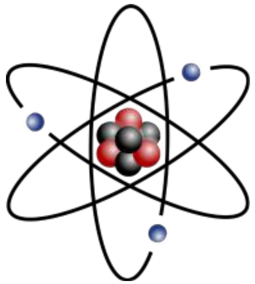
An OWL 2 Ontology is formally expressed in a persistent form by axioms declarations following a specific syntax (e.g. ASCII file with Turtle syntax)




```
@prefix : <http://www.semanticweb.org/emanuele/ontologies/example#> .
@prefix owl: <http://www.w3.org/2002/07/owl#> .
@prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#> .
@prefix xml: <http://www.w3.org/XML/1998/namespace> .
@prefix xsd: <http://www.w3.org/2001/XMLSchema#> .
@prefix rdfs: <http://www.w3.org/2000/01/rdf-schema#> .
@base <http://www.semanticweb.org/emanuele/ontologies/example> .

<http://www.semanticweb.org/emanuele/ontologies/example> rdf:type owl:Ontology .

###  http://www.semanticweb.org/emanuele/ontologies/example#hasColor
:hasColor rdf:type owl:ObjectProperty ;
          rdfs:subPropertyOf owl:topObjectProperty ;
          rdfs:range :Color .

###  http://www.semanticweb.org/emanuele/ontologies/example#Car
:Car rdf:type owl:Class ;
     rdfs:subClassOf [ rdf:type owl:Restriction ;
                       owl:onProperty :hasColor ;
                       owl:someValuesFrom :Color
                     ] .

###  http://www.semanticweb.org/emanuele/ontologies/example#Color
:Color rdf:type owl:Class .

###  http://www.semanticweb.org/emanuele/ontologies/example#Flower
:Flower rdf:type owl:Class ;
        rdfs:subClassOf [ rdf:type owl:Restriction ;
                          owl:onProperty :hasColor ;
                          owl:someValuesFrom :Color
                        ] .

###  http://www.semanticweb.org/emanuele/ontologies/example#Red
:Red rdf:type owl:Class ;
     rdfs:subClassOf :Color .

###  http://www.semanticweb.org/emanuele/ontologies/example#Yellow
:Yellow rdf:type owl:Class ;
        rdfs:subClassOf :Color .

###  http://www.semanticweb.org/emanuele/ontologies/example#a
:a rdf:type owl:NamedIndividual ,
            :Car ;
   :hasColor :r .

###  http://www.semanticweb.org/emanuele/ontologies/example#b
:b rdf:type owl:NamedIndividual ,
            :Car ;
   :hasColor :y .

###  http://www.semanticweb.org/emanuele/ontologies/example#f
:f rdf:type owl:NamedIndividual ,
            :Flower ;
   :hasColor :y .

###  http://www.semanticweb.org/emanuele/ontologies/example#r
:r rdf:type owl:NamedIndividual ,
            :Color .

###  http://www.semanticweb.org/emanuele/ontologies/example#y
:y rdf:type owl:NamedIndividual ,
            :Color .
```

https://www.w3.org/TR/owl2-syntax/#Introduction

The Importance Of Ontologies



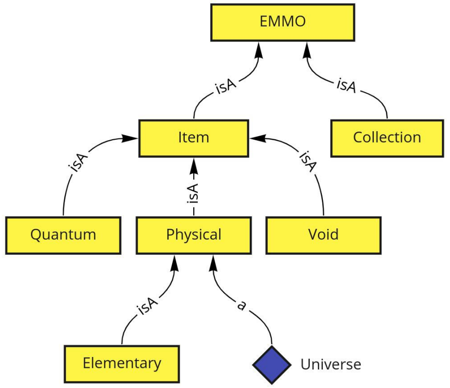
PHYSICS

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

MATH

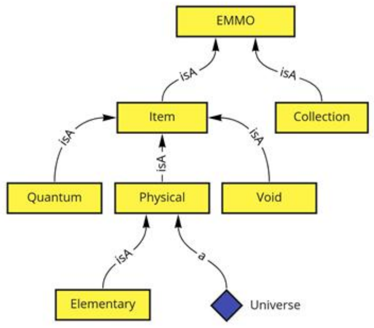
=

INDUSTRY



ONTOLOGY

The Importance Of Ontologies



ONTOLOGY

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

MATH

Universal Language
(i.e. transcend linguistic differences)

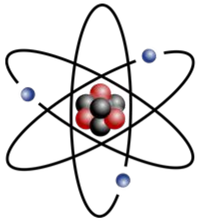
Hard to learn
(i.e. requires adequate training)

Able to Perform Logical Reasoning
(i.e. infer new knowledge from existing one)

Provides Models of the World
(i.e. let us play with abstractions instead of material things)

When It Works, It Can Be Hidden
(i.e. things using it may confine its complexity behind the user interface layer)

The Importance Of Ontologies



PHYSICS

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

MATH

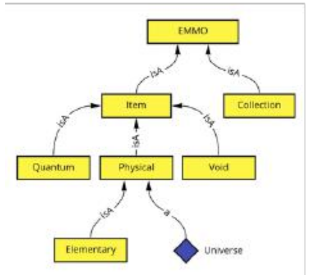
Math has been the key for the highest achievements in **Physics**

(e.g. Newton, Maxwell, Einstein, Schrodinger, Standard Model)

Ontologies can be the key for a quantum leap in **Industry**

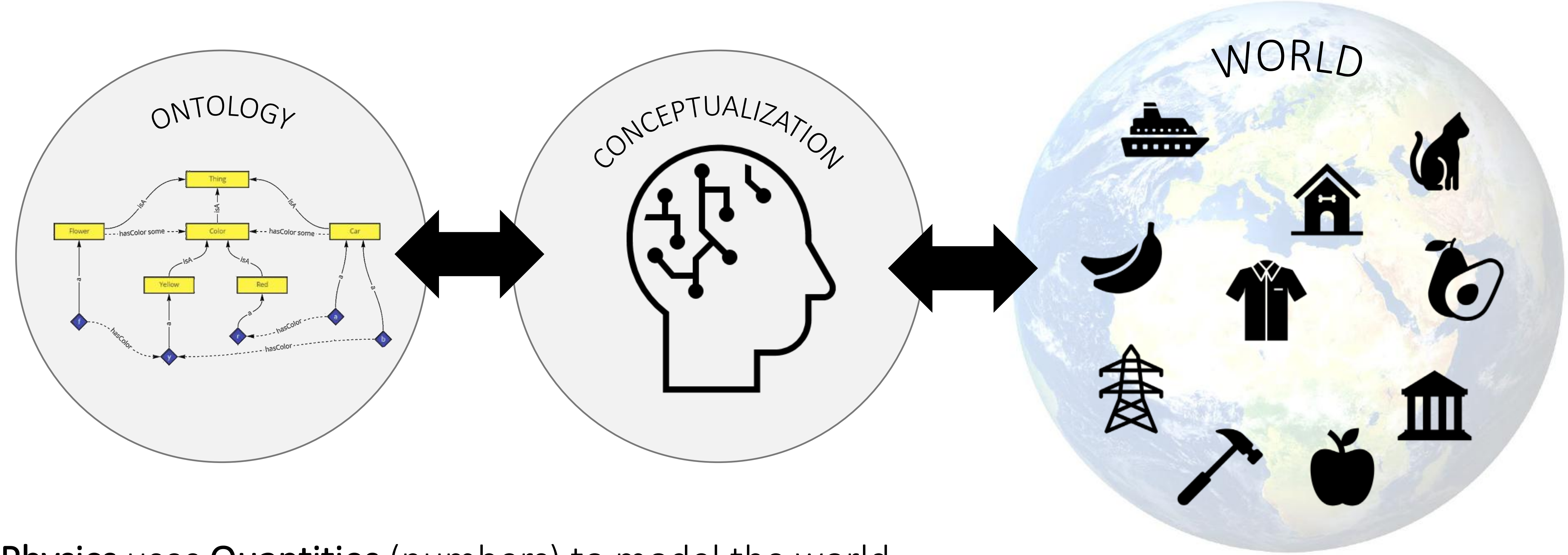
(e.g. pervasive digitalization, knowledge sharing, Industry 4.0 to 5.0)

INDUSTRY



ONTOLOGY

A New Language to Talk to Machines



Physics uses **Quantities** (numbers) to model the world

Ontologies use **Concepts** to build a **(onto)-logical representation** of the world

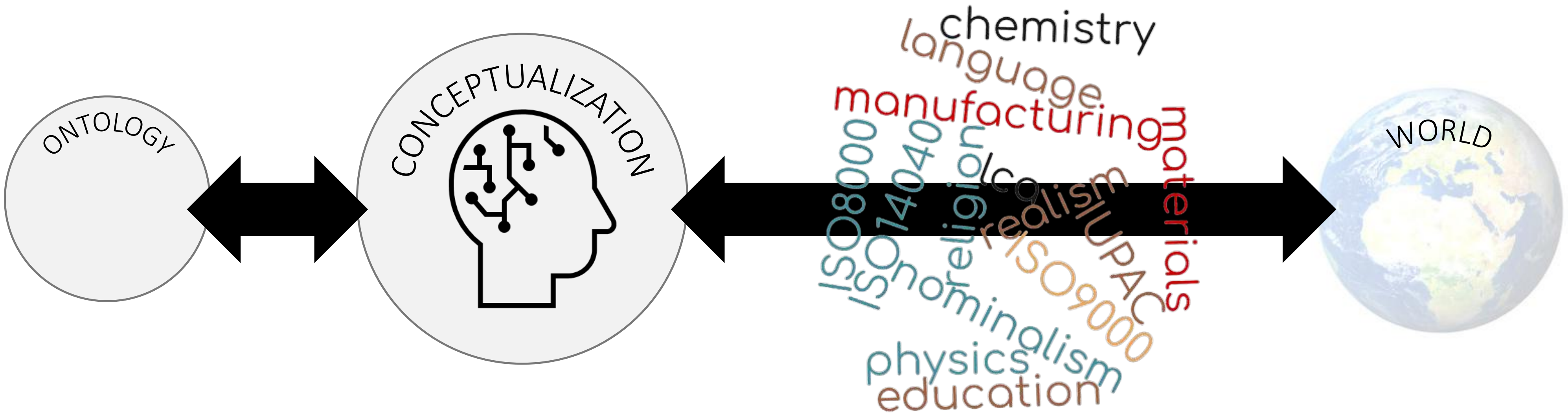
A New Language to Talk to Machines

Machines understand the logical language of ontologies (e.g. FOL, OWL-2), and already can be used to:

- **document data** (e.g. dcterms, DCAT)
- infer **new knowledge** (e.g. resoners)
- support **AI** (e.g. ontology assisted AI)

Bottlenecks: The Human Factor

Jumping from Ontology to World requires **Interpretation**



Several conceptualizations exist for **the same things**, so that almost each human being is going to provide a different definition for a single term.

(physics is not affected since it works with quantities, and solve the issue with well defined measurement practices)

What Is Pluralism?

Etymology

From Latin *pluralis* ("of or belonging to more than one, belonging to many", adjective), from *pluris* ("more") + *-alis*.

Definition

To embrace a diversity of views or stands rather than a single approach or method.

Epistemological Pluralism

There are **many different ways of knowing the same thing**, depending on the epistemological approach (as opposed to **monism**, for which there is only one and one way)

Ontological Pluralism

There are **different modes of being**, so that there is no overarching, sin… fundamental ontology, but only a **patchwork of overlapping interconnected ontologies** ineluctably leading from one to another (see Ludwig Wittgenstein).

Is There Pluralism in Industry?

ISO 9000

Quality management systems

3.7.5

output

result of a **process** (3.4.1)

Note 1 to entry: Whether an output of the **organization** (3.2.1) is a **product** (3.7.6) or a **service** (3.7.7) depends on the preponderance of the **characteristics** (3.10.1) involved, e.g. a painting for sale in a gallery is a product whereas supply of a commissioned painting is a service, a hamburger bought in a retail store is a product whereas receiving an order and serving a hamburger ordered in a restaurant is part of a service.

3.7.6

product

output (3.7.5) of an **organization** (3.2.1) that can be produced without any transaction taking place between the organization and the **customer** (3.2.4)

Note 1 to entry: Production of a product is achieved without any transaction necessarily taking place between **provider** (3.2.5) and customer, but can often involve this **service** (3.7.7) element upon its delivery to the customer.

Note 2 to entry: The dominant element of a product is that it is generally tangible.

Note 3 to entry: Hardware is tangible and its amount is a countable **characteristic** (3.10.1) (e.g. tyres). Processed materials are tangible and their amount is a continuous characteristic (e.g. fuel and soft drinks). Hardware and processed materials are often referred to as goods. Software consists of **information** (3.8.2) regardless of delivery medium (e.g. computer programme, mobile phone app, instruction manual, dictionary content, musical composition copyright, driver's license).

3.7.7

service

output (3.7.5) of an **organization** (3.2.1) with at least one activity necessarily performed between the organization and the **customer** (3.2.4)

Note 1 to entry: The dominant elements of a service are generally intangible.

ISO 14040

Environmental management — Life cycle assessment

3.9

product

any goods or service

Note 1 to entry: The product can be categorized as follows:

— services (e.g. transport);

— software (e.g. computer program, dictionary);

— hardware (e.g. engine mechanical part);

— processed materials (e.g. lubricant).

Note 2 to entry: Services have tangible and intangible elements. Provision of a service can involve, for example, the following:

— an activity performed on a customer-supplied tangible product (e.g. automobile to be repaired);

— an activity performed on a customer-supplied intangible product (e.g. the income statement needed to prepare a tax return);

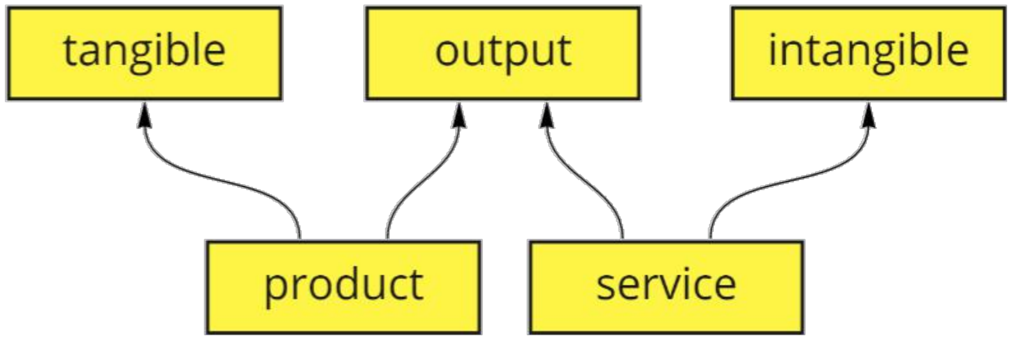
— the delivery of an intangible product (e.g. the delivery of information in the context of knowledge transmission);

— the creation of ambience for the customer (e.g. in hotels and restaurants).

ISO vs ISO

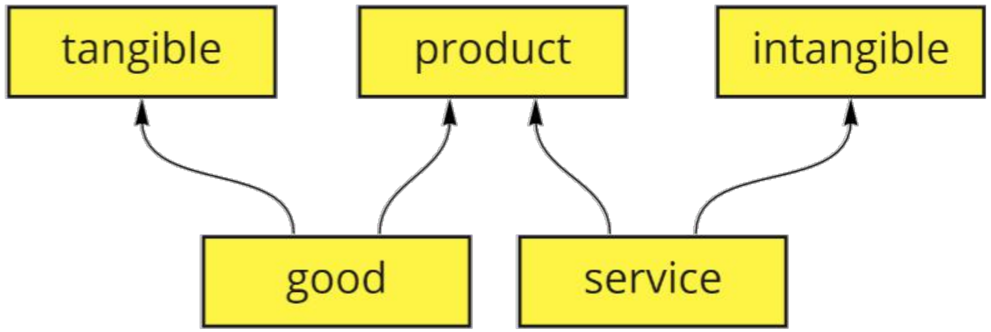
ISO 9000

Quality management systems



ISO 14040

Environmental management — Life cycle assessment



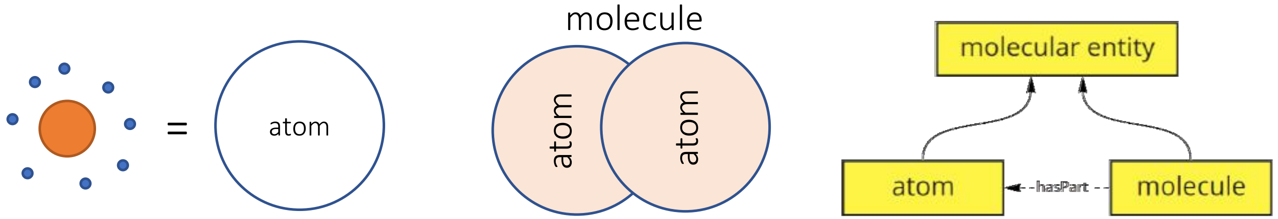
It seems that the definitions of product in ISO 9000 and ISO 14040 **are somewhat incompatible**, and for an ontology embracing one ISO means that the other ISO will be no more representable.

Chemistry vs Physics

<u>IUPAC Definitions (Chemistry)</u>

An **Atom** is a nucleus of Z positive charge and Z electrons

A **Molecule** is an electrically neutral entity consisting of more than one atom



<u>Chemical-Physics Definitions</u>

A **Molecule** is an electrically neutral entity consisting of nuclei and electrons (no atom involved here: atom is a singular type of molecule)

Chemistry and Chemical-Physics are two different approaches the lead to a **different definitions of atoms and molecules** and hence different parthood relations between their concepts.

Pluralism Seems the Rule (not the exception)

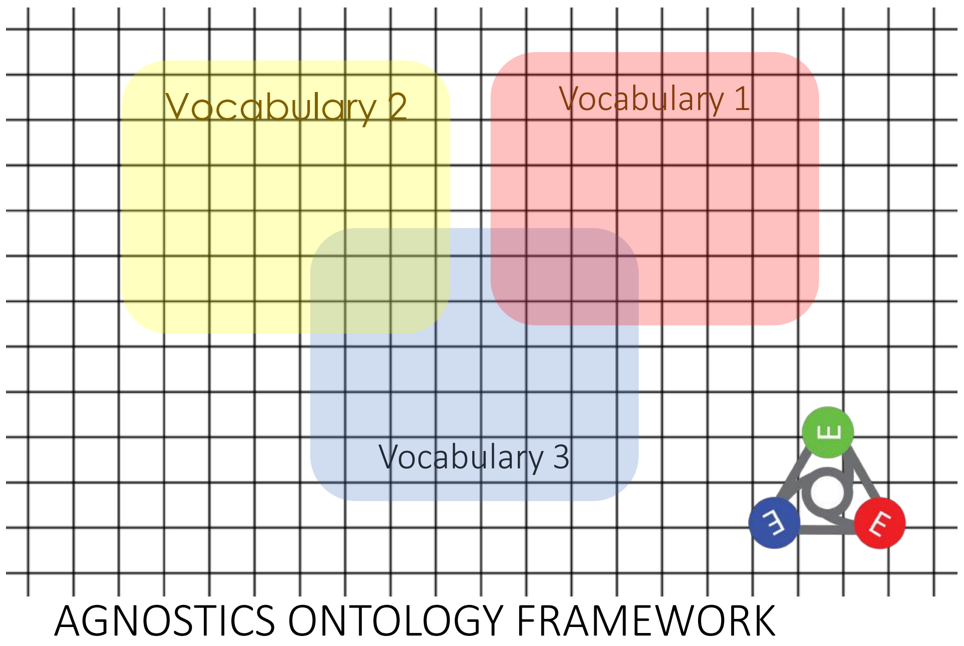
Pluralism seems the rule when dealing with domains knowledge, given that the domain fields of human knowledge are so vast and deep that every one of them developed its own conceptualization for things.

There are two ways to deal with the de-facto pluralism in human knowledge:

- The <u>rule-them-all</u> approach, that forces the user to embrace a **single perspective** for the world description by proposing a single ontological approach (from Top Level to Domains). However, the large amount of TLOs should suggest that there is not an agreement even on the fundamentals of knowledge formalization.

- The <u>pluralistic</u> approach, that proposes a long and enormously difficult journey to find **similarities** and **differences** between diverse Top Level Ontologies and find a way to host more than one perspective for the same domain within the same framework

Pluralism



A true **human centric** approach, leading to Industry 5.0, occurs when a **pluralistic approach** is used.

Ontology development should embrace pluralism, in the form of allowing **multiple representations for the same real world object**.

A pluralistic ontology is the **gateway** to **human-to-machine** and **machine-to-human** interaction.

EMMO Experience

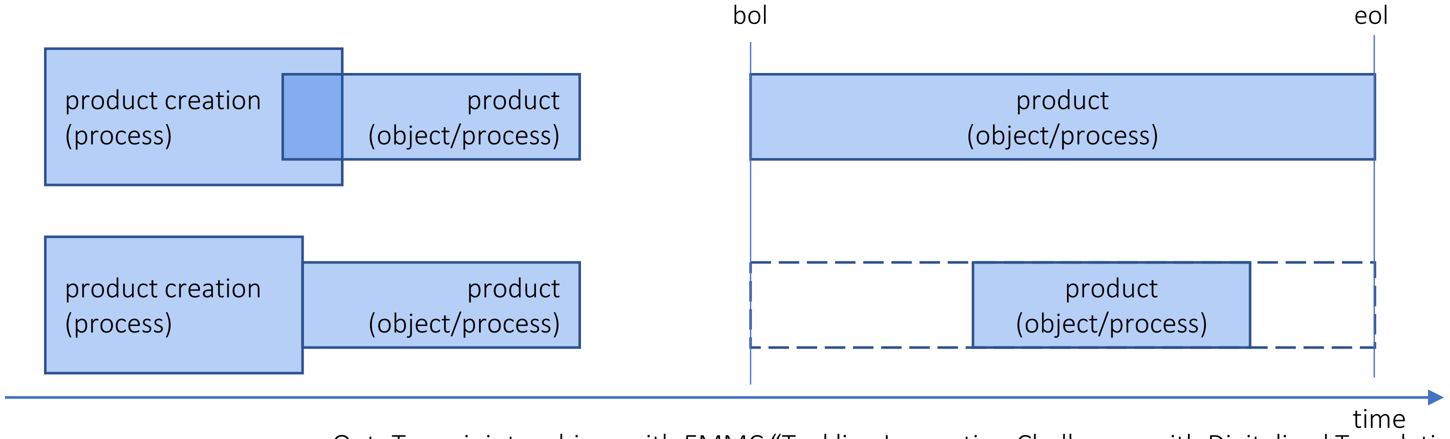
So, what is a product?

- Is it a process or an object?
- Which are its mereotopological relations with its process creator (is an output overcrossing its creating process)?
- Is product concept encompassing the overall lifetime (in a LCA view) or can it refer to an interval of its lifetime?

EMMO has been used in several projects to represent **innovation cases**, including manufacturing, commercialization, modelling, and workflow representation.

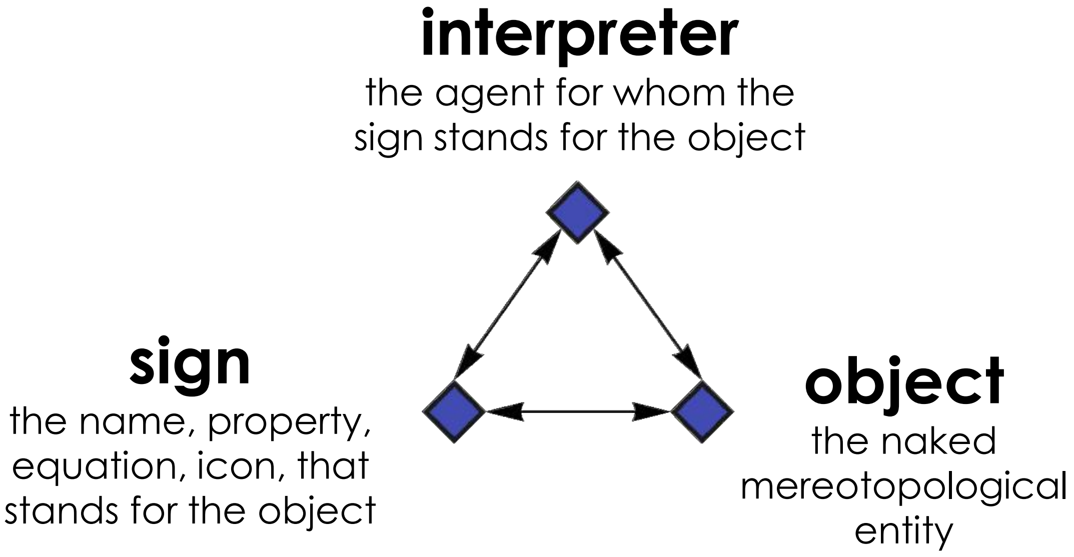
The idea is to build an ontology that enables the representation of all this cloud of concepts in a very detailed way, and provide dedicated annotations (e.g., labels, elucidations) that link the concepts to existing approaches (e.g., ISO 14040 and ISO 9000) without totally committing to a single one.

Focus on concepts, not on names!



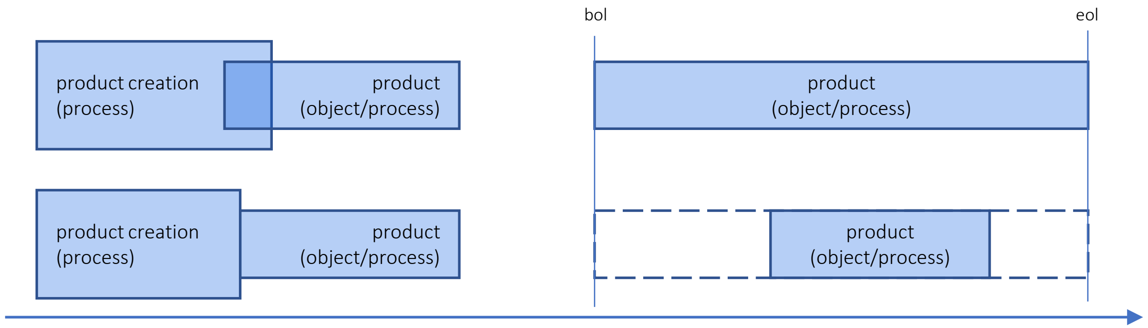
EMMO Pluralism

Semiotic approach to knowledge representation (in-ontology pluralism)



Mereotopology to fill (not to substitute) the sloppiness of existing vocabularies.

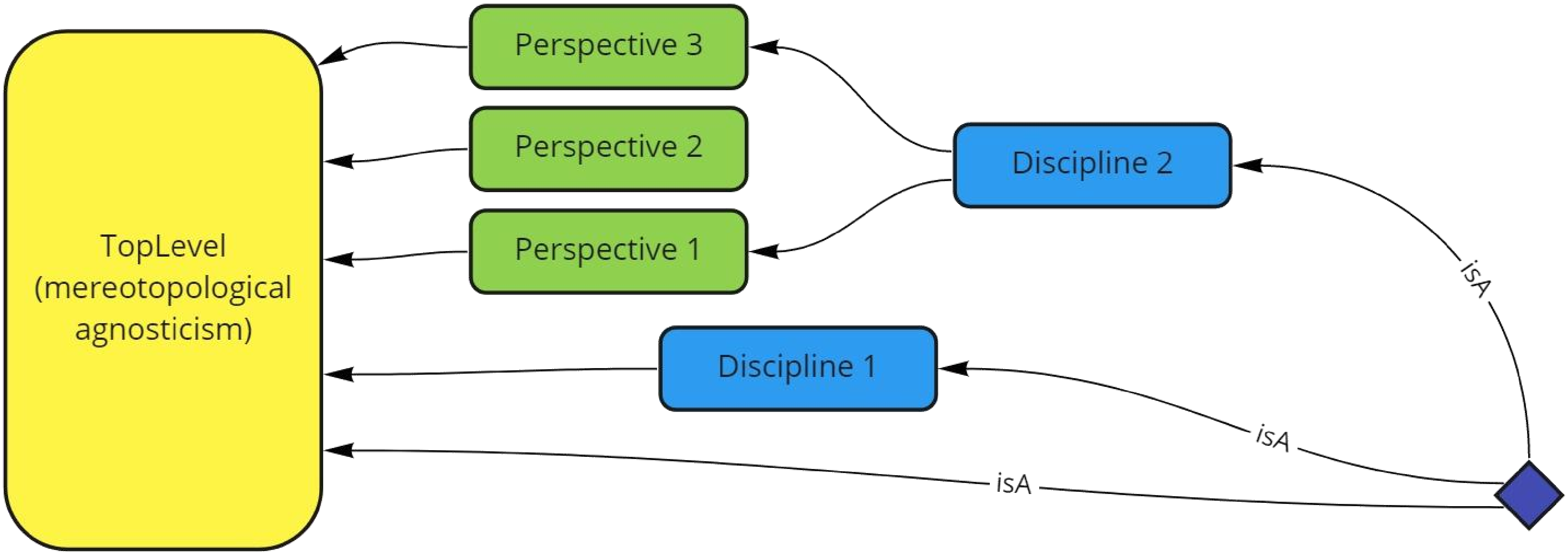
Provide a **deeper level of detail** to existing standards.



Gaps in existing standards lead to questions like:
Does a product overlaps its creation process? Does a product definition encompasses all the lifetime?

EMMO Environment Structure

General Perspective Concepts
(ontological pluralism -> MLO, covering axioms)

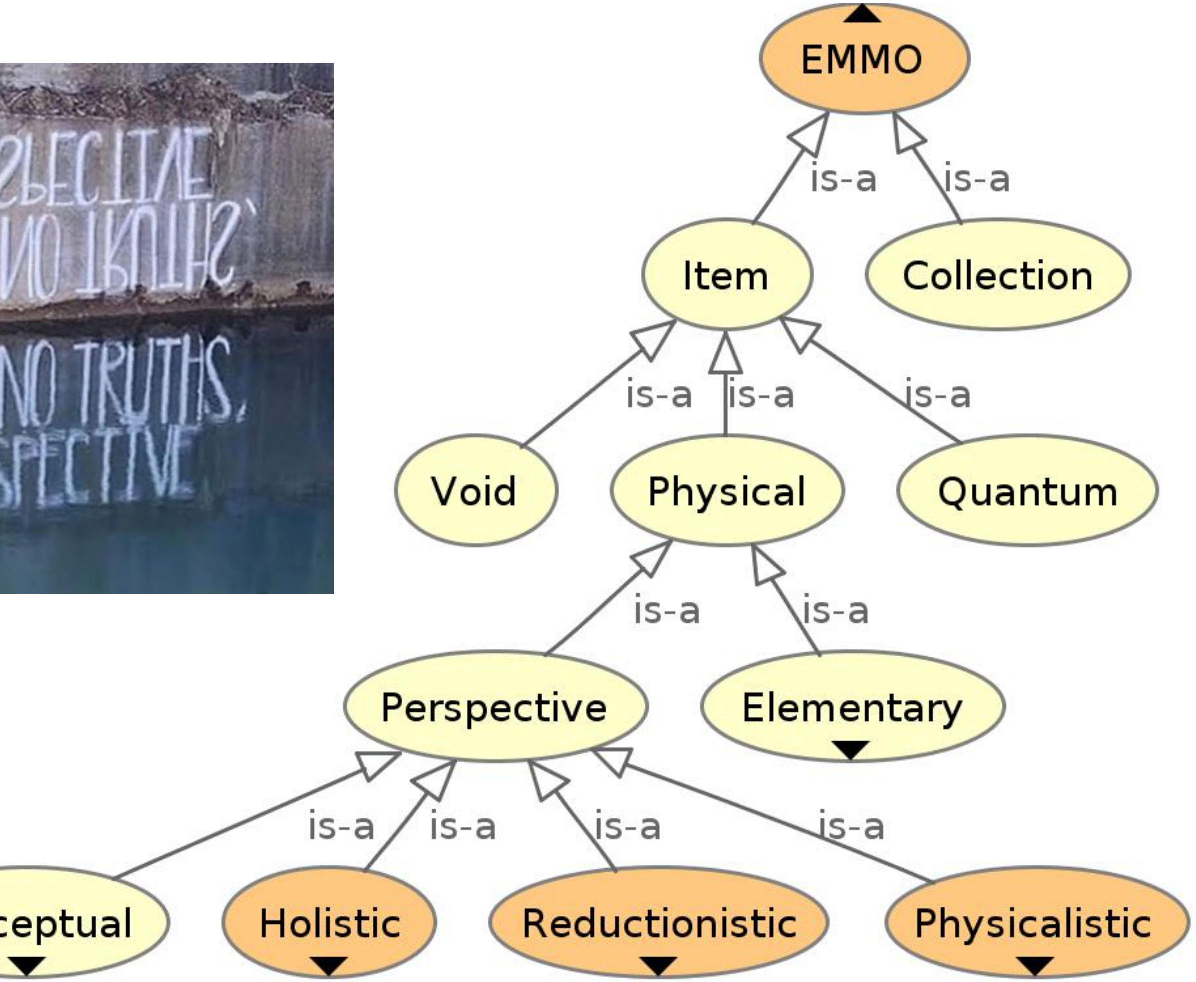


Mereotopology
(parthood, causality)

Practical Disciplines
(domain and application pluralism -> DLO, no covering axioms)

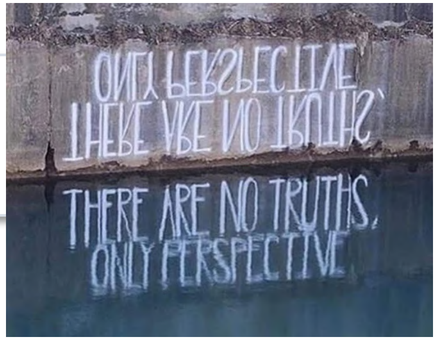
Perspectives

The most powerful feature of the EMMO is the commitment about the fact that there are no absolute definitions of the ontological nature of objects excepts for the Universe and the single indivisible quantum elements of which it is made up.



The Top Level of the EMMO respect this fact, and hosts a branch for perspectives that categorizes things in many different ways.

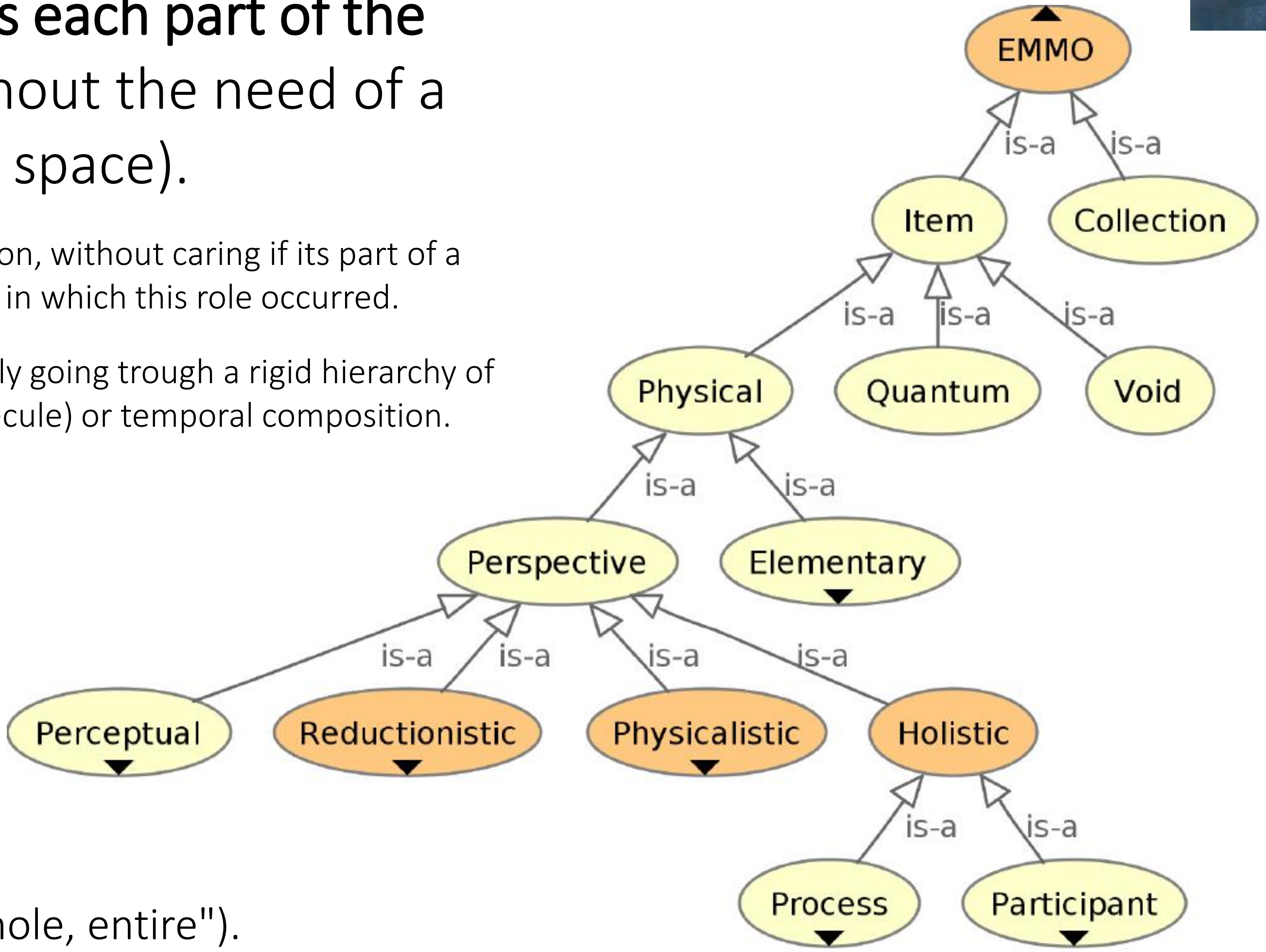
Holistic



An **Holistic** perspective **considers each part of the whole as equally important**, without the need of a granularity hierarchy (in time or space).

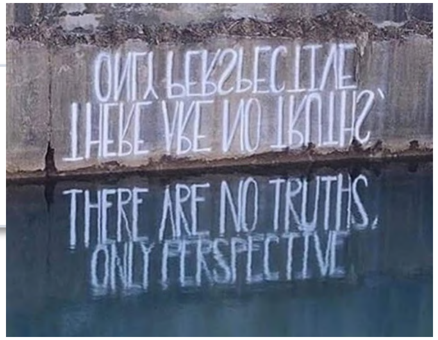
A molecule of a body can have role in the body evolution, without caring if its part of a specific organ and without specifying the time interval in which this role occurred.

This class allows the picking of parts without necessarily going trough a rigid hierarchy of spatial compositions (e.g. body -> organ -> cell -> molecule) or temporal composition.

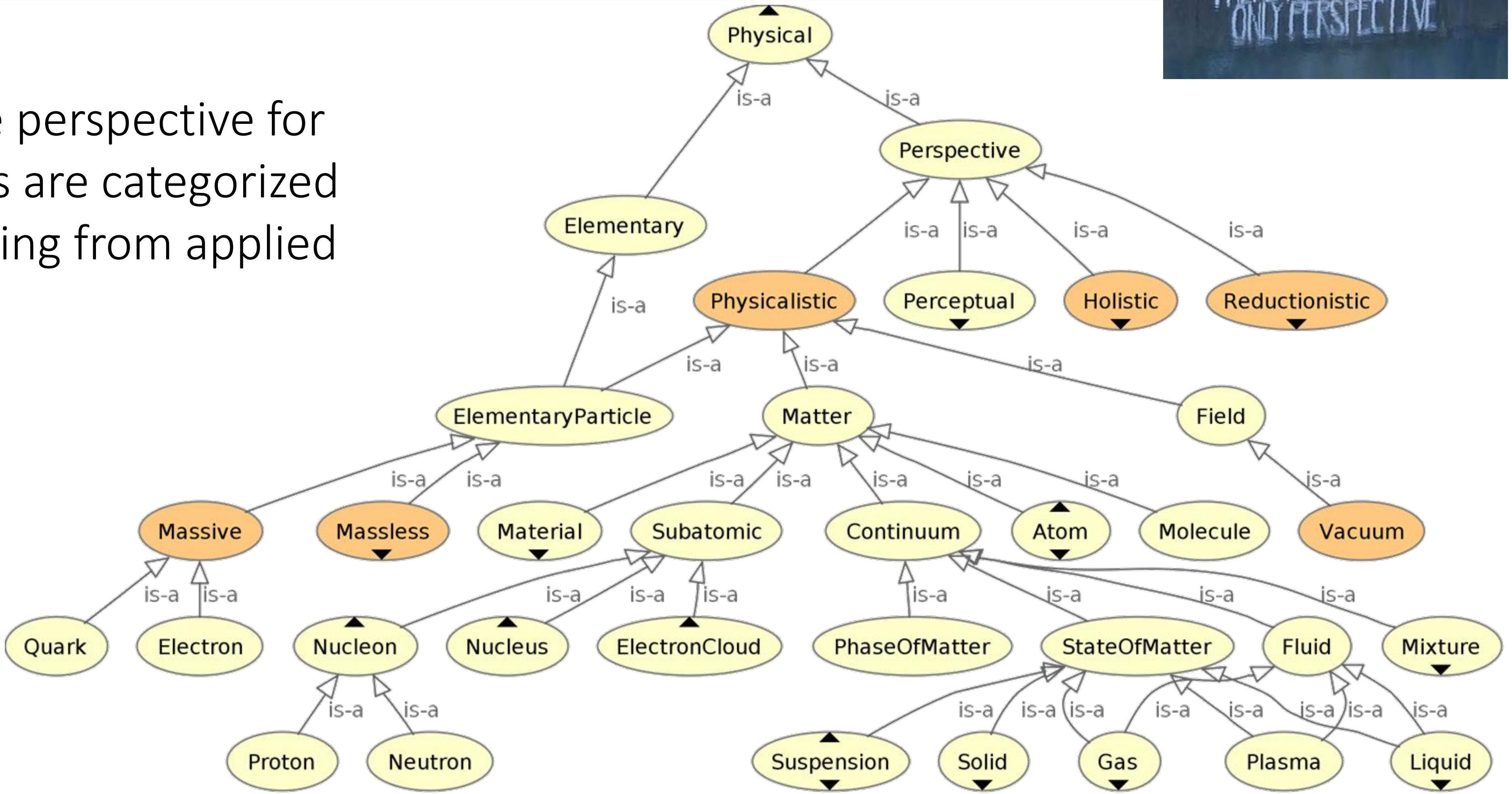


Holism (from Greek ὅλος holos "all, whole, entire").

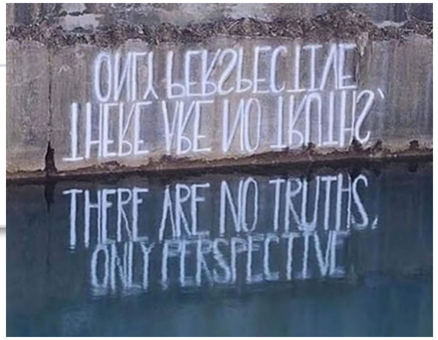
Physicalistic



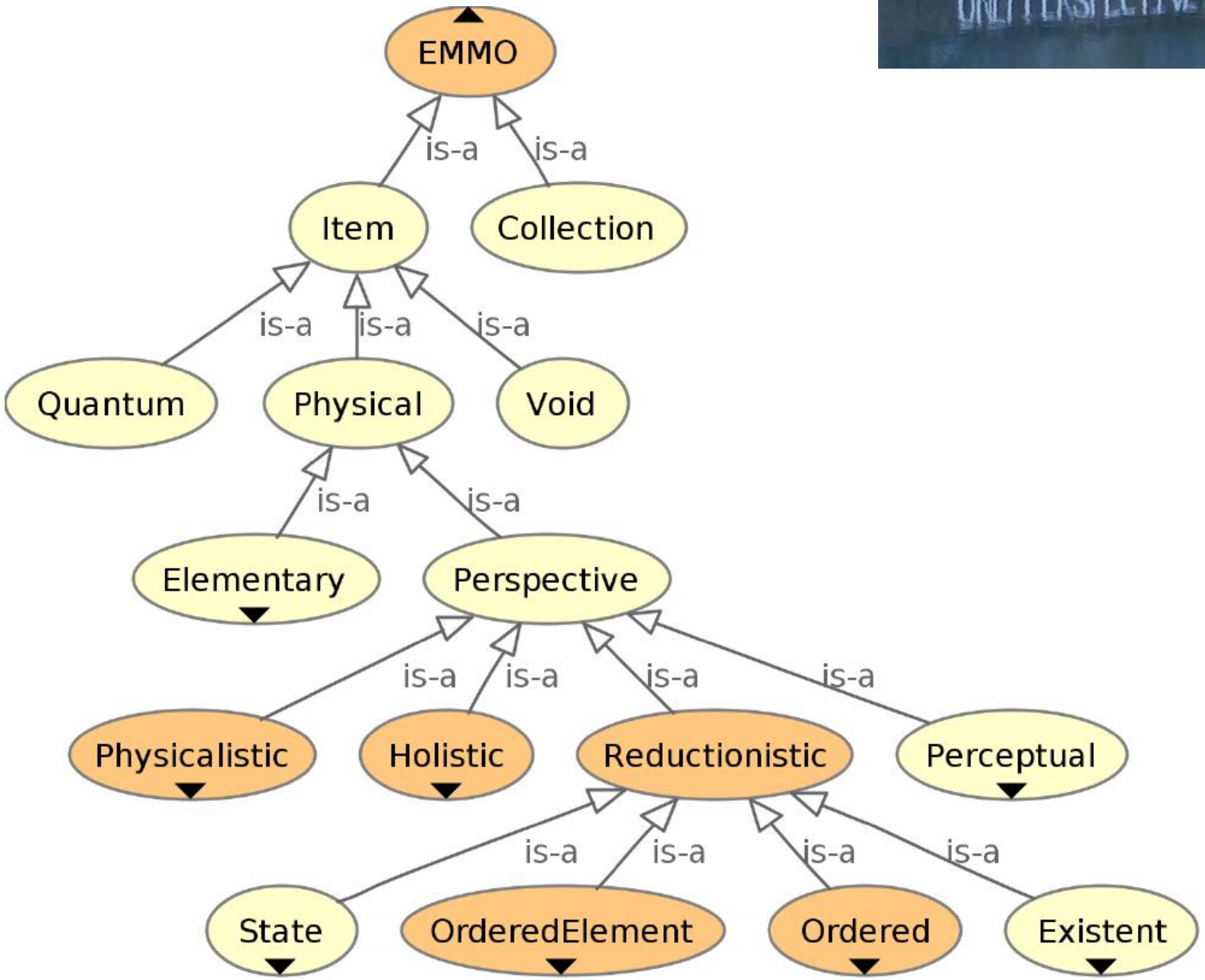
The **Physicalistic** is the perspective for which physical objects are categorized only by concepts coming from applied physical sciences.



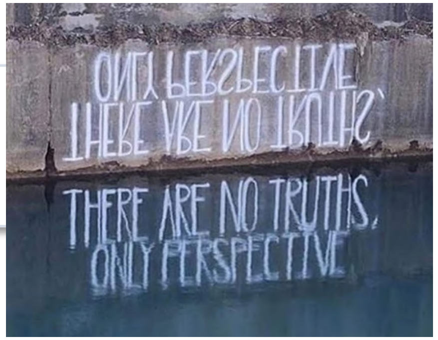
Reductionistic



The **Reductionistic** is the perspective devoted to categorize 'Physical'-s according to their granularity relations, first in terms of time evolution (Existent) and then in terms of their composition (State), up to the spatial a-tomistic element (Elementary).



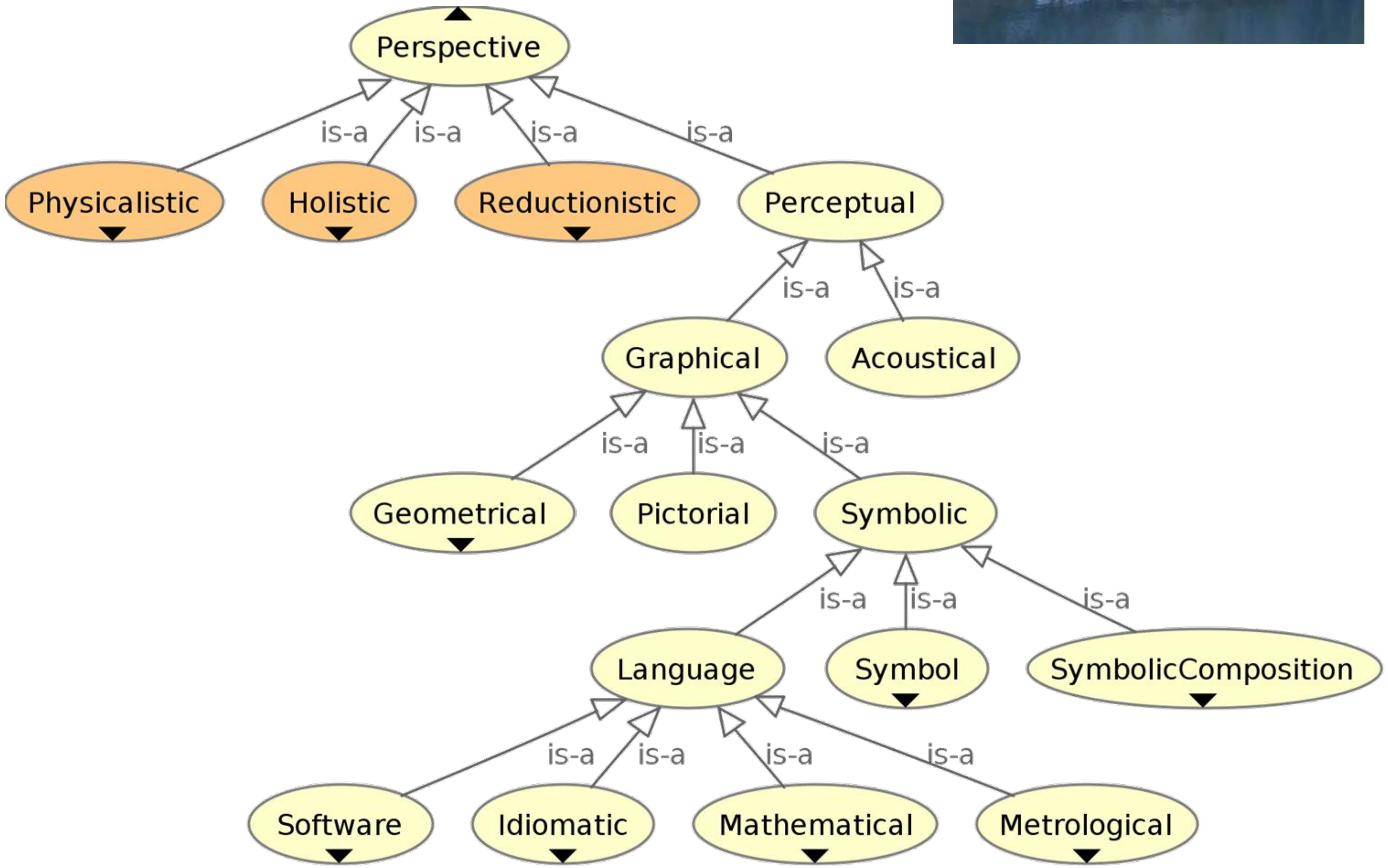
Perceptual



A **Perceptual** is a Physical which stands for a real world object that can stimulate a perception (e.g. a mental impression, the excitation of a sensor) to an interpreter (human or non-human).

Perceptuals include real world objects that:

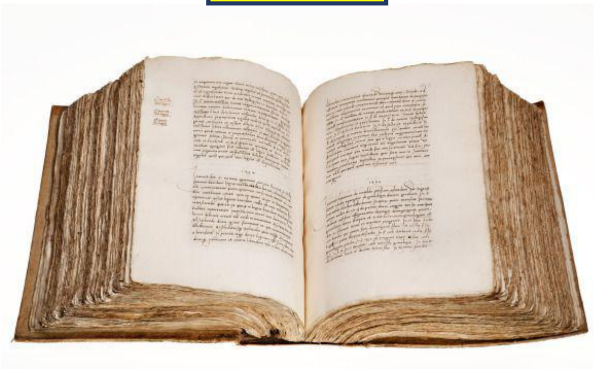
- are part of a **communication system** (e.g. words, speech, alphabets)
- are not part of a communication system, but can be identified and referred by an interpreter



From Latin perceptiō ("a receiving or collecting, perception, comprehension"), from perceptus ("perceived, observed").

Multiperspective

Book



Physicalistc
A solid which is an aggregate of organic and inorganic molecules

Holistic	Persistence
A whole and an object	

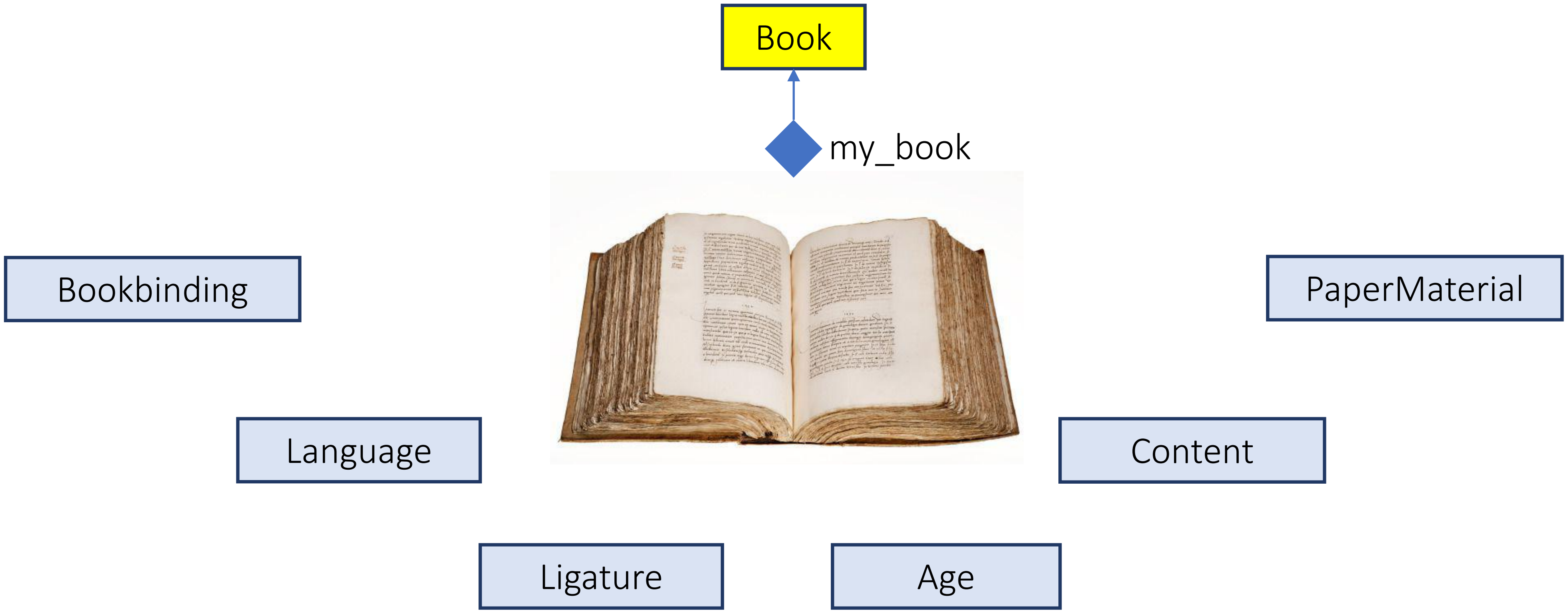
Physicalistic	Reductionistic
A hierarchy of physical entities book -> pages -> paper -> fiber -> ...	

Semiotics
A sign that stands e.g. for the life of a person

Symbolic	Reductionistic
A hierarchy of book -> chapters -> pragraphs -> words -> symbols	

Disciplines Book Example

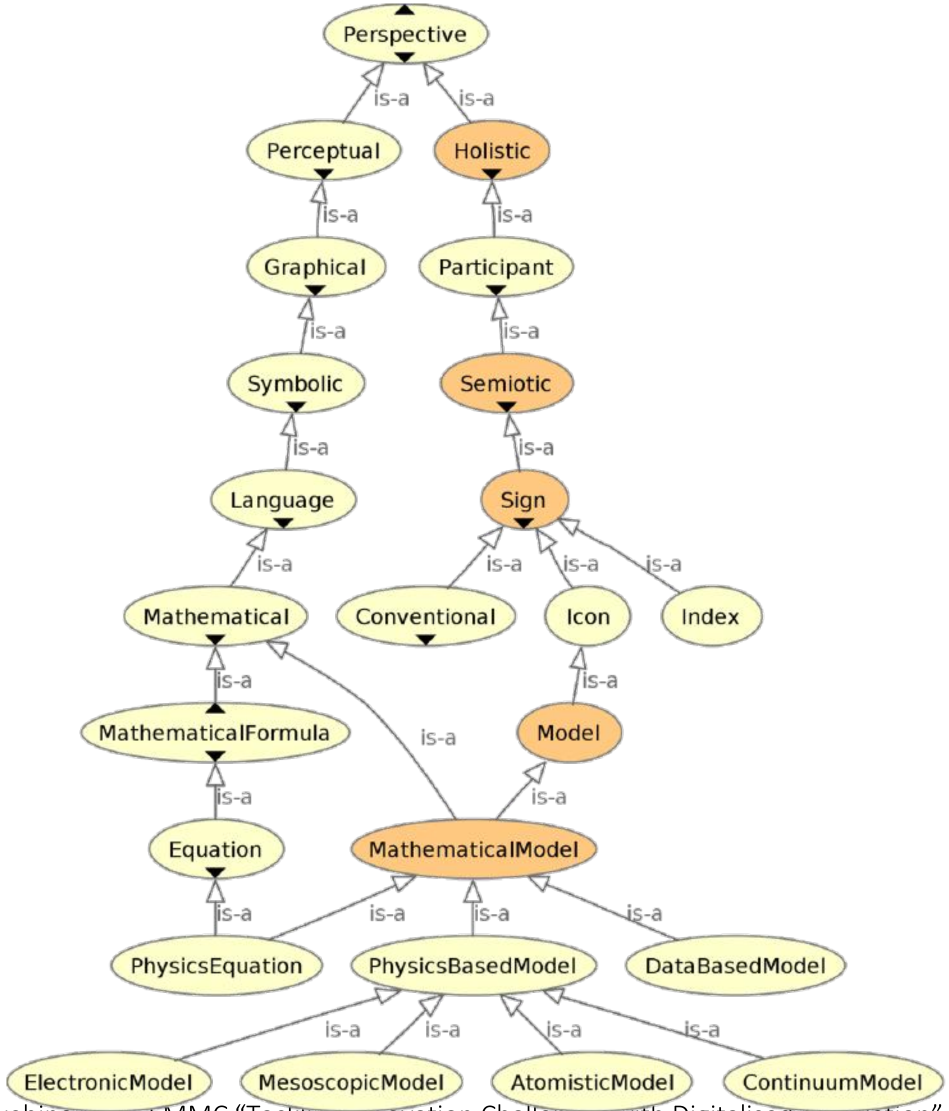
Disciplines have no ambition to cover the overall real world objects categories (no covering axioms), just to **channel the interpretation** of an entity towards a specific domain of interest.



Examples: Models

A **model** is a **sign** (**icon**) that not only stands for a **physical** or a **process**, but it is also a simplified representation, aimed to assist calculations for its description or for predictions of its behaviour.

A **model** represents a **physical** or a **process** by direct similitude (e.g. small scale replica) or by capturing in a logical framework the relations between its properties (e.g. mathematical model).



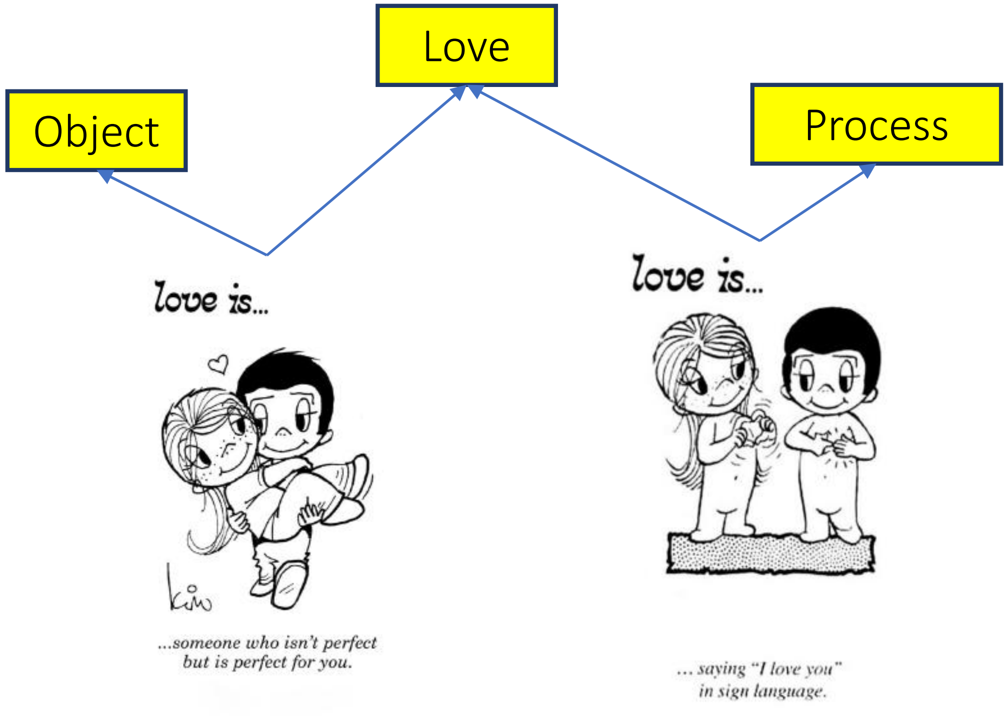
Material

Only material entities exist:

Ontologist: *"I love you"*
EMMO: *"Prove it!"*

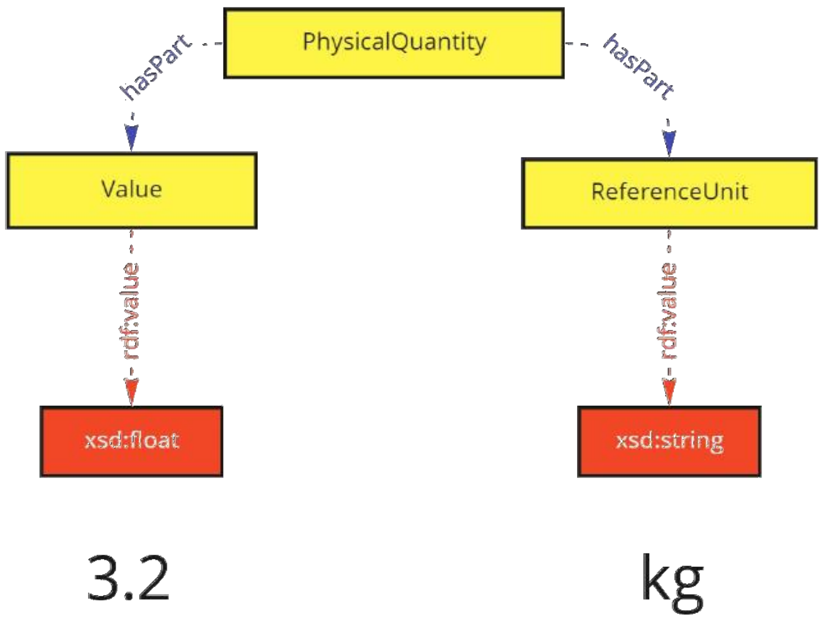
Abstract concepts role is taken by **classes**.
Individuals only refers to **material entities**.

Such sort of materialism (or physicism) forces ontologist to be **accurate in their declarations**, avoiding ambiguities that are typical for abstract concepts.

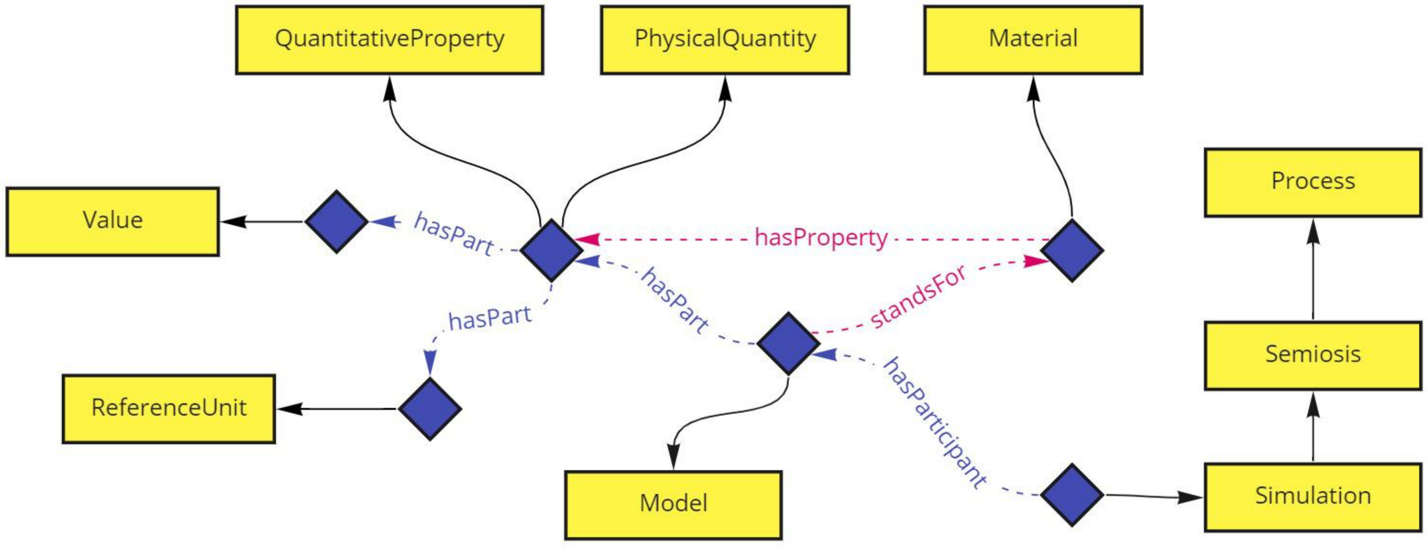


Examples: Quantities Properties

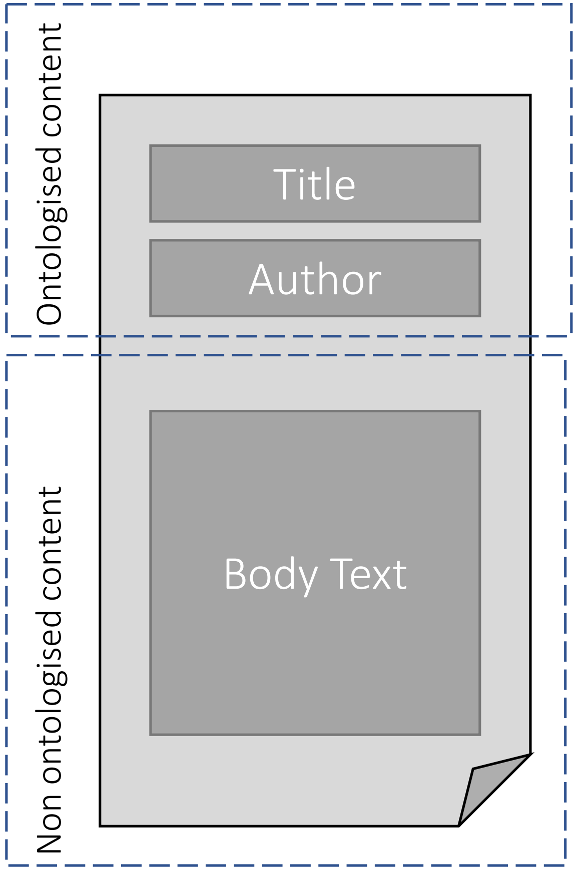
Physical Quantities are represented as syntactical structures of numbers and strings, and stored in RDFS format.



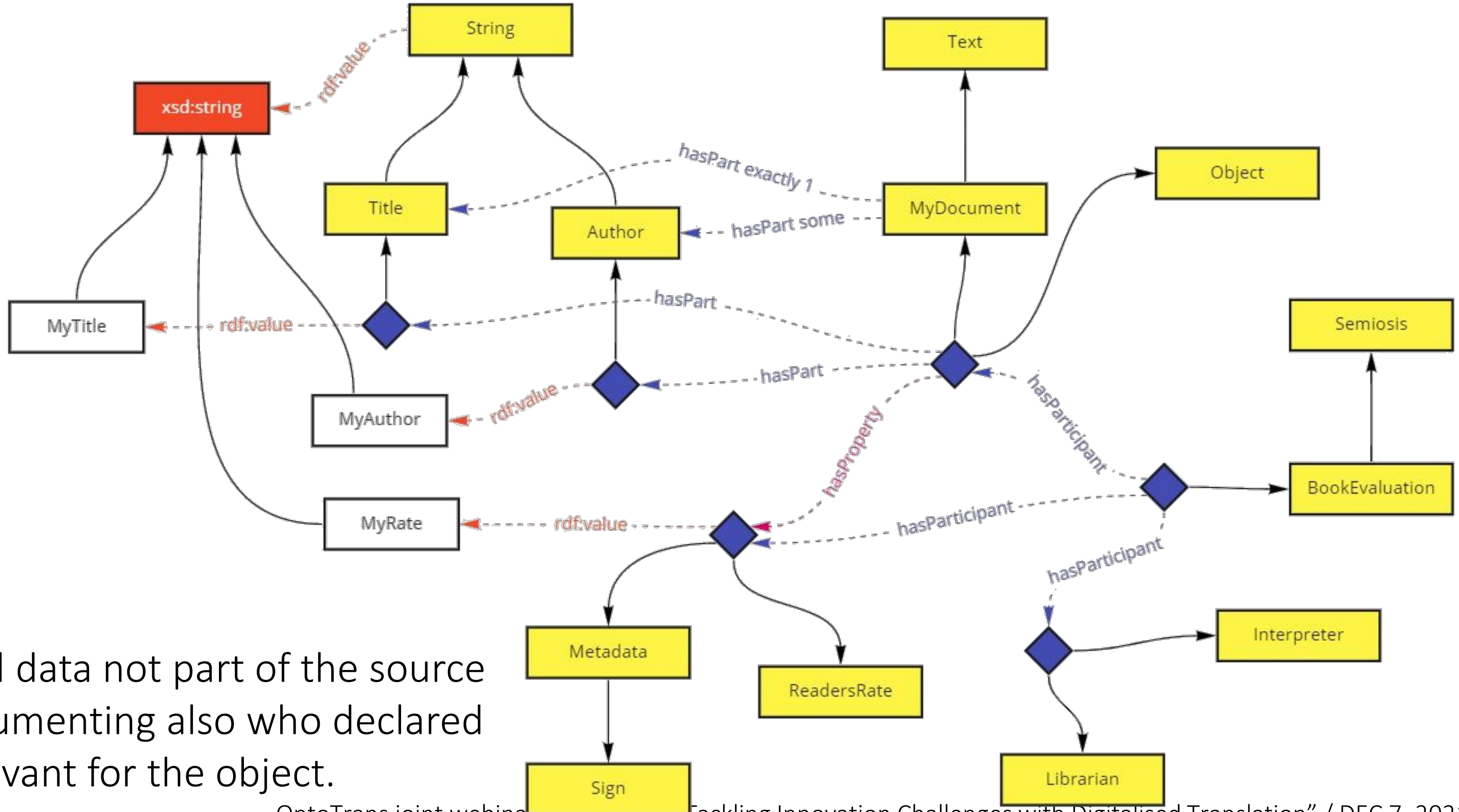
QuantitativeProperties are physical quantities that are connected to a material through a semiotic process of simulation.



Examples: Data Documentation



Using parthood we can extract some relevant data from the source (e.g. title), while leaving the bulk of the data outside the ontology.



Using semiosis we can add data not part of the source (e.g. book rating) and documenting also who declared that particular data as relevant for the object.

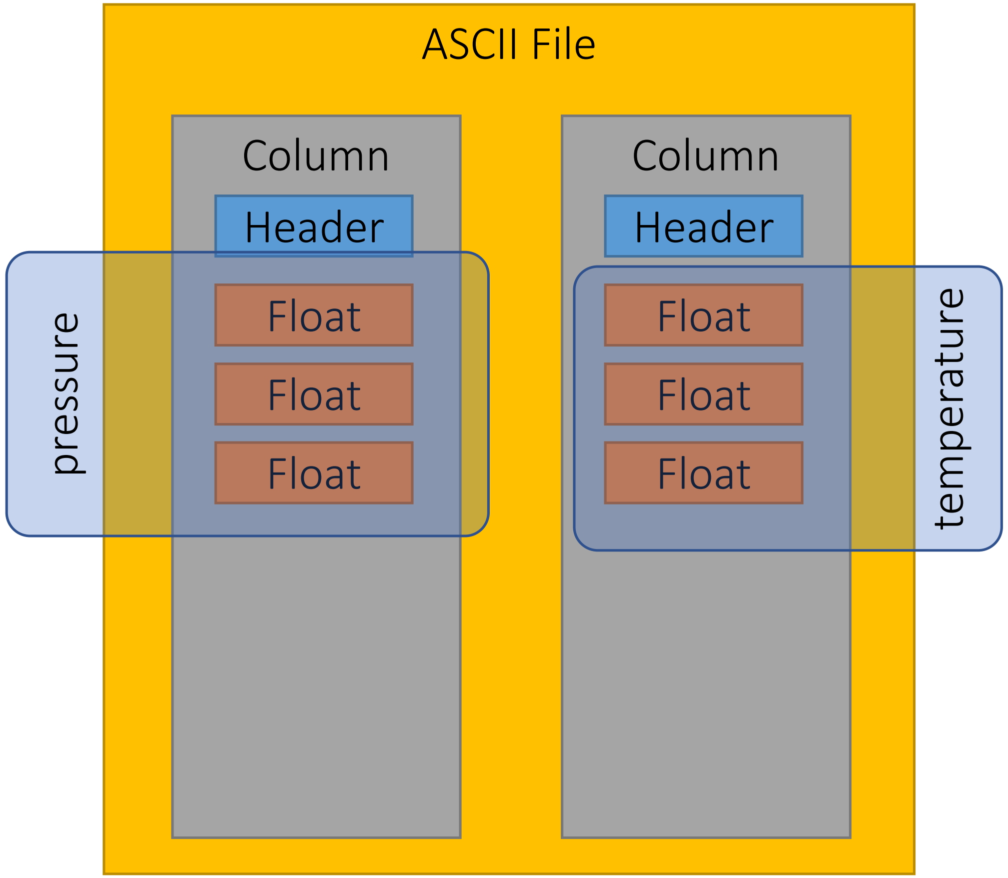
Examples: Data Documentation

Using **reductionism** we can declare the **structure of a data set** and provide **mapping from syntax to semantics**

ASCII file

press. atm	temp. K	density kg/m^3	mol. wt. kg/mol	sonic vel. m/s	enthalpy J/kg	spec. heat J/kg/K	gamma
1.00	300.0	1.5109E+00	3.7202E-02	3.2459E+02	2.6237E+02	6.1459E+02	1.5714E+00
1.00	400.0	1.1332E+00	3.7202E-02	3.7451E+02	6.1794E+04	6.1632E+02	1.5689E+00
1.00	500.0	9.0652E-01	3.7202E-02	4.1811E+02	1.2357E+05	6.1947E+02	1.5644E+00
1.00	600.0	7.5544E-01	3.7202E-02	4.5717E+02	1.8572E+05	6.2357E+02	1.5586E+00
1.00	700.0	6.4752E-01	3.7202E-02	4.9279E+02	2.4830E+05	6.2816E+02	1.5523E+00
1.00	800.0	5.6658E-01	3.7202E-02	5.2573E+02	3.1136E+05	6.3288E+02	1.5459E+00
1.00	900.0	5.0362E-01	3.7202E-02	5.5655E+02	3.7487E+05	6.3738E+02	1.5400E+00
1.00	1000.0	4.5326E-01	3.7202E-02	5.8567E+02	4.3882E+05	6.4138E+02	1.5348E+00
1.00	1100.0	4.1206E-01	3.7202E-02	6.1338E+02	5.0313E+05	6.4485E+02	1.5304E+00
1.00	1200.0	3.7772E-01	3.7202E-02	6.3977E+02	5.6778E+05	6.4822E+02	1.5262E+00
1.00	1300.0	3.4866E-01	3.7202E-02	6.6499E+02	6.3277E+05	6.5157E+02	1.5221E+00
1.00	1400.0	3.2376E-01	3.7202E-02	6.8917E+02	6.9810E+05	6.5496E+02	1.5180E+00

Reductionism + Symbolic + Semiosis

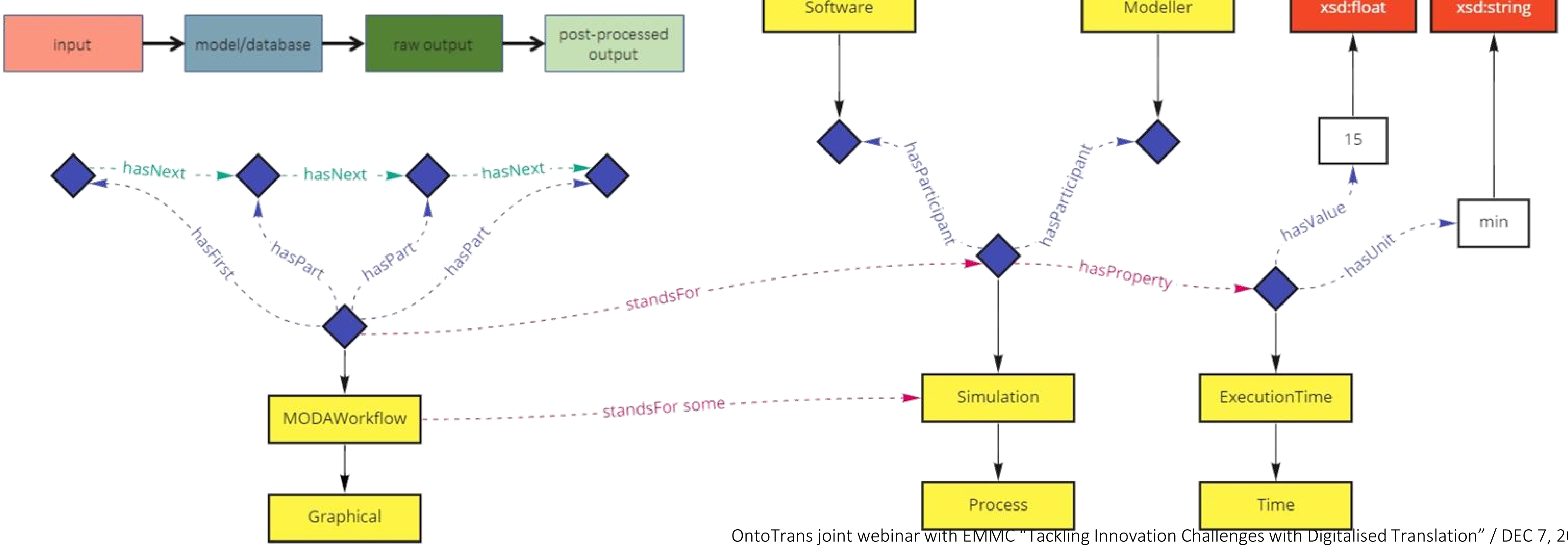


Examples: Workflows and Simulation

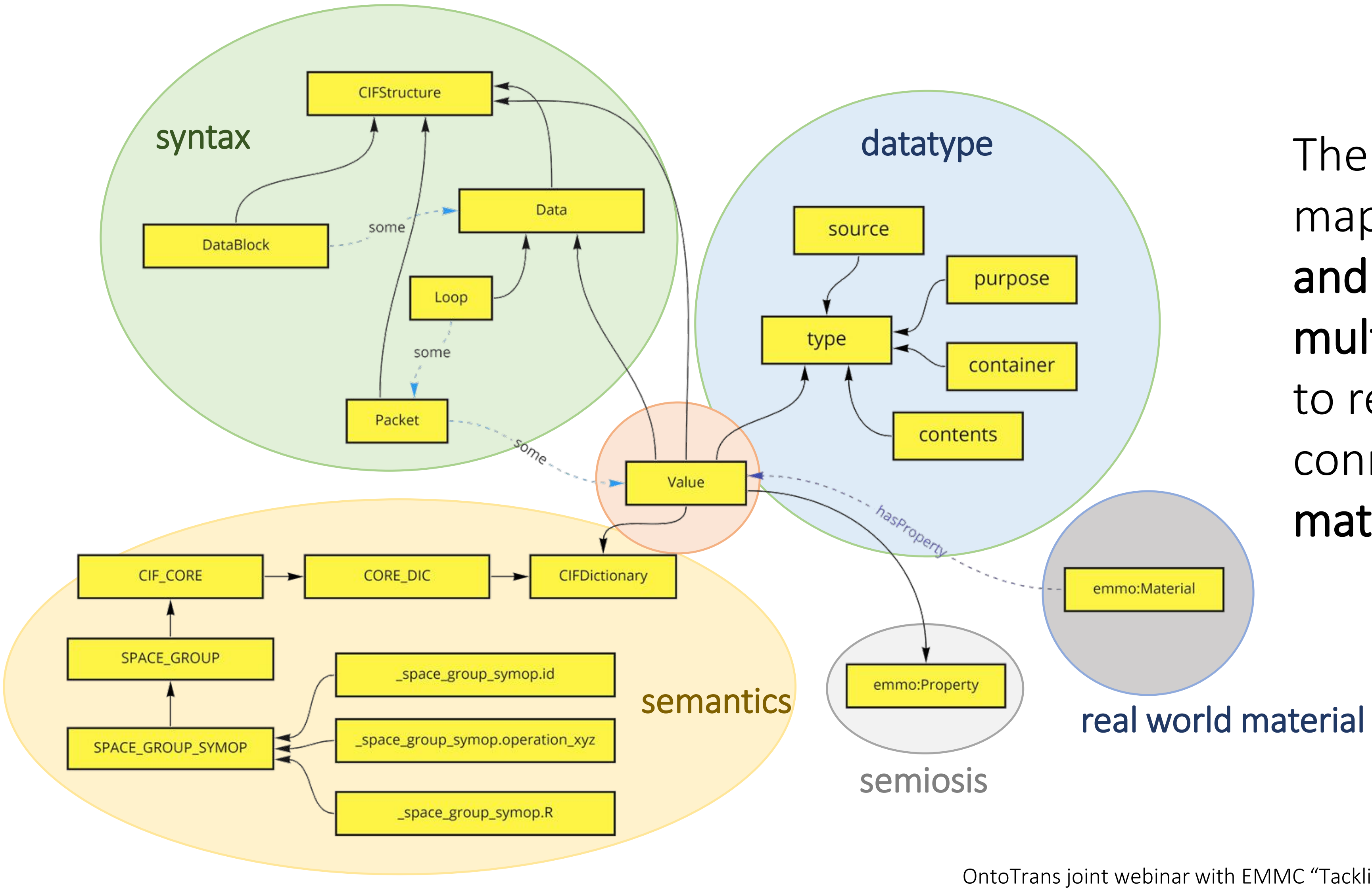
Algorithms can be represented as graphical workflows within the ontology, so **that the user can design his simulation directly within the ontology**.

Then the workflow can be **executed** one or more time as simulation, and the **properties of its execution (e.g. time, cost) can be stored** to document the process.

MODA Workflow



Examples: EMMO CIF Ontology



The EMMO CIF ontology maps **all concepts of CIF-DDL and CIF-CORE** and provides a **multiperspective approach** to represent CIF data and to connect them to **real world materials**.

BOTTLENECKS: MULTIDISCIPLINARITY GAP

We experienced the **difficulty to grasp** the complexity of the scenarios, competencies and technologies.

There are **strong resistances** from each community against visions that goes outside their **conceptual comfort zones**

Ontology community tries to put together these people…

Philosophers are driven by curiosity, and have difficulty to bend their view to applications.

Ontologist (logics) are strongly committed to rigid deterministic systems, not really open to compromises

Computer scientists would happily drop logical complexity to a minimum in order to make the machine run

Applied scientists don't believe in ontologies: they already have mathematics

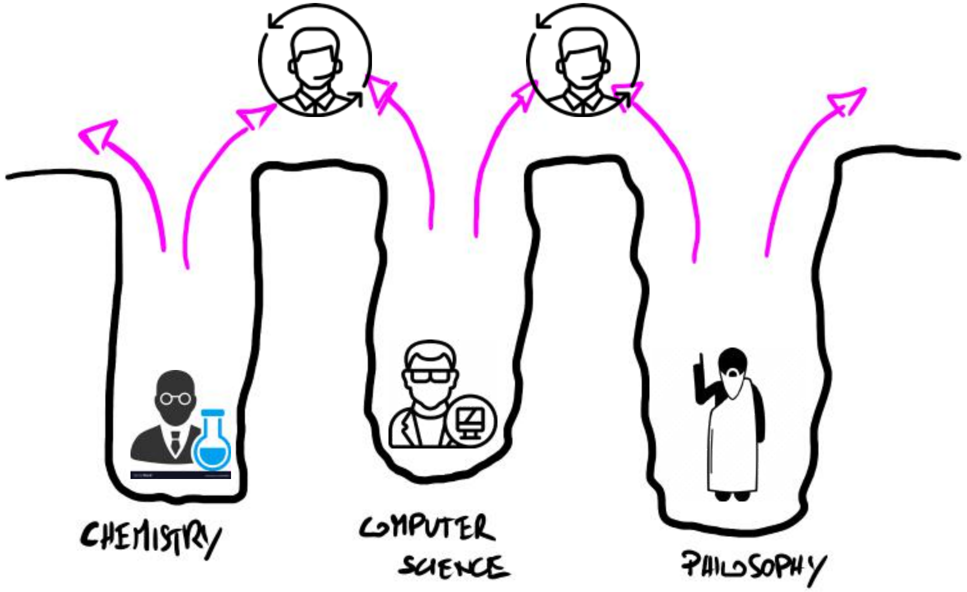
Engineers would like ontologies but at the same time don't want to abandon well established standards towards a new one.

However, is by requiring such multidisciplinarity that Ontologies may provide a **huge level of innovation** (and this is within the nature of our good old Europe!!!)

Invest in Multidisciplinary Actions

Suggestions:

- Require **strong multidisciplinary approach** in the future work progamme calls
- **Propose ontologies** as a way to force such multidisciplinary approach
- Push for **education approaches** that introduces **specialization only in the very last years**, with a strong amount of **human sciences for all education curriculum**
- Invest in the figure of **Translators** (as defined by **EMMC** and **OntoCommons**) as way to bridge the gaps between disciplines



Extraction of knowledge from each single discipline is **more and more difficult**: innovation comes from **multidisciplinarity**.

Conclusion: Embrace complexity

The **importance** of **semantic approach to knowledge** is that is provides **a new language, digitally and machine friendly**, that can **push for the transition towards Industry 5.0**.

Bottlenecks come mainly from **compartimentalized human approach to knowledge** (there's also the need to develop tools, but its in my opinion secondary).

The solutions may be to propose initiative that helps EU citizens to **embrace and manage complexity, and not to fight it** (as it seems the case for social media and some political views).

Push towards **multidisciplinary in education, science and engineering** seems the right direction, and **this attitude may be reflected in the next WPs**, by requiring multidisciplinarity in each HE project.

Ontologies are a field in which **multidisciplinary is acting in its best**, and should be **incentivated** in their many aspects as **catalyst toward multidisciplinarity**.

Multidisciplinarity is something **that is culturally in the DNA of European citizens**, and can be something that may give us a **distinct advantage against other international actors.**

Conclusions

The EMMO is more about **Pluralistic Parallelism** (represent things in many different and coexisting ways) instead of **Serial Stratification** (things are represented in a one and one only way).

The focus for EMMO development is on **capturing the multiple** ways in which a real world object is expressed by communities.

A distinction between **Perspectives** (MLO) and **Disciplines** (DLO) is proposed, using **covering axiomatisation** for Perspectives, leading to a hierarchy of Disciplines with a combination of parallel/serial dependencies.

Ongoing Initiatives

SimDOME — Open Simulation Platform

ONTOTRANS — Open Translation Environment

Open Model — Material Modelling Innovation Platform

DOME 4.0 — Industrial Data Marketplace

ONTO COMMONS (Ontology-driven data documentation for industry commons) — Ontology Ecosystem

Elementary Multiperspective Material Ontology

Some of the ongoing EMMO Efforts:

- Crystallography ontology
- Mechanical testing
- Atomistic
- Chemistry
- Chemical Kinetics
- Battery interfaces
- Algorithm (diagrams) representation

https://github.com/emmo-repo

Ongoing Initiatives

The EMMO is:

Emanuele Ghedini (UNIBO)

Jesper Friis (SINTEF)

Gerhard Goldbeck (GCL)

Adham Hashibon (UCL)

Georg Schmitz (ACCESS)

… and many more!

Elementary
Multiperspective
Material Ontology

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