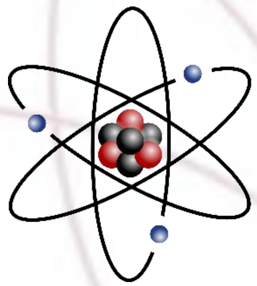
ONTOTRANS

Ontology of Innovation Cases

Approach and Process from Innovation Case via Conceptualisation to Ontology

Emanuele Ghedini – UNIBO

Ontology As Language



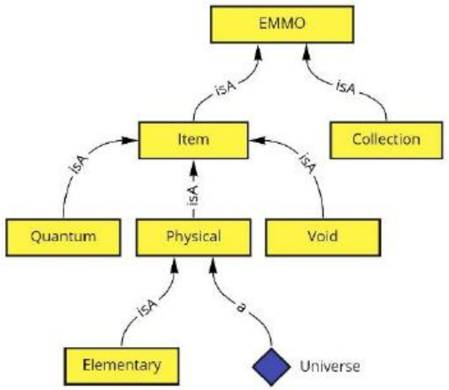
PHYSICS

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

MATH

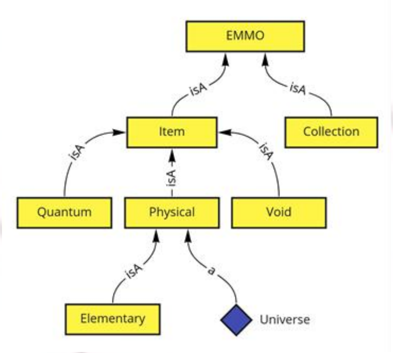
=

INDUSTRY



ONTOLOGY

Ontology As Language



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)

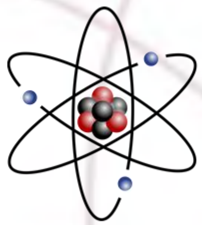
Provides Models of the World

(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)

Ontology As Language



PHYSICS

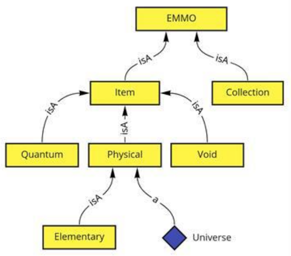
$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

MATH

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

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

INDUSTRY



ONTOLOGY

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

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

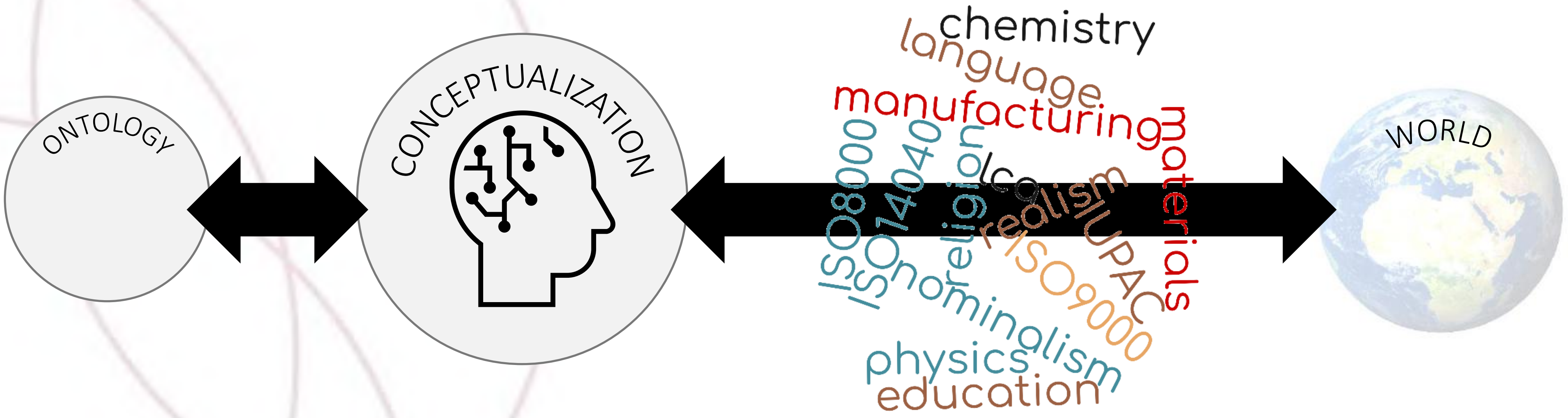
Talking to Machines

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)

Talking to Machines

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)

Talking to Machines

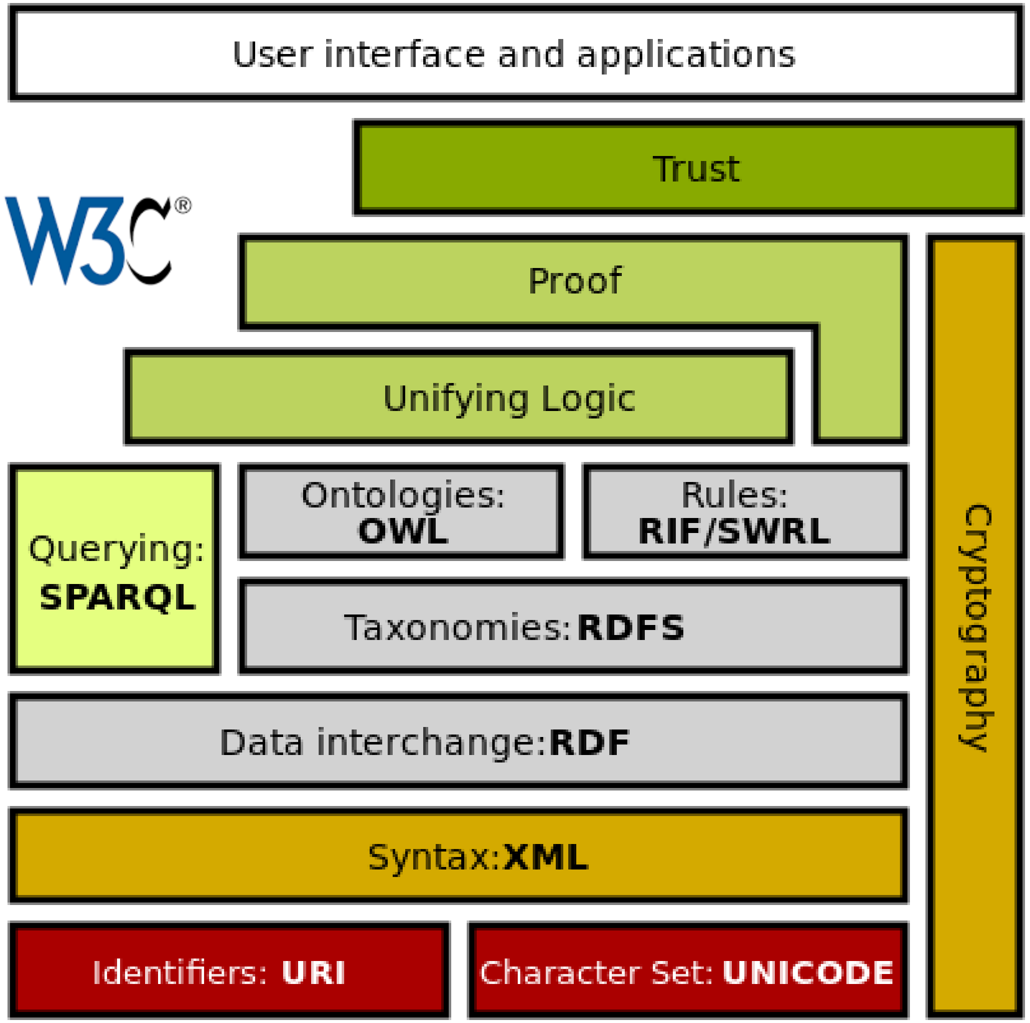
A great boost towards the use of formal ontologies in practice came in the ‘90 from the Semantic Web extension of the World Wide Web, thanks to the W3C standardization activities.

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!



Talking to Machines

Ontology Entities

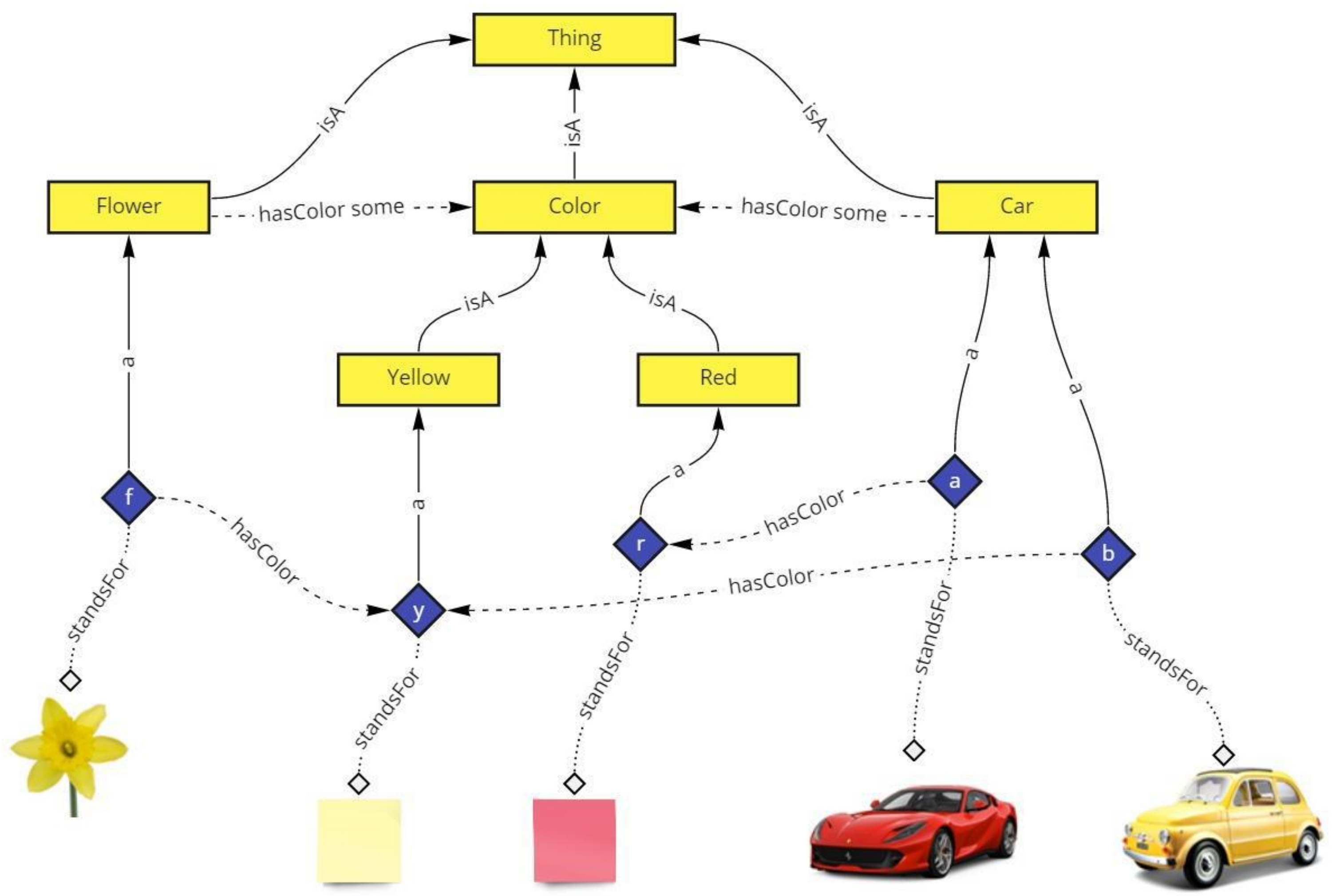
class relation individual

Example of axioms:

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

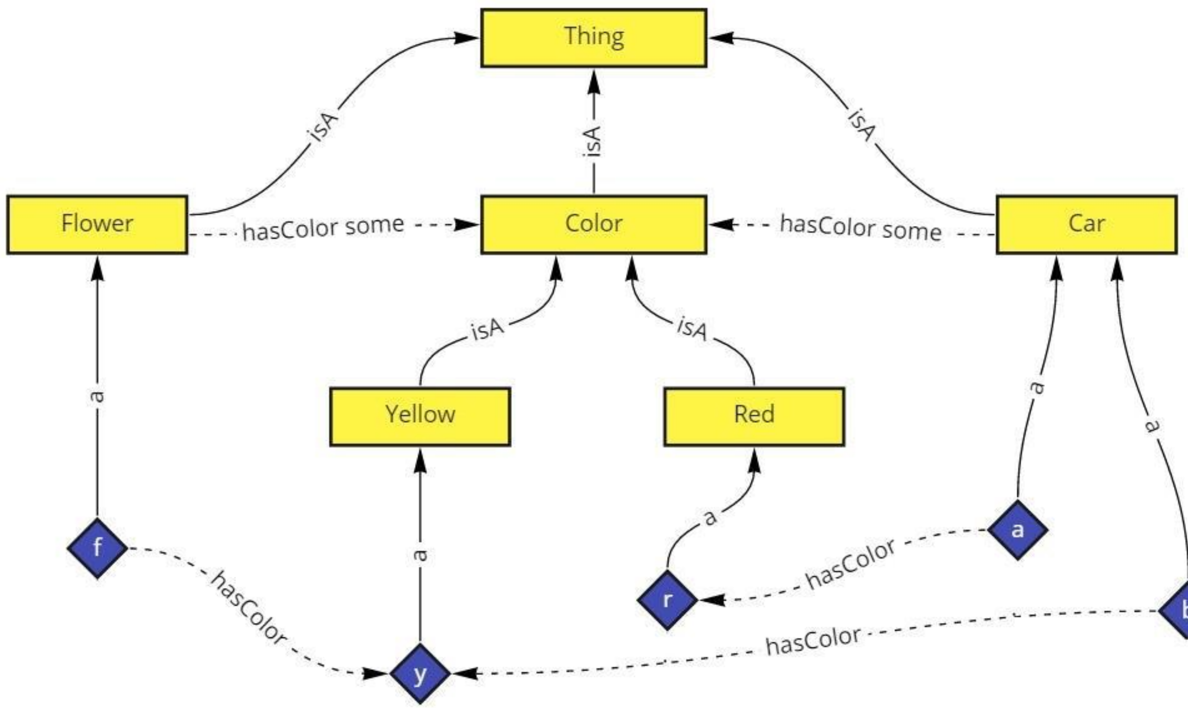
Real-world objects

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



Talking to Machines

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 .
```

Terminology I (how we understand each others…)

Innovation Challenge: the high level innovation objective addressed by specific cases expressed in natural language (e.g. master the process parameters, agile response to product, market and regulatory requirements)

Innovation Case (or Application): a specific class of cases (e.g. design, manufacturing, sales) for which the challenge applies, involving processes and material objects and expressed in some human readable form (e.g. diagrams, flow charts).

User Case: a specific implementation of an innovation case for the user (e.g. a step in the manufacturing of a specific product, a manufacturing line of a company).

Workflow: data workflow expressed using MODA (or MODA-like) graphs representing the combination of methods for the prediction of properties of our objects/processes of interests (the totality or part of the user case).

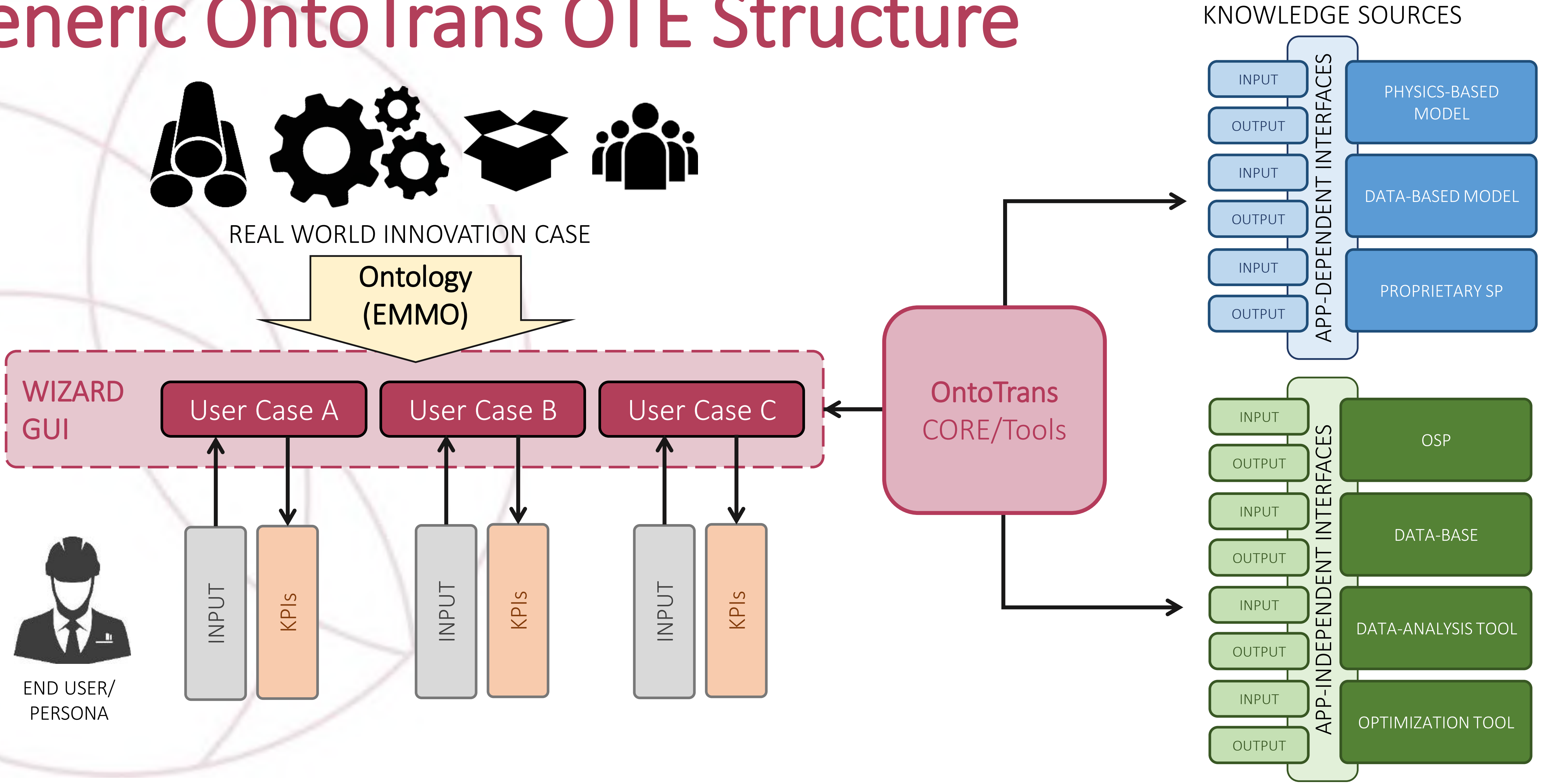
Terminology II (how we understand each others…)

APP: the software module of the OTE (one for each Innovation Challenge) used to declare the components of a specific User Case, to build the workflow by selecting available solutions (e.g. models, database, other cases data, machine learning approaches) and to connect the available tools together (passive or active)

Knowledge Source: everything that can be used to provide new knowledge from existing one. It needs an INPUT (e.g. case set up for simulation, query for a database) and provide an OUTPUT.

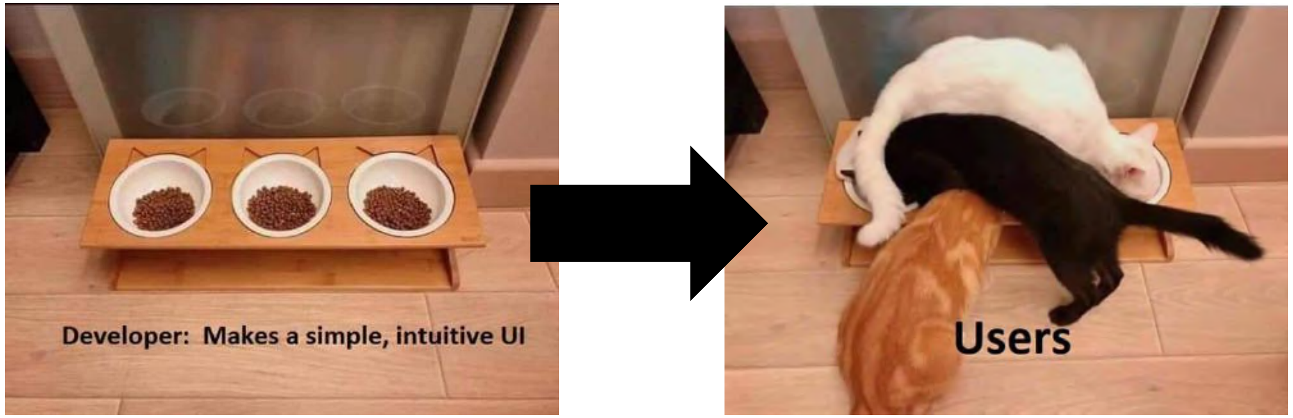
> Knowledge Generator: a knowledge source that generate new non-existing knowledge (e.g. a model that provides calculated properties for an object, the INPUT is the setup case and the OUTPUT are the properties)
>
> Knowledge Repository: a knowledge source that provides already-existing knowledge (e.g. a database of properties, the INPUT is the name of the substance and OUTPUT is the desired property)

Generic OntoTrans OTE Structure

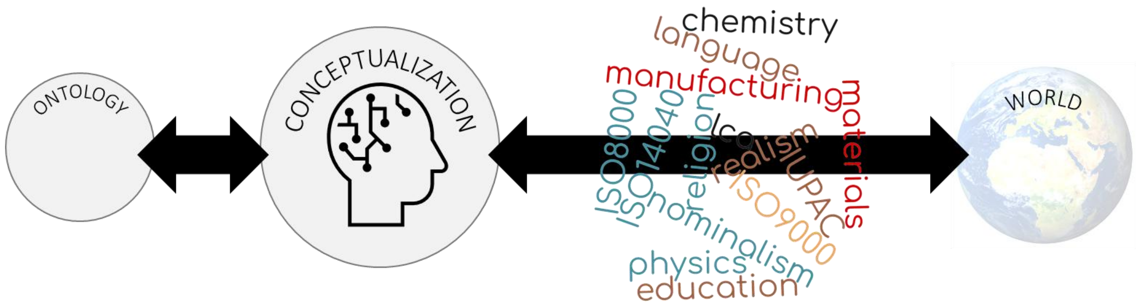


Facilitate Users’ Life

How to avoid this?



By building the ontological description of the innovation cases around the user.



Facilitate Users' Life

TRANSLATORS

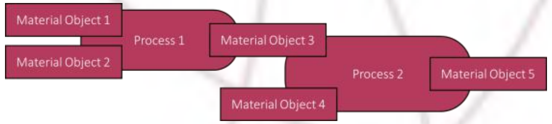
INDUSTRIAL USERS

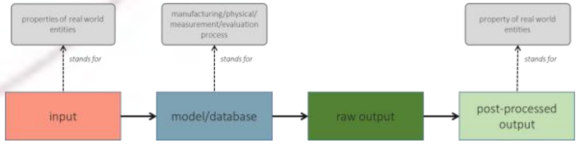
ONTOLOGISTS

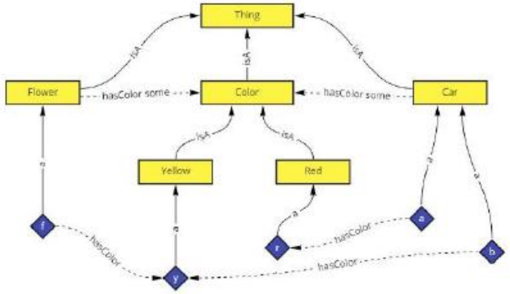
Human Friendly Template

Graphical Conceptualisation

Formal Ontology





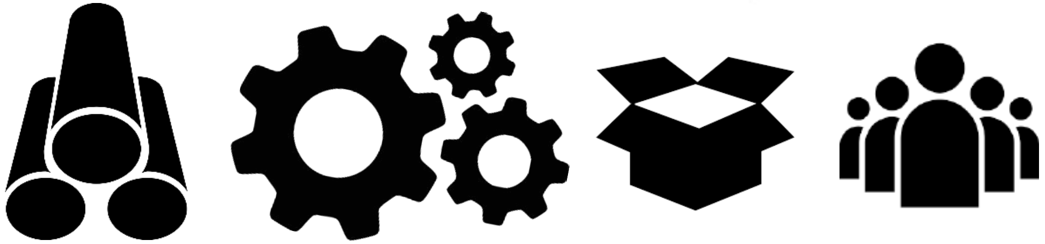


Innovation Case Template

Human Friendly Template

- Collect all the relevant information regarding each **Innovation Challenge** for the design of the OntoTrans components
- Information is collected using tables describing each aspect of the **Innovation Case**.

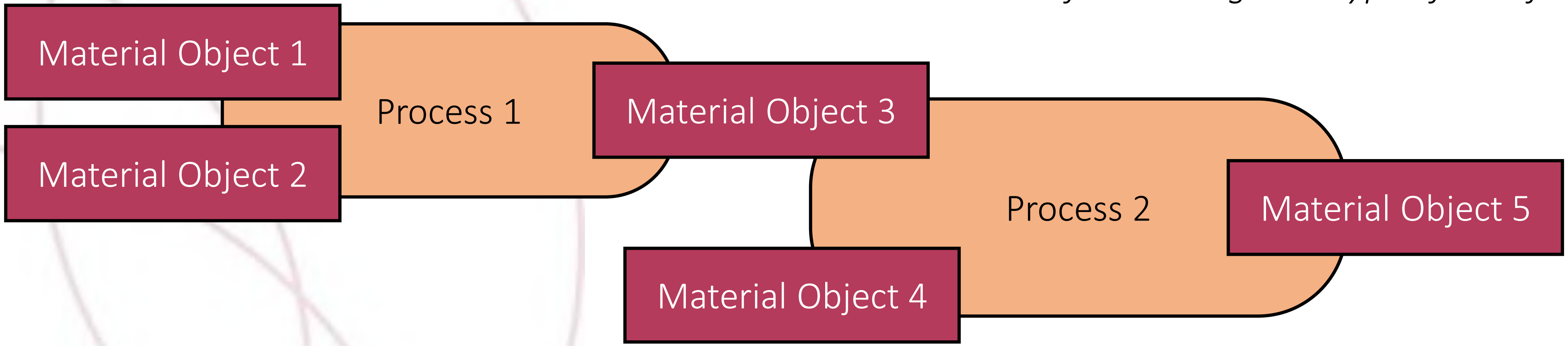
Innovation Case



- Describe, in terms of material objects (e.g. raw materials, product, components) and processes, all the steps that constitutes the **Innovation Case**, from raw materials to on-the-shelf product (e.g. lamination, packing, selling) as expression of an **Innovation Challenge**
- The Innovation Case clearly defines its boundaries, identifying its Cradle-to-Gate and Gate-to-Consumer temporal parts, including also the Consumer Feedback when needed
- Each material object and process must provide a list of relevant properties (i.e. descriptors of their state) and the measurement procedures used to obtain them (e.g. measurement device, consumer feedback)
- KPIs are relevant properties identified by the user as indicators of the targets to be achieved.

Innovation Case

EMMO: Causality and not time is the criteria for creating such type of workflows.



An **innovation case** is formalised as an **ontological entities workflow** with the purpose of identifying all the entities that play a role in the case to be referenced by properties and models.

A simplified object/process approach is chosen to facilitate understanding by users without experience in ontologies.

Innovation Case

List of all Objects and Properties with their description in natural language

Object	Description
Object 1	*(natural language description)*
Object 2	*(natural language description)*

Process	Description
Process 1	*(natural language description)*
Process 2	*(natural language description)*

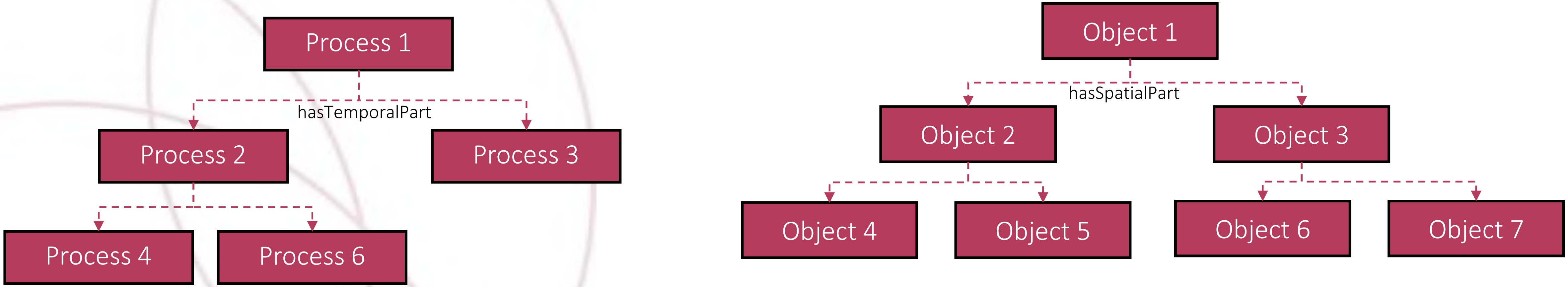
Innovation Case

List of all properties we need to deal with, for each innovation case.

Please consider that in the EMMO everything we know about an entity must come as a property, which is a symbolic representation of the object itself defined for a specific class of interpreters within a well defined observation process.

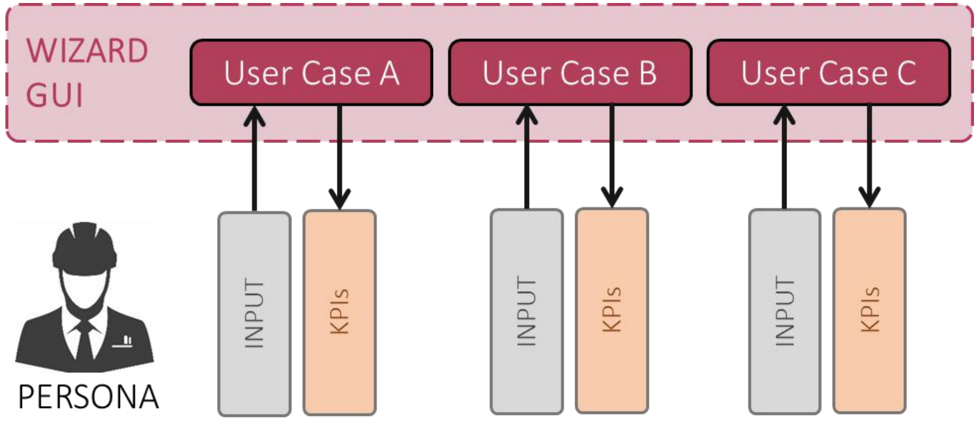
	Property Names	Property Description (semantics)	Data Description (symbolic)				Potential Interpreters				Source Data File Format
			Data Type	Data Range	Units	Reference Physical Quantity	Measured by	Modelled by	Assigned by	Other	

Innovation Case



Use mereological concepts to express wholes and parts, with both temporal and spatial partitioning.

User Cases



- User Cases are subsets of a specific Innovation Case, expressing the different user approaches to address the Innovation Challenge

- Different User Cases for the same real world innovation case can be proposed, each one focusing on different set of properties or level of details of the objects, according to specific design objectives

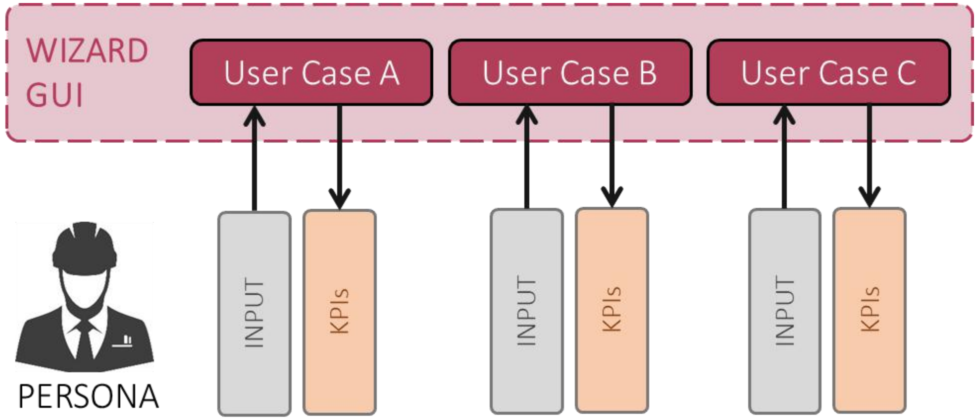
- User Cases are represented like the Innovation Case, by selecting objects (or macro objects), processes and properties of interest

- Properties of real world objects/processes must be defined as problem inputs or KPIs, for each User Case

Workflows

Workflows are intended as <u>**data workflow**</u>.

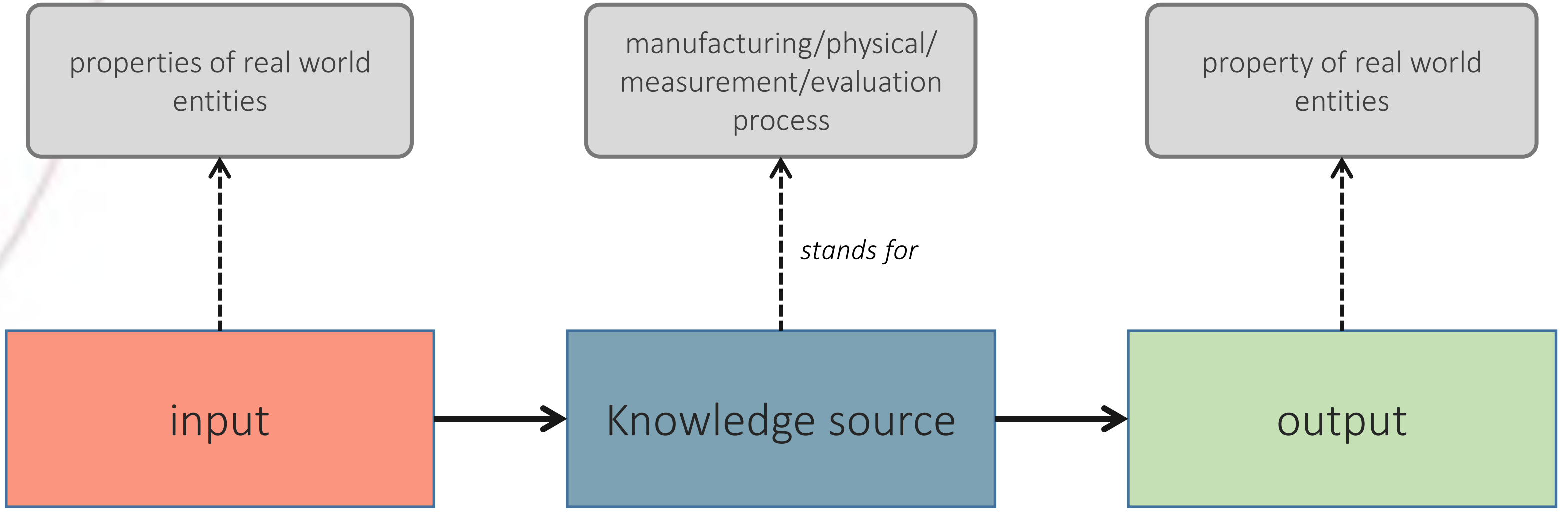
Workflows describe how **properties** are obtained by means of **tools** (e.g. simulation software) or **methodologies** (e.g. measurement).



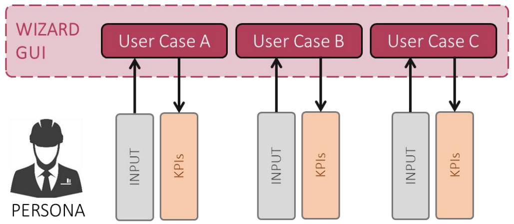
Wokflows are made of a connected **sequence** of **knowledge sources** (e.g. models, databases, experiment).

A knowledge source **stands for** (i.e. substitute, act as, predict the outcome of) a real process.

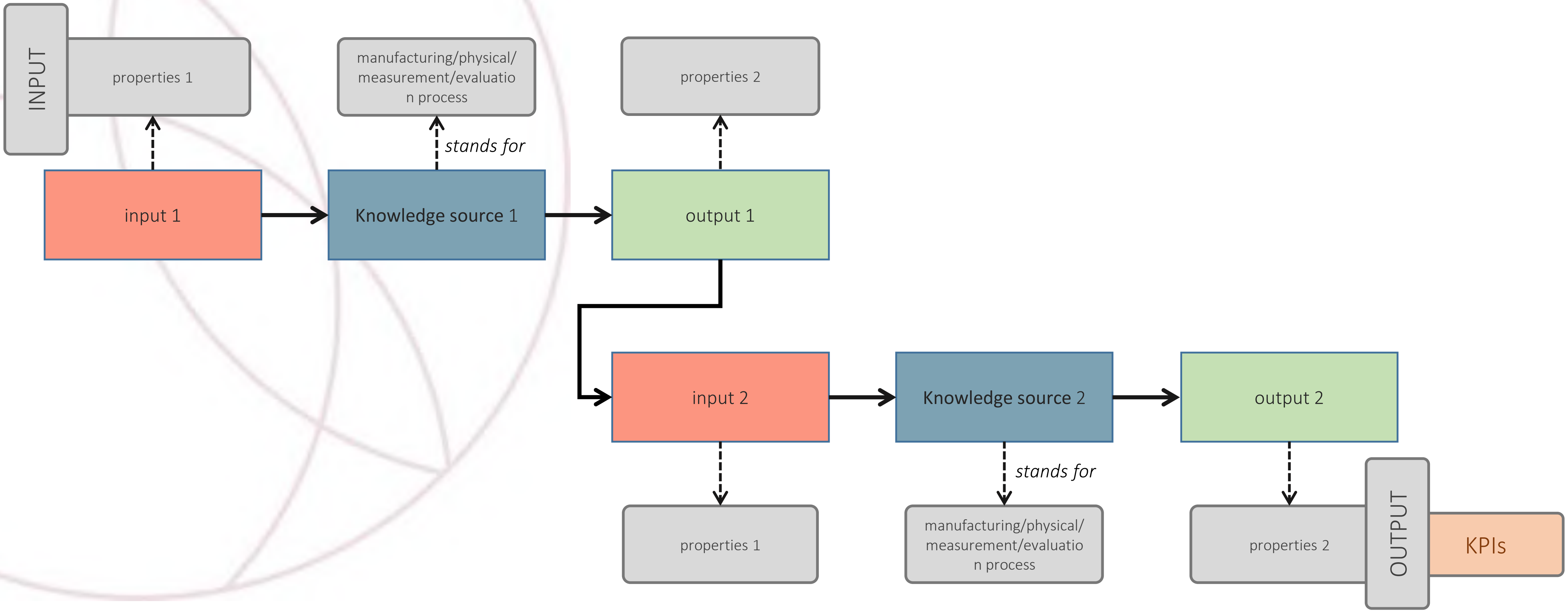
Workflows must be represented using **MODA-like** graphs, and refers in each step the real world properties and real world processes of the user case



Workflows



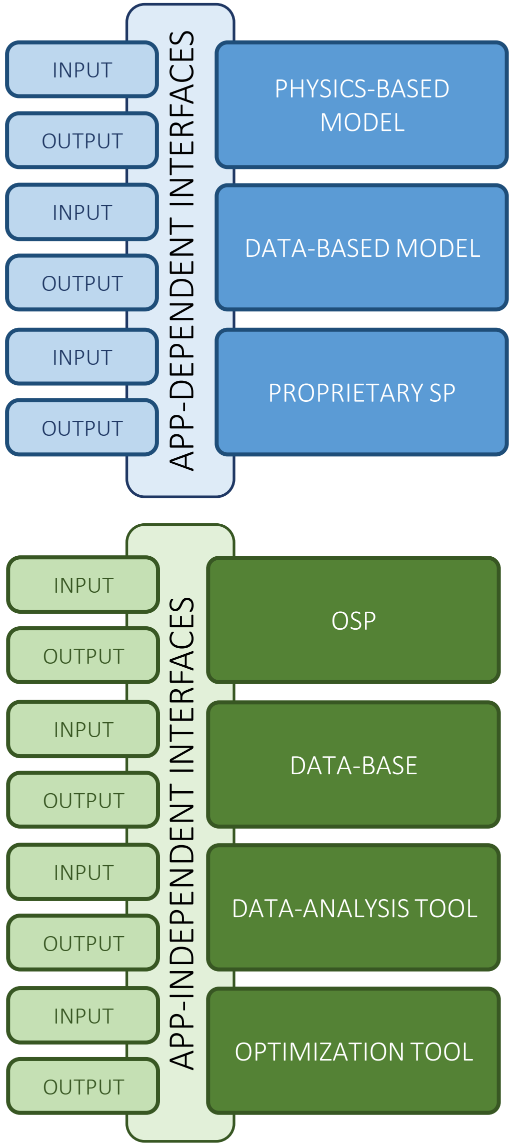
Build one or more potential data workflow connecting data representing properties of real world entities part of the user case



Knowledge Sources

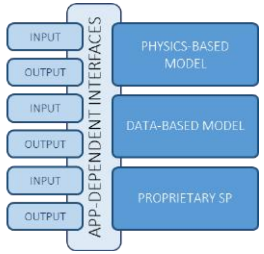
- Knowledge Sources potentially needed by each User Case to build Workflows must be listed, together with the expected Input/Output to facilitate interface design
  i.e. what I need to provide to the tool (input) in order for it to provide me an answer (output)

- The software that provides Models used in the MODA workflow must be listed and categorized in order to build the necessary interfaces, together with the expected data stream between the OTE and the software



The interfaces are not intended to run complex software (e.g. ANSYS) exploiting all their capabilities (they would grow too complex), but they are tailored towards specific problems setup (e.g. monospecies laminar flow).

Knowledge Sources

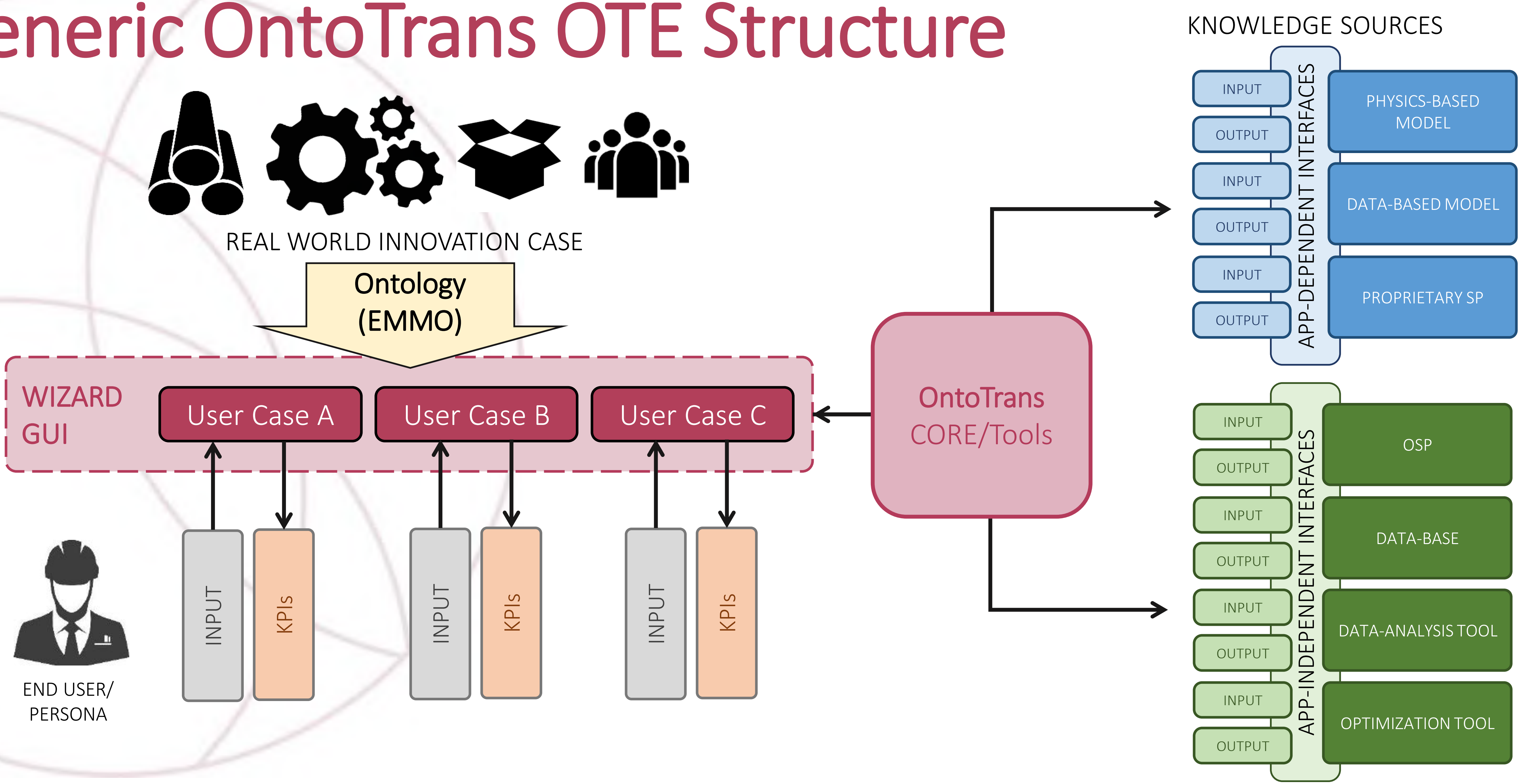


For each Knowledge Source we need to know details about I/O and expected usage by the OTE

Name	*Name of the Knowledge Source*
Type	*Software, Database, Proprietary Workflow Manager,…*
Refers to	*A manufacturing step, a physical process, a customer evaluation, …*
App-Dependent or Independent	…
License	…
Static/Dynamic	*Run internally by the OTE or externally by the user*
Digitalization Status	*Digitalization status of the knowledge source (e.g. raw data on paper, consumer opinions not yet collected, technical knowledge in the form of human skill or experience). Highlight the level of human intervention for data collection and interpretation.*
…	…

I/O	Property	DataType
INPUT		*e.g. STEP file*
		e.g. SQL query
		e.g. custom P&G XML format
OUTPUT		*e.g. VTK data file*

Generic OntoTrans OTE Structure

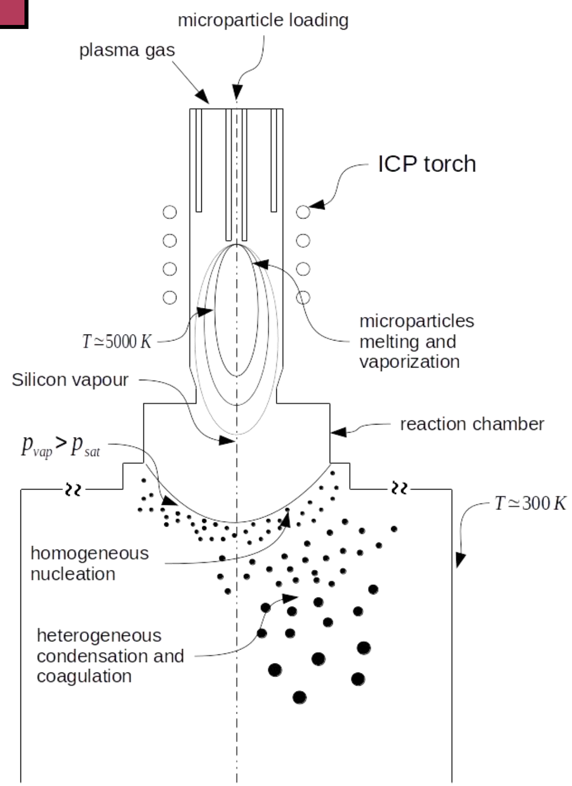


Generic Example

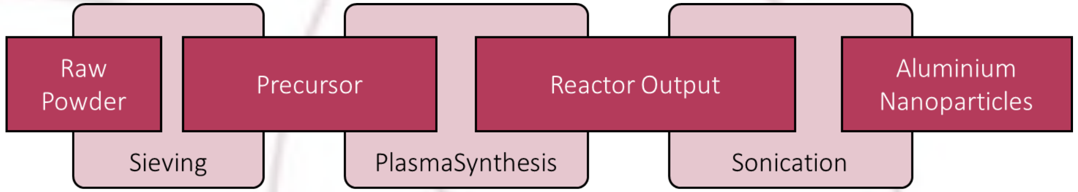
Raw Powder → Sieving → Precursor → PlasmaSynthesis → Reactor Output → Sonication → Aluminium Nanoparticles

Object	Description
Raw Powder	*Micrometric aluminium particles*
Precursor	*Size controlled aluminium particles*
Reactor Output	*Aluminium nanoparticles aggregates coming from the reactor*
Final Product	*Sonicated aluminium nanoparticles*

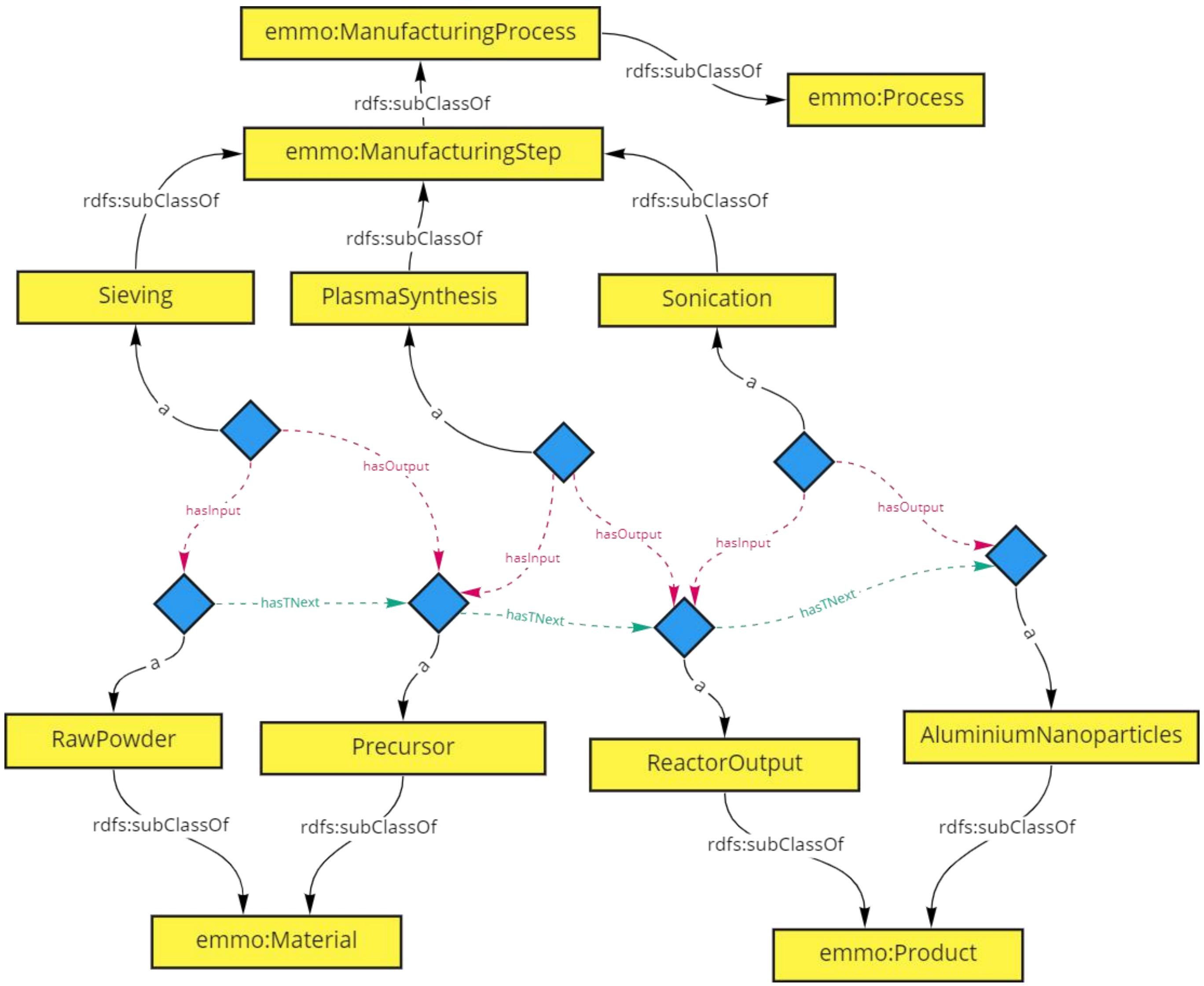
Process	Description
Sieving	*The process of selecting particles according to…*
Plasma Synthesis	*Vaporisation of materials through a plasma reactor for …*
Sonication	*Application of sound energy to break nanoparticles aggregates into smaller…*



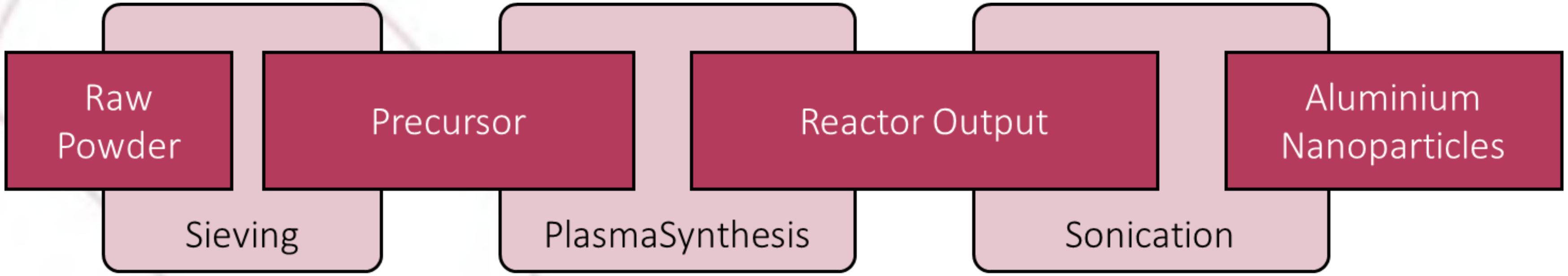
Generic Example



An **ontology-like representation** can be provided to link the concepts developed in the innovation case with the EMMO higher level concepts, and to draw the **boundary between T-Box and A-Box**.

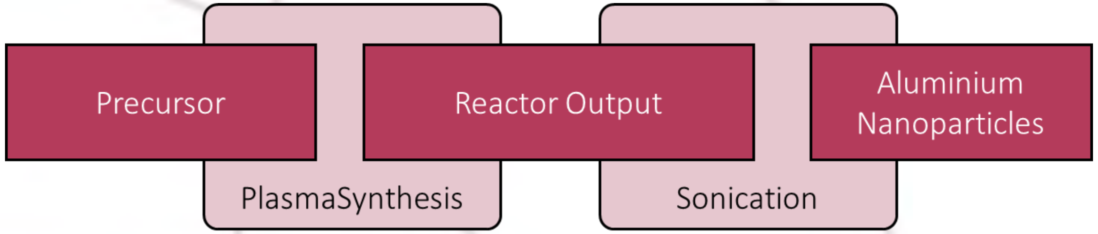


Generic Example



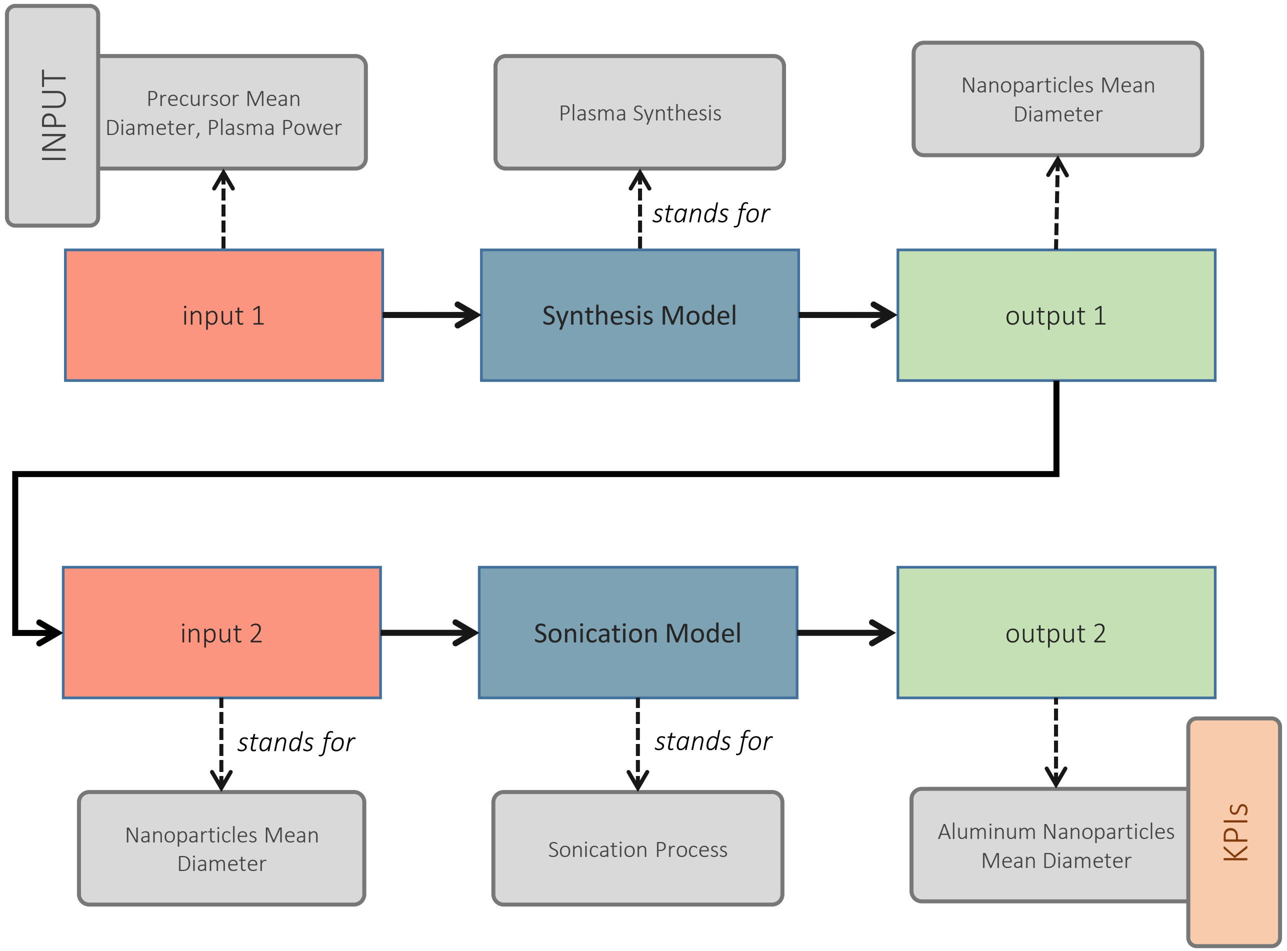
Entity	Property Names	Property Description (semantics)	Data Description (symbolic)				Potential Interpreters			
			Data Type	Data Range	Units	Reference Physical Quantity	Measured by	Modelled by	Assigned by	Other
Raw Powder	Powder's mean diameter	The mean diameter of powder's particles.	Real scalar	Positive	m	Diameter	-	-	Seller	-
	Powder's Price	The mass price of the powders	Real scalar	Positive	€/kg	Price per kg	-	-	Seller	-
Reactor Output	Nanoparticles mean diameter	The mean diameter of nanoparticles collected after the synthesis.	Real scalar	Positive	m	Diameter	Internal Lab	Synthesis Model	-	-
Aluminium Nanoparticles	Aluminum nanoparticles mean diameter	The mean diameter of nanoparticles collected after the sonication.	Real scalar	Positive	m	Diameter	Internal Lab	Sonication Model	-	
Plasma Synthesis	Treatment time	The process time.	Real Scalar	Positive	s	Time	Device Timer	-	-	
	Plasma Power	The power of the plasma torch in the reactor.	Real Scalar	Positive	W	Power	Reactor instrumentation	-	Operator	
Sonication	Sonication power	The power of the sonicator.	Real Scalar	Positive	W	Power	Sonicator instrumentation	Sonication ML model	Operator	

Generic Example

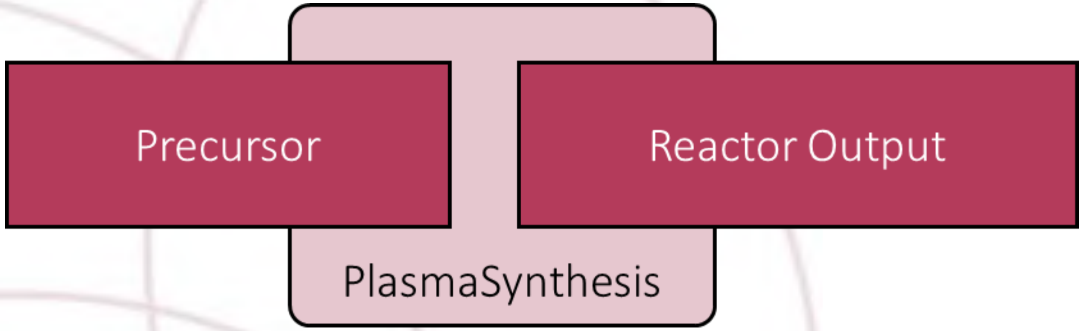


Innovation Challenge:
Produce Al nanoparticles of selected diameter

KPI:
Al nanoparticles mean diameter

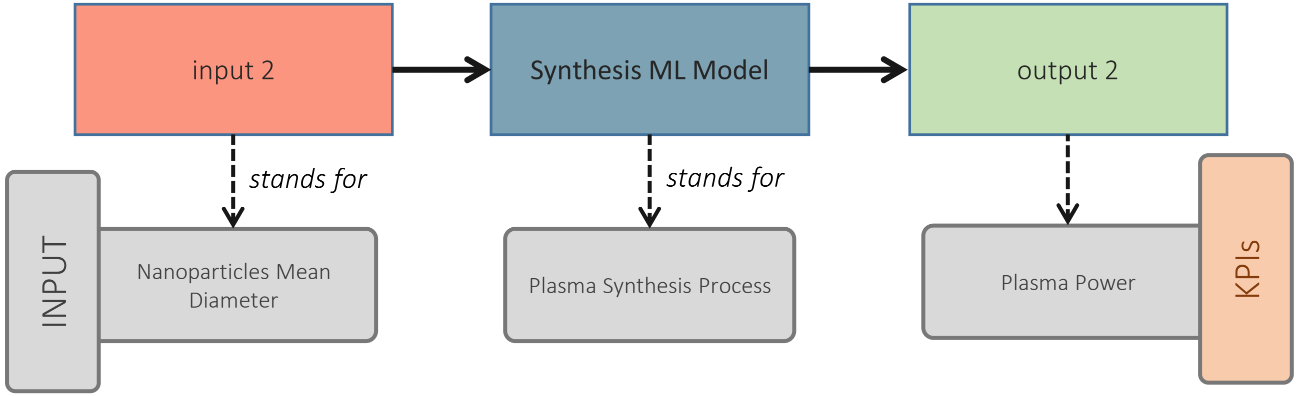


Generic Example



Innovation Challenge:
Produce Al nanoparticles of selected diameter

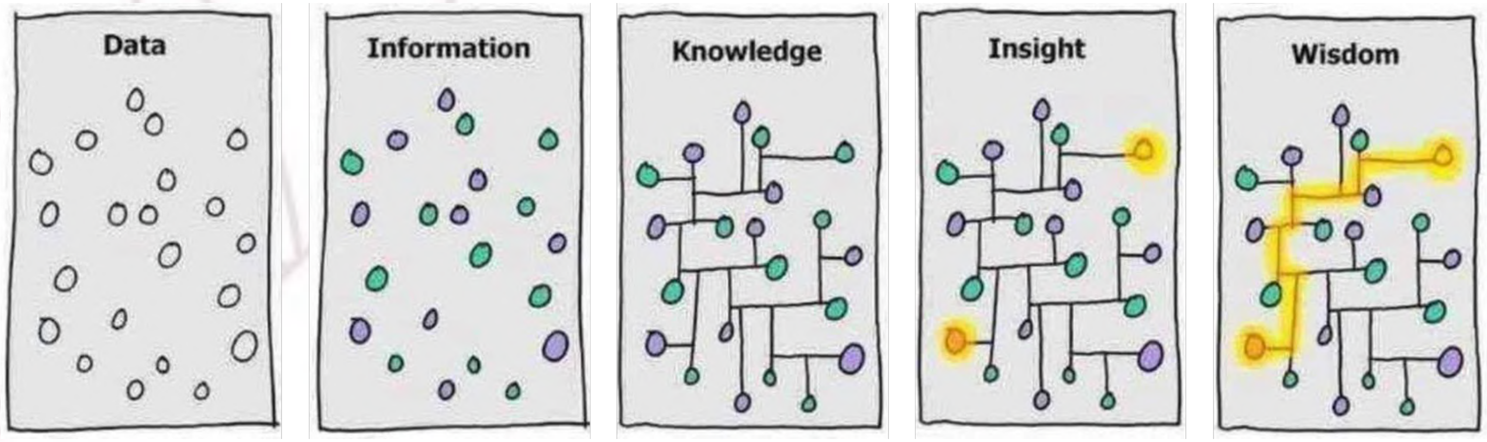
KPI:
Plasma Power (e.g. the focus in on minimising process power)



In Layman Terms…

The ontology is expected to represent, to document and to connect together:

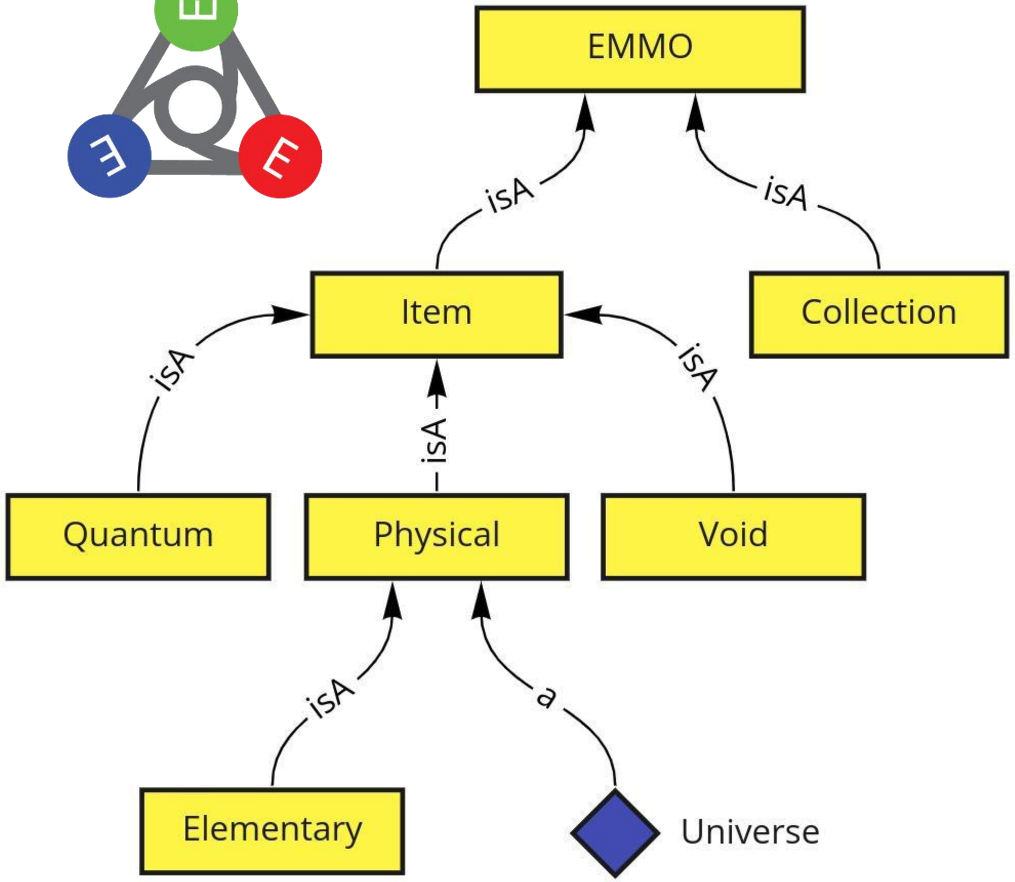
- the **innovation** and **user case** (i.e. the things: object and processes)
- their **properties** (i.e. the data that describes the things)
- the **tools** used to generate (e.g. models, characterisation) or retrieve (e.g. databases) the required properties (i.e. the knowledge sources)
- the **data workflow** used to generate the desired properties (i.e. the KPIs)



EMMO

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.

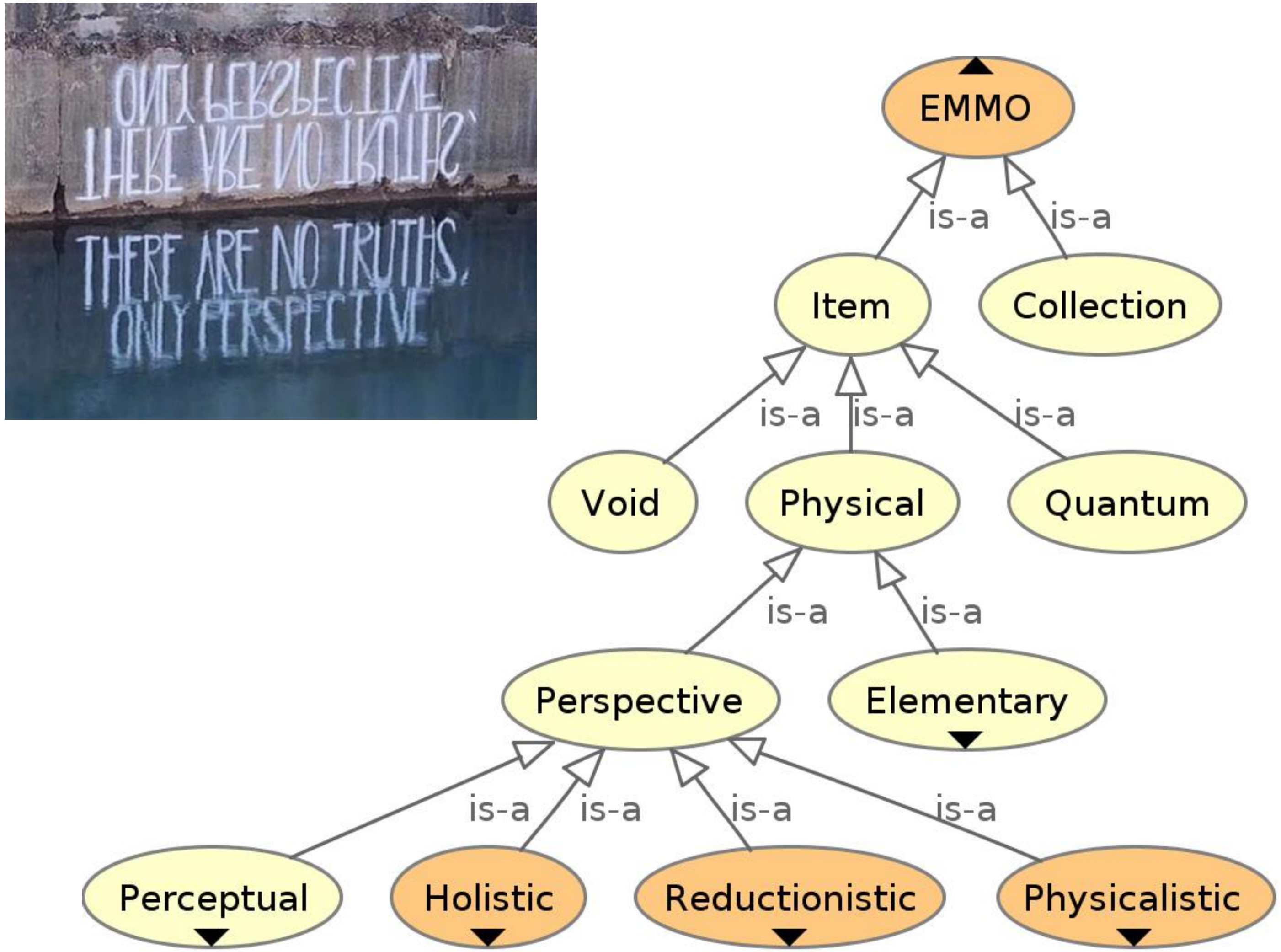


EMMO

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.

http://emmo.info



Conclusions

- The use of ontologies as **human-to-machine** and **machine-to-human** interfaces requires an approach that facilitates the participation of industrial users in the **conceptualisation step** (i.e. OntoTrans template)
- **Human Translators** are needed to guide the industrial users and formalise the user case in ontological form.
- The EMMO is used to build ontology modules to represent all the steps of Innovation Case to **design**, **execution** and **documentation**.
- Ontological representation is used to populate a **knowledge base (OntoKB)** that can be navigated by agents to harvest existing data, or used as training set for AI approaches towards **automated decision making** or **workflow design**.

Thank you!

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