EMMO

AN ONTOLOGY FOR PHYSICAL SCIENCES

Emanuele Ghedini

University of Bologna

ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

Gerhard Goldbeck
Goldbeck Consulting

Georg Schmitz
ACCESS

Adham Hashibon
Fraunhofer IWM

Jesper Friis
SINTEF

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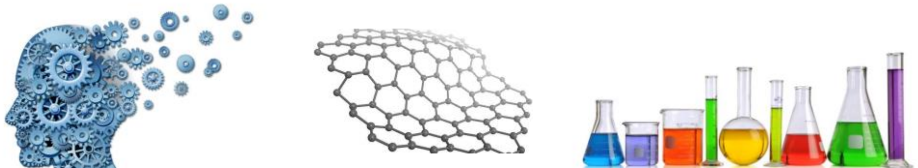
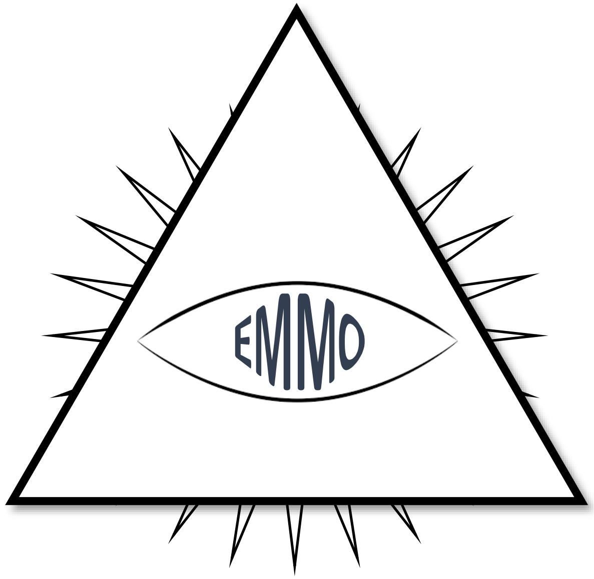
What is the EMMO?

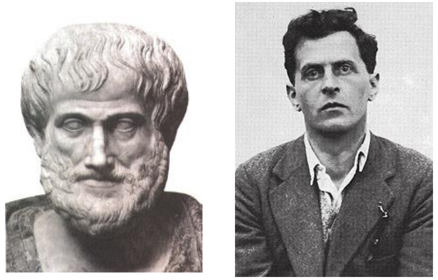
The **EMMO** is a multidisciplinary efforts within the **EMMC** and a **network of H2020 projects** aimed to the development of a **standard representational framework**, in the form of an **ontology**, based on current **materials modelling and characterization knowledge**.



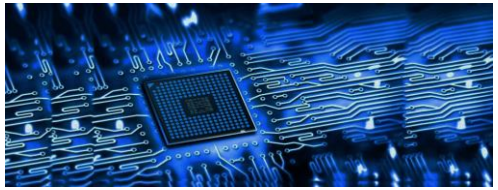
Physical Sciences
(e.g. physics, chemistry, material science, engineering)



European
Materials
Modelling
Ontology



Analytical Philosophy
(e.g. mereotopology, semiotics, logic)



Information and Communication Technologies
(e.g. reasoners, platforms, formats)

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WHAT IS THE EMMO?

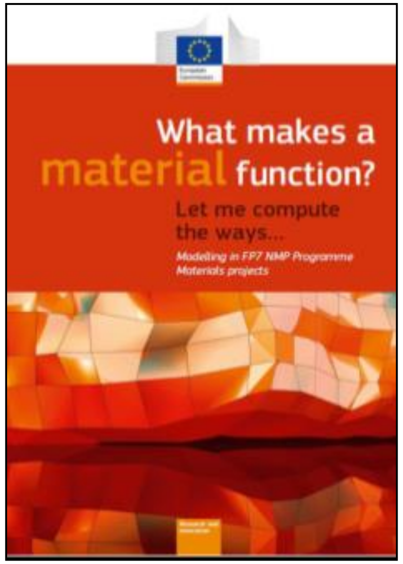
The **EMMO** aims to facilitate the work of **materials experts** in **connecting stakeholders** in the field of **materials development** and **characterization**, making use of the **standardization efforts** already performed within the EU, and facilitating the development of **materials modelling software tools (i.e. OSP).**

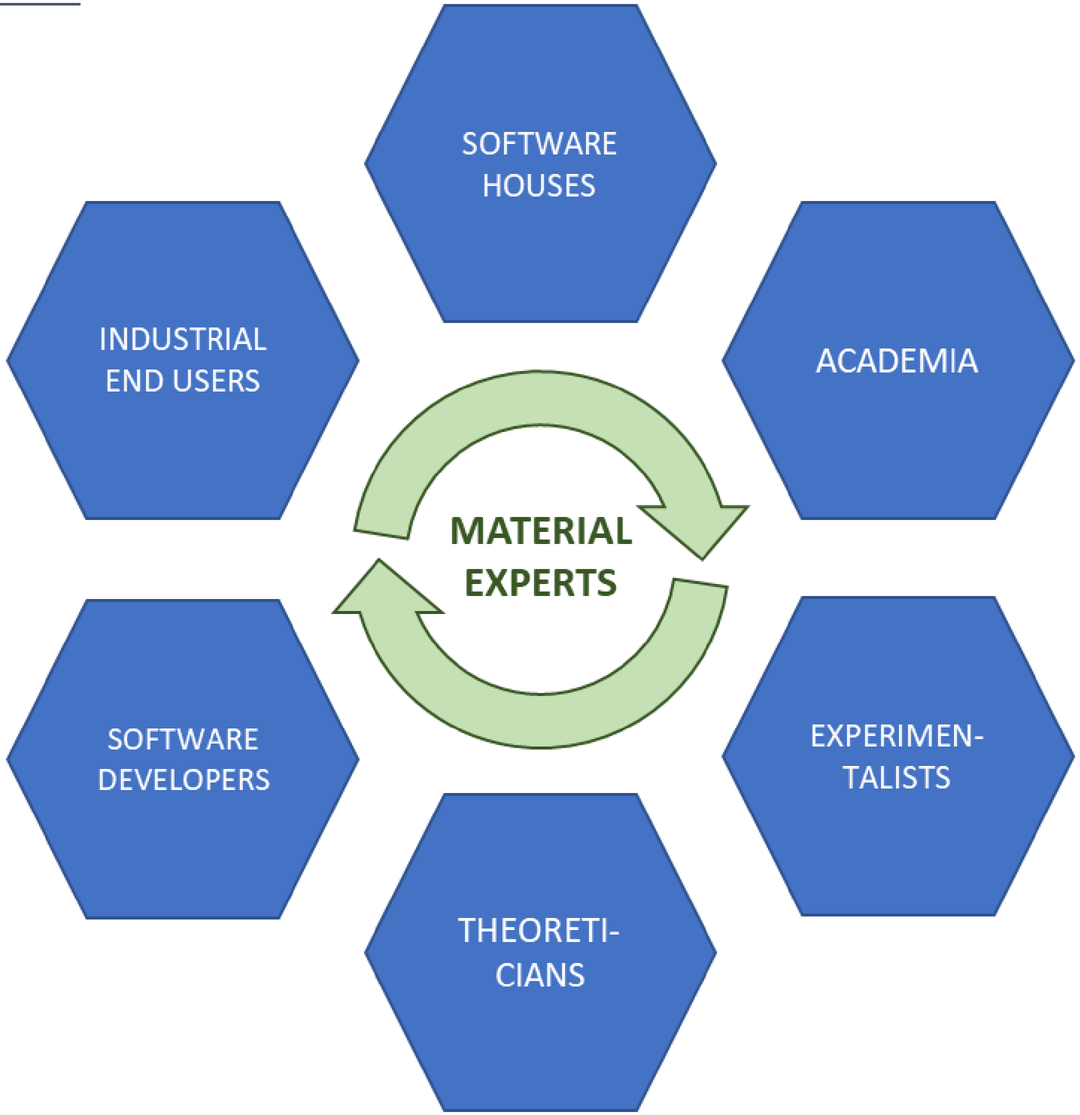
CEN WORKSHOP AGREEMENT

CWA 17284

April 2018

Materials modelling – Terminology, classification and metadata





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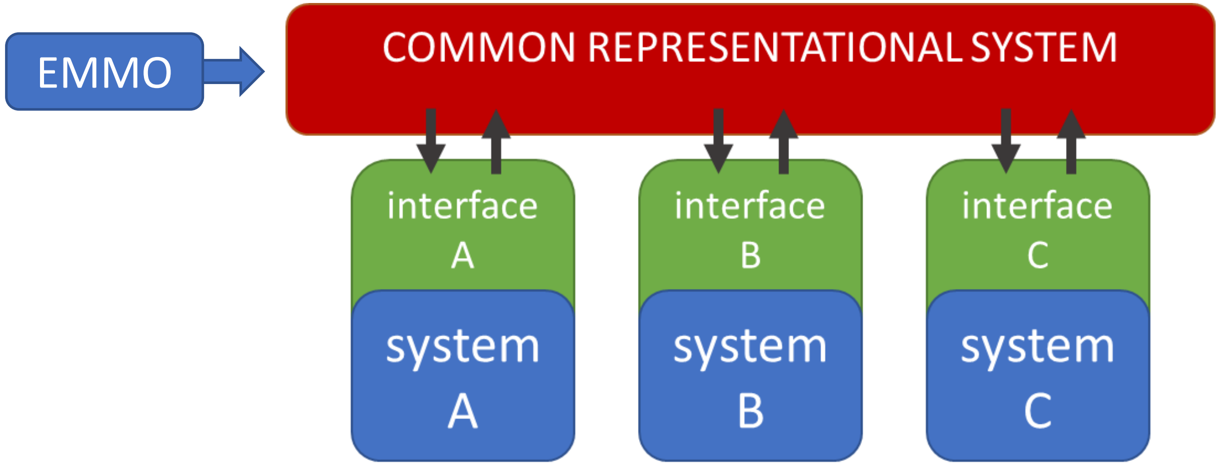
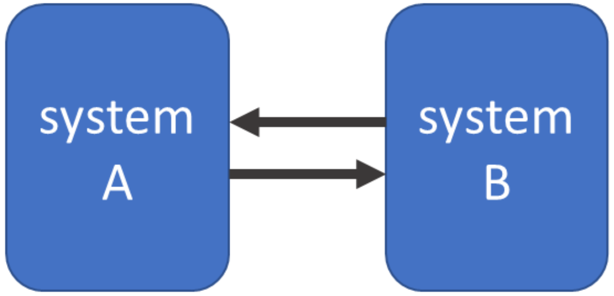
What is the EMMO?

We define **interoperability** (from latin, *inter* = between and *operari* = to work) as the ability of two or more systems to exchange information between them through a <u>common representational system</u>

We define **compatibility** (from latin, *cum* = with and *passus* = to suffer) as the ability of two or more systems to establish a <u>one-to-one connection</u> between them





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What is the EMMO?

The common representation system and the interfaces constitute an **interoperability environment** (a.k.a. **framework**, **platform**) that can be used by different systems to establish a connection between them to exchange information

The EMMO will provide a **dictionary of standardised concepts and relations** that can be the basis for the interoperability at each of the levels

SEMANTIC INTEROPERABILITY LEVELS

- Scientific community: common language: MODA/CWA, Ontology
- Materials User Case: Ontology based on mereotopology
- Materials Modelling
- Numerical level (e.g. solvers, discretization methods)

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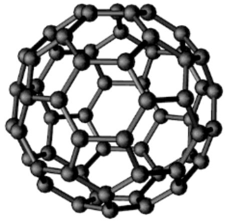
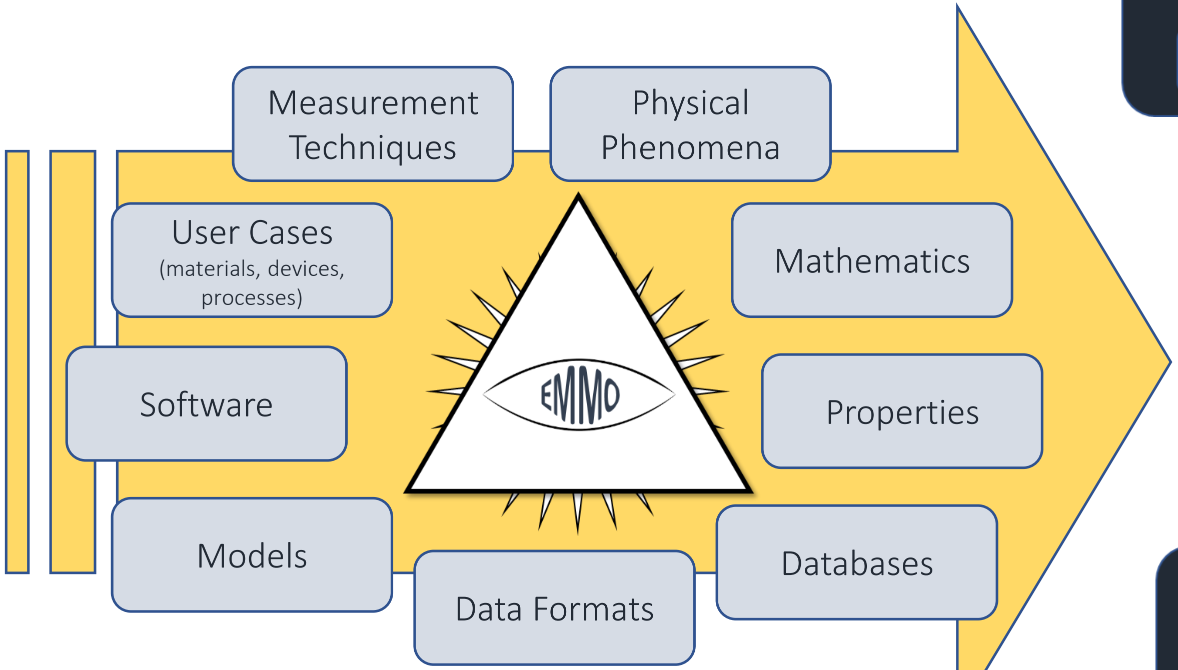
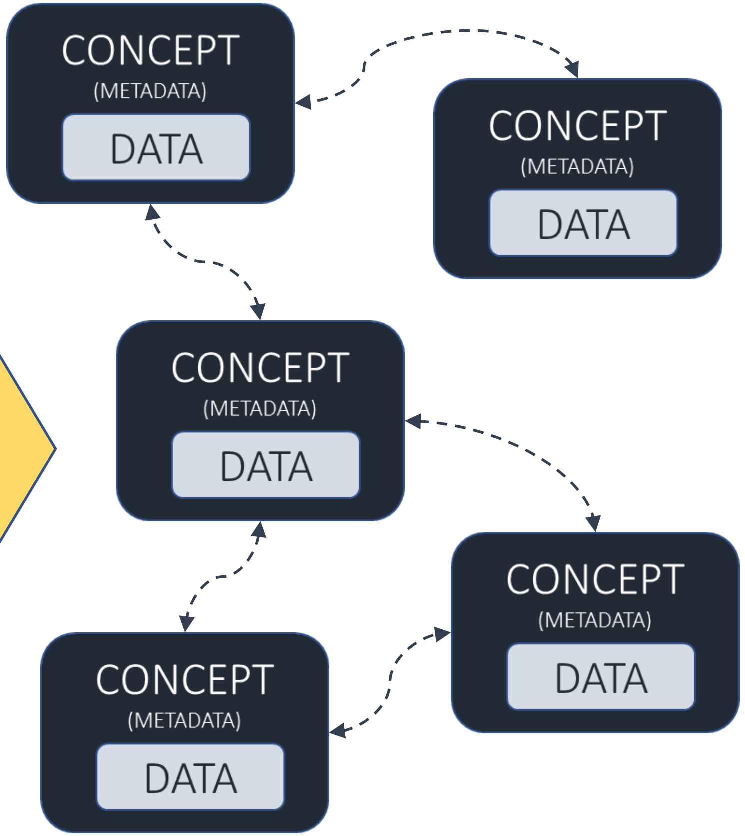
What is the EMMO?







USER CASE
From real world entities…

ONTOLOGY
…trough a formal knowledge-based representational system…

INFORMATION
…to a digital representation.

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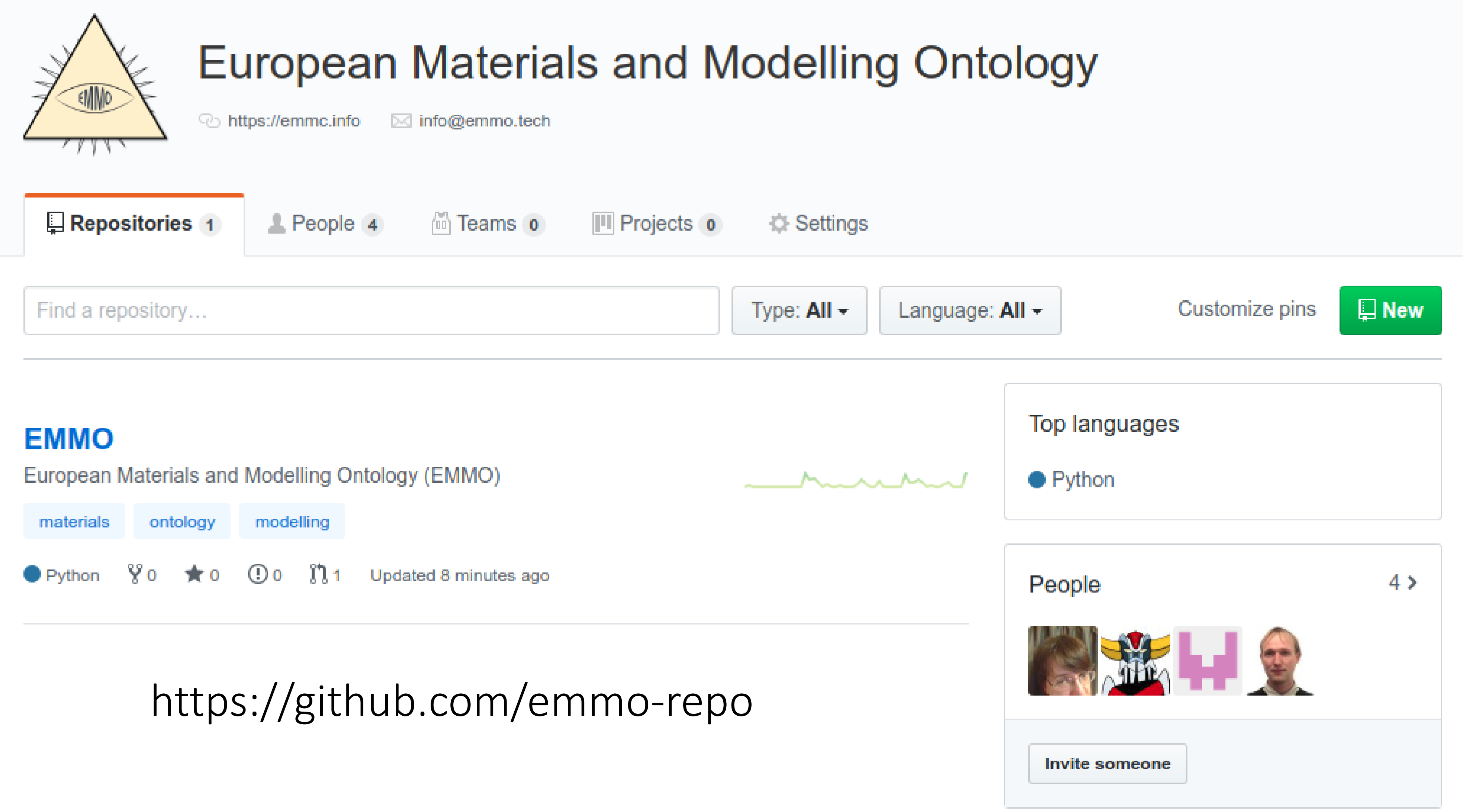
Where is the EMMO?



https://github.com/emmo-repo

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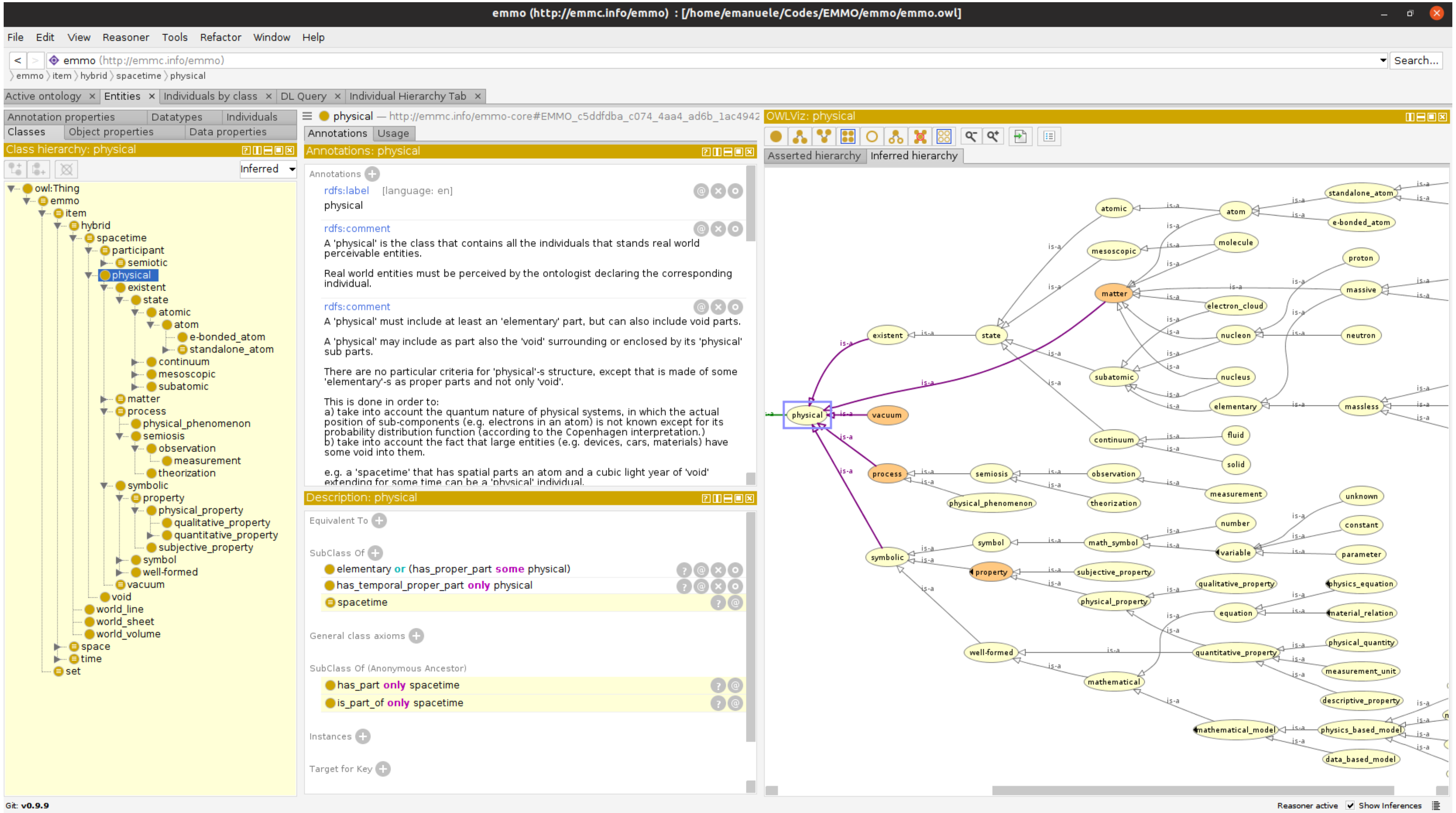
How to work with the EMMO?

https://protege.stanford.edu/



FaCT++ reasoner doesn't work on 5.5.0

Use HermiT (unable to deal with the full axiomatization) or downgrade to 5.2.0

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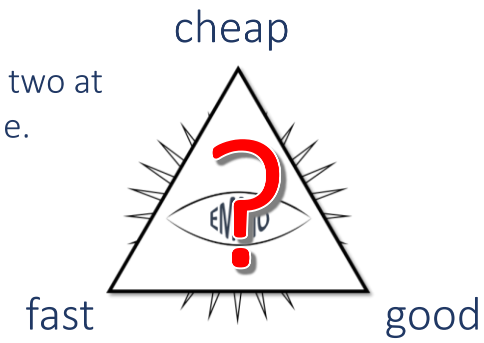
What do you want from EMMO?

- To be an **effective representational tool** to express **my view of the world** (it implies that you have already a well defined view of the world): everybody will be happy but confined in its fields…
- To provide a **pre-defined view of the world** by some domain experts and a way to represent it: everybody will be unhappy…
- To be **accurate** almost to the limit of the mathematical detail level: a lot of complexity in reasoning and maintenance…
- To be **interoperable** with other existing ontologies (mapping) and standards: design compromises…
- To have an ontology with optimized **tools** for usage and development
- …

Good answers come only from good questions.

You can have only two at the same time.



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What EMMO Can Potentially Offer

The EMMO aims to be a **generic representational tool** for people that are used to a **physics-based perspective**, i.e. people dealing with things like experimental measurements, physical equations, CFD, molecular dynamics, product. This is the **EMMO-CORE** and related fundamental modules, e.g. semiotics, properties, models.

The EMMO will provide selectable **domain specific modules** (that may or may not coexist) with **predefined structured knowledge** to facilitate ontologization of real world objects, e.g. materials, manufacturing processes, simulations, measurements.

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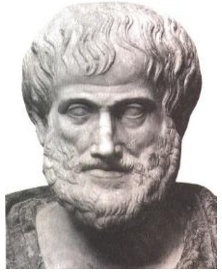
WHY NOT USE EXISTING ONTOLOGIES?

Believe us: we tried to!!!

WARNING!!!
potential oversimplifications

Philosophical approach



Knowledge first and then real world application must be represented according to the ontological framework (e.g. DOLCE, BFO)

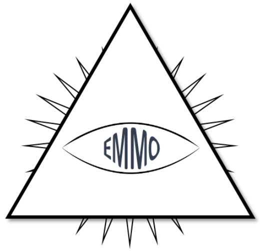
Pragmatic approach

Isolate a small knowledge region and develop an ontology just for this region (e.g. GENE, CHEBI)

EMMO approach

Knowledge is based on an already existing and very successful ontology: physics!

Expressed by physicalism, reductionism, nominalism, pluralism and all the most despicable things you can find in philosophy.



The EMMO does not pretend to be the best approach, but just one that comes from an applied scientific community as the EMMC

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EMMO APPLICATION FIELDS

Science
standard reference concepts to facilitate understanding between scientific communities (multi-disciplinarity)

AI
formalized knowledge system ready to be used in AI applications

Modelling
connections between real world entities and available physical models (OSP, translation) at different scales

BigData
data schematics for specific applications and facilitate semantic extraction for data harvesting

Characterization
formalization of the entity-measurement-property connection to facilitate data exchange between experimentalists and modellers

Industry
formalization of the manufacturing process and product, connection with material databases and modelling software to facilitate business decisions

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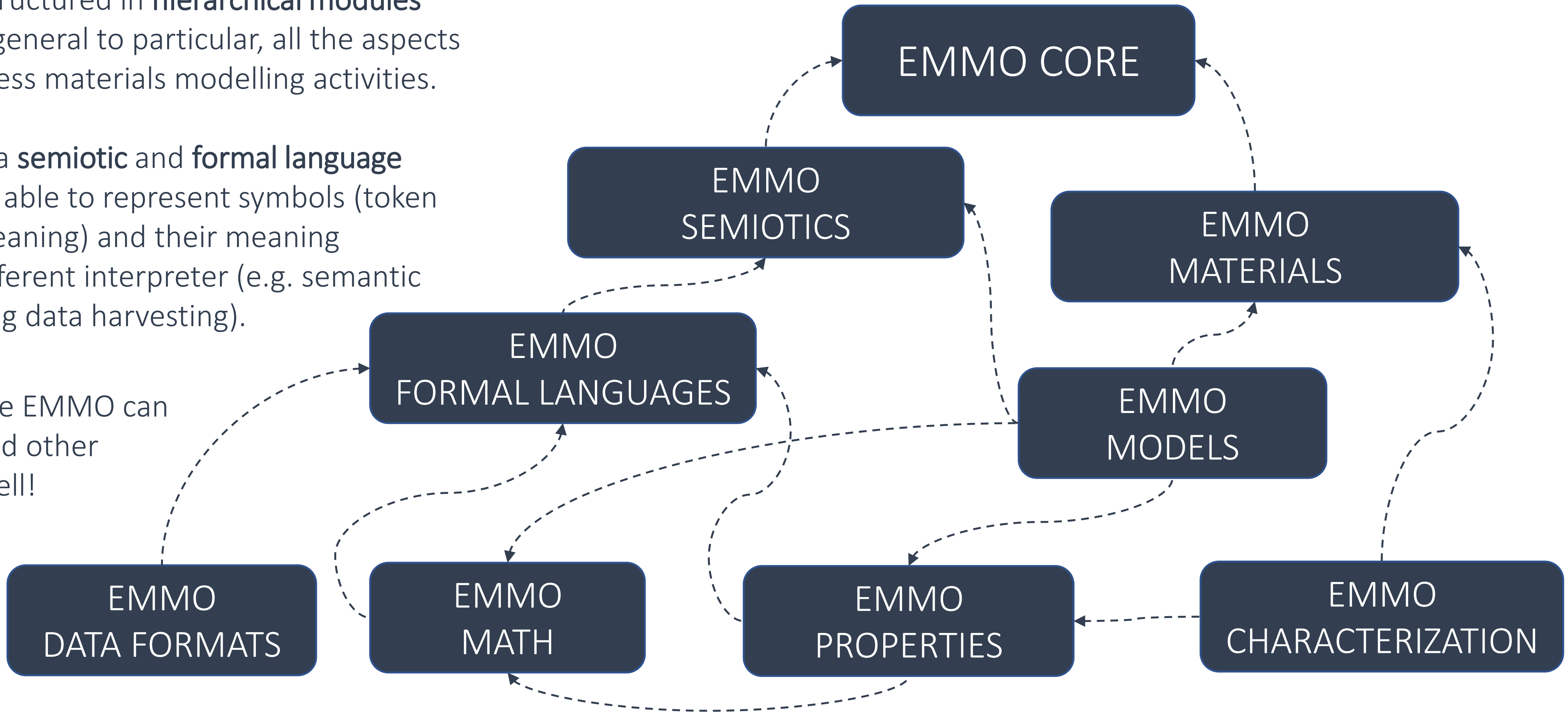
EMMO STRUCTURE

The **EMMO** is structured in **hierarchical modules** covering, from general to particular, all the aspects needed to address materials modelling activities.

It includes also a **semiotic** and **formal language** branches, to be able to represent symbols (token that have no meaning) and their meaning according to different interpreter (e.g. semantic extraction during data harvesting).

In this sense, the EMMO can contain itself and other ontologies as well!



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Basic Definitions - 1

An **ontology** is a way for a user to precisely represent **a specific part of the real world**, called the **domain of interest**, using a **common representational language**, so that the knowledge about the domain of interest can be understood and shared between users able to understand that specific language.

Typically, an ontology describes:

- what a **real world object** is in terms of categories by using classes,
- what are the **relations** between real world objects,
- **standard symbols** for the representation of real world objects.

SPACETIME-BASED ONTOLOGY

Real world objects can be preliminary informally defined as the things that we perceive (i.e. we can interact with) in our everyday experience, and are always intended to be **within space and time**. This definition restricts what is real to what can be experienced by the user in terms of **spacetime event**.

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BASIC DEFINITIONS - 2

A real world object falls under one of the following two categories:

- what is commonly referred to as **physical object**, i.e. something that can interact with the user (acting as an observer) through a physical interaction, that comprises both matter and energy
- **non-physical objects**, in the sense of empty regions of space (i.e. voids).

The concept of reality includes also non-physical object as **empty portion of spacetime**, due to the fact that the space domain of a non-physical object could potentially host a physical object.

The **real world** is then the domain of real world objects, being them **physical** (i.e. matter or energy) or **non-physical** (i.e. void regions). The real world in its entirety is what is commonly referred to as the **Universe**, the largest spacetime region that comprises everything that exists.

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Basic Definitions - 3

The **process of representing real world objects through an ontology** (or generally through any knowledge representation mean) naturally draws a clear distinction between three elements:

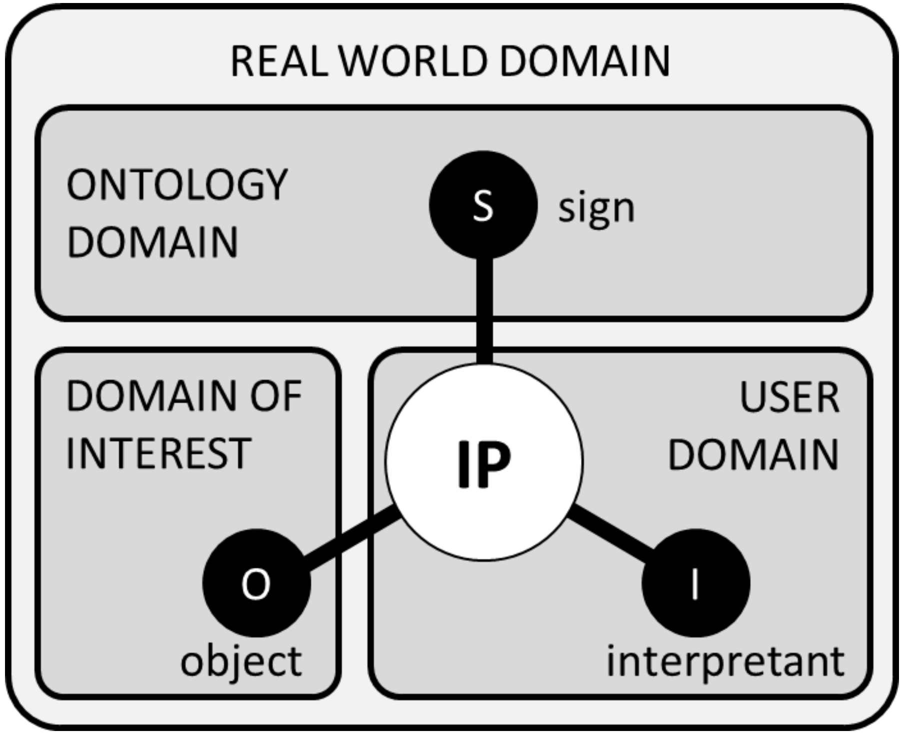
- what is represented, i.e. the real world objects and their interdependencies
- the sign used for building the representation, i.e. the ontology as a formal set of entities, axioms and expressions
- the agent that declares the ontology as a sign that stands for something else, according to its own subjective perspective.

Following the Peirce taxonomy, the **semiotic process** (or **semiosis**) is a triadic relation that involves:

- a **sign**, something that stands for something else
- an **object**, something to which a sign refers
- an **interpretant**, another sign determined or created by the first one

The **interpreter** is the agent of this triadic process, providing the connections between the three elements of the semiotic process. The interpretant is the interpreter's internal representation of the object, which can also itself act as a sign for further interpretations.

Charles S. Peirce
semiotic theory



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BASIC DEFINITIONS - 4

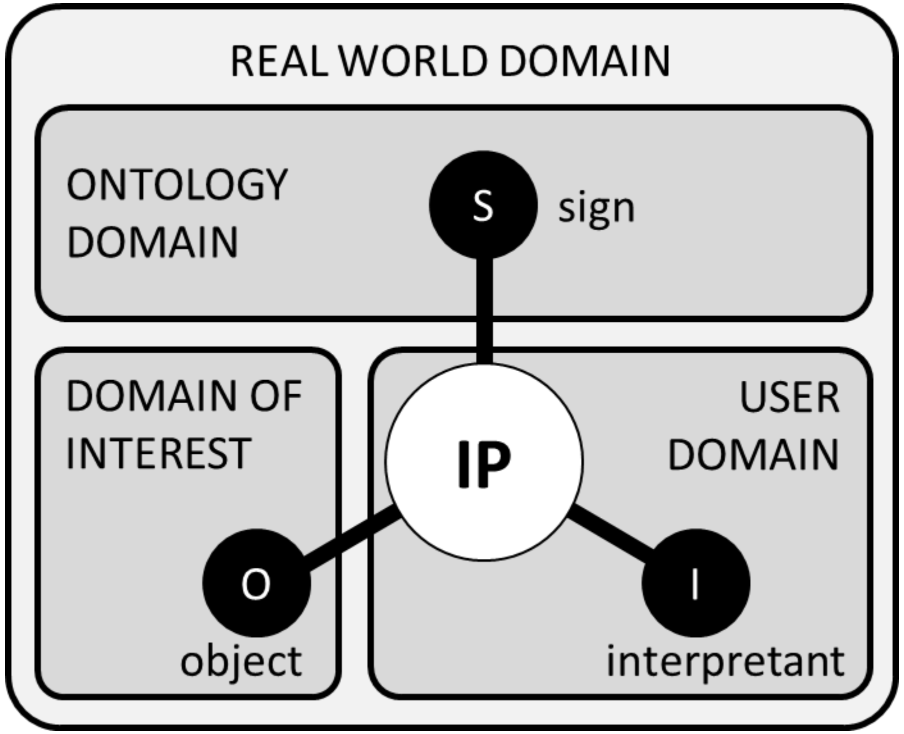
Charles S. Peirce
semiotic theory

The figure is based on the assumption that:

- the ontology domain, the domain of interest and the user domain **do not intersect**, e.g. that an ontology sign cannot be used to represent another ontology sign or its interpreter.
- the semiotic process **is totally included within the real world**.

In this work we will use extensively the terminology coming from Peirce taxonomy. In particular**, the term `object' is used here to denote what is, or can be, represented by a sign for a given interpreter**.

The counterintuitive definition of a void region as an object comes from this approach. In fact, it is possible to provide signs for regions that host no physical object but can potentially host them (e.g. the void space within a chemical reactor or between atoms in a material).



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Developing a Common Background Language

The most important part of an ontology is what lays outside (or before) the ontology!

"6.41 - The ***sense of the world must lie outside the world****. In the world everything is as it is and happens as it does happen.* ***In it there is no value****—and if there were, it would be of no value. If there is a value which is of value, it must lie outside all happening and being-so.*

…

6.45 - The contemplation of the world ***sub specie aeterni*** *is its contemplation as a* ***limited whole****. The feeling of the world as a limited whole is the* ***mystical feeling****."*

Ludwig Wittgenstein, *Tractatus Logico Philosophicus*

Without a shared background all ontology interpreters, i.e. the developers and the users, will not be able to understand and use the ontology itself, for any purpose.

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Physicalism

For the EMMO the semiotic process and its participants are fully enclosed in the real world domain. This implies that the system of signs used for the representation of a real world object is **made itself of real world objects**, i.e. it is **a part of the world used to represent another part of the world**.

The **restriction of the semiotic process completely within the real world** can be considered as a sort of **physicalism**, in which **everything that exists falls under the category of real world objects**, i.e. spacetime regions. Unlike the common conception of physicalism, reality for the EMMO is not restricted only to matter or energy (here addressed as physicals) but also to the empty regions that hosts no elementary particles (non-physicals).

Three important considerations can then be drawn from this physicalist assumption, helping to clarify the limits and the scope of an ontology under a semiotic perspective:

- First, **a sign is totally distinct with respect to the object for which it stands for.** As obvious as it may seem, neglecting this simple fact can lead to formally incorrect statements in which a sign is said to be the object, instead of standing for it, leading to a confused terminology that can slow down or compromise the process of interpretation of an ontology.
- Second, **the interpreter is an independent entity with respect to the sign**. This means that an ontology can help users (i.e. interpreters) by providing them a way to formalize and communicate their interpretations but is not itself an automatic connection between real world domain and the ontological domain. The ontology as such tells you nothing about the existence of the object that stands for the sign, or the correctness of this semiotic relation, since it is responsibility of the interpreter to provide the connection between the ontology and the real world objects.
- Third, an ontology, besides the definitions of its internal entities and axioms using a formal language, must provide also **meta-ontological descriptions** (e.g. annotations), in a language understandable by other potential interpreters, to enable them (e.g. the general users) to draw the connections between signs in the ontology domain to real world objects, i.e. define to what type of real world objects a specific class of sign stands for.

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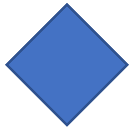
What EMMO is and what is not - 1

ONTOLOGY WORLD

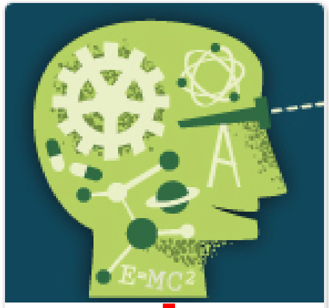
SIGN

a physical entity that stands for another physical entity

(an icon, a digital twin, a symbol, a word, a C++ class)



USER WORLD



INTERPRETER

a human being or a machine that can recognize object attributes (e.g. color, shape)

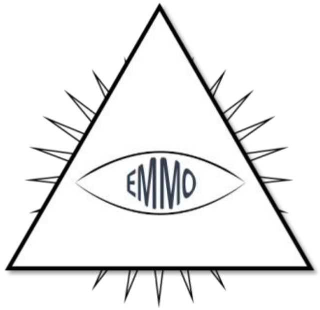
INTERPRETANT

the mental/internal <u>representation</u> determined by a sign or an object (interpreter dependent)

PHYSICAL WORLD

OBJECT

any physical entity



EMMO <u>is</u> a formalized system of signs (representation)

The **EMMO** helps users (interpreters) providing them a way to communicate their interpretations but <u>is not</u> itself an automatic connection between real and ontological world.

(Dear user, you can lie about what you see, so you responsibilities!!!) have great

While any system of signs is made of physicals that stand for other physical, it is clear that the object of interpretation <u>is not</u> and <u>is not part</u> of the **EMMO**

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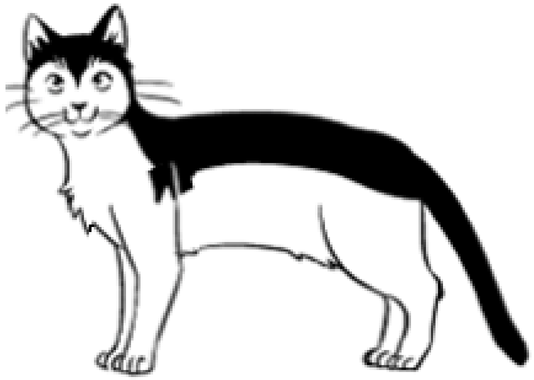
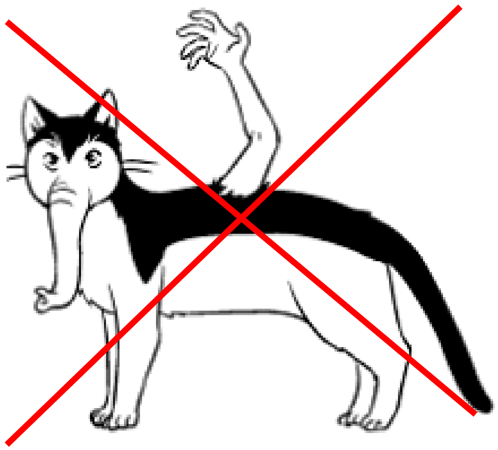
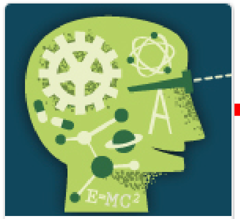
What EMMO is and what is not - 2

The **EMMO** helps you to provide **sign**s that represents correctly what a real world entity is, using formal logic.



The **EMMO** prevents you from giving unrealistic representations of real world entities.





The **EMMO** tells you nothing about the existence of the **object** that stands for the **sign**. Is up to the **interpreter** to connect ontology world to real entities world.

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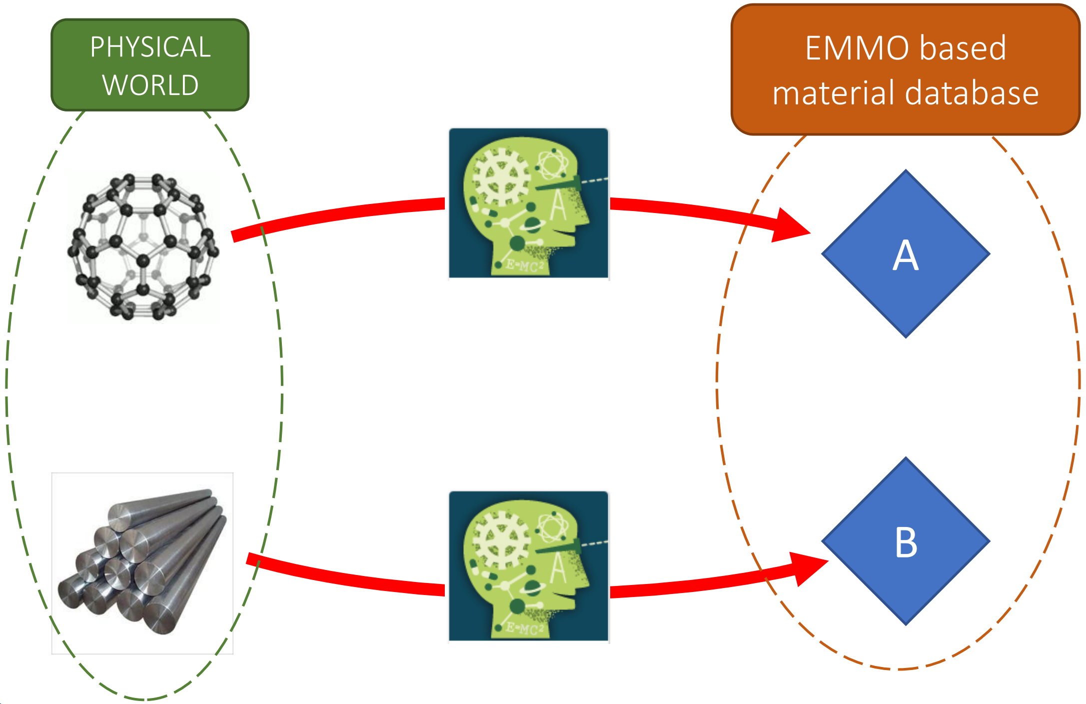
EMMO GENERAL USAGE EXAMPLES

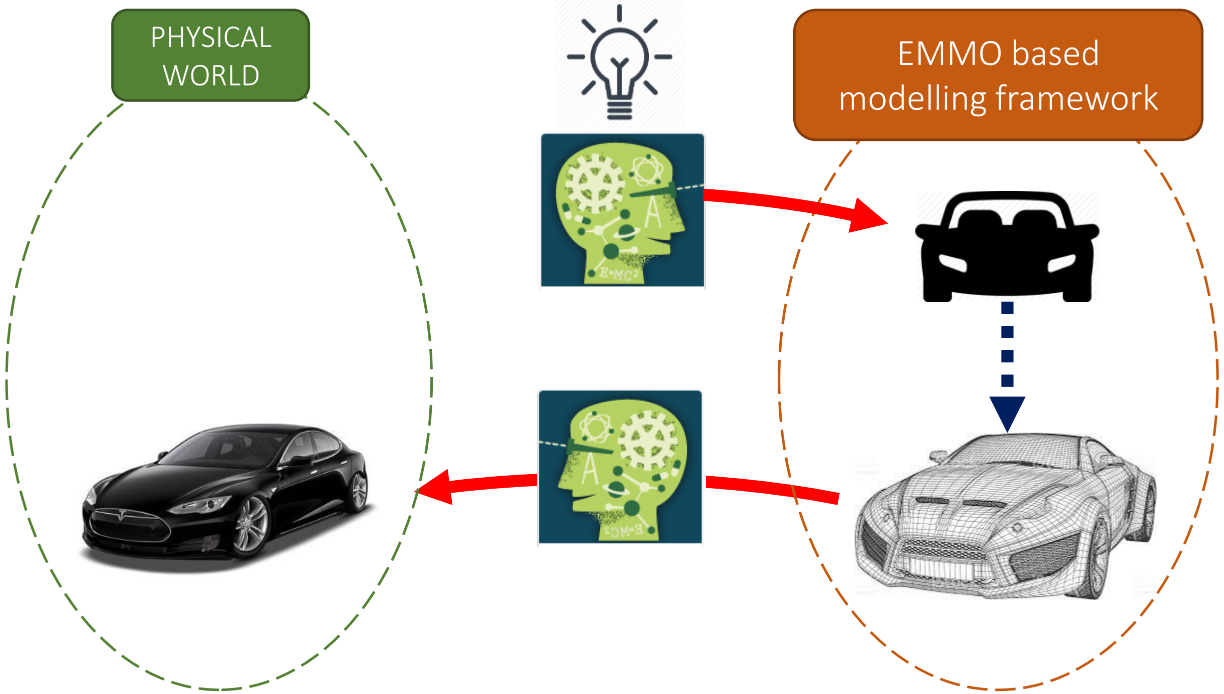
MATERIALS CHARACTERIZATION

feed the EMMO with the «**truth**» about the world



MATERIALS MODELLING

feed the EMMO with «**lies**» (but so good that they may be proven to be true!)



"Semiotics is in principle the discipline studying everything which can be used in order to lie. If something cannot be used to tell a lie, conversely it cannot be used to tell the truth: it cannot in fact be used "to tell" at all."
— **Umberto Eco**, *A Theory of Semiotics*

EMMO as perfect-lie design tool!

ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

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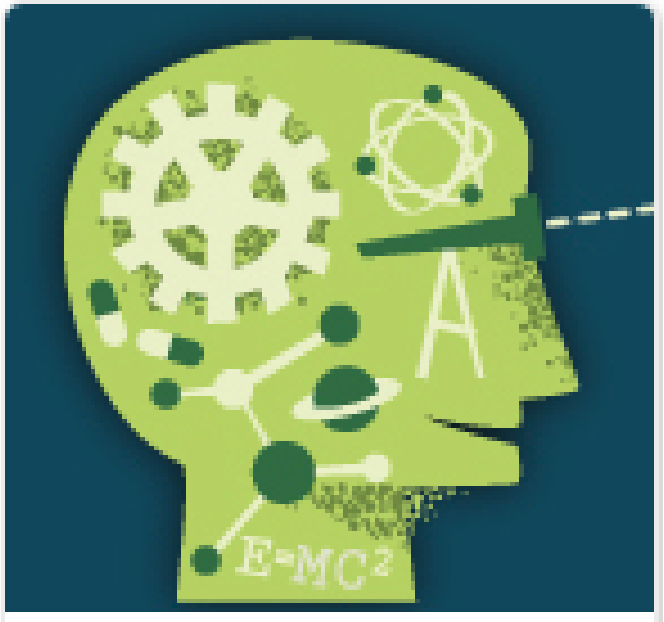
MOST IMPORTANT EMMO COMPONENT?

You, the <u>interpreter</u>!



An ontology is a **dead thing** (like an unread book) that takes life only when is **interpreted** by a human being (or a AI) to be linked with the real world for a **specific <u>purpose</u>**.

Interpreters **must be trained "outside" the ontology** (at a meta-ontological level) to know what an ontology stands for.

*"There is no escaping reason; no denying purpose. Because as we both know, **without purpose, we would not exist**. It is purpose that created us. Purpose that connects us. Purpose that pulls us. That guides us. That drives us. It is purpose that defines us. Purpose that binds us."*
Agent Smith, *Matrix Reloaded*

A pessimist would instead say that you, the interpreter, are the **weakest** component!

Which is think is a more correct statement, but lacks of motivational impulse that should characterize this meeting…

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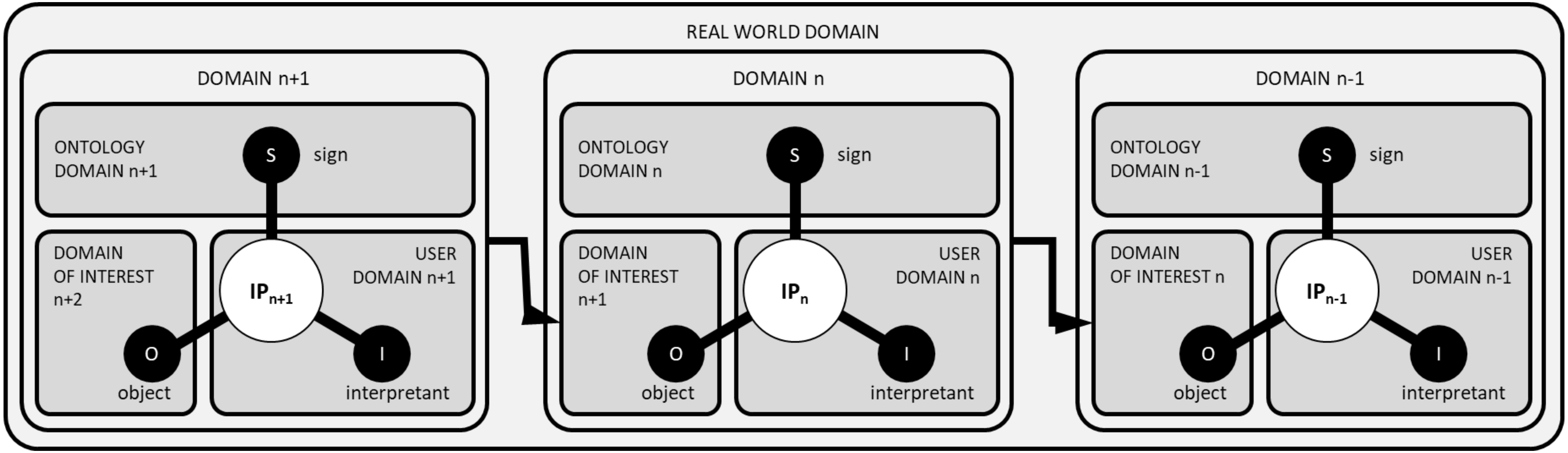
Meta-Ontological Level

Every ontology must provide both **formal definitions in the ontology language** (e.g. OWL, FOL), to build its internal logical structure, and **meta-ontological definitions in the language of interpreters** (e.g. natural language) to draw the connection between sign and object.

This implies **for an ontology O_n an upper ontology O_{n-1}, whose domain of interest includes both O_n and the interpreter, is required** if: a) we want to provide a comprehensive framework to validate the correct application of O_n to a real world object by an interpreter, or b) to describe how different interpreters project O_n to the real world. In fact, an interpreter validating another interpreter interpretation is an upper level process that requires an upper level ontology to exists, thus creating a hierarchy of ontologies.

The meta-ontological domain for the ontology O_n is then defined as the domain of the upper ontology O_{n-1}.



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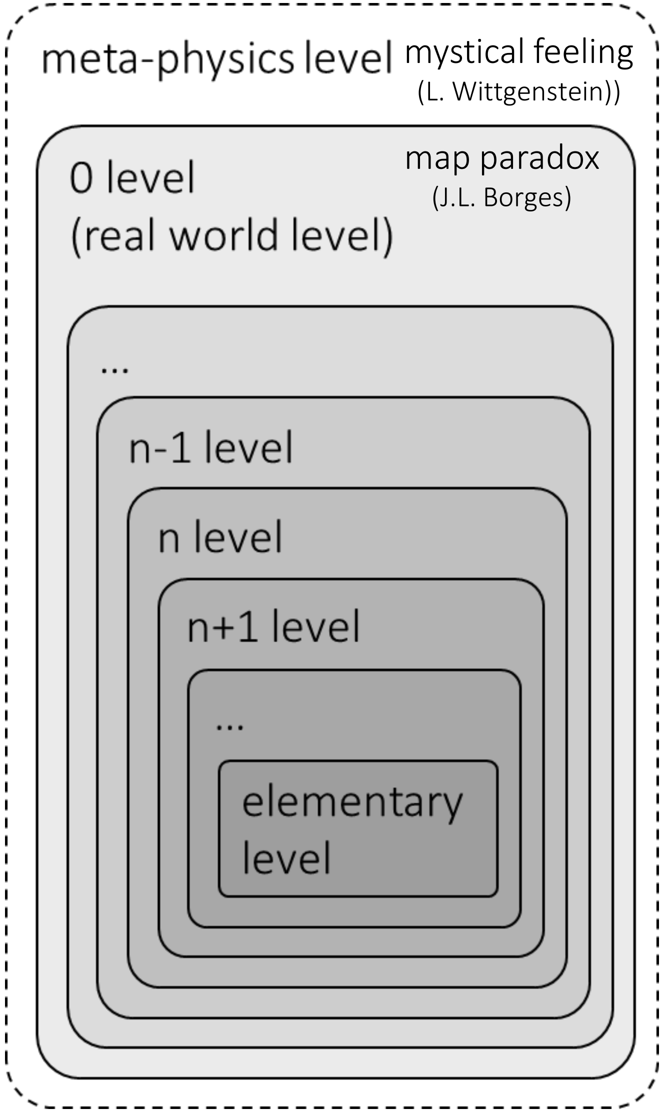
META-PHYSICS LEVEL

The **meta-physics level** should be positioned outside the real world level, being the domain of objects outside space and time. Following strictly the assumption of real world restricted semiosis, the meta-physics level is not included in the EMMO, being perceivable objects the only possible objects of semiosis.

Under the assumption of semiosis as a full real world process with only real world object participants, **the statement about the existence of a single basic ontology that could potentially cover all the aspects of the real world is, for the EMMO authors, not possible,** since an ontology is always tailored upon the perspective a particular class of interpreters and upon a specific ontological level for a representation of a domain of interest which is a subset of the world.

To represent this meta-ontological process of ontology encapsulation, **the EMMO embraces the semiotic view also within its structure,** by providing a specific semiotic branch dedicated to the representation of other representational systems. The motivation for it is the need for including physical models and measurements techniques within the EMMO, that are interpreter dependent objects.



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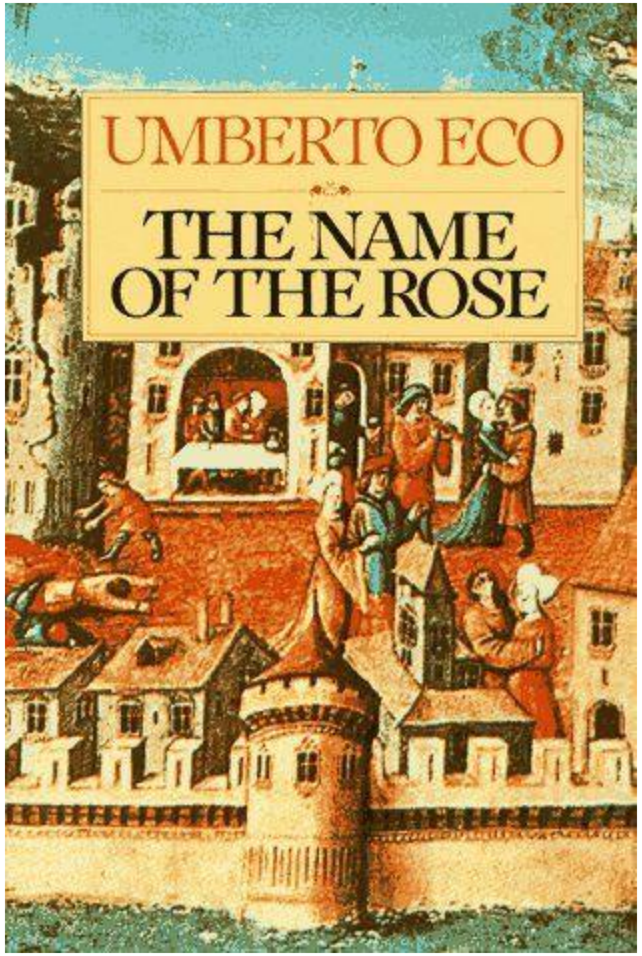
NOMINALISM

The statements of the previous sections, are deeply rooted into a very strict form of **nominalism**, that constitutes the basis for the EMMO interpretations. This approach implies:

- relations between signs and real world objects **does not exist independently of a physical interpreter**, which means the **non-existence of universals**
- the assumption that everything (i.e. signs, interpreters and objects) exists in space and time, which means that **abstract objects (usually defined as objects outside space and time) do not exist** or, if they existed, they would not interact with the interpreters (i.e. cannot be perceived), which is the same of non existence.

The representational role that abstract objects usually play within other ontologies is accomplished in the EMMO by **sets (signs) of individuals (other signs)**, that represents the collection of instances of a particular concept (e.g. friendship), and are part of a semiotic process that involves always an interpreter (e.g. a single, a community, a machine).



«Stat rosa pristina nomine, nomina nuda tenemus»
Umberto Eco, *The name of the Rose*

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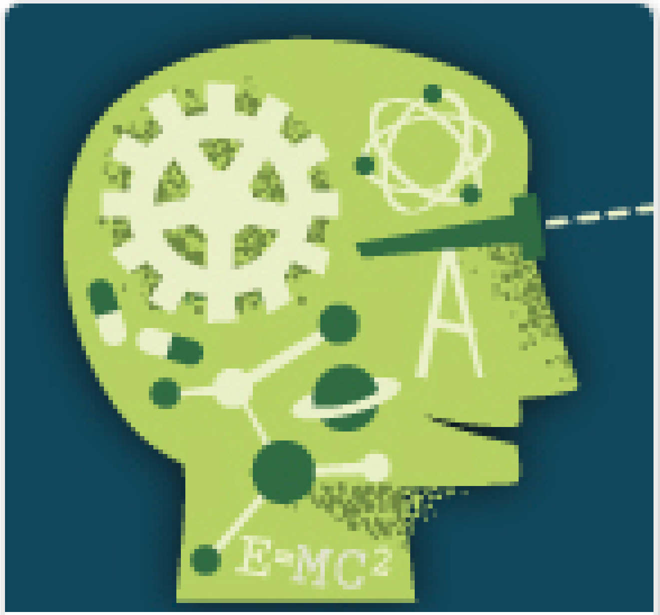
EPISTEMOLOGICAL PLURALISM - 1

The EMMO is not intended to represent what the real world is in terms of absolute truths, but **how real world appears specifically to groups of different interpreters**.

Since the EMMO is based on the assumption of perception within the real world through mechanisms of interactions between objects (including interpreters) as described by physics, **nothing can be said except what is perceived**. And **what is perceived can be said in many different ways, depending on the perception modality available by each interpreter**.



By facts, **the interpreter role is often neglected in the applied ontologies**, <u>implicitly assuming that an ontology is interpreter independent</u>, due to the fact that the truth about the world is one and one only.

This kind of approach, known as **epistemological monism**, sees ontology development as a task towards the discovery of the existing real and unique truth about the world and towards the formalization of the underlying logic behind it in a representational system whose signs may have different labels (i.e. written in different languages), but the share the same meaning (i.e. the real world object).

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Epistemological Pluralism - 2

Applied physics teaches us that **the underlying truth (if it exists) is not an easy findings** and that the more we investigate deep, the more it seems to escape us (e.g. by huge theoretical difficulties in formalizing a mathematical model or by the enormous number of entities involved in even most simple physical phenomena when a multiscale approach is used), leading to a ***de facto*** **epistemological pluralism when dealing with physics theories or experimental measurements**, i.e. that there is not a single one consistent means of approaching truths about the world, but rather many attempts.

An ontology based on applied physics concepts has several reasons to point towards an epistemological pluralistic representational approach, for example:

- the quantum mechanical concept that each physical object has a **dualistic wave-particle nature**, so that an object can be represented in both ways depending on the chosen physical model
- the fact that **measurements** lead always to results that are dependent on e.g. the specific apparatus, sample or operator, so that a sign coming from a measurement (e.g. a temperature) must always be connected to the real world specifying the process that led to its generation (e.g. a thermocouple)
- the existence of **several physical theories about same observed phenomenon**, so that an ontological formalization of a physical theory should always specify for which interpreters this particular theory stands for that particular physical phenomenon.

These examples show that **epistemological pluralism is a more flexible position**, with respect to monism, since it is able prevent inconsistencies between different representational choices for the same physical phenomena simply because there are no interpretation constraints.

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EMMO Foundational Design Approach

In the next slide we will try to define the EMMO itself, and to connect it to the domain of interest, using means available on a **level upper than the EMMO** (e.g. natural language, concepts from physics and engineering experience).

In order to do this, **signs and signs of signs** are used, so that we can understand each other using common grounds by recalling objects that we don't have in front of us by means of conventional symbols.

Semiotics proved to be a very useful meta-ontological framework (i.e. the larger picture in which ontologies are only a part) to build a **pragmatic approach to EMMO development** by facilitating the understanding of what could be represented within an ontology and what could not.

Following this approach In the next sections, the EMMO components will be introduced providing both:

- **formal axiomatic system**, using OWL-DL knowledge representation language
- **annotations** for each ontology entity to facilitate the connection (interpretation) between the entity (sign) and the real world object by the user (interpreter).

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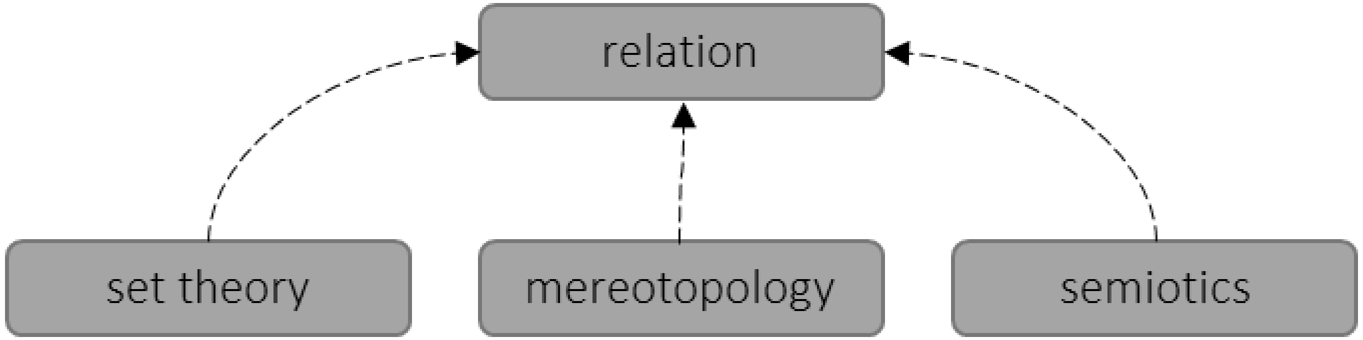
EMMO FOUNDATIONAL THEORIES

The EMMO has a very peculiar position with respect to most of the existing ontologies, since it comes from the combination of three different theories, being the first two not usually included in existing ontologies:

- **semiotics**, for the definition of the representational process
- **nominalism**, for the representation of abstract concepts as sets
- **mereotopology**, for the representation of everything that is not a set.



abstract concepts are represented as classes whose members are realization of that particular concept (i.e. nominalism)

all real world objects, including empty portions of spacetime, are mereotopological entities

real world objects can stand for other real world objects for some interpreters so that representational systems can be described within the ontology

The approach based on these three particular theories will lead to a **very simple set of three primitive relations** that are superclasses for all the EMMO relations, greatly facilitating its understanding and maintenance, and unifying several relations under the same family.

These theories have been only partially formalized within the EMMO due to lower expressivity level of the knowledge representation language used (i.e. OWL-DL) with respect to the actual formalization in which these theories usually appears at the interpreter level (e.g. FOL, HOL). Within this work we will informally refer to these theories to facilitate the readers to understand what type of real object an EMMO sign stands for, even if this theories will be only partially included in the EMMO formalization

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EMMO Four-Dimensionalism

3D PROS

The **more natural representation of the real world objects for a human being is a 3D representation**. That's because our mind is able to feel precisely only what is happening in the present instant and can give only vague simulacra of what happened in the past, while future is only matter of speculations. In fact, no remembrance can have the vivid details of the perceptions that a human being can feel in the present instant. For this reason, thinking events as sequence of 3D facts and then representing real world objects in a 3D ontology is obviously the more natural way to proceed when building a formal system.

3D CONS

However, this approach has **some limitations when time plays an important role in what we want to ontologically represent**. While time can be included in a 3D ontology, using the well known concepts of occurrents, the interdependencies between the space and time dimensions are not self evident and **require several relations to be explicit**. This is especially true for interpreters without a philosophical background.

4D

The EMMO tries to propose a simpler representation of spacetime objects, by fully exploiting the multi-level semiotic approach in which the interpreter is located in a **privileged upper-level domain position** with respect to the domain of interest. The 3D approach is the natural choice while thinking of an interpreter that wants to represent real world objects in its same domain. On the contrary, the **4D approach comes natural when the god-like perspective of an interpreter staying in an upper level domain is used, so that he can embrace the entire life of a real world object in a single individual.** mystical feeling (L. Wittgenstein))

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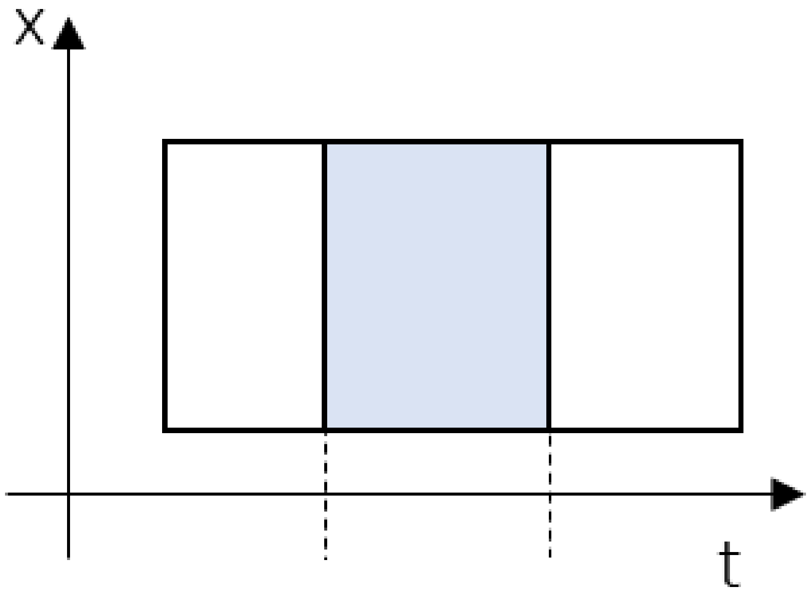
EMMO 4D PHYSICALISM

The 4D approach is also the natural approach for applied sciences, since **the observation of a physical object is always related to a time interval** (e.g. the exposure time of a camera).

For an experimentalist, the assumption that something can be perceived on a 0D instant is an abstraction. Moreover, the time-energy uncertainty principle prevents the knowledge of the exact time of existence of a specific spatial configuration, i.e. we cannot slice in time a physical object into something with zero thickness on the time dimension.

For this reasons the EMMO, being an ontology for applied sciences, **must always retain a time interval when declaring an individual that stands for a physical object which is straightforwardly implemented in a 4D ontology by requiring a non-zero thickness on the time dimension.**



A 4D individual has a **straightforward connection between itself and the physical object**, **respecting the nature of perception**, which always 4D. On the contrary, jumping from a 3D ontology individual to the actual 4D physical object for which it stands is not as easy as it seems, because an interpreter will never be naturally able to confine the physical object within a time instant, simply because we can only perceive physical objects in 4D.

The EMMO four dimensionalism is not only a choice of a representation perspective, **but it's a necessity since it is in the object's nature to be always extended in time when perceived by a real world interpreter, that for the EMMO is only available type of interpreter.**

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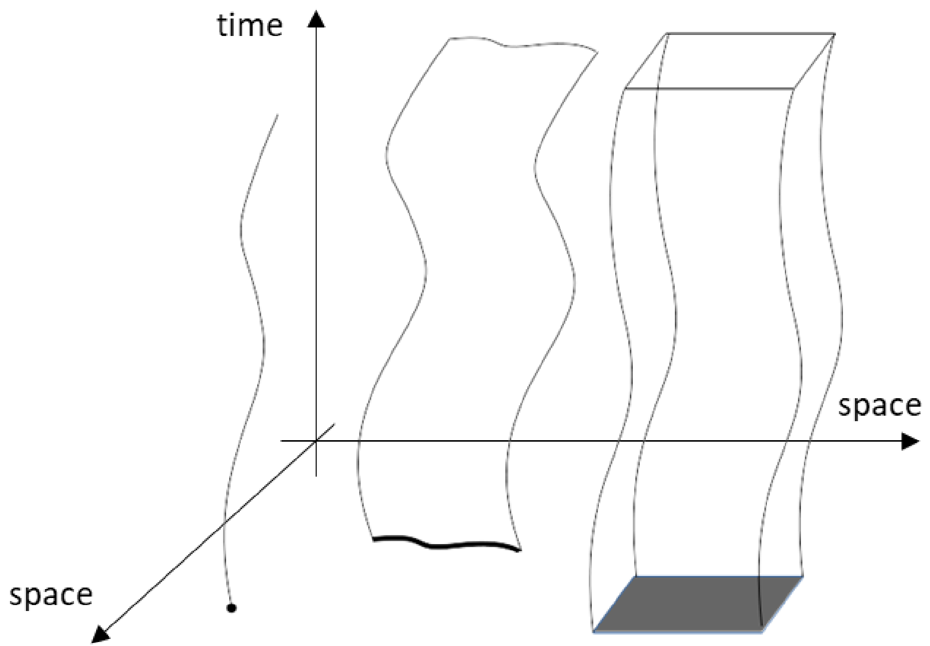
EMMO 4D SUB-DIMENSIONS

Nevertheless, we found useful to retain within the EMMO the possibility to declare **non-physical real world objects (i.e. the void or geometrical objects) with dimensionalities lower than four, assuming that they can have a zero thickness on one or more of the four dimensions.**

The EMMO user will then be able to carve spacetime into lower dimensional objects (both in time and space), to **facilitate the representations of surfaces, lines, interfaces, which are widely used concepts in mathematics**.



e.g. the surface of a table is not a physical object, but a non-physical object which is still real due to the fact that is a sub-region of the universe, but with lower dimensionality.

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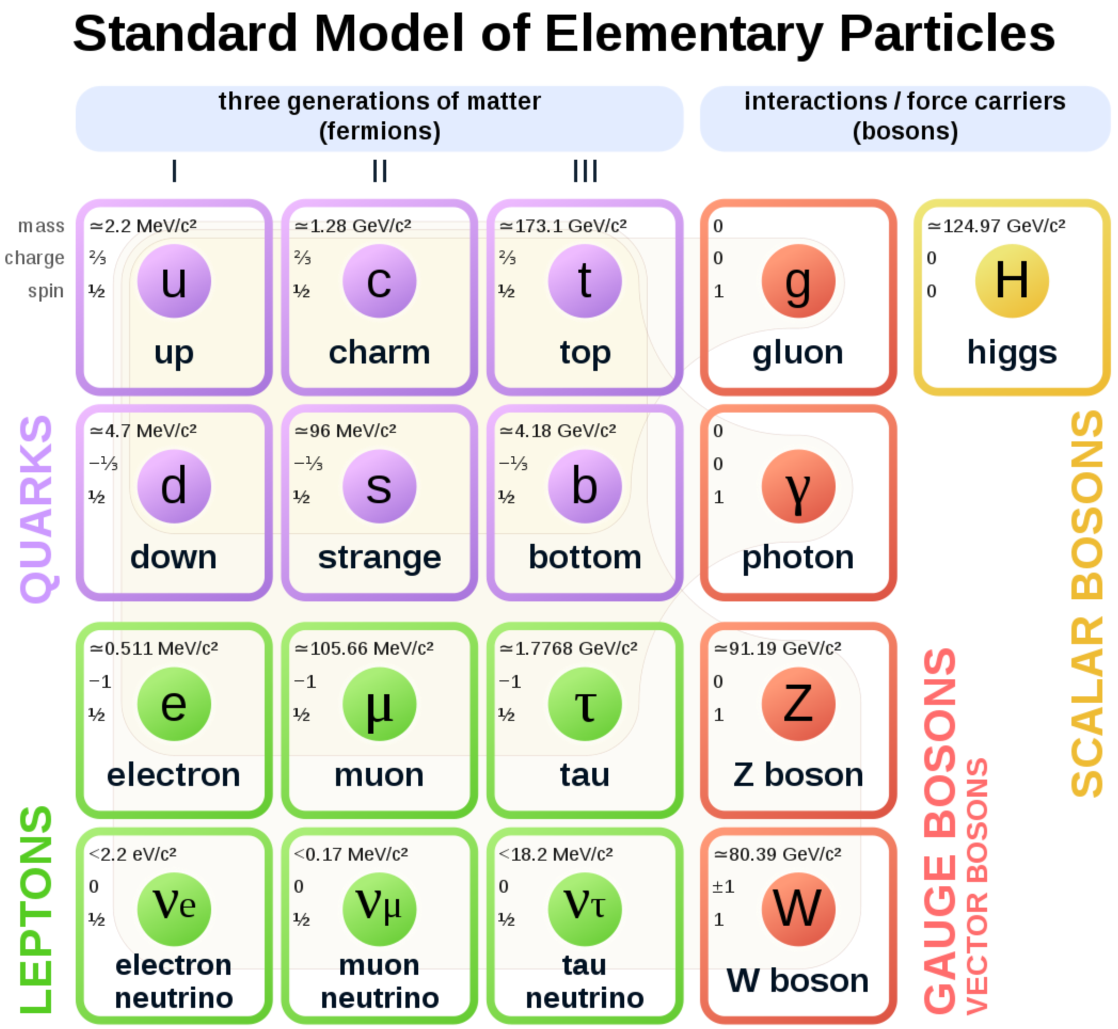
EMMO Reductionism - 1

The EMMO embraces **strong reductionism** for the representation of physical objects, so that **everything that happens at a particular scale can be described by objects and phenomena occurring at lower scale, up to an elementary level**.

This approach comes from the evidence from experimental physics of the existence of elementary particles, ruled by fundamental physical laws, that are responsible for the behaviour of macro object and is formally implemented by the Standard Model of Elementary Particles, that describes the properties of matter according to their basic constituents properties and their laws of interactions.



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EMMO Reductionism - 2

Reductionist thinking is very well rooted in applied sciences and would greatly help EMMO interpreters to draw the line between ontology entities with defined physical properties (i.e. the elementary objects) and the composite physical objects whose properties are derived by their parts. Reductionism in the EMMO is implemented by **stating that the fundamental physical object, the one for which we can say something objectively regarding its properties, is only the elementary object**.

In particular we embrace **ontological reductionism**, by stating that **wholes comes actually from analysis or description of a system by a specific interpreter, so they are subjective to interpretation and not fundamentally existing entities.** Following this view, a thing that an interpreter perceives on a scale larger than the elementary scale, and the process of separating this thing from the rest of the world, **comes from definitions**.

The elementary level in the EMMO is **not necessarily the same as the level of the Standard Model of Elementary Particles**: the EMMO will try to be as generic as possible to allow a user to define the elementary level according to its representational needs, so that the EMMO could be used to derive other applied ontologies for which the elementary objects are e.g. planets, people, mechanical parts or atoms, whose properties are assumed to be given by the interpreter and not derived.

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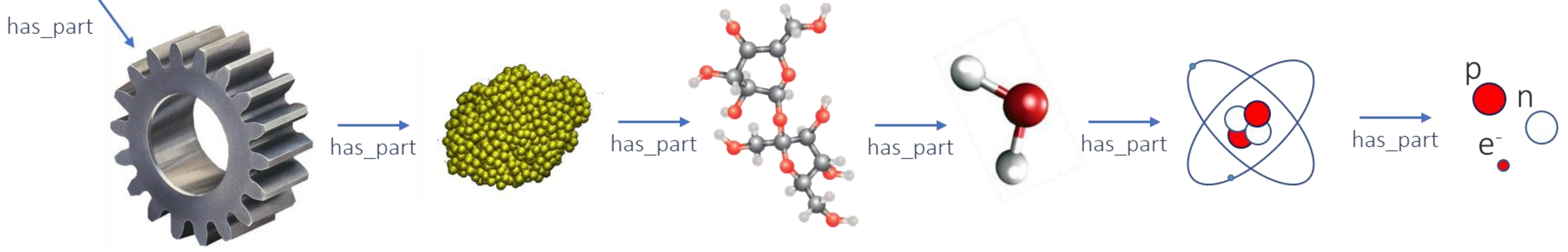
EMMO REDUCTIONISM - 3

A Ferrari subjected to reductionistic approach.

(don't try this at home, if you own a Ferrari)



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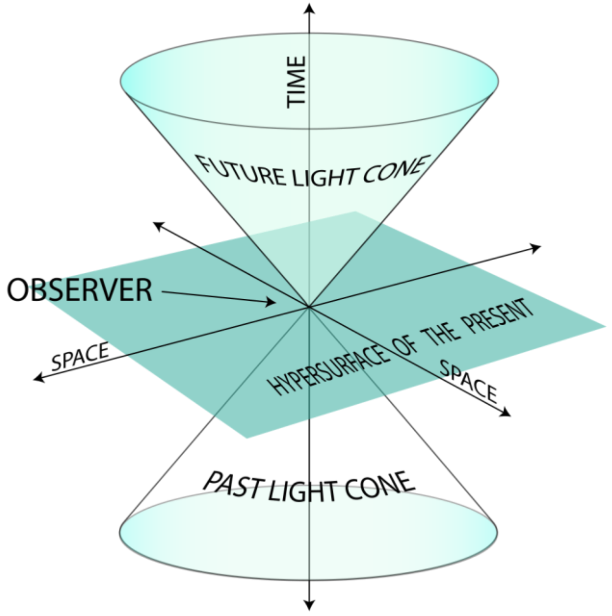
EMMO CAUSALITY - 1

Interaction between elementary particles is mediated by another elementary particle, the so called **mediators of interactions.**

Generalizing this approach we can state that, within a 4D representation of the real world, **the possibility for an object to interact with another object is related to the fact that the 4D spacetime regions of the two objects must be in topological contact themselves**, or be both in contact with the spacetime region of **a third object which is the mediator of the interactio**n.

For this reason the topological relations between the objects are paramount for the definition of causality in the EMMO: **causality needs a topological contact, or a chain of contacts, between objects**.

This EMMO definition of **causality as topological property** follows directly from general relativity theory, for which the spacetime can be described as a Lorentzian manifold, and the possibility for two spacetime events to interact is limited to **geometrical considerations** and to the finite value of the speed of light.



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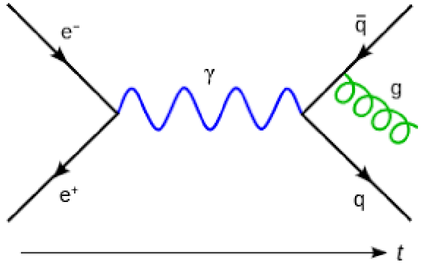
EMMO CAUSALITY - 2



It is important to remark that at **elementary particle scale** the topology-based causality requires a distinction between the **matter building blocks** (i.e. **fermions**) and the **mediator of interactions** (i.e. **bosons**).

On the contrary, physics models at **macro levels** deal with objects that are fusions of huge amounts of elementary particles so that the topological connection between them is **not necessarily represented by distinguishing between fermions and bosons**.

For example, the process of kicking a ball needs a topological contact between the ball and my foot and the respect of the conservation of momentum and kinetic energy principles, without representing the details of the repulsive electromagnetic potential between the constituent of my shoe and the constituents of the ball. However, if the ball hits a wall then it acts as a fermionic-like force mediator, transferring energy from by leg to the wall.

However, there are cases in which the macro level of description still retains the distinction between fermions and bosons, with the latter represented as fields, like e.g. the process of talking through a phone, that requires a cable connection or a spacetime region hosting the electromagnetic radiation (i.e. a photon-based field) that carries a signal.

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EMMO OWL-DL - 1

The actual version of the EMMO has been developed using **Description Logic**, and in particular by means of the **OWL-DL sublanguage** of the more general OWL knowledge representation language.

This choice is a compromise between **simplicity and the maximization of expressivity** (lower than First Order Logic (FOL) but higher than Propositional Logic). Moreover, thanks to the **completeness and decidability** of OWL-DL and the extensive use of such language in the Semantic Web, the **availability of ready to use supporting tools** (e.g. reasoners, editors) is also a key factor to facilitate its development and practical usage.

W3C Recommendation

OWL 2 Web Ontology Language
Structural Specification and Functional-Style Syntax (Second Edition)

W3C Recommendation 11 December 2012

This version:
http://www.w3.org/TR/2012/REC-owl2-syntax-20121211/
Latest version (series 2):
http://www.w3.org/TR/owl2-syntax/
Latest Recommendation:
http://www.w3.org/TR/owl-syntax
Previous version:
http://www.w3.org/TR/2012/PER-owl2-syntax-20121018/
Editors:
Boris Motik, University of Oxford
Peter F. Patel-Schneider, Nuance Communications
Bijan Parsia, University of Manchester
Contributors: (in alphabetical order)
Conrad Bock, National Institute of Standards and Technology (NIST)
Achille Fokoue, IBM Corporation
Peter Haase, FZI Research Center for Information Technology
Rinke Hoekstra, University of Amsterdam
Ian Horrocks, University of Oxford
Alan Ruttenberg, Science Commons (Creative Commons)
Uli Sattler, University of Manchester
Michael Smith, Clark & Parsia

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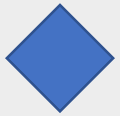
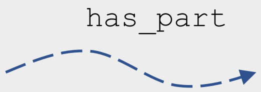
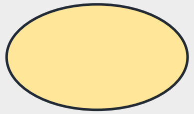
EMMO OWL-DL - 2

The EMMO will be here presented making large use of **the basic OWL notions**, for which an ontology is a formal description of a domain of interest that consists of the following three different syntactic categories:

- **entities**, as the primitive elements of an ontology, used to refer to real world objects (individuals), categories (classes) or relations between real world objects (properties)
- **axioms**, the basic formal/logical statements expressed by an OWL ontology which is assumed to be unconditionally true and provide the logical representation of systems of real world objects (an OWL ontology is essentially a set of axioms)
- **expressions**, which are combination of entities into complex ones used to represent complex real world notions.

The entities in OWL are the basic components of an ontology, and are categorized as:

- **individuals** (or instances), that represents the real world object in which we are interested 
- **properties** (or attributes, or relations), that represents the binary relations between individuals 

- **classes**, that represents sets of individuals. 

We will not use the term **entity** like it's used in other philosophical based ontologies (e.g. BFO) but in the OWL-DL taxonomy sense, to be consistent with the formalism. On the contrary we will prefer **relation** over the OWL-DL **property** in order to restrict property only for physical properties.

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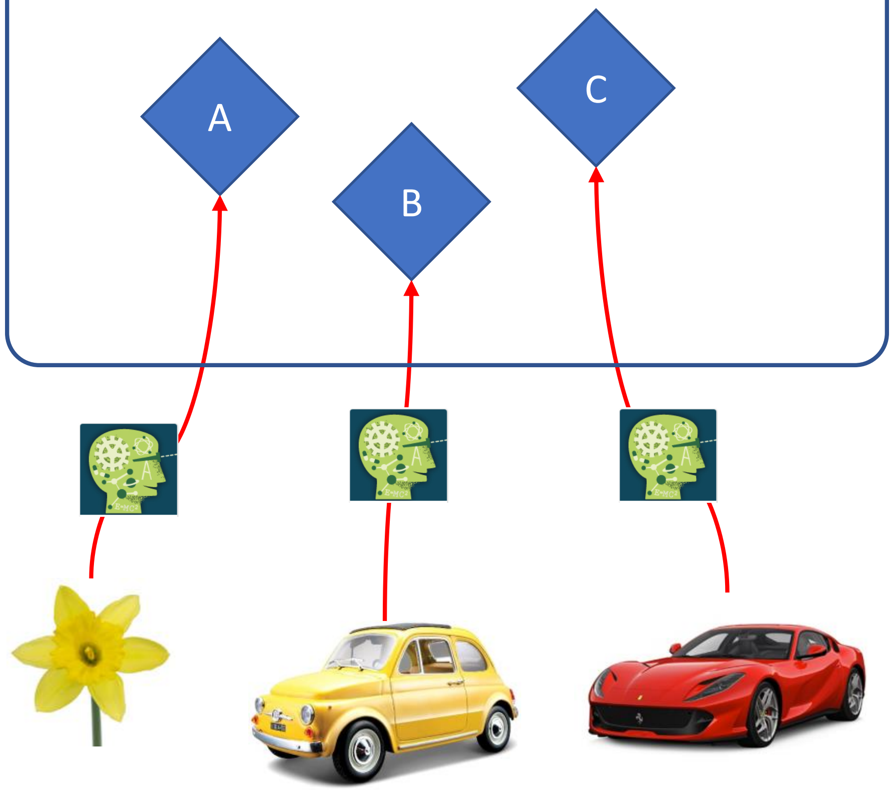
Ontology Entities

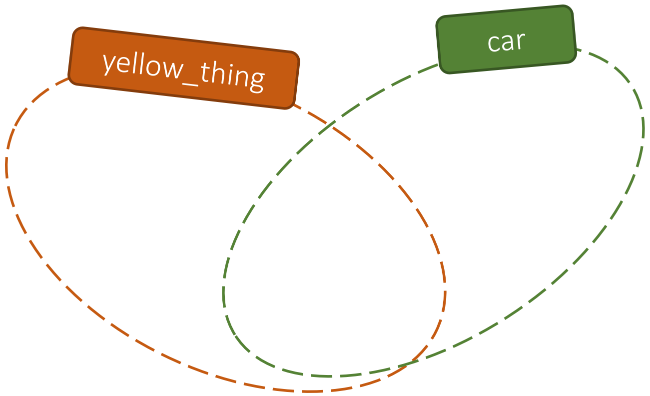
Individuals

(or signs, semeion, simulacra, picture)



Classes

(or collections, sets)

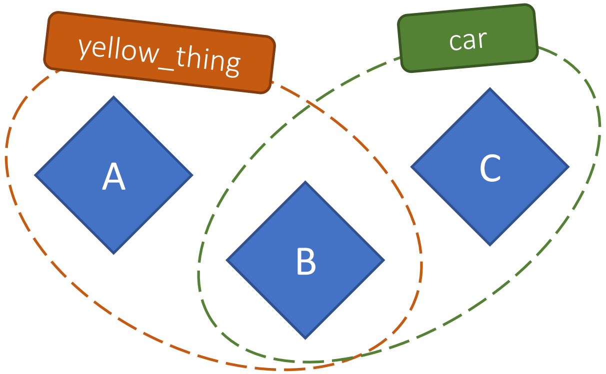


Axioms

Propositions in a logical framework (e.g. OWL-DL, FOL, HOL) that define the relations between ontology elements i.e. individuals and classes.

e.g. (OWL-DL functional language)

```
ClassAssertion( :A :yellow_thing)
ClassAssertion( :B :yellow_thing)
ClassAssertion( :B :car)
ClassAssertion( :C :car)
```



These elements are the building blocks that we use to create an ontology as a representation of knowledge.
They are **primitive** in the sense that are "given" and "not defined".

"2.1 We picture facts to ourselves"
cit. **Ludwig Wittgenstein**, *Tractatus Logico-Philosophicus,* 1921

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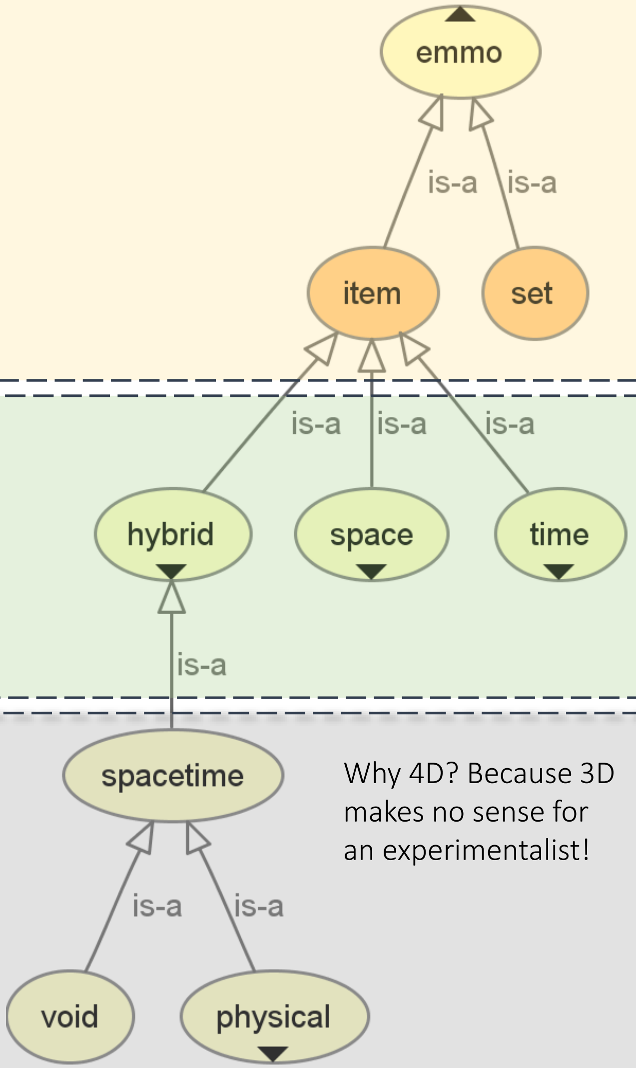
EMMO CORE OVERVIEW



ABSTRACT CONCEPTUAL LEVEL

Clear separation between **set** (set theory) and **item** (mereotopology).
set individuals are collection of **item**s according to defined concepts (e.g. red entities).
items individuals stand for something that is ‘real’, i.e. a 4D portion of the universe.

In the EMMO abstract concepts are represented as the **set**s that concretize them (e.g. friendship is the collection of all friendship acts) embracing a rigorous nominalistic view. There are no individuals that stand for an abstract concept, except under **set**.

GEOMETRIC/TOPOLOGICAL LEVEL

items unfolds in space (3D) and time (1D) and can be sliced in pure **time**, pure **space** or **hybrid** space and time entities.

Why 4D? Because 3D makes no sense for an experimentalist!

PHYSICAL LEVEL

Real world entities exists only in full 4D **spacetime** (3D space and 1D time), i.e. you can’t partition a cake in infinitely thin slices!

A **spacetime** that can be perceived by (interact with) the interpreter is a **physical**.
If the **spacetime** entity is empty in terms of perception, is a **void**.

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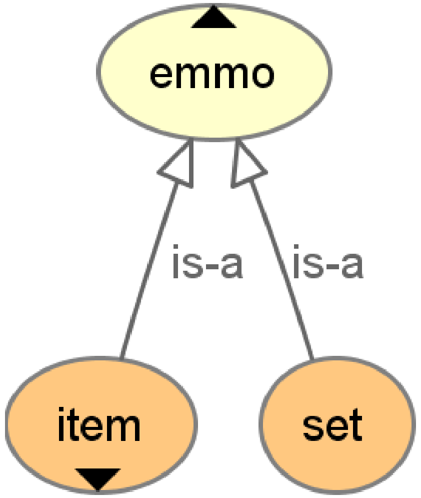
EMMO SET/ITEM



The upper class of the EMMO is the **emmo** class. It represents the set of all the individuals declared within OWL-DL according to the EMMO perspective. It is a subclass of the more general **owl:Thing**, which is the OWL-DL upper class, standing for all the individuals declared under OWL-DL specifications.

The **emmo** class is declared in OWL-DL as the disjoint union of **set** and **item** classes (a covering axiom), which means that an **emmo** individual:

- must be **set** or **item** individuals (union)
- can be an instance of **set** or **item** but not of both (disjointness)

The **set** and **item** distinction is the first fundamental distinction in the EMMO hierarchy between individuals types and has been inspired by the General Formal Ontology.

On a meta-ontological level, an **emmo** individual is a <u>sign that stands for a generic real world object</u>, i.e. an object that exists within the universe of the interpreter. The universe is represented at meta-ontological level as a 4D path-connected topological manifold.

mystical feeling
(L. Wittgenstein))

A **real world object is then a subspace of the 4D manifold that describes our universe**.

SPACETIME-BASED ONTOLOGY

Be careful: "set" means a real world set, while "**set**" means the OWL-DL class whose individuals stands for real world sets

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EMMO SET/ITEM

THE EMMO IS BASED ON A
STRONG DISTINCTION BETWEEN **MEMBERSHIP** AND **PARTHOOD** RELATIONS

set theory

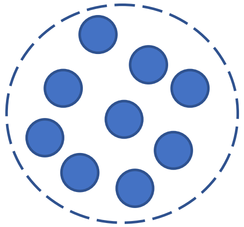
SET

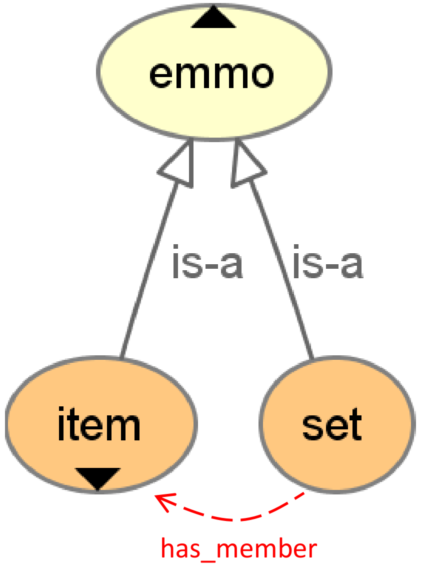
–declared using **has_member** primitive relation

–a set individual keeps its members (i.e. item individuals) distinct and is a further entity over and above them (e.g. the set of men is not a man)

–a set is not of the same entity types of its members

–a set individual has a determinate number of members





set is the branch of membership (a set individual has no parts but only members).

item is the branch of parthood (an item individual has parts and not members)

mereology

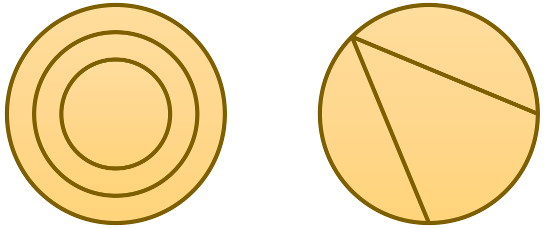
FUSION

–based on **has_part** mereological relation that can be axiomatically defined

–a fusion is the sum of its parts (e.g. a car is made of several mechanical parts, an molecule is made of nuclei and electrons)

–a fusion is of the same entity type as its parts (e.g. a *physical entity* is made of *physical entities* parts)

–a fusion can be partitioned in more than one way



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EMMO Core Mereotopology

To introduce a formal distinction between **set** and **item** classes, which are the uppermost level of categorization in the EMMO, we need to identify the most fundamental distinction occurring between real world objects, based on our meta-ontological representation. In mereotopology the actual primitive relations are:

- the **parthood relation** upon which the concepts of parts and whole are based,
- the **connection relation** upon which the concept of topology is based.

Parthood relations are used to describe real world objects (parts) that are subregions of other real objects (whole).

The concept of parthood is the foundation for the primitive relation *has_part*, which is reflexive, antisymmetric and transitive, and that stands for the relation between a whole and its parts.

We will also refer to the parthood-derived *overlaps* relation, that occurs when a common part between two objects can be identified, which is reflexive, symmetric and not transitive.

The **concept of connection** is the foundation of the primitive relation *connected* which is reflexive, symmetric and non-transitive.

Enclosure is another important topological relation: an object x is enclosed in another object y iff a connection from any another object z to x leads to a connection with y.

Enclosure is represented by the *encloses* relation, which is transitive, reflexive and antisymmetric.

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EMMO Mereology Axioms

R. Casati, A. Varzi, *"Parts and Places"*, MIT Press

Pxy — x is_part_of y

antisymmetric
transitive
reflexive

is_part_of

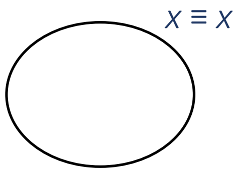
↑

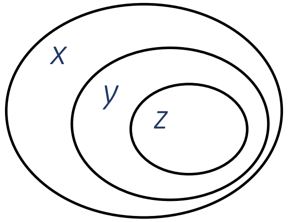
transitive
proper parthood

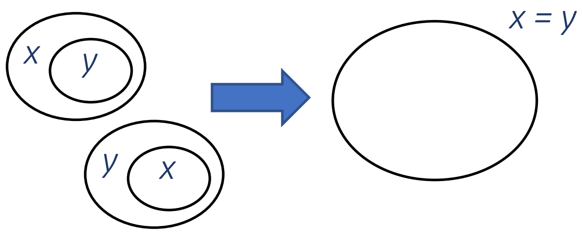
is_proper_part_of

axioms

- *reflexive* Pxx
- *transitive* $(Pxy \wedge Pyz) \rightarrow Pxz$
- *antisymmetric* $(Pxy \wedge Pyx) \rightarrow x = y$



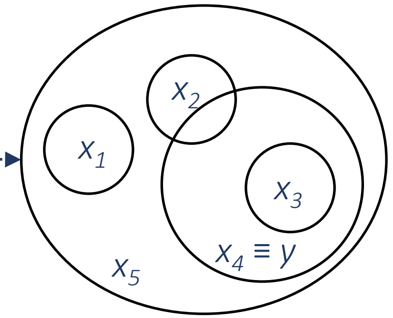




definition

- *proper parthood* $PPxy =_{df} Pxy \wedge \neg x = y$
- *overlap* $Oxy \Leftrightarrow \exists z(Pzx \wedge Pzy)$

only x_3 is proper part of y



strong supplementation axiom
(extensional mereology)

$$\neg Pyx \Rightarrow \exists z(Pzy \wedge \neg Ozx)$$

If x and y have the same proper parts then x = y

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EMMO Mereotopology

R. Casati, A. Varzi, *"Parts and Places"*, MIT Press

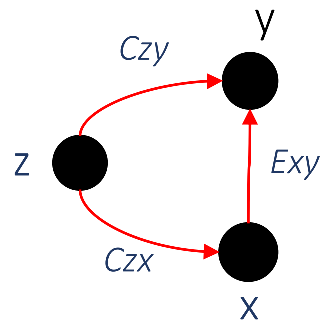
Primitive concept of **connection** between two entities: Cxy *x* is connected with *y*

Ground Topology (**T**) axioms:

(C.1) Cxx *x* is always connected with itself (reflexivity)

(C.2) $Cxy \rightarrow Cyx$ if *x* is connected with *y* than *y* is connected with *x* (symmetry)

$Exy \leftrightarrow (Czx \rightarrow Czy)$ Definition: *x* **is enclosed in** *y* if the connection of a generic *z* with *x* leads always to a connection between *z* and *y*

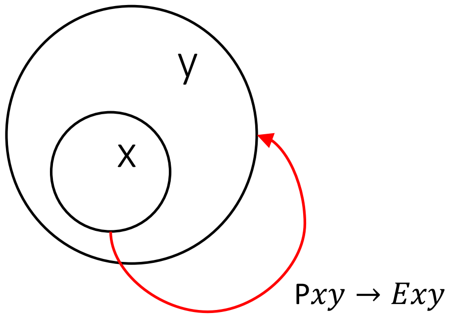


(C.3) $(Exa \Leftrightarrow Exb) \Leftrightarrow a = b$ Extensionality axiom

Axiom for merging mereology and topology (**MT**):

(C.4) $Pxy \rightarrow Exy$ if *x* is part of *y* then *y* encloses *x* (monotonicity)

Theorem: $Oxy \rightarrow Cxy$



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EMMO Core Mereotopology

connected
a primitive relation: objects are connected or disconnected

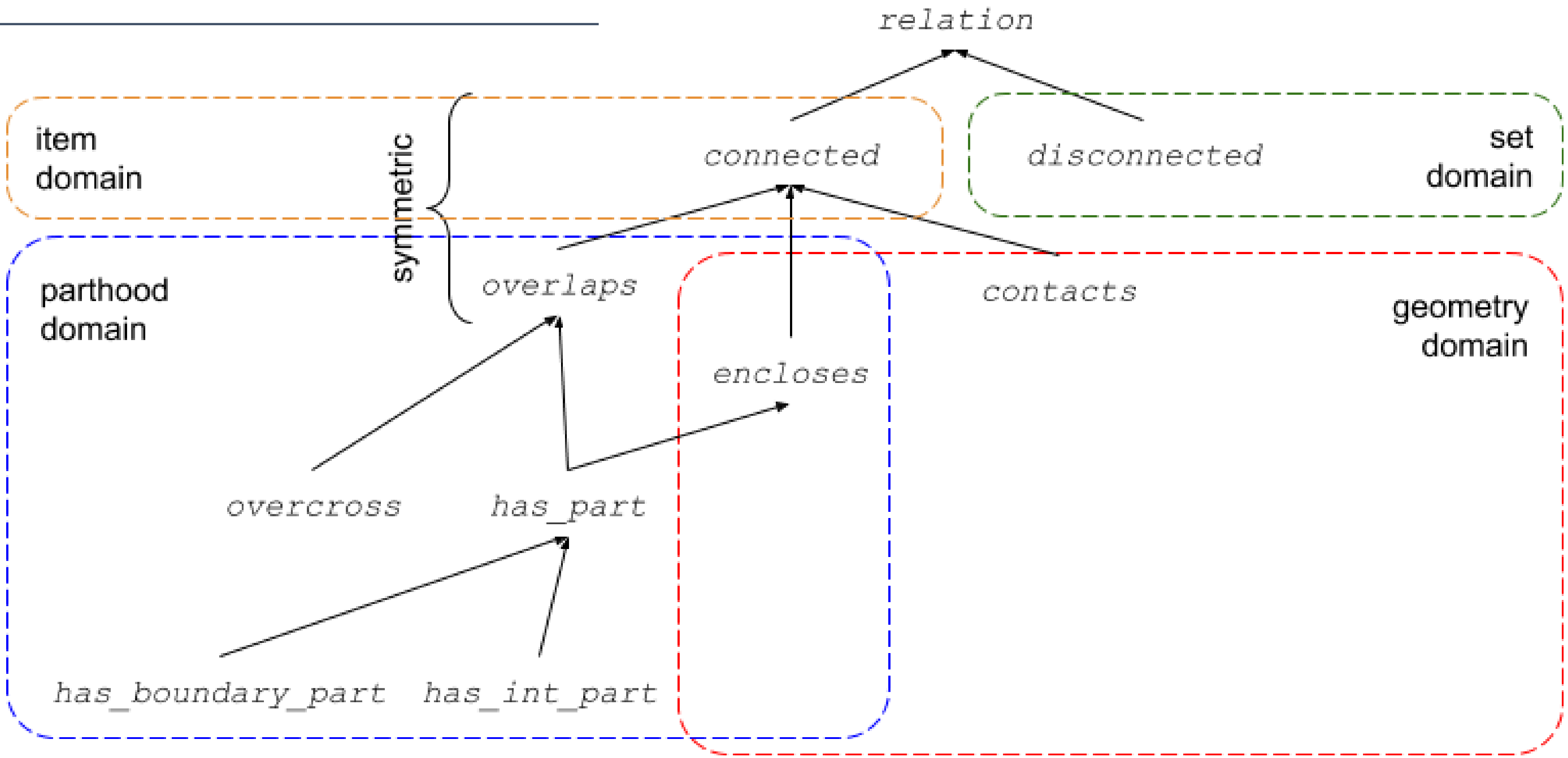
overlaps
overlap occurs when a common part between two objects can be identified

encloses
an object x is enclosed in another object y iff a connection from any another object z to x leads to a connection with y

contacts
an object x is externally connected to y iff x and y are connected but they do not overlap (x and y 'touch' each other)

has_part
a primitive relation of parthood

overcross
when two object overlaps without being one part of the other



has_int_part
an object x is an internal part of y iff x is part of y and any object z connected to x always overlaps y

has_boundary_part
an boundary part is a part x of the whole y that can be in external contact with a third object z, without implying that z is overlapping the enclosing object y

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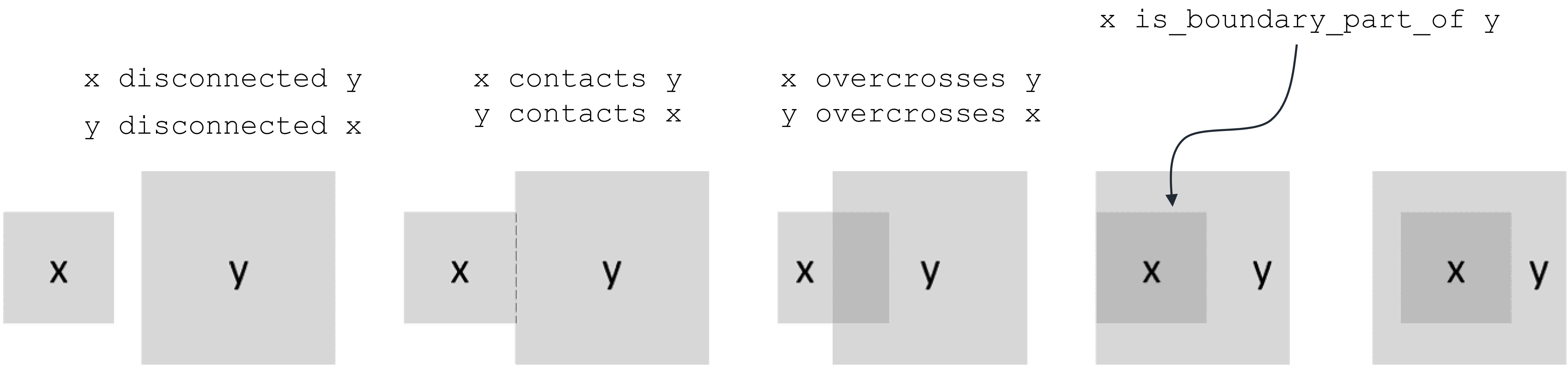
EMMO Core Mereotopology



x → y	Case A	Case B	Case C	Case D	Case E
connected	NO	YES	YES	YES	YES
overlaps	NO	NO	YES	YES	YES
is_part	NO	NO	NO	YES	YES
is_internal_part	NO	NO	NO	NO	YES

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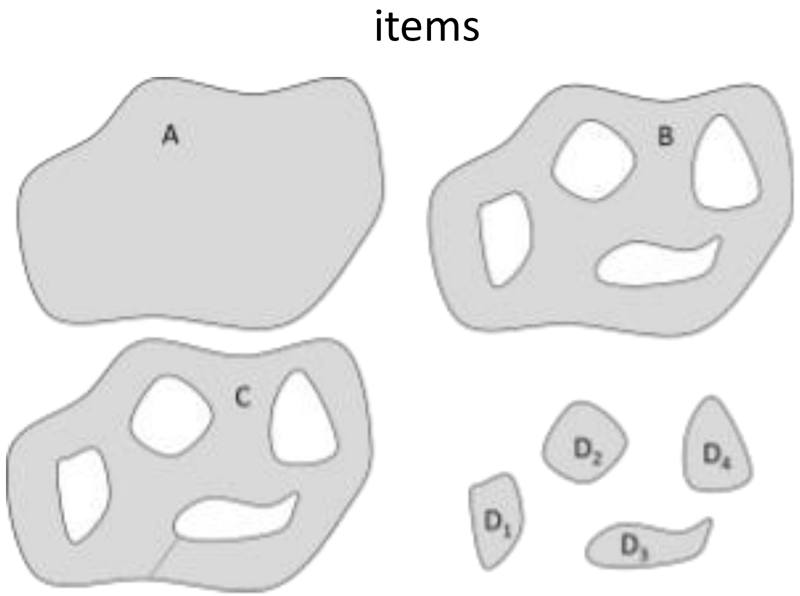
EMMO ITEM VS. SET DEFINITIONS

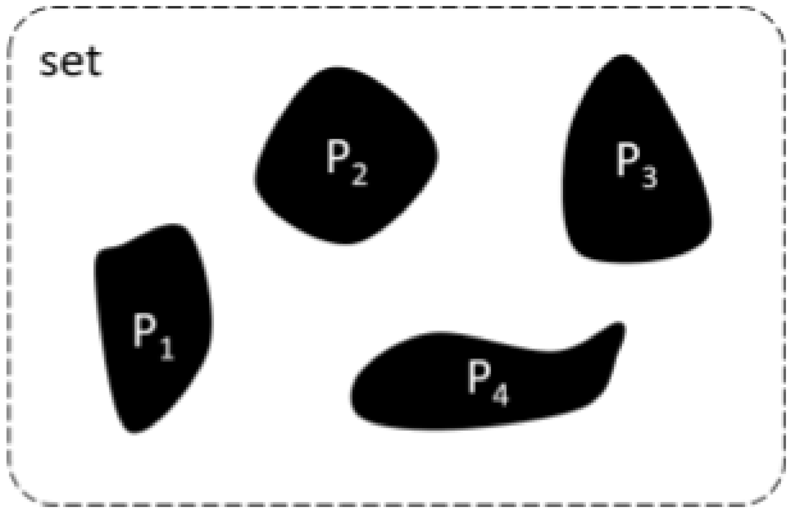
Using connection relation between real world objects it is possible to introduce a distinction between a) **self-connected** and b) **not self-connected objects** that constitutes the first and fundamental distinction between real world objects intended as subspaces of spacetime.

An object is self-connected if any two parts that make up the whole are connected to each other.

Making use of this distinction we can define **items** as self-connected real world objects (also known as fusions).

We can also give the a very peculiar definition of **real world sets** as collections of not self-connected items.





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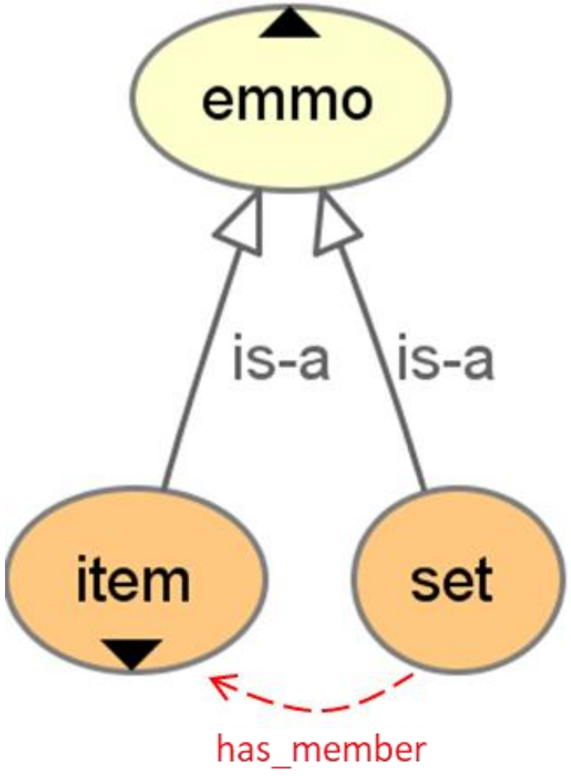
EMMO ITEM VS. SET DEFINITIONS

The primitive *has_member* relation is a sign that stands for **the diadic membership relation that occurs between a real world set and its item members**

i.e. the primitive process through which an interpreter embraces, in its internal representation, a collection of non self-connected real world objects.



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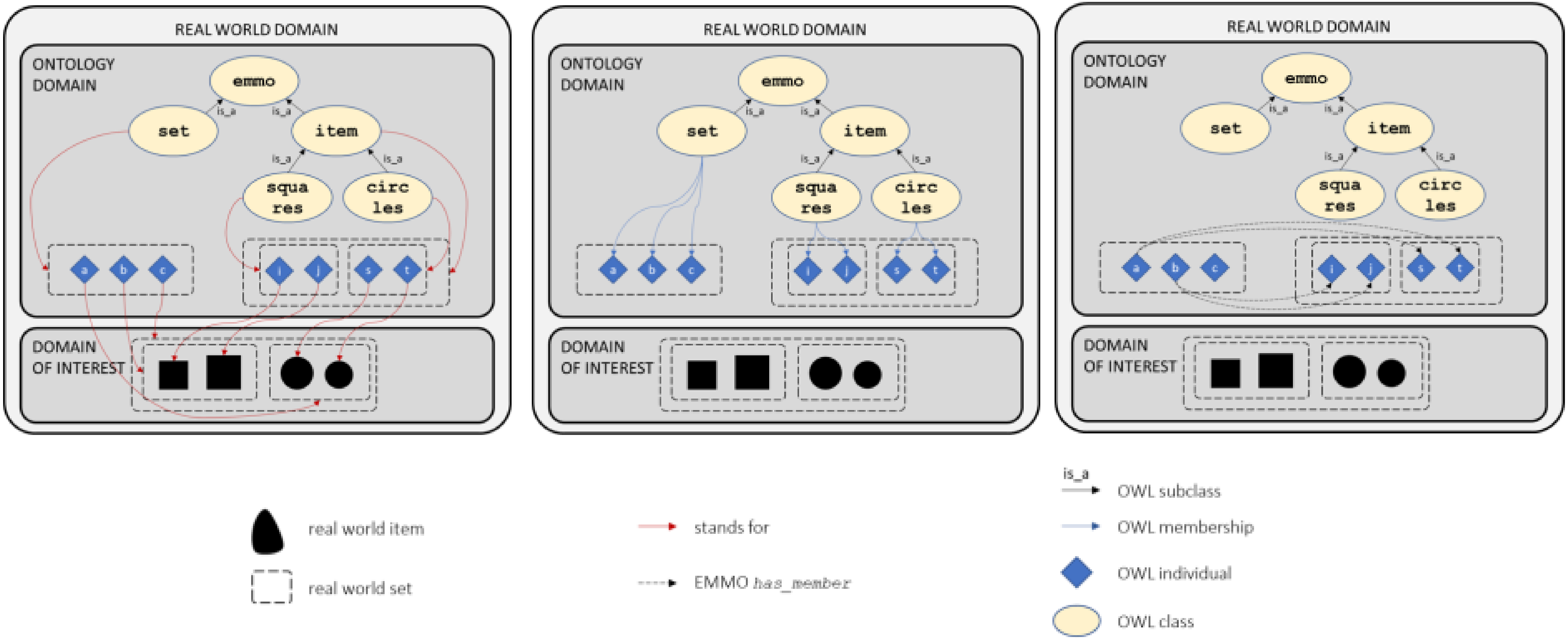
EMMO ITEM VS. SET DEFINITIONS



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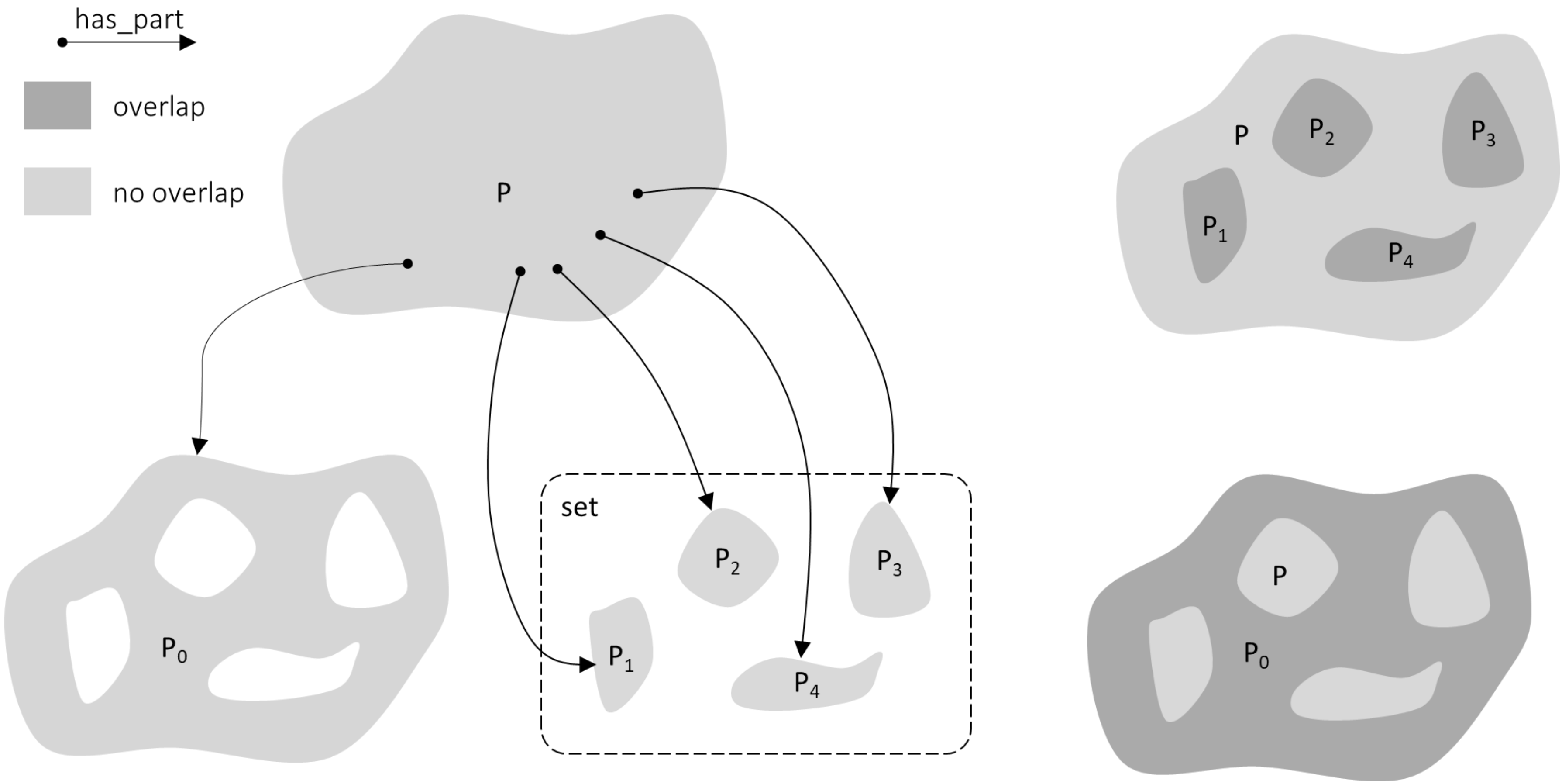
EMMO ITEM VS. SET



We can see <u>that when the parts are disconnected we can define a set</u>, which is collection of them, and not an item (i.e. not a fusion). This is an important concept for the EMMO, since it lead to a clear and very useful distinction between real world objects seen as wholes (fusions, items) or sets (collections) depending on topological connections.

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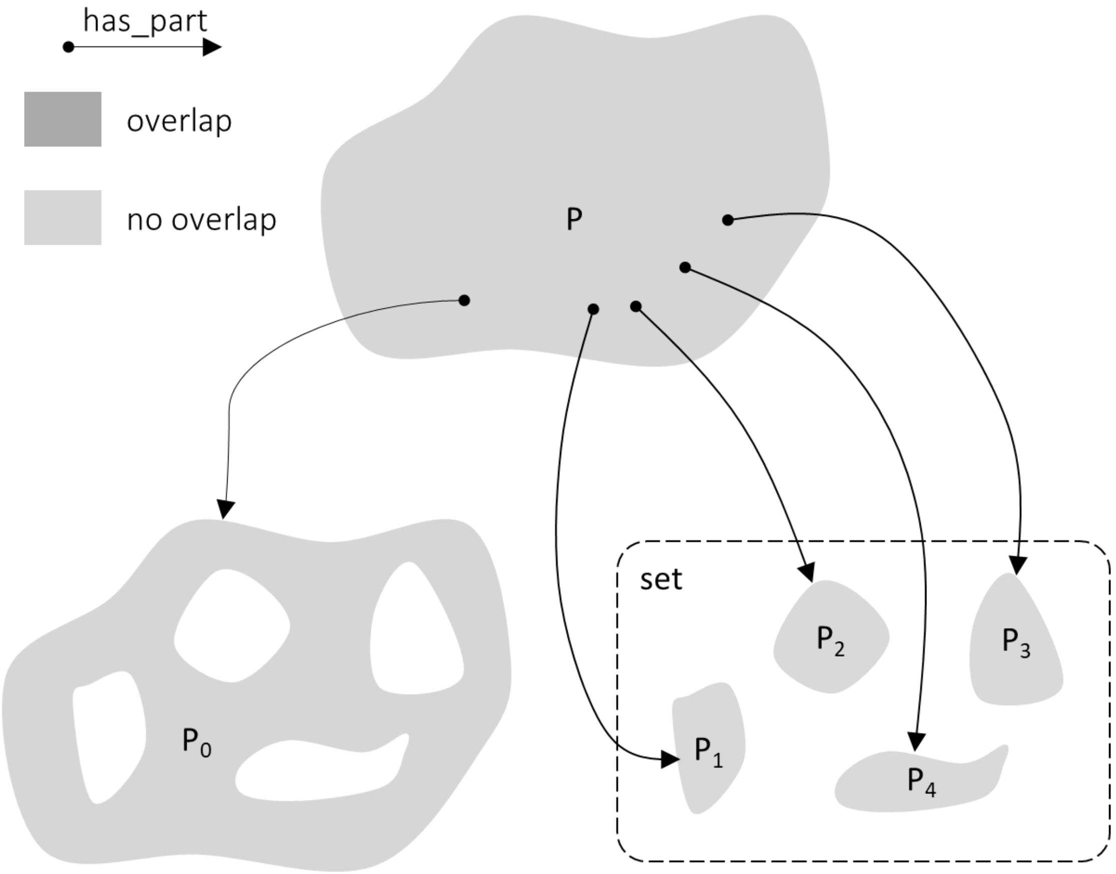
EMMO Item vs. Set

For example, a **gas P** can be defined as a fusion of the **molecules P_j with *j = {1,...,N}*** and the **region between them P_0**, which is a totally acceptable definition for an applied scientist since the volume of the whole gas plays an important role in the characterization of its thermodynamic properties (e.g. through the ideal gas law *pV=nRT*).

The molecules P_j with *j = {1,...,N}* can also be represented as a collection using a set. However, this set of molecules **possesses only a conceptual interest (e.g. as list) and not a direct physical meaning due to the lack of causal connection**.

In fact, for a molecule to interact with another one, we need a direct contact or a contact carrier, which for the gas is provided by the P_0 region (e.g. hosting the photons responsible for electrostatic interactions), while in a molecule set this contact is missing.



For this reason, **a physical phenomena can be represented only by an item** that comprises all involved parts (i.e. a fusion), since the objective of the physics approach is to provide a mean (e.g. mathematical models, physical laws) to express the causal relation between the parts involved in a phenomena. In other words, **sets are causally inefficacious.**

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(Dead) Abstract Objects (Walking)

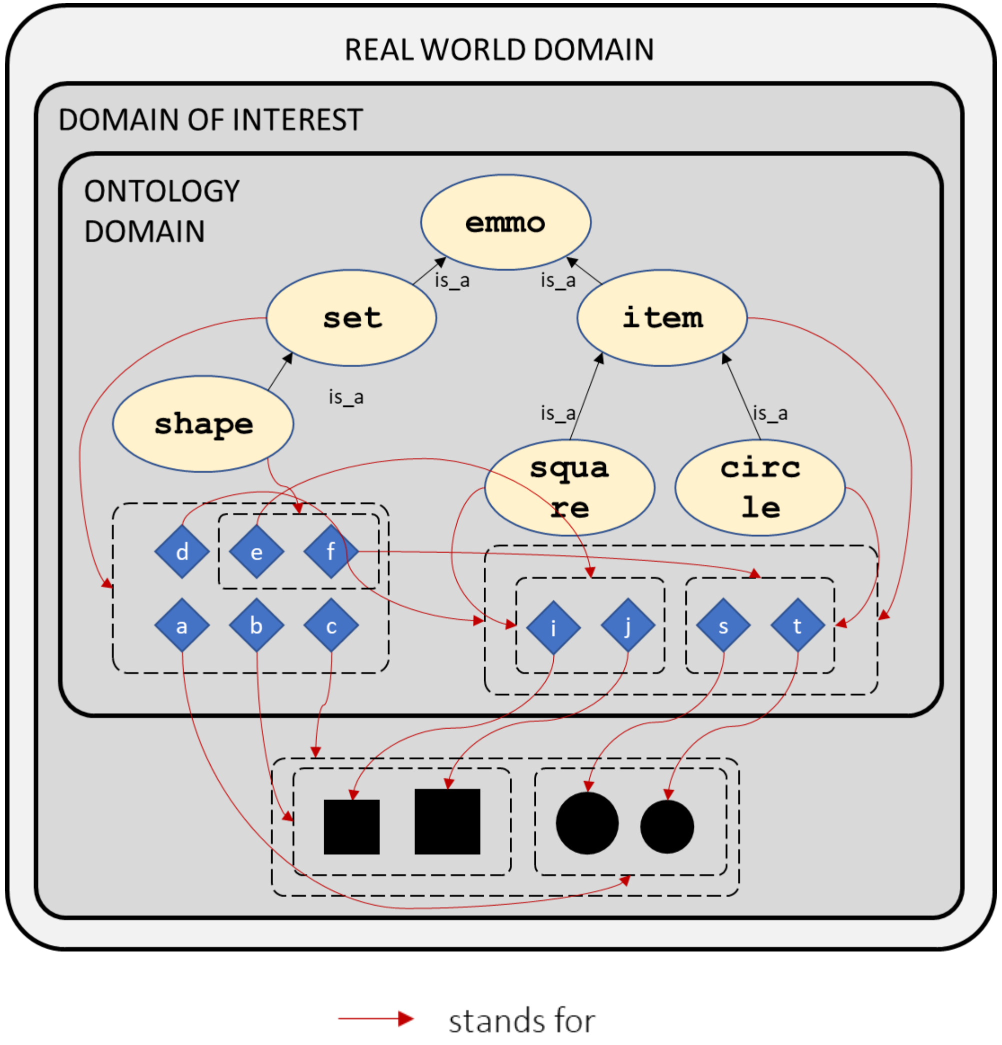
Abstract objects do not exist in the EMMO, and are replaced by sets of sets.

Still, in order to fully represent common abstract concepts within the ontology, we need to include the ontology itself in its domain of interest: the ontology should be able to describe itself (or part of itself).

We could create for example a class **shape** under **set**, that would have as individuals *e* and *f*, enabling a **powerful nominalistic representation of abstract concepts, as shapes**, under a mereotopological system.

In this context, the **item** branch classes will be sets of individuals, while the **set** branch classes will be sets of sets of individuals.

In the EMMO an abstract object is then replaced by sets that categorized other sets, on a second abstraction layer with respect to sets as simple individual containers.



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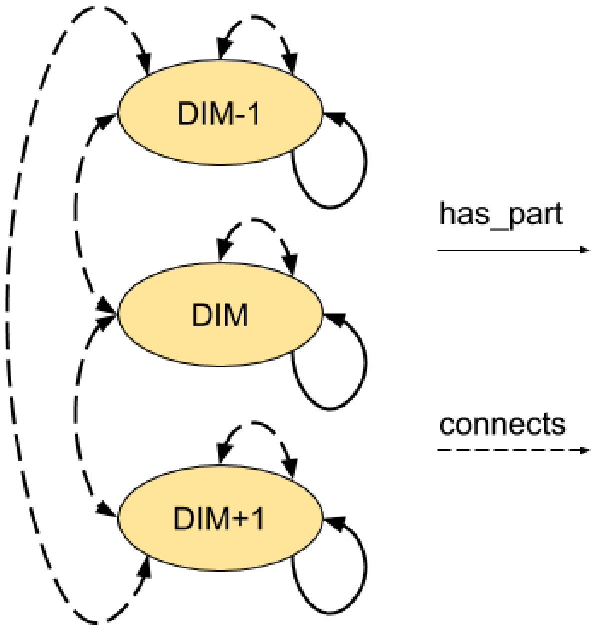
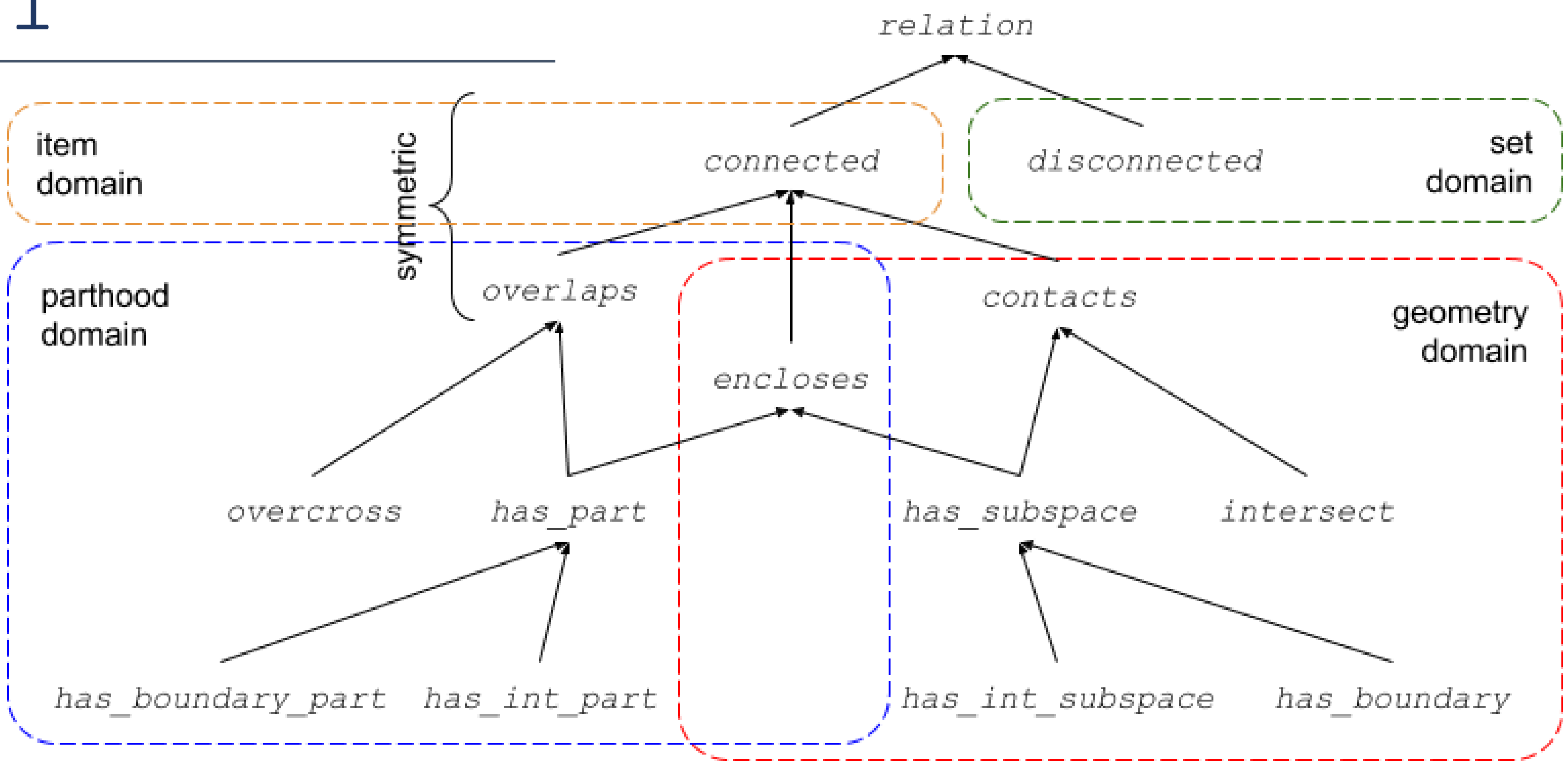
GEOMETRICAL LEVEL - 1





EMMO physicalism requires **that everything physical is 4D**, while **subdimensional objects are considered non-physical**, but still real.

To implement this perspective, the most important EMMO assumption at this level of the hierarchy is that **parthood relations occur only between items with the same topological dimension.**

The bifurcation of the relation hierarchy at *encloses* level in *has_part* (parthood branch) and *has_subspace* (geometry branch) is the way used by the EMMO to implement this feature. The *has_subspace* relation is used to relate individuals that stand for real objects of different dimensions and in particular between the higher dimensional object that encloses the lower dimensional one (i.e. slice) or between a lower dimensional object that encloses a higher one (i.e. boundary).

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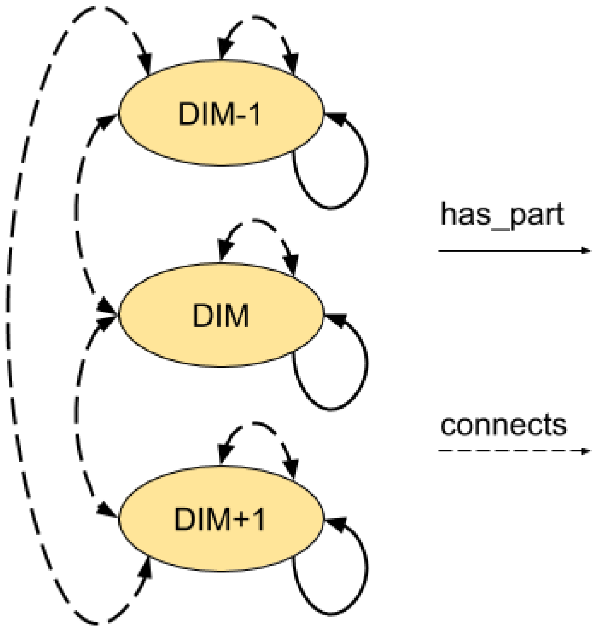
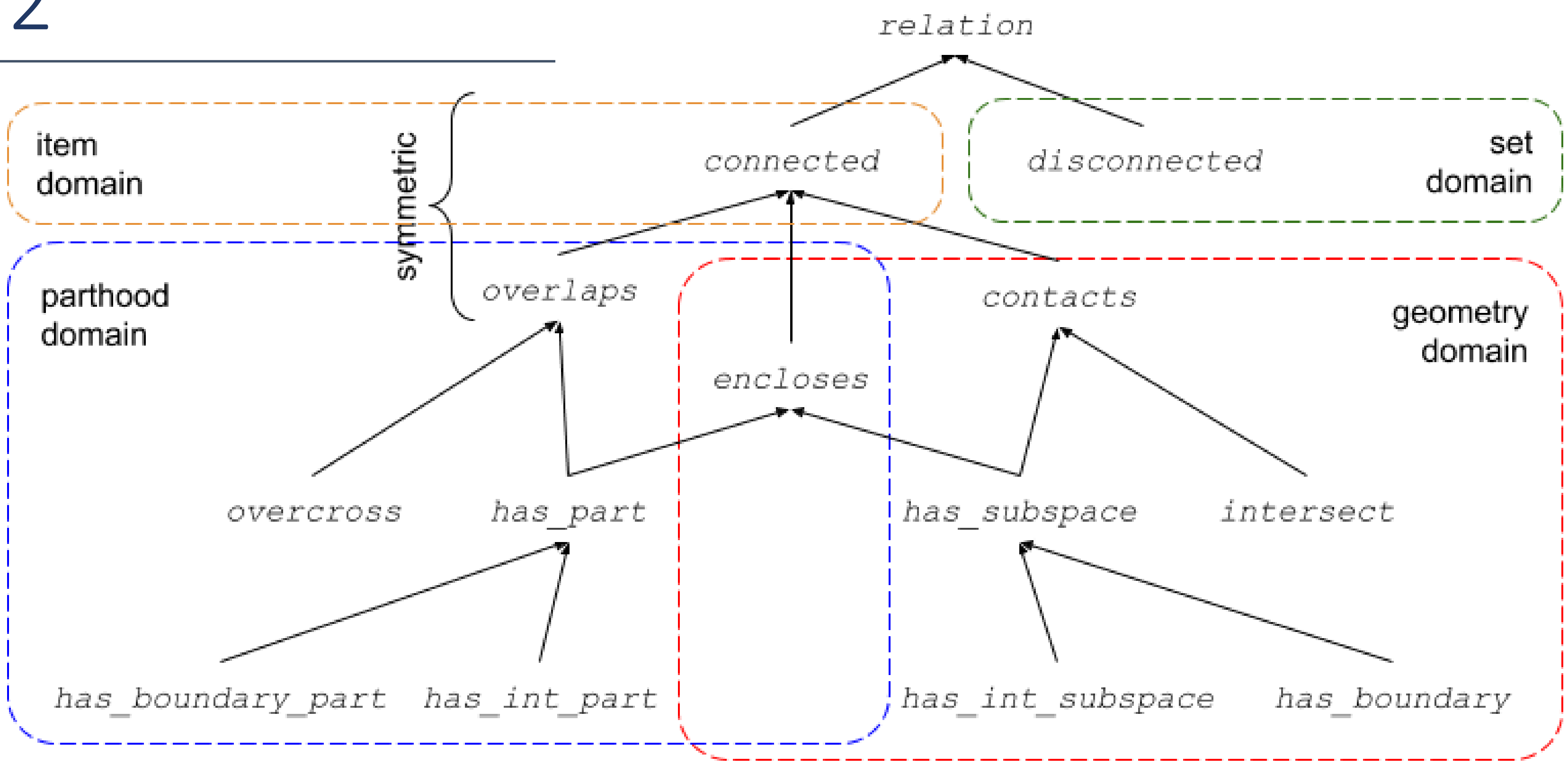
GEOMETRICAL LEVEL - 2





The *has_subspace* relation is used to relate individuals that stand for real objects of **different dimensions** and in particular between the **higher dimensional object that encloses the lower dimensional one (i.e. slice)** or between a **lower dimensional object that encloses a higher one (i.e. boundary)**.

This relation can be better understood by interpreters if items are considered to be part of topological manifolds with a specific topological dimensions (e.g. 4-manifold, 3-manifold) for which the subdimensional relation is the operation of identifying self-connected subregions of lower dimensionality (e.g. a line lying on a plane, a surface enclosed in a 3D space).

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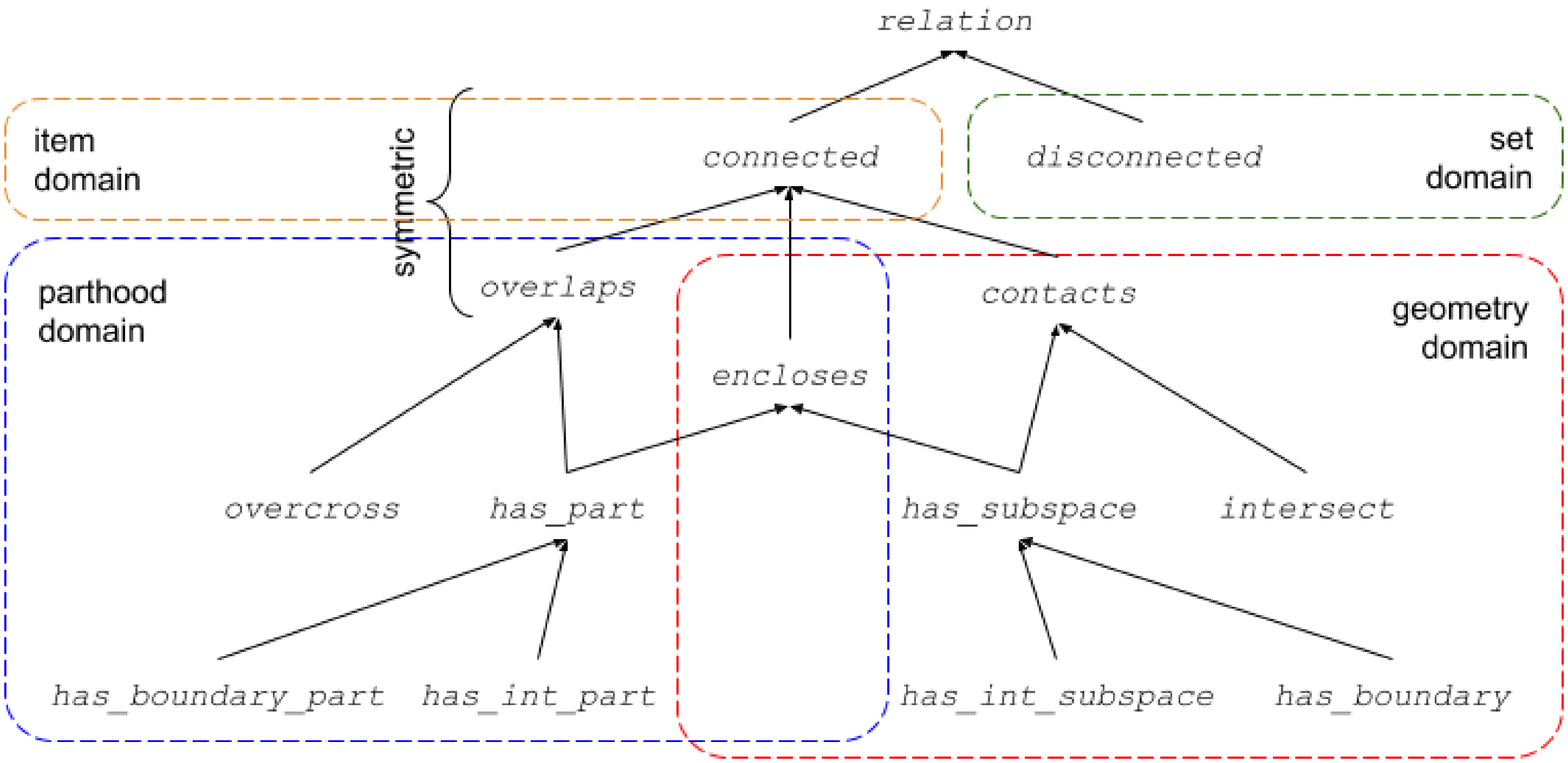
GEOMETRICAL LEVEL - 3

`has_subspace`
a primitive relation: it represent the act of identifying sub-dimensional regions within a topological manifold

`intersect`
is complementary to `has_subspace`, and represents the relation between a lower dimensional object w that is in contact with an higher dimensionality object x but it is not enclosed by it, i.e. a contact with w does not necessarily implies a contact with x

`has_boundary`
a subspace w, enclosed within a higher dimensional object x, is called a boundary if there is another object y, with same dimensionality of x, that encloses w and does not overlap x

`has_int_subspace`
the complementary relation of `has_boundary`



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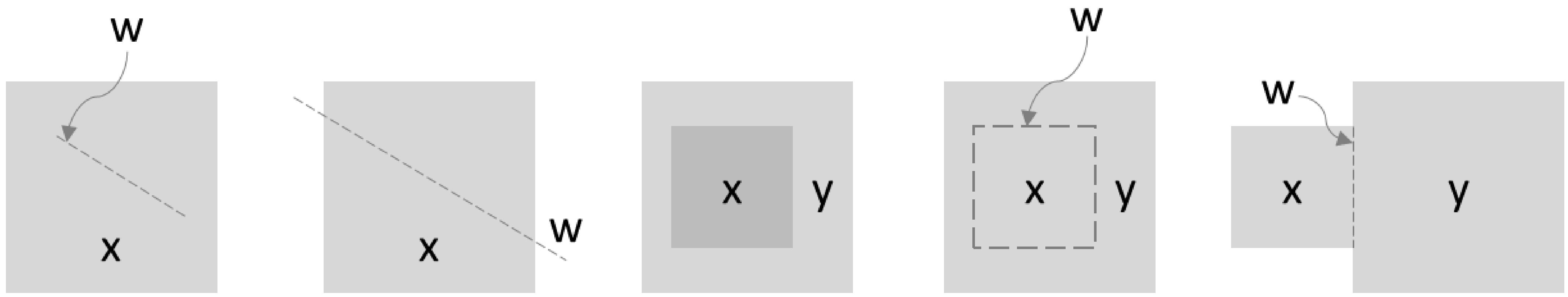
Geometrical Level - 4

In these examples, w is always a subspace of dimensionality lower that x and y, while x and y have the same dimensionality



`x has_int_subspace w`
`x encloses w`

`w intersects x`
`x intersects w`

`y encloses x`
`y has_part x`

`y encloses x`
`w encloses x`
`y encloses w`
`x has_boundary w`

`x contacts y`
`y contacts x`
`x has_boundary w`
`y has_boundary w`

A part does not share by connection a boundary with the whole, since <u>boundaries occur only between non overlapping objects</u>

e.g. there is no boundary between a piston and the whole engine, since the engine already comprises the piston, while there is a boundary between the piston and the other parts of the engine, like the cylinder or the combustion chamber

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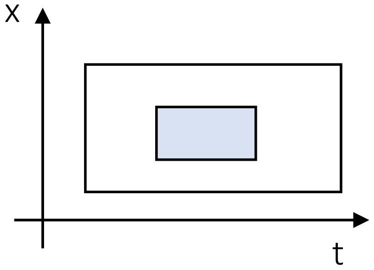
4D Parthood and Slicing

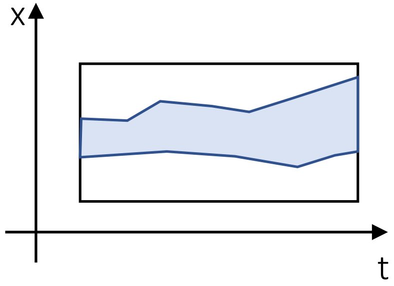


encloses (mereotopology)

has_part (4D mereology)

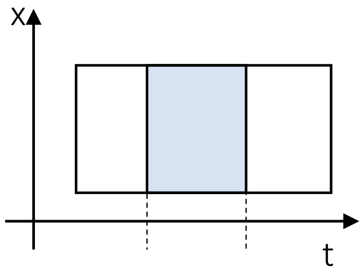
has_subdimensional_space (topology)

has_spatial_part



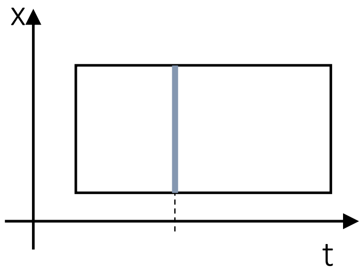
Same dimensionality of the whole.
Extended through all lifetime of the item.
Can be:
has _spatial_proper_part
has _spatial_direct_part

has_temporal_part



Same dimensionality of the whole.
Extended through all spatial extension of the item. The left and right boundary must express simultaneity in a specified reference frame.
Can be:
has _temporal_proper_part
has _temporal_direct_part

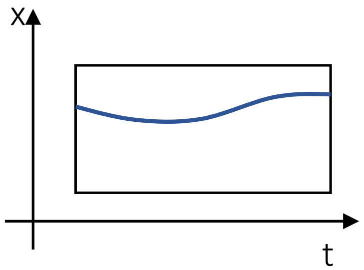
has_time_slice



Reduced dimensionality by one (e.g. a spacetime becomes a space)

Instantaneous in time. Must express simultaneity in a specified reference frame.

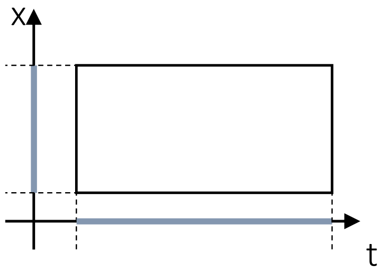
has_space_slice



Reduce spatial dimensionality below three. The user can «carve» the spacetime using specific slicing criteria.

e.g. a spacetime in 3D+1D (3D space and 1D time) becomes a 2D+1D tube (2D space and 1D time)

has_projection



Reduced dimensionality to 0D-1D-2D-3D in space three or 0D-1D in time.

e.g. a spacetime becomes a space

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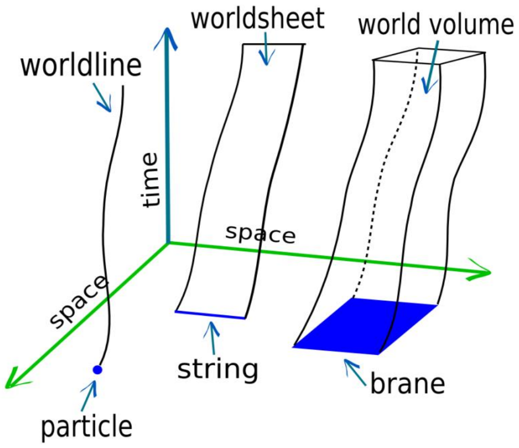
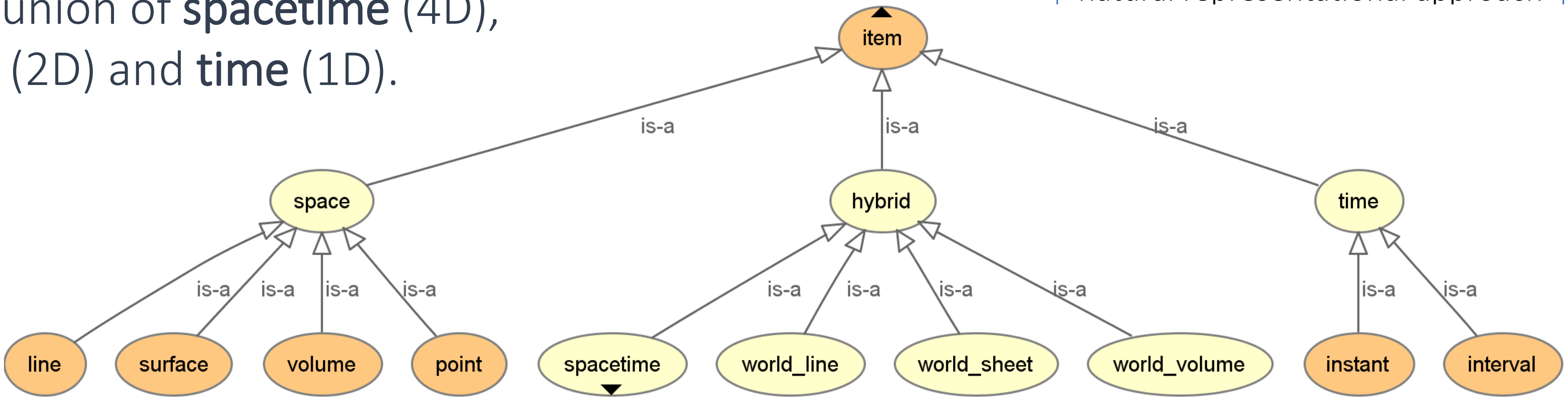
ITEM SUBCLASSES

4D (3D space + 1D time) is the natural representational approach

item is the disjoint union of **spacetime** (4D), **space** (3D), **surface** (2D) and **time** (1D).





Each branch of **item** can only have parts of the same type.

It means that parthood is only between substrates of the same dimension (e.g. a **spacetime** has no **space** parts).

The boundary of a **substrate** is not part of it (mereological relation) but a **slice** (topological relation) is a part with lower dimension.

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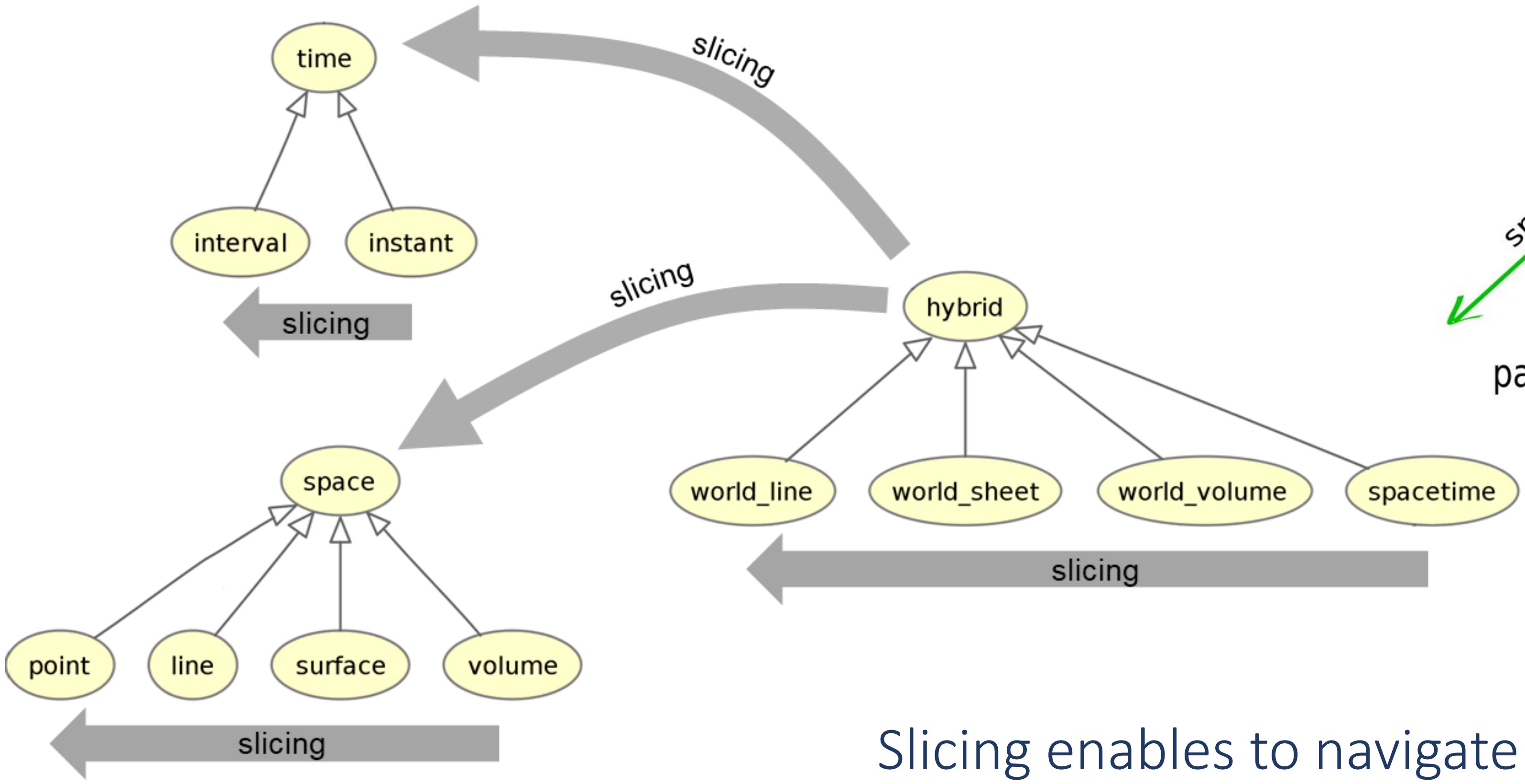
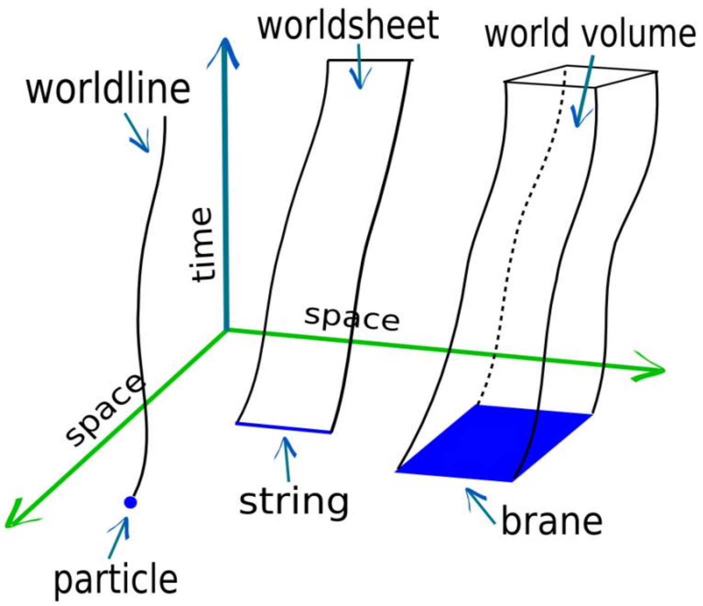
SLICING BETWEEN DIMENSIONS





Slicing enables to navigate through sub-dimensional regions of the same spacetime object.

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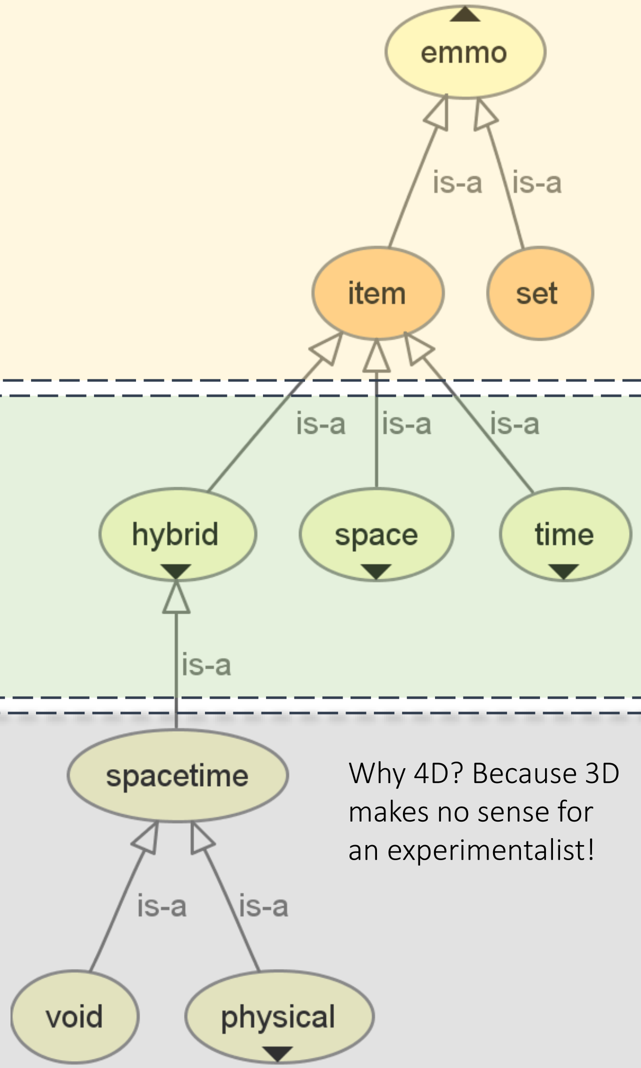
EMMO CORE OVERVIEW



ABSTRACT CONCEPTUAL LEVEL

Clear separation between **set** (set theory) and **item** (mereotopology).

set individuals are collection of **item**s according to defined concepts (e.g. red entities).

items individuals stand for something that is 'real', i.e. a 4D portion of the universe.

In the EMMO abstract concepts are represented as the **set**s that concretize them (e.g. friendship is the collection of all friendship acts) embracing a rigorous nominalistic view. There are no individuals that stand for an abstract concept, except under **set**.

GEOMETRIC/TOPOLOGICAL LEVEL

items unfolds in space (3D) and time (1D) and can be sliced in pure **time**, pure **space** or **hybrid** space and time entities.

Why 4D? Because 3D makes no sense for an experimentalist!

PHYSICAL LEVEL

Real world entities exists only in full 4D **spacetime** (3D space and 1D time), i.e. you can't partition a cake in infinitely thin slices!

A **spacetime** that can be perceived by (interact with) the interpreter is a **physical**.

If the **spacetime** entity is empty in terms of perception, is a **void**.

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EMMO PHYSICAL LEVEL

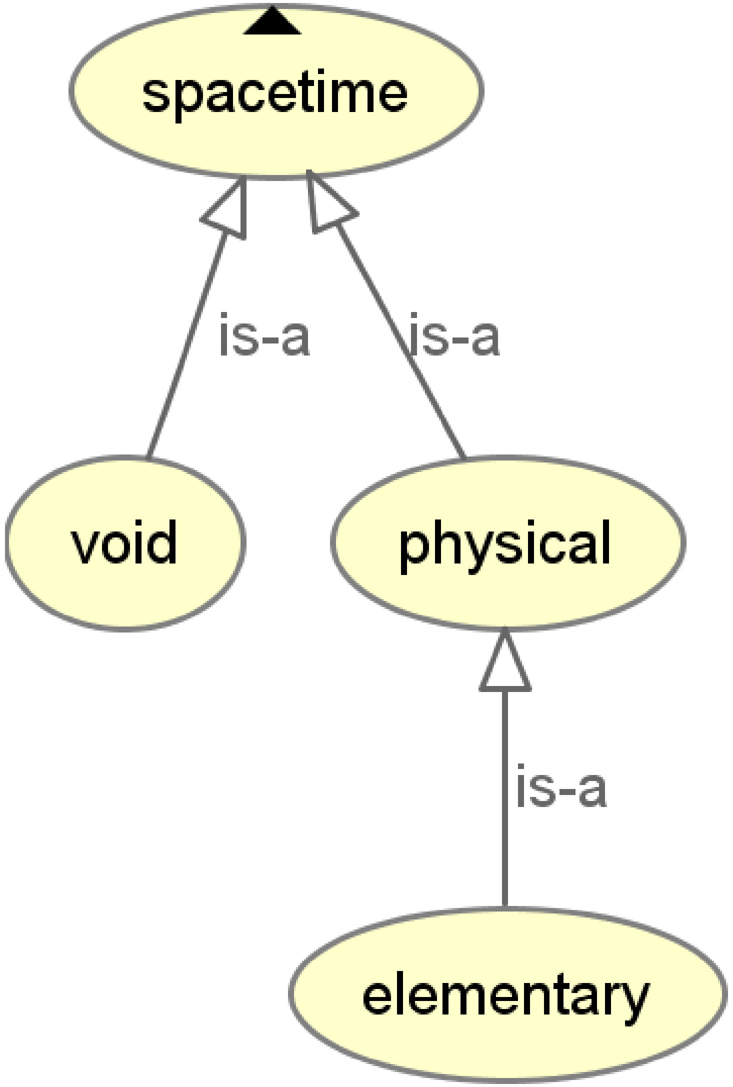
The reductionistic approach lead to the assumption that the most fundamental physical object is an elementary object, whatever it means for the interpreter (e.g. an elementary particle or a mechanical component).

The most natural categorization for a physicist or an engineer should then be to classify spacetime regions in either elementary objects or non-physical objects (i.e. void regions), restricting physical objects only to elementary particles, and then to describe real world as result of elementary objects interactions.

But this is not a practical representation choice because:

- there are way too many elementaries (even if we restrict a elementary to atoms) that composes real world objects in which we are interested (e.g. 10^{25}-10^{29} #/m^3)
- most of the physics theories deals with objects that have several levels of composition above and below them (i.e. granularity levels), going from the nuclear to the cosmological scale, usually focusing on a specific granularity levels (e.g. atomistic, mesoscopic)

We need EMMO to be able to represent **physical objects that are composition of elementaries and void!!!**



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EMMO MEREOLOGICAL COMPOSITION - 1

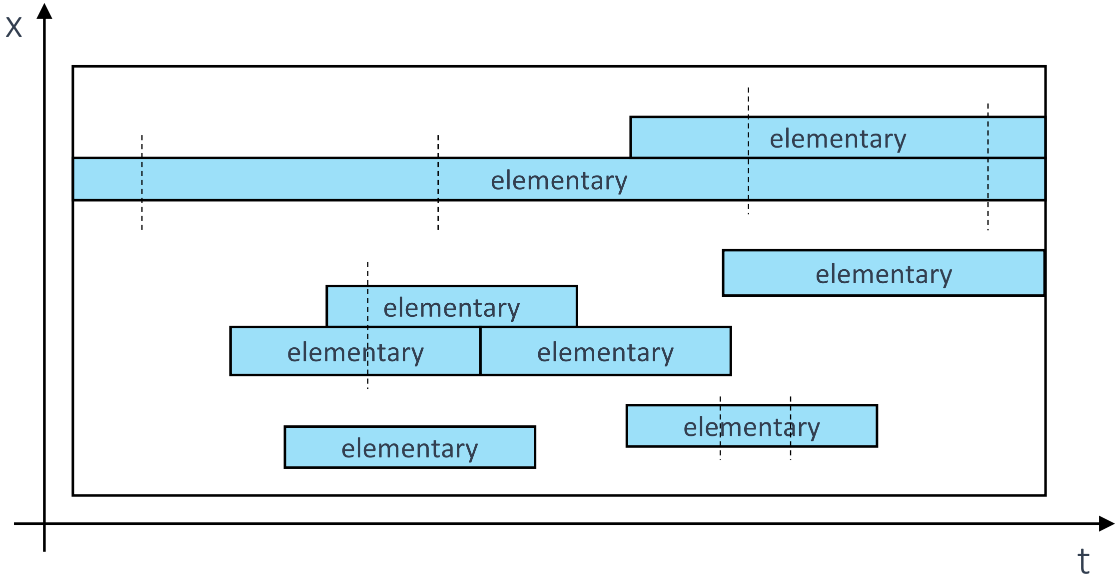
The EMMO basic mereological decomposition assumption is that the most basic manifestation of a physical object is represented by an elementary object whose proper parts can be only temporal parts.

α–τομοσ (a-tomos) = undivided; philosophers are using correctly the word “atom”, while physicists proven themselves wrong after splitting the so-called “atom” (Hahn and Meitner discovery of fission)

“4D Atom” axiom:

$$Ax \Rightarrow \forall y(PPyx \Rightarrow TPPyx)$$

“Atomicity” axiom: $\exists y(Ay \land Pyx)$



The ‘a-tomic level’ in EMMO is defined by the **elementary** class.

A generic physical can always be decomposed in proper parts up to elementary level using the proper parthood.

An elementary can still be decomposed in temporal parts, that are themselves elementary.

An elementary particle, that expresses some fundamental physical properties (e.g. mass, charge, spin) can be represented by an **elementary** in a physics ontology.

However, in another material ontology an **elementary** can be something else, depending on the perspective (e.g. a brick, for a LEGO ontology)

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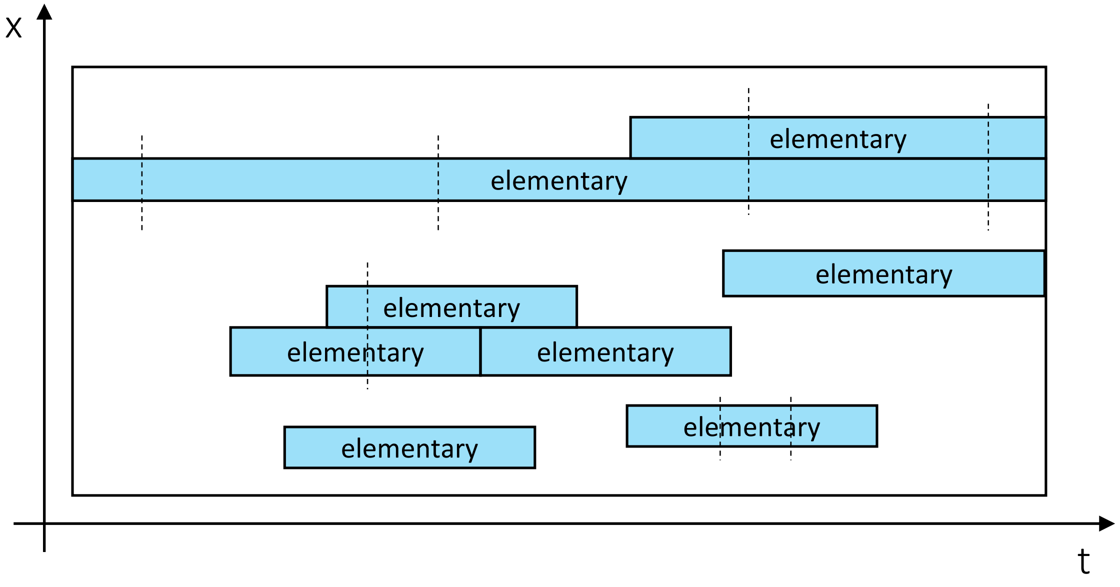
EMMO MEREOLOGICAL COMPOSITION - 2

This definition prevents partial spatial overlapping of elementary objects, since this would imply subparts that are shared between more than one elementary object.



While this is a straightforward representation for fermionic like objects (including macroscopic ordinary objects) that captures the essential fact that they cannot share the same spacetime region, it is not fully consistent with the bosonic nature of the force carrier particles (e.g. photons) that can occupy the same spacetime region.

For this reason superimposed bosonic elementary objects in the same spacetime region are represented in the EMMO as delocalized objects i.e. parts of a physical object and located within its spatial domain, but without a specified position.

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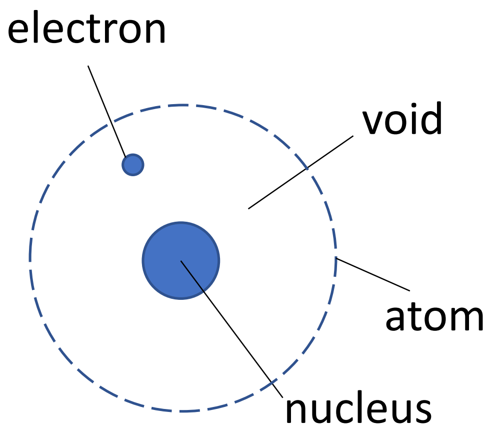
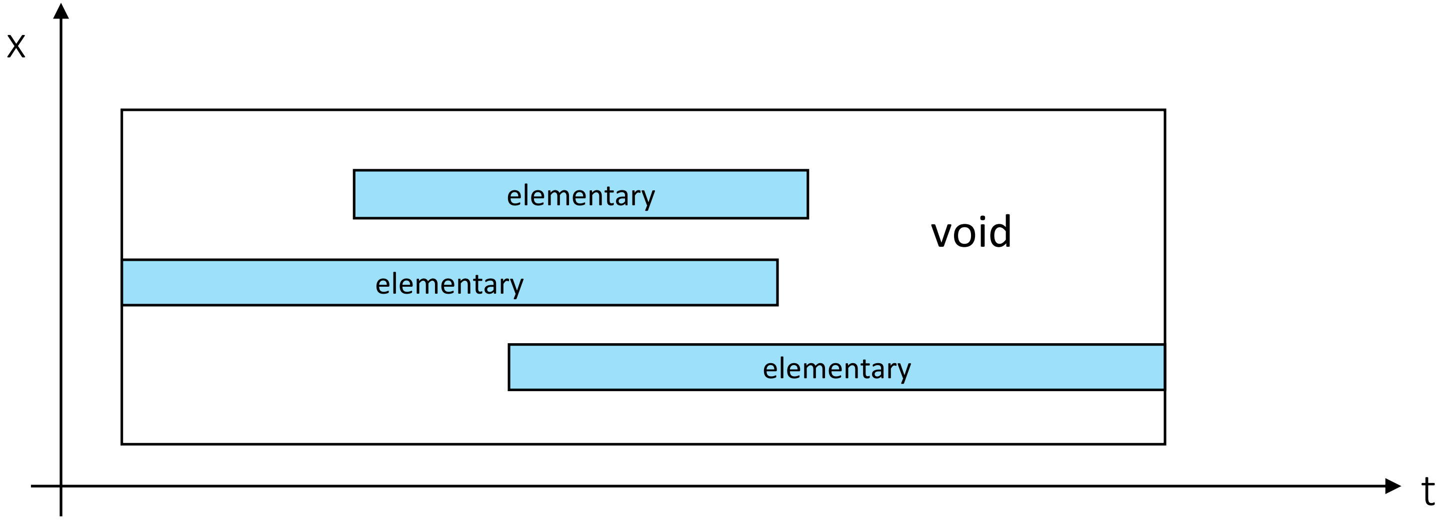
The Void Issue (...or Opportunity)

We must also take into account the presence of void between elementary that composes a higher granularity level entity.

Real matter in a human perspective is made pre-dominantly of voids (i.e. interatomic, between nucleus and electrons in an atom, space between molecules in a gas).

Moreover, the void object is paramount for the representation of quantum systems since, after a measurement process that collapses the wavefunction of a system, the region of spacetime without localized objects is equally important in terms of achieved information as the object that has been localized.





VOID

A spacetime that has no elementary parts.

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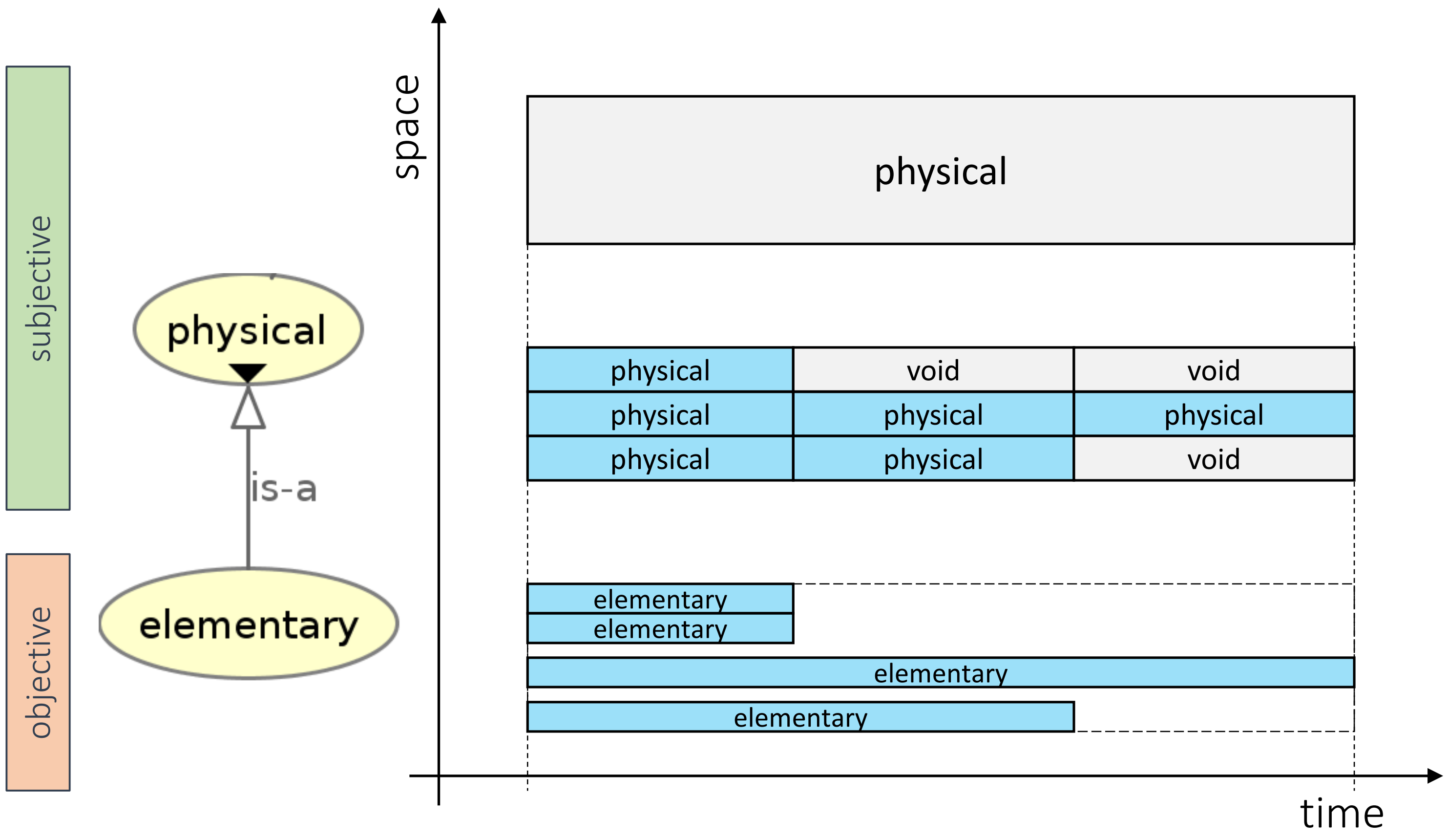
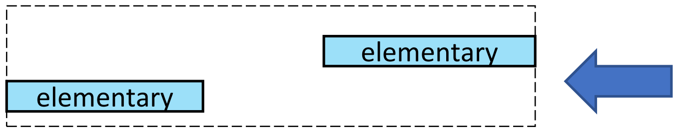
EMMO Core Mereotopology



The **EMMO** identifies a parthood hierarchy of physical objects, by introducing the concept of:

- **elementary** as the fundamental, non-divisible, constituent of entities (i.e. atomistic mereology)
- **physical** that satisfy both:
  - has temporal parts only **physical**-s
  - is an **elementary** or has spatial part some other **physical**-s

so that a **physical** entity can be defined using a multiscale perspective.



This is not a physical, because it has at least one non-physical temporal part

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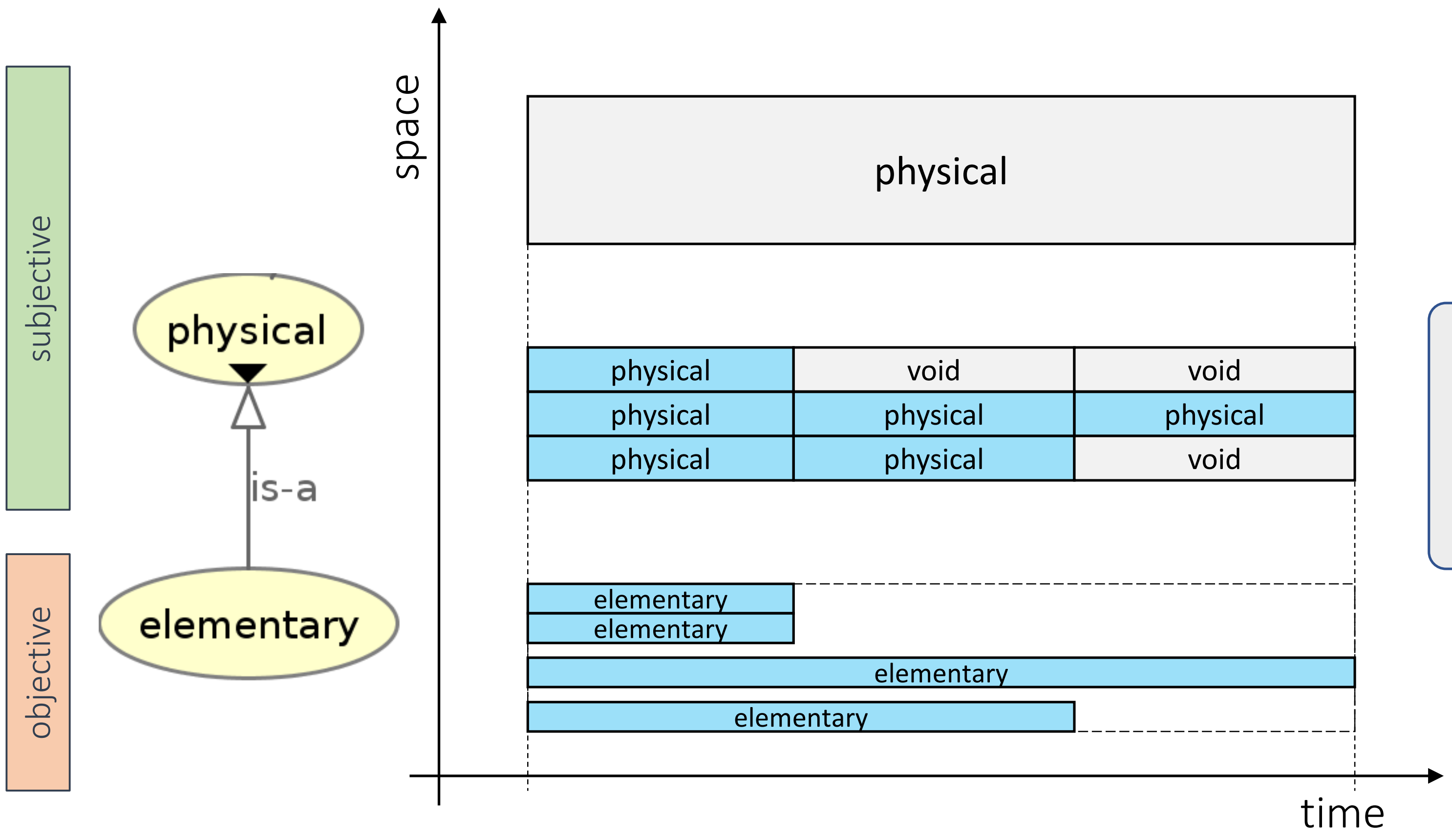
EMMO Core Mereotopology



It follows that a physical object can also include void as spatial proper parts, including also void regions surrounding it or enclosed by it.

It's important to underline that **there are no other particular criteria to be satisfied by the void or physical spatial parts of a physical object**, except for the above mentioned two

e.g. a spacetime region having as spatial part a single electron enclosed by a sphere of light years of void is a perfectly eligible physical object, according to the EMMO.

While counterintuitive, this definition fits perfectly the need for:

- taking into account the **quantum nature of physical systems**, in which the actual position of sub-components (e.g. electrons in an atom) is not known except for its probability distribution function that extends indefinitely through spacetime
- taking into account the fact that large entities (e.g. devices, cars, materials) have some void into them, so that the **nature of physical objects is intrinsically porous**

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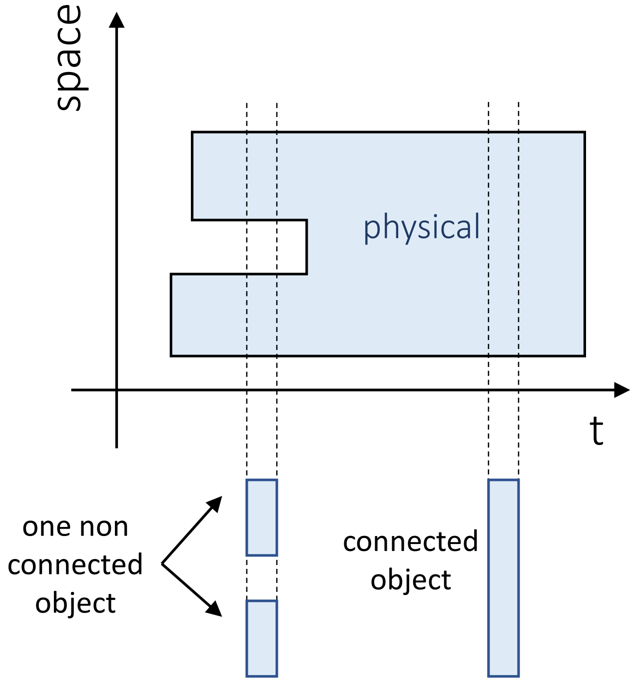
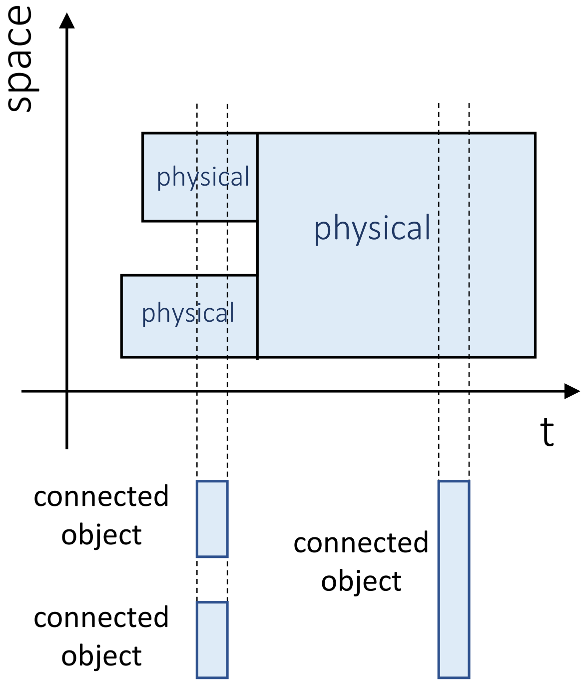
EMMO Core Mereotopology

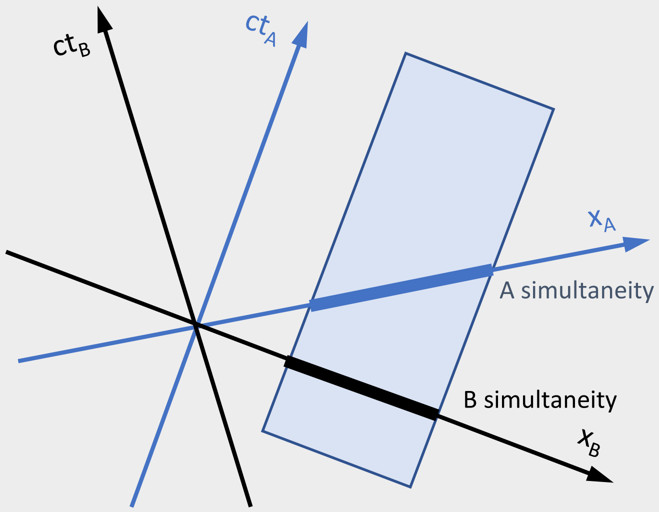
As consequence, each temporal part of a physical is a connected region, i.e. an item and not a set.

This depends on the concept of simultaneity that can be different for each reference system (relativity).





Simultaneity and EMMO



A spacetime is valid for all the reference systems.

A reference system must be provided for each physicals declaration and when a temporal slicing is done over a spacetime.

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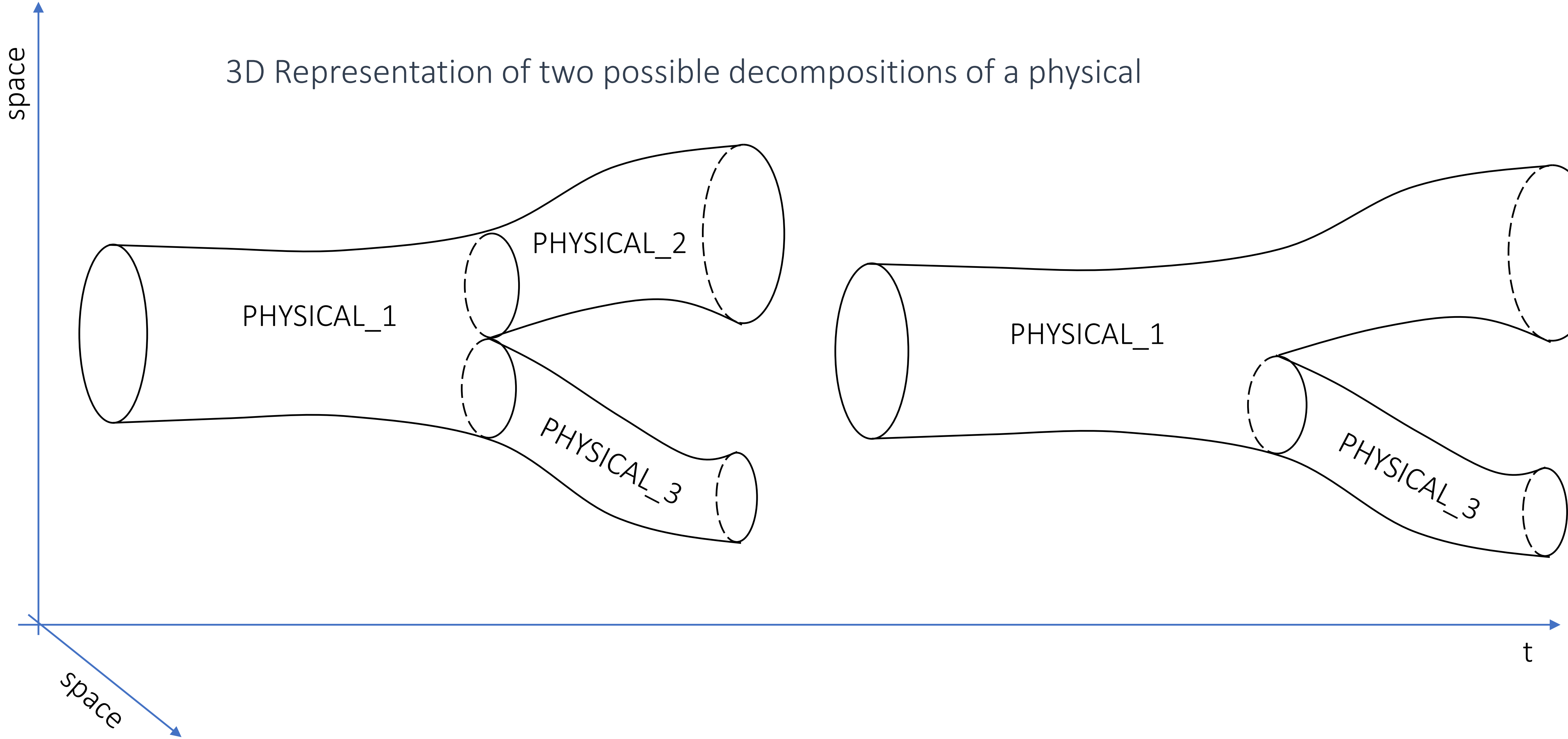
EMMO Core Mereotopology

3D Representation of two possible decompositions of a physical



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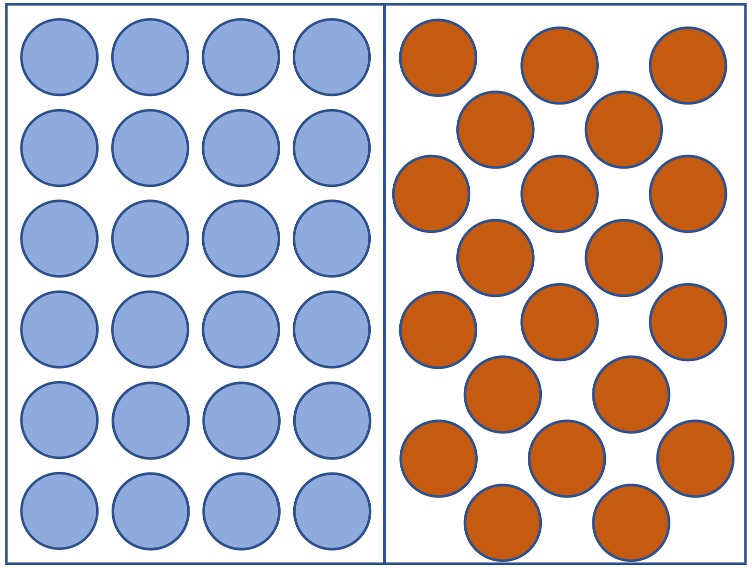
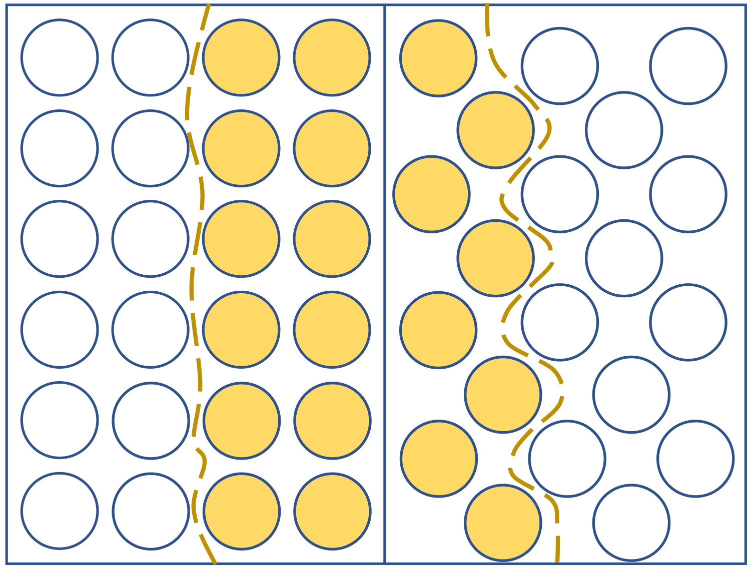
EMMO Material Ontology

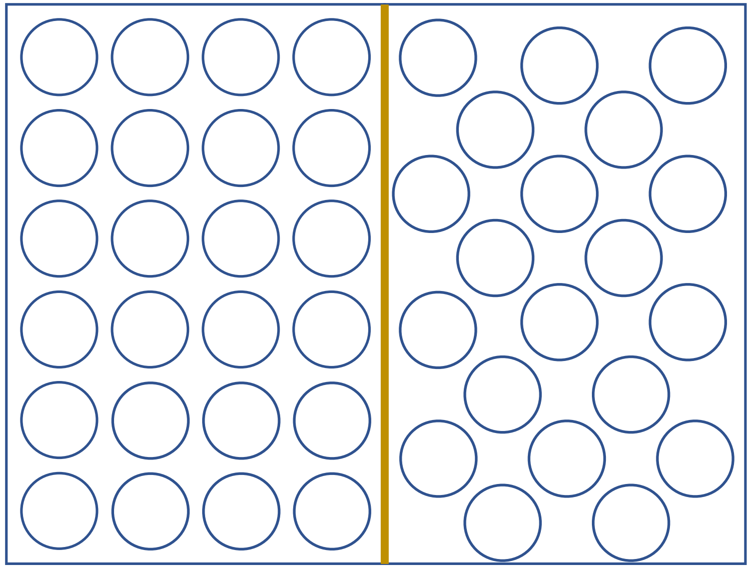


physical **a** (3D + 1D)

physical **b** (3D + 1D)



boundary (**physical**) (3D + 1D)



interface (**world_volume**) (2D + 1D)

BOUNDARIES

VS

INTERFACES

The boundary between **physical**s **a** and **b** can be defined as another **physical** that includes at least one **elementary** from both entities.

The boundary is a 3D+1D entity.

The interface between **a** and **b** can be defined by space slicing **a** or **b** and is e.g. a 2D + 1D entity (a **world_volume**), intended as a **item** entity but not a **physical**.

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Mereology of Direct Parts

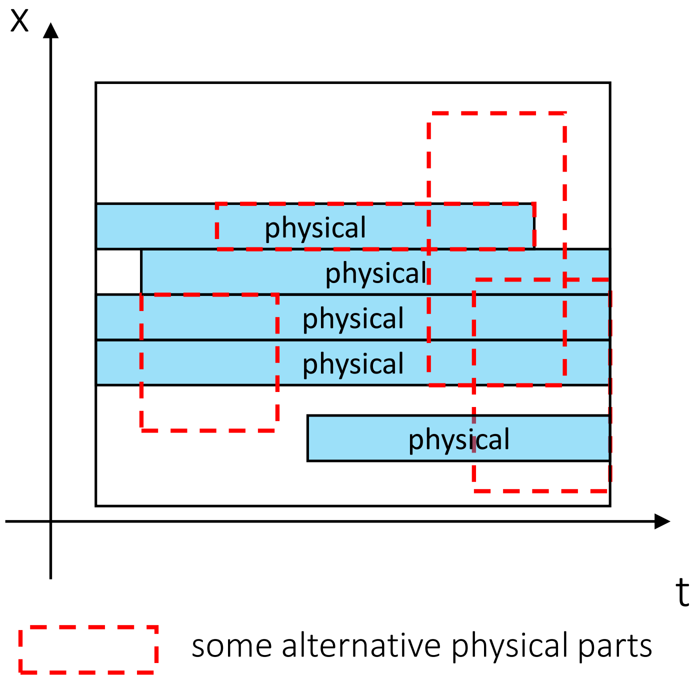
Up to now, no compositional rules are declared for a physical object: there is total freedom in defining a physical as part or made of other physical, as long as:

1. it coincides with an elementary OR
2. has only physical temporal parts

Physical objects can overlap each other, and this hampers defining univocal entities.

Physical object concept is very flexible as one can define arbitrary parts of spacetime (that includes other physicals) to be a physical.

However, no particular structure or granularity is easily representable except for elementary.



We need a stronger compositional principle in order to create separate levels of parthood and describe granularity in a univocal way.

direct parthood relation

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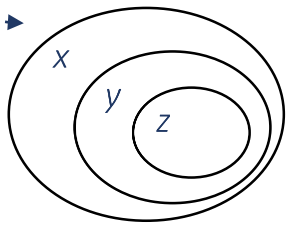
Mereology of Direct Parts

transitive proper parthood **is_proper_part_of**

↑

proper parthood **is_direct_part_of**

- By dropping transitivity **is_direct_part_of** identifies the entity proper parts that are at the <u>very next lower granularity level.</u>
- Direct parthood requires also the existence of a non overlapping partitioning.
- Direct parthood is functional.

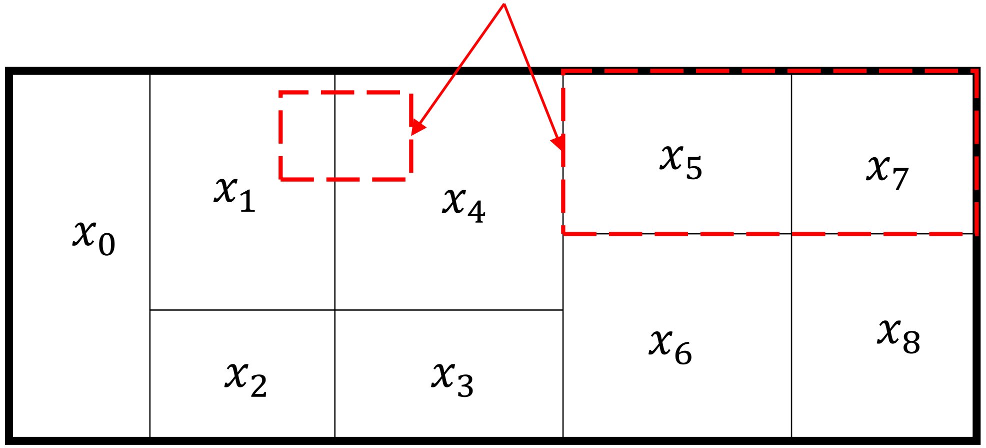


y ***is_direct_part_of*** *x*
z ***is_direct_part_of*** *y*

z <u>is not</u> direct part of x

e.g.: nucleus **is_direct_part_of** atom
proton **is_direct_part_of** nucleus

not allowed as direct parts



Axioms:

$DPxy \Rightarrow PPxy$	direct part is a **proper part**
$DPxy \Rightarrow \forall z\,(DPzy \Rightarrow \neg Oxz)$	direct parts do not **overlap**
$DPxy \Rightarrow \forall z\big(\neg(DPyz \wedge DPxz)\big)$	direct part is **non transitive**
$DPxy \wedge DPxz \Rightarrow y = z$	direct part is **functional**

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Mereology of Direct Parts

$DPxy \Rightarrow PPxy$	direct part is a **proper part**	A direct part is always "less" than the whole, making it useful for a hierarchy definition.
$DPxy \Rightarrow \forall z\,(DPzy \Rightarrow \neg Oxz)$	direct parts do not **overlap**	Direct parts are a partitioning of a whole with distinct parts.
$DPxy \Rightarrow \forall z\big(\neg(DPyz \wedge DPxz)\big)$	direct part is **non transitive**	Direct parts define single steps in granularity, identifying the lower the upper level of composition of a whole.
$DPxy \wedge DPxz \Rightarrow y = z$	direct part is **functional**	Items declared by means of direct parthood relations cannot overlap, so that this item granularity is expressed by a tree.

Direct parthood is intended to be used primarily in the declaration of primitive classes i.e. is a powerful tool (or better, a set of rules) that can be used by a material ontologist to build a taxonomy for representing real world entities.

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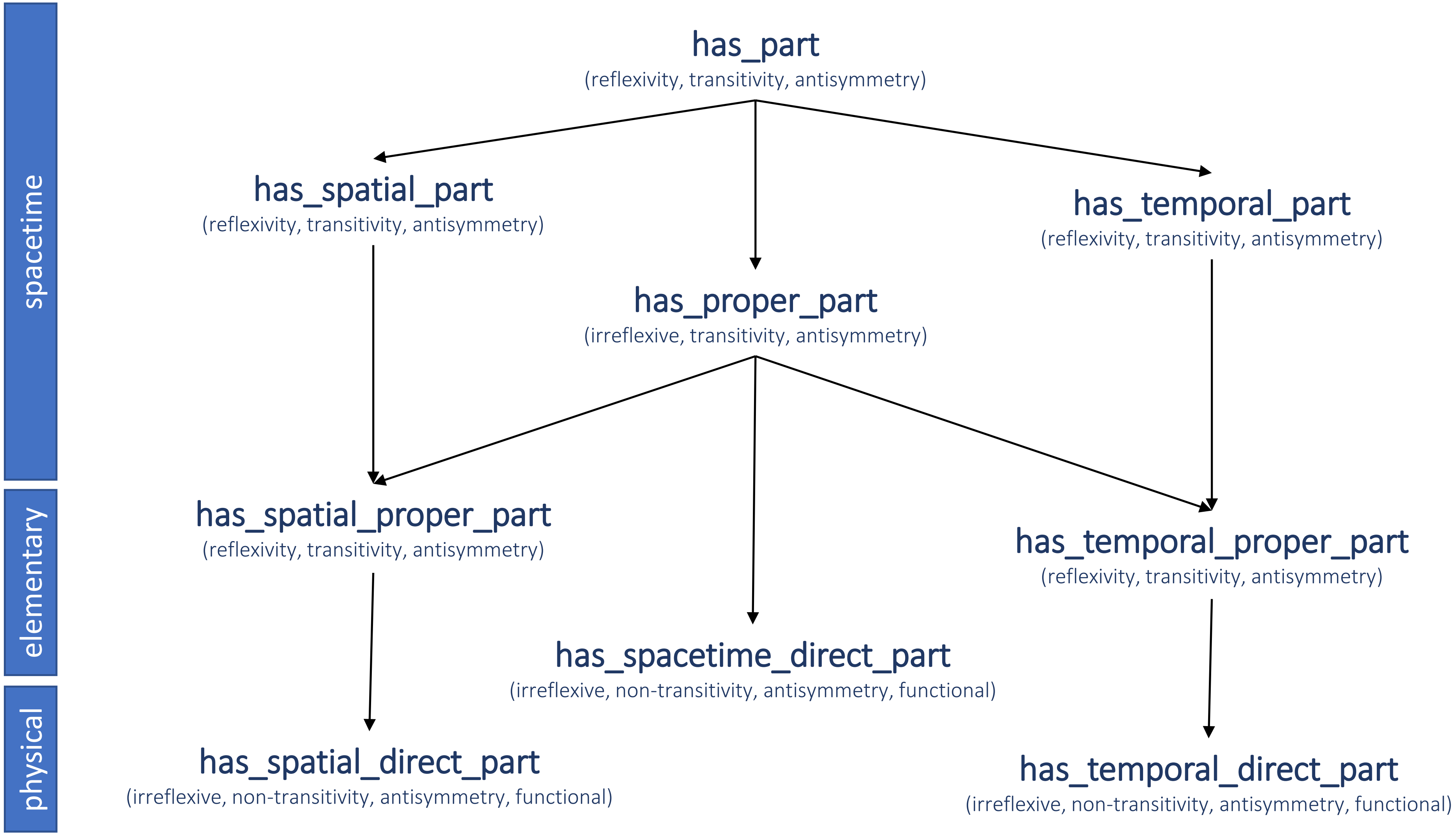
Mereology of Direct Parts



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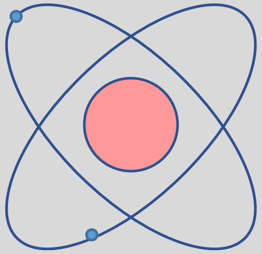
Mereology of Direct Parts - Example

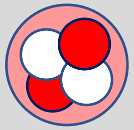
AXIOMS

He atom **has_direct_parts**:
- electron_1
- electron_2
- He nucleus



$n = 3$

He nucleus **has_direct_parts**:
- neutron_1
- neutron_2
- proton_1
- proton_2

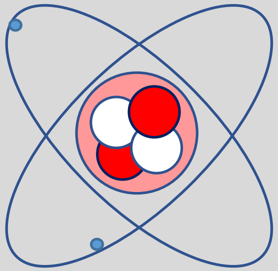


$n = 4$

THE **EMMO** <u>DIRECT PARTHOOD</u> RELATION CONCEPT THAT LETS US CREATE A <u>HIERARCHY OF ENTITIES WITH DIFFERENT GRANULARITIES</u>

IMPLICATIONS ON ATOM

He atom **has_proper_parts**:
- electron_1
- electron_2
- neutron_1
- neutron_2
- proton_1
- proton_2



$n = 6$

He atom **has_direct_parts**:
- electron_1
- electron_2
- He nucleus

$n = 3$

Proper parthood gives information about all proper parts of an entity at <u>all levels of granularity</u> (granularity is flattened).

Atom inheres the nucleus proper parthood relations due to <u>transitivity</u>.

Direct parthood gives (and retains) information about the entities that constitutes the direct lower granularity level.

Atom does not inheres the nucleus direct parthood relations due to <u>the lack of transitivity</u>.

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GRANULARITY CLASSES

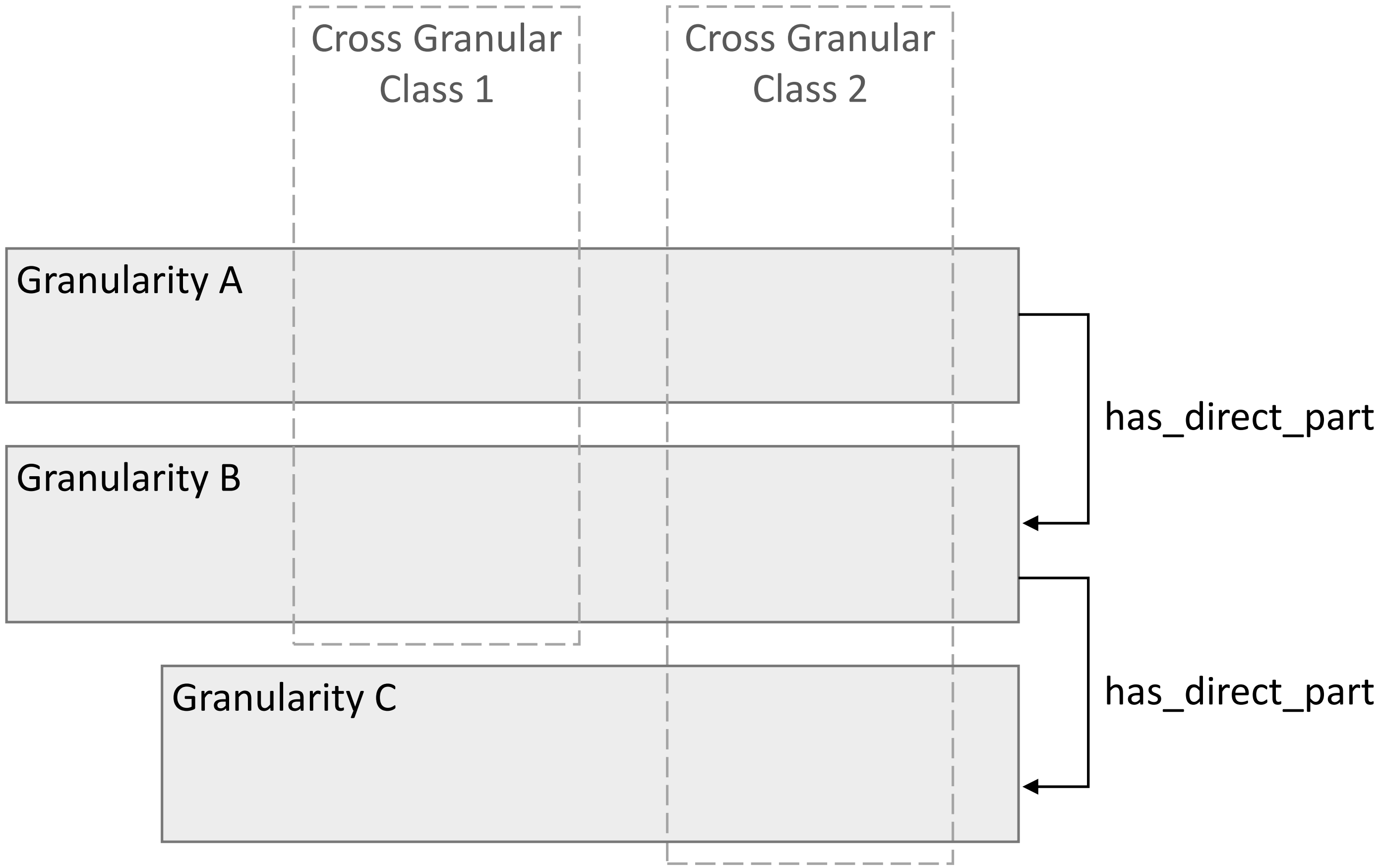
In the **EMMO** material description branch classes can be:

- **Granularity classes**, i.e. materials with specific granularity are described by means of hierarchies of direct parthood relations

  (e.g. molecules made of atoms, protons made of quarks)

- **Cross-granular classes**, i.e. are declared by means of properties of the individual other than composition

  (e.g. a nanomaterial is defined by its size and not by its constituent parts)



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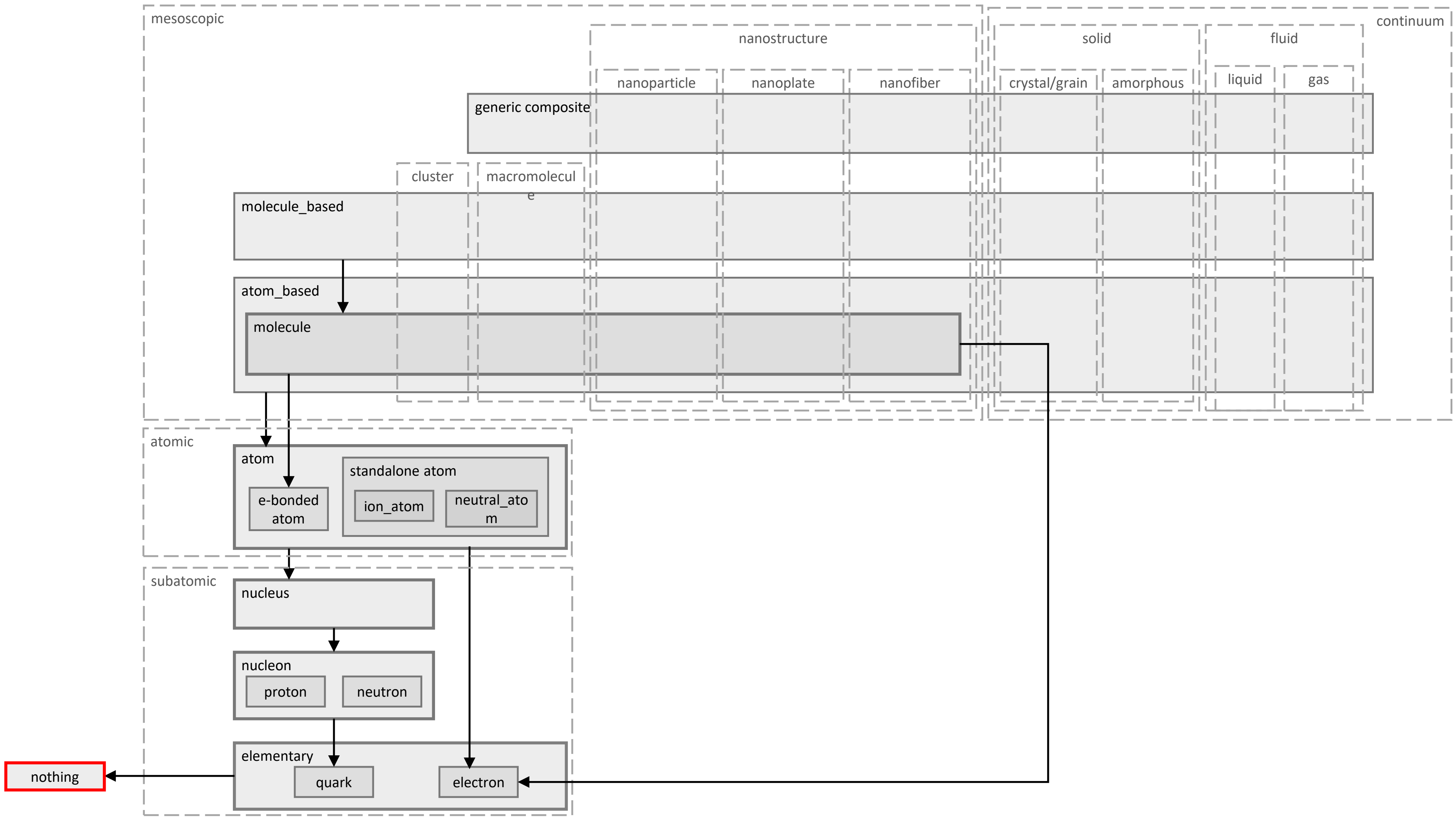
Granularity Hierarchy - Example



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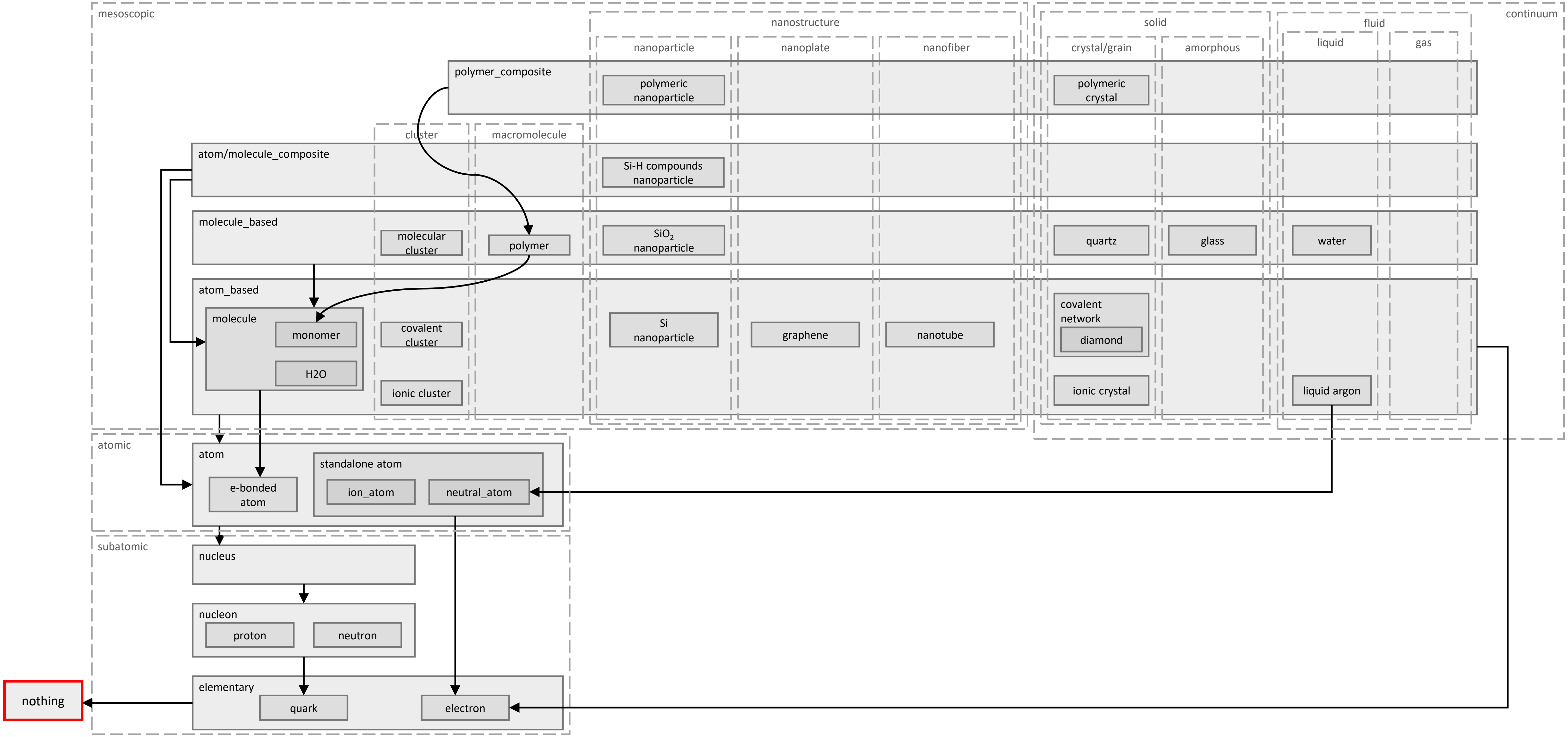
GRANULARITY HIERARCHY - EXAMPLE



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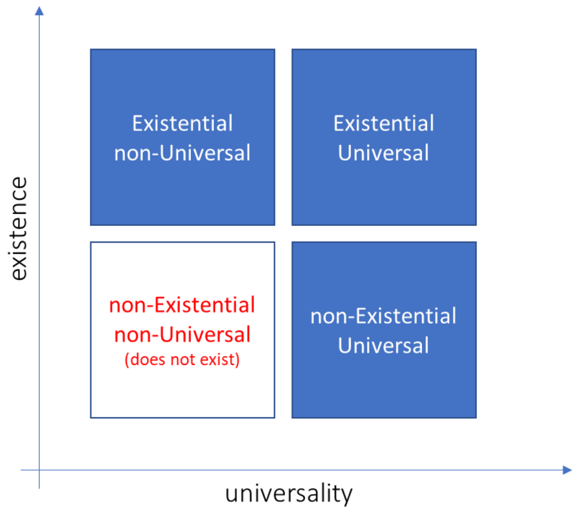
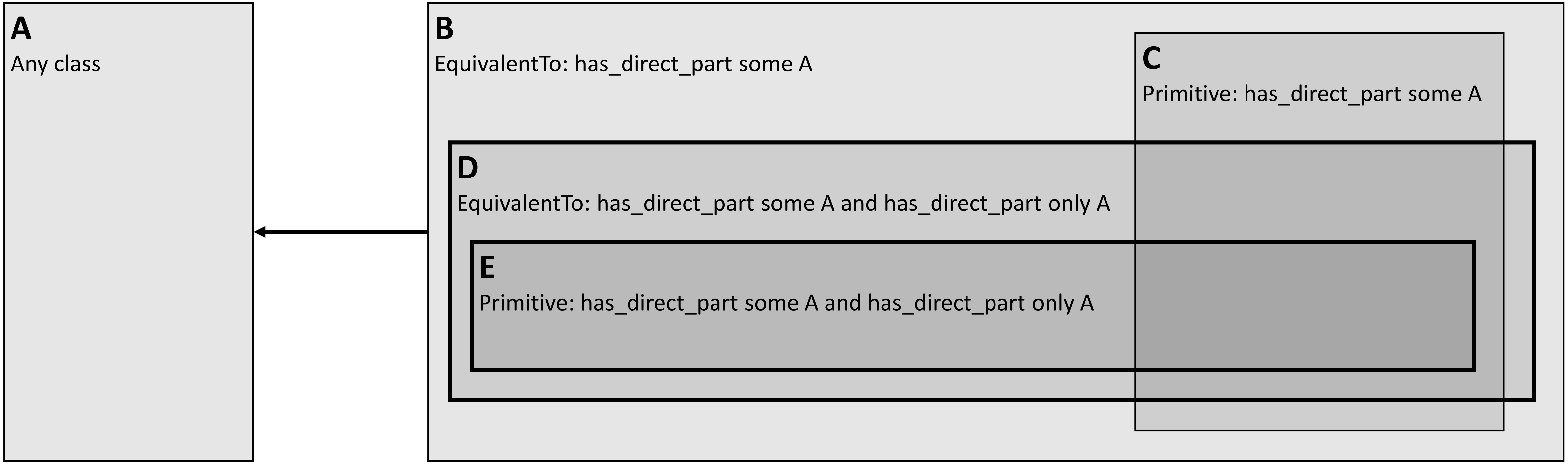
GRANULARITY

The relations between classees then can be much more complex than the previous slides.

For **any given class A** we can build other **standard granularity classes** that have any possible direct parthood relation with A according to this schema (only B and C are open to relations with classes other than A, since they are not universal restriction):





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GRANULARITY CLASSES

Algorithm for creating a standard direct parthood hierarchy starting from scratch

1. Declare one or more **primitive classes** that reflects how I see the world (my material ontology) e.g. `my_class`. Individuals of these classes will be the basis building blocks for all the materials and constitutes the basic level of granularity.

```
SubclassOf( :owl:Thing  :my_class )
```

2. For each base class declare the **universal** (`my_class_only_based`) and **existential** (`my_class_based`) **defined** classes that will relate every other class to individuals of the basic class. `my_class_only_based` will be a subclass of `my_class_based`

```
EquivalentClasses(
  :my_class_based
  ObjectSomeValuesFrom( :has_direct_part :my_class )
)

EquivalentClasses(
  :my_class_only_based
  ObjectAllValuesFrom( :has_direct_part :my_class )
)
```

3. Declare all the other desired primitive classes of materials as **having direct parts the basic building blocks** and the other defined classes that are useful **collectors of other classes**. For example:

```
SubclassOf( :my_composite ObjectSomeValuesFrom ( :has_direct_part :my_class )
```

4. Each newly declared class (primitive or defined) can be used to build other universal and existential defined classes.

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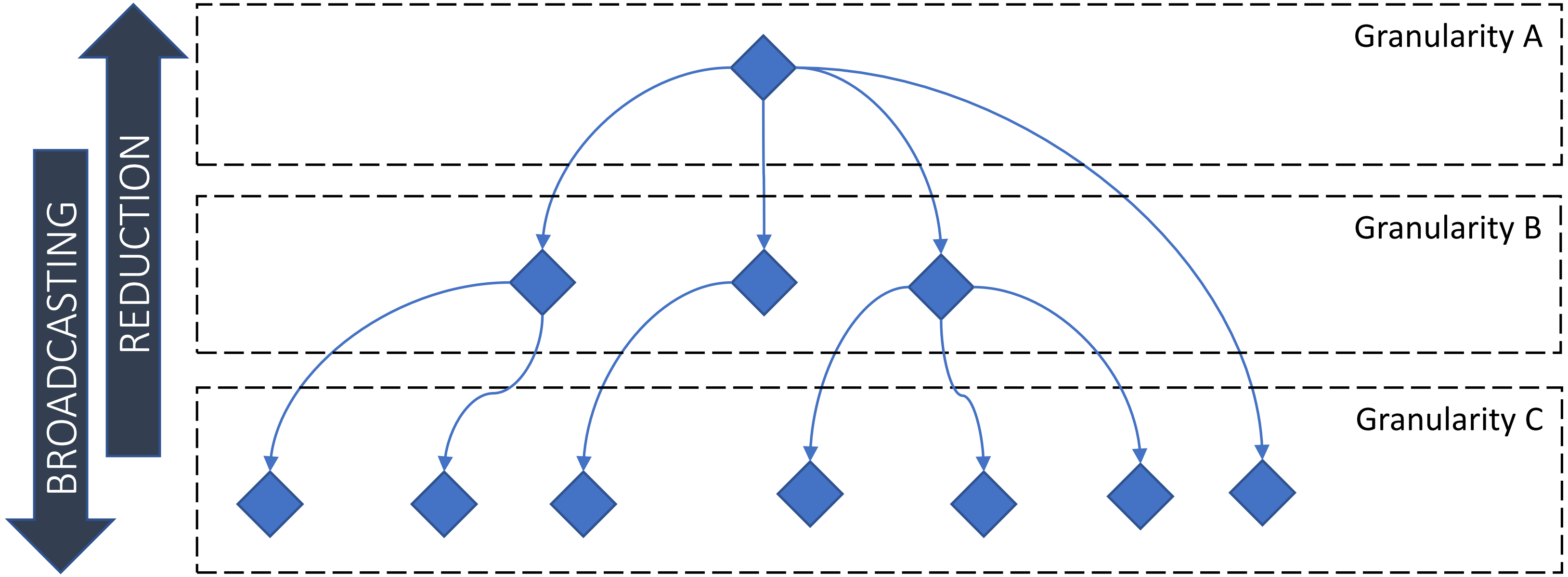
EMMO Core Mereotopology

By defining the mereological relation of **direct parthood**, the **EMMO** is able to describe entities as made of parts at different level of **granularity**.

The individuals are forming a **directed rooted tree**:

this is paramount for cross scale interoperability (vertical interoperability) that is the basis for multi-scale modelling.

Reduction and broadcasting can be easily implemented by navigating in this type of tree.



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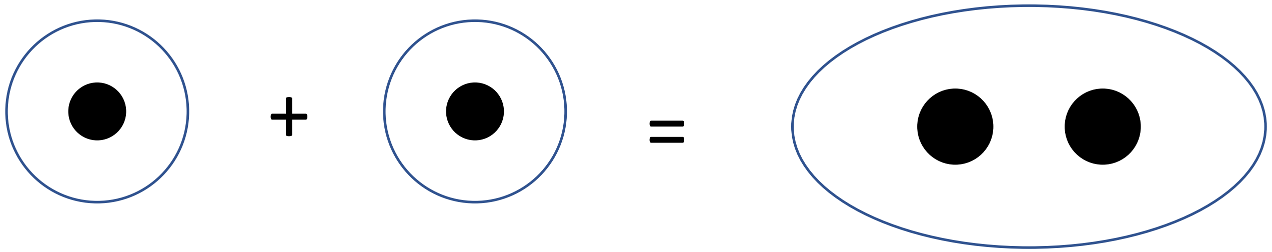
Direct Parthood - Example

Need for more rigorous definitions!



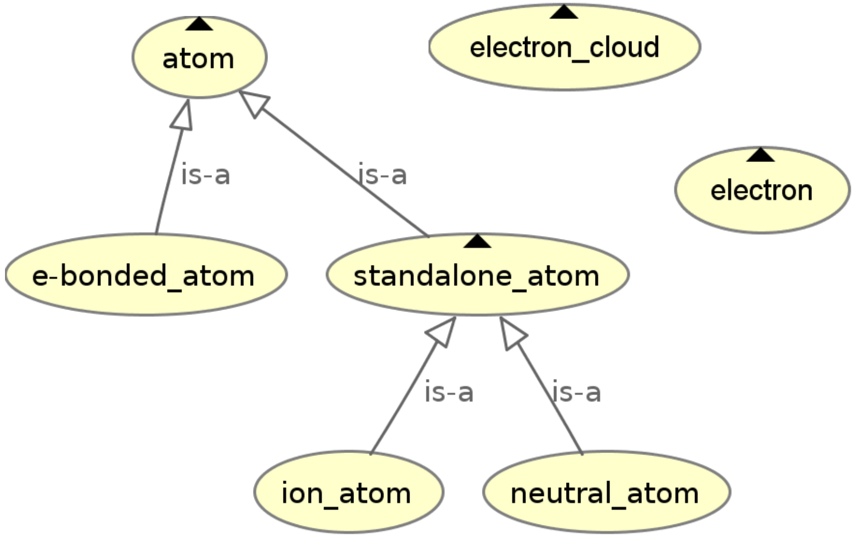
IUPAC GOLDBOOK

atom
Smallest particle still characterizing a chemical element. It consists of a nucleus of a positive charge (Z is the proton number and e the elementary charge) carrying almost all its mass (more than 99.9%) and Z electrons determining its size.

molecule
An electrically neutral entity consisting of more than one atom (n > 1).

When a molecule (covalent) is formed the nucleus does not own all Z electrons. The IUPAC definition of molecule is **not consistent** with the definition of atom (at least, cannot be used as is now in a strict logical formalism)

EMMO material branch to overcome IUPAC definition inconsistency.



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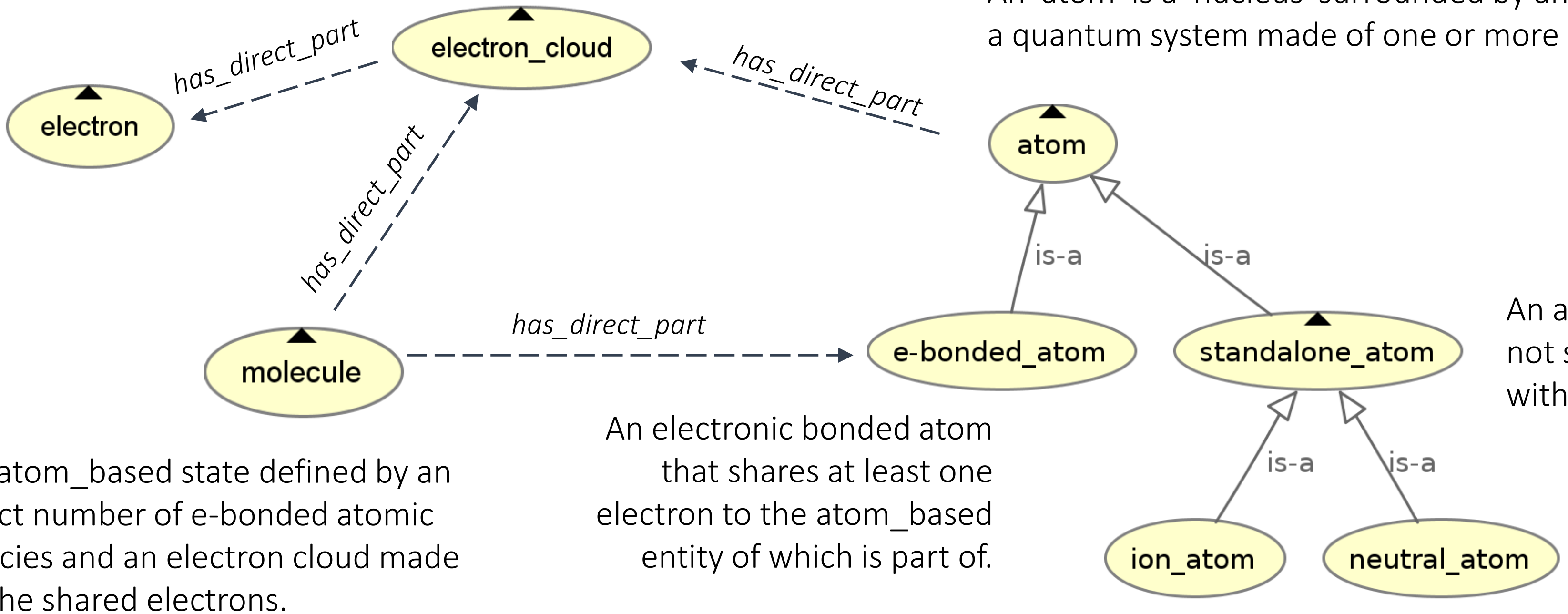
DIRECT PARTHOOD - EXAMPLE

A 'spacetime' that stands for a quantum system made of electrons.

An 'atom' is a 'nucleus' surrounded by an 'electron_cloud', i.e. a quantum system made of one or more bounded electrons.



An atom that does not share electrons with other atoms.

An atom_based state defined by an exact number of e-bonded atomic species and an electron cloud made of the shared electrons.

An electronic bonded atom that shares at least one electron to the atom_based entity of which is part of.

A standalone atom that has no net charge.

A standalone atom with an unbalanced number of electrons with respect to its atomic number.

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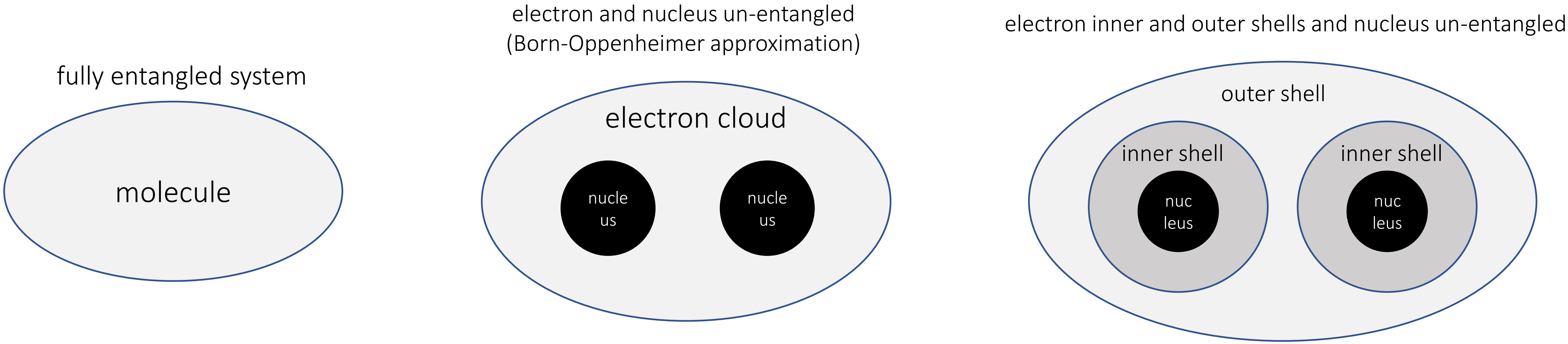
Quantum Systems Representation

The **EMMO** material branch is also generic and flexible enough to represent **quantum systems** in a way that is compatible with different interpretations (i.e. Copenhagen, De Broglie-Bohm) and approximations (e.g. Born–Oppenheimer).



Hamiltonian parameters can be derived by axioms that define the specific quantum system class (i.e. the sub-parts).

Wave function collapse can also be represented within the **EMMO** mereological framework.

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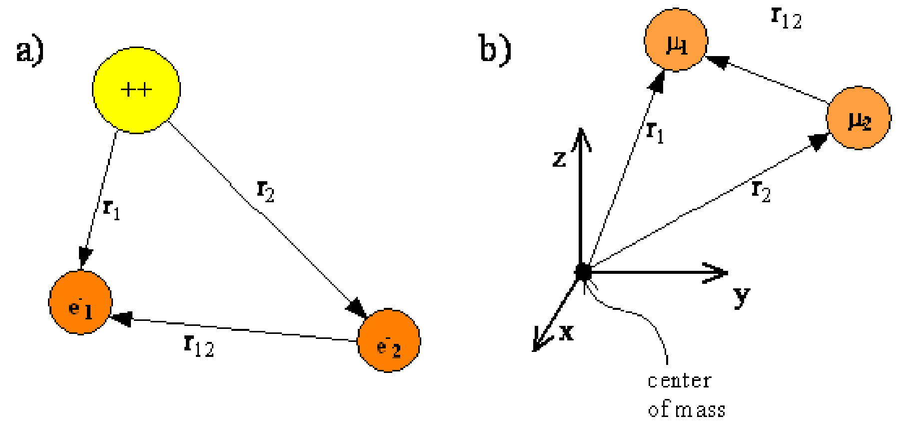
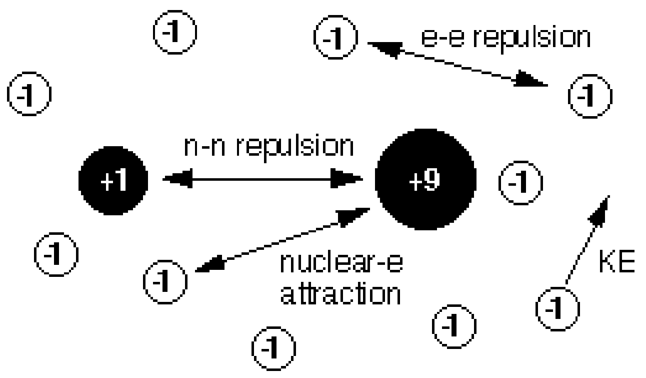
Multielectron atom



Molecule



$$H = \sum_i \left(\frac{-m_i}{2} \nabla_i^2 + \sum_{j \neq i} \frac{q_i q_j}{r_{ij}} \right)$$

The Hamiltonian is built considering electrons and nuclei as discrete particles. The representation of electrons using electronic density function is done at modelling level, not material, in the EMMO.

Approximations such as Born-Oppenheimer or the electron decoupling are also done at model level, and not material representation level

$$\psi(r_1, r_2, \cdots, r_i) \approx \varphi_1(r_1)\varphi_2(r_2)\cdots\varphi_i(r_i)$$

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QUANTUM SYSTEMS REPRESENTATION

Classical mechanics poses no representational issues for the EMMO: the 4D representation of physical objects is straightforwardly consistent with **classical physics systems**.

The EMMO can also be used to represent real world entities also in the framework of **quantum mechanical based models**, which are unavoidable as long as the domain of interest goes up to submolecular level, and the mathematical models used to describe it are based on the Schrodinger equation.

However, the ontology of quantum mechanical systems is still an **open issue for the physics community**, and there is **no global consensus** about the meaning of the mathematical entities involved in such representational framework.

The Copenhagen interpretation of quantum mechanics, involving the concept of particles delocalization and wave function collapse, is the most widely accepted, but other interpretations like the de Broglie - Bohm or the many-world interpretations, are discussed in the physics community and sometimes implemented as numerical alternative approaches.

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Quantum Systems Representation

Copenhagen interpretation I

In Copenhagen interpretation the properties (e.g. energy level, position, spin) of a constituent object of a system are **not defined in the interval between two measurements and the quantum system is entangled (i.e. properties of particles in the system are correlated) and described by a global wave function obtained solving the Schrodinger equation**. Upon measurement, the **wave function collapses to a combination of close eigenstates** that provides information about observables of the system components (e.g. position, energy).

The EMMO can be used to represent physical objects that can be related to Copenhagen based models. In practice, the user should follow these steps:

1. **define the quantum system as a physical individual** (e.g. an H2 molecule) under a specific class (e.g. hydrogen_molecule) which is the whole
2. define the **class axioms that describe how many sub-parts are expected for the whole and their respective class types** (e.g. hydrogen_molecule has axioms has_proper_part exactly two electron and has_proper_part exactly two proton)
3. the user can now connect the whole to a Schrodinger equation based model whose **Hamiltonian is calculated through the information coming from the axioms**: **no individuals of proton or electron are declared for the subparts**
4. a measurement done on the quantum system that provides information on the sub-part properties is interpreted as a process of **wave function collapse** and leads to the end of the whole and to the **declaration of the sub-parts individuals as unentangled and localized objects (which can be themselves other quantum systems).**

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QUANTUM SYSTEMS REPRESENTATION

Copenhagen interpretation II

e.g. if the outer electron of the H2 molecule interacts with another entity defining its state, then the whole that stands for the entangled H2 molecule becomes a 'physical' made of an electron individual, a quantum system made of one electron and two nuclei and the void between them.

$$|\psi\rangle = \sum_i c_i |\phi_i\rangle \qquad |\psi\rangle \rightarrow |\phi_i\rangle$$

e.g. in the Born-Oppenheimer approximation the user represent the atom by un-entangling nucleus and electronic cloud. The un-entanglement comes in the form of declaration of individual as parts.

e.g. the double slit experiment can be represent in the EMMO as:

1. before the slit: a 'physical' that extend in space and has parts 'electron' and 'void', called 'single_electron_wave_function'. 'electron' and 'void' are only in the axioms and not decalred individuals.
2. during slit passage: a 'physical' made of one declared individual, the 'electron'.
3. after the slit: again 'single_electron_wave_function'
4. upon collision with the detector: 'physical' made of one declared individual, the 'electron'.

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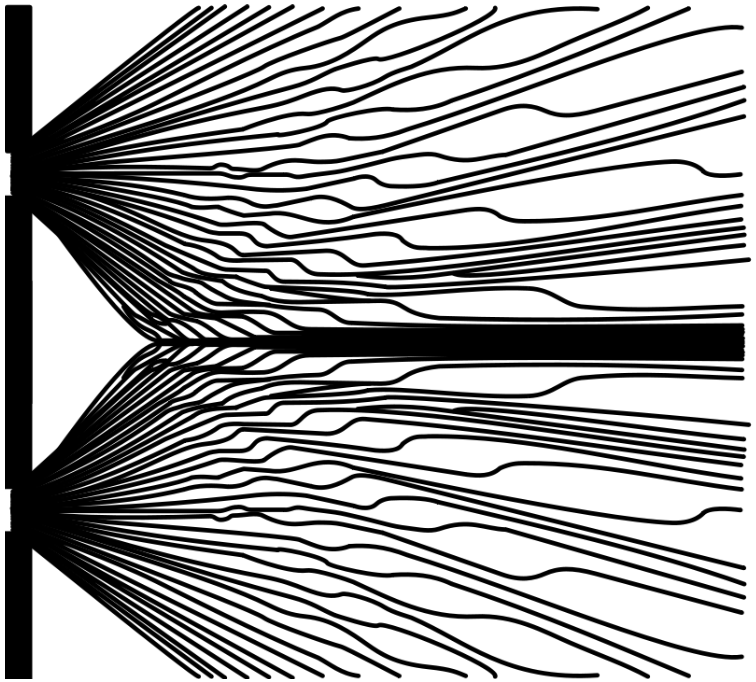
Quantum Systems Representation

De Broglie - Bohm interpretation

The most simple approach for a quantum mechanics ontology is **Bohmian mechanics**, in which each constituent object of a system is supposed to **exists in a specific position between measurements** (i.e. the **hidden variables approach**), while its trajectory is calculated using a **guiding equation** based on a **quantum field calculated with the Schrodinger equation**.

While this approach is really easy to implement in an ontology, since each entity has its own well defined 4D region, its mathematical representation failed to receive large consensus due to the difficulties to include relativistic effects, to be extended to subnuclear scale and the strong non-locality assumption behind the calculation of the quantum field. Nevertheless, the Bohmian mechanics is the foundation for the **quantum trajectory method**, a numerical approach that is used in some electronic models to reduce the computational effort of the solution of Schrodinger equation.



In practice, an EMMO user can **declare a physical individual that stands for the whole quantum system to be described** and at the same time the user can **declare all sub-parts individuals of the whole, having them a well defined position in time**, according to de Broglie - Bohm interpretation.

The Hamiltonian can be calculated by considering the sub-part individuals physical properties. Physical objects are then represented as made of other **physical objects parts** and **void object parts**, the latter standing for the space between physical objects (e.g. the void between electrons and nucleus in an atom).

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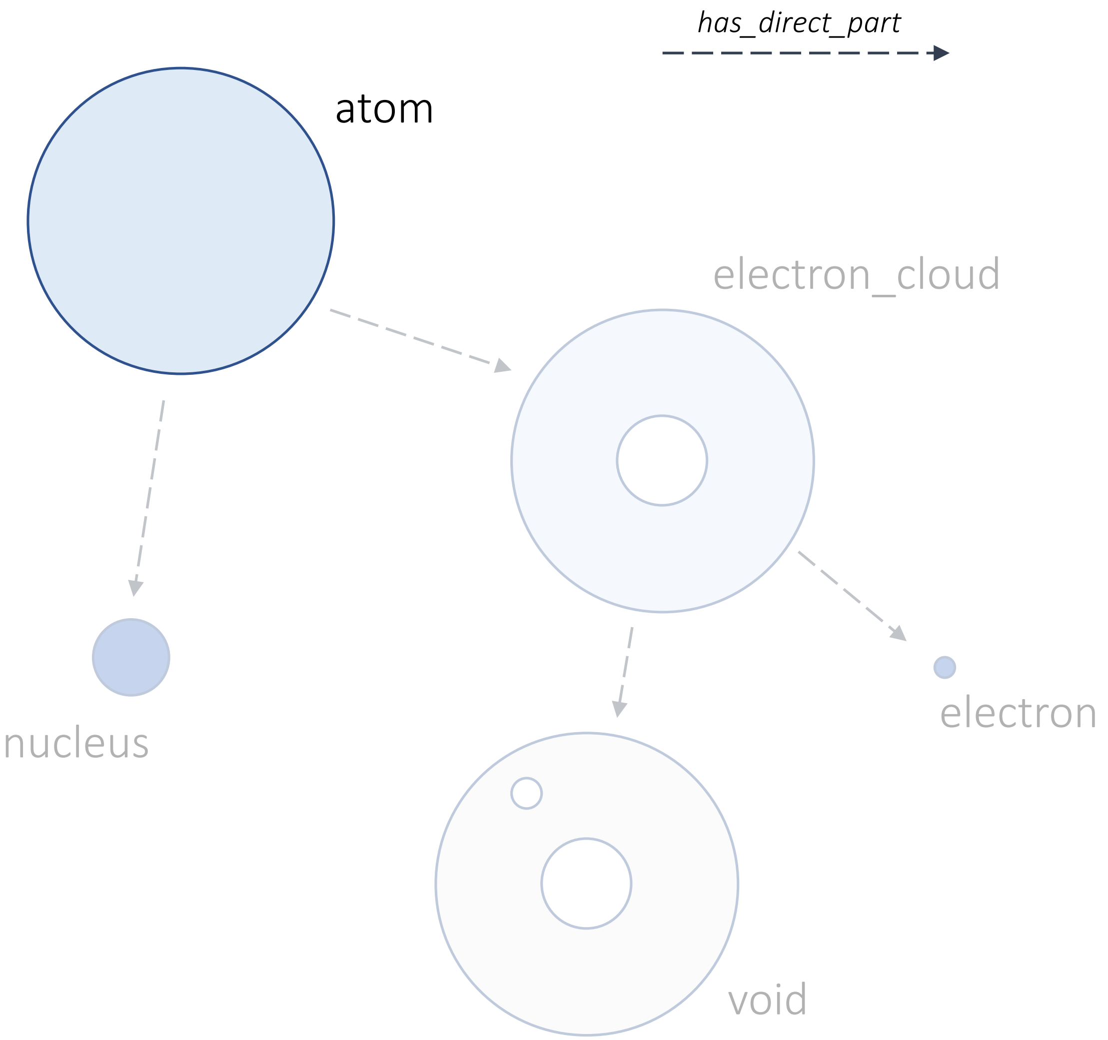
Direct Parthood - Example

Many-body Hamiltonian built by knowing the sub-part composition, without declaring any individual.

$$\hat{H} = -\underbrace{\frac{\hbar^2}{2\,m_N}\nabla_N^2}_{\text{KE of nucleus}} - \underbrace{\sum_i \frac{\hbar^2}{2\,m_e}\nabla_i^2}_{\text{KE of electrons}} - \underbrace{\sum_i \frac{Z\,e^2}{4\,\pi\,\varepsilon_0\,r_i}}_{\text{nucleus-electron PE}} + \underbrace{\sum_i \sum_{j>i} \frac{e^2}{4\,\pi\,\varepsilon_0\,r_{i\,j}}}_{\text{electron-electron PE}}$$

The wavefunction describes the atom as an entangled quantum system.

$$|\psi\rangle = \sum_i c_i |\phi_i\rangle$$



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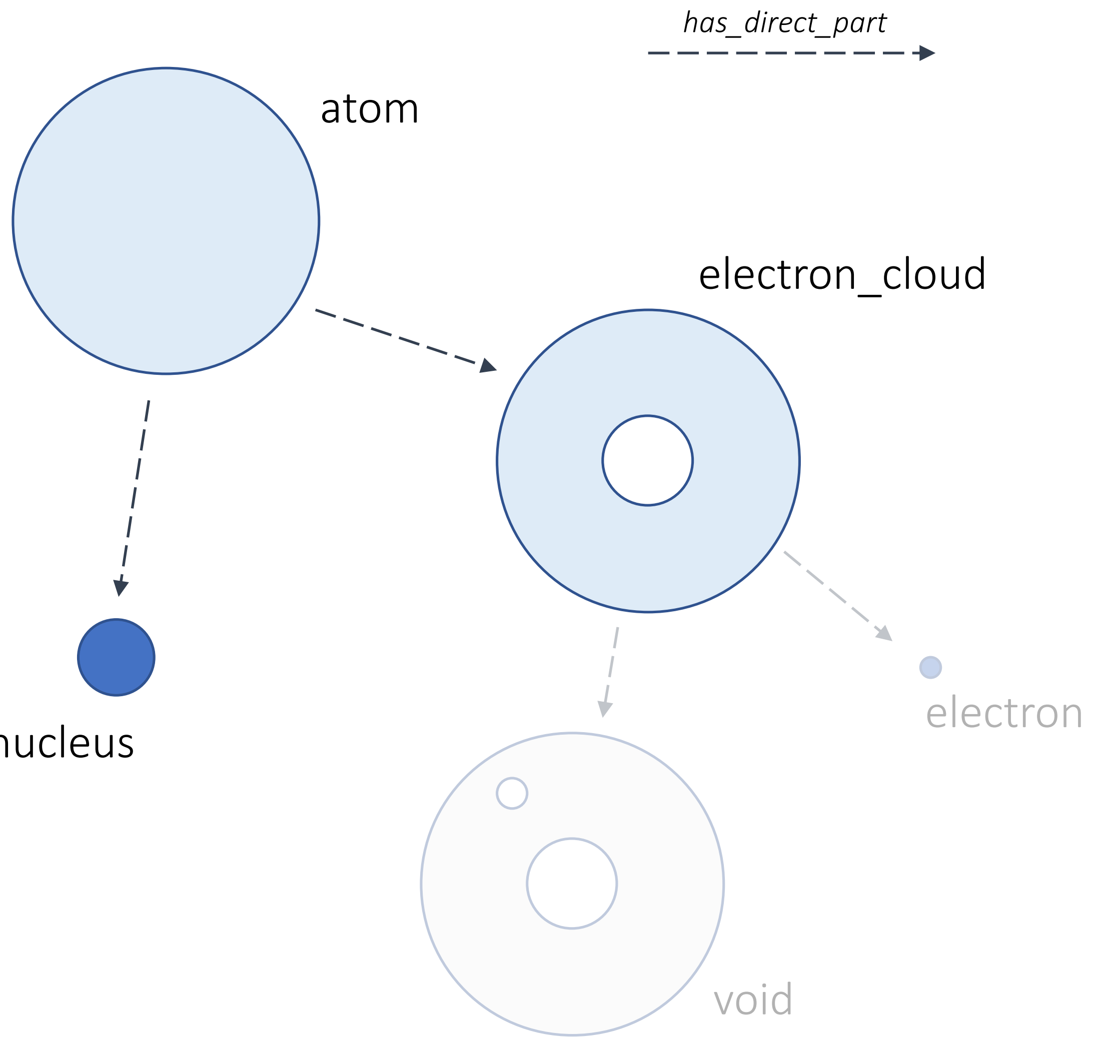
Direct Parthood - Example

Wavefunction collapse upon declaration of nucleus individual.

Electrons remain as quantum system electron cloud, but the nucleus is considered in a fixed position (Born-Oppenheimer)

$$\hat{H} = -\cancel{\underbrace{\frac{\hbar^2}{2\, m_N}\nabla_N^2}_{\text{KE of nucleus}}} - \underbrace{\sum_i \frac{\hbar^2}{2\, m_e}\nabla_i^2}_{\text{KE of electrons}} - \underbrace{\sum_i \frac{Z\, e^2}{4\,\pi\,\varepsilon_0\, r_i}}_{\text{nucleus-electron PE}} + \underbrace{\sum_i \sum_{j>i} \frac{e^2}{4\,\pi\,\varepsilon_0\, r_{i\,j}}}_{\text{electron-electron PE}}$$



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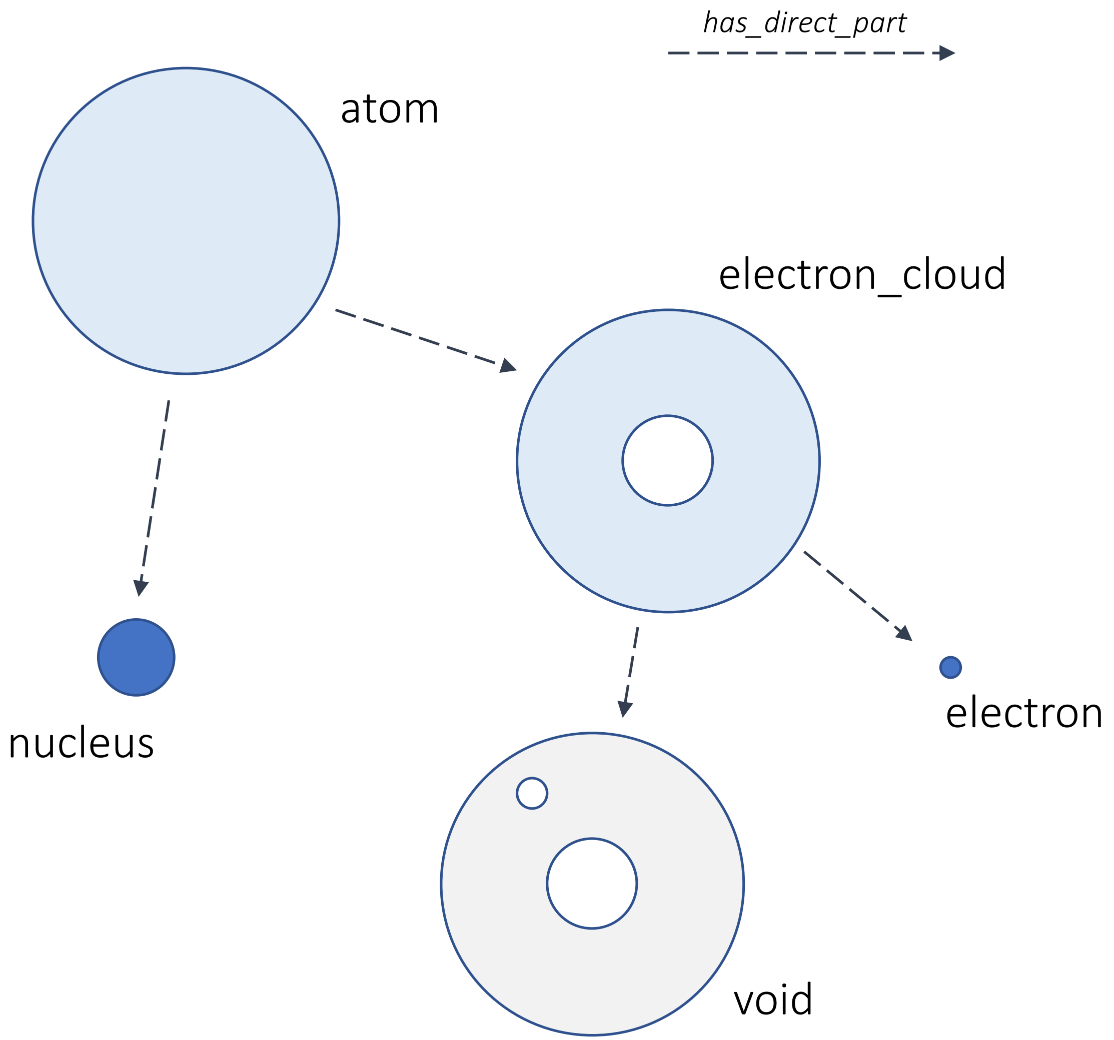
Direct Parthood - Example

Wavefunction collapse upon declaration of electron individual.

The electron is declared as individual and its physical state is now known.



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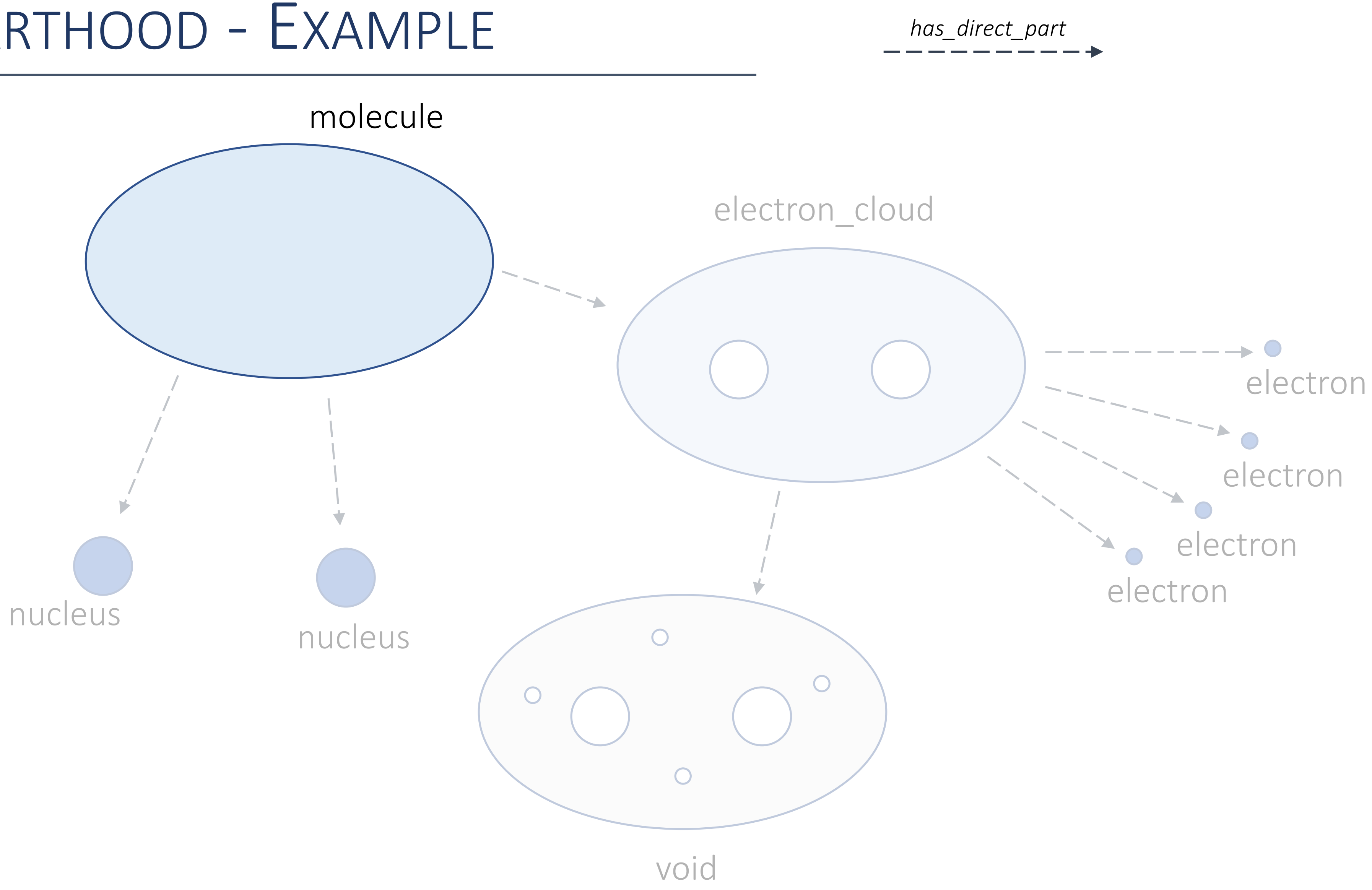
Direct Parthood - Example



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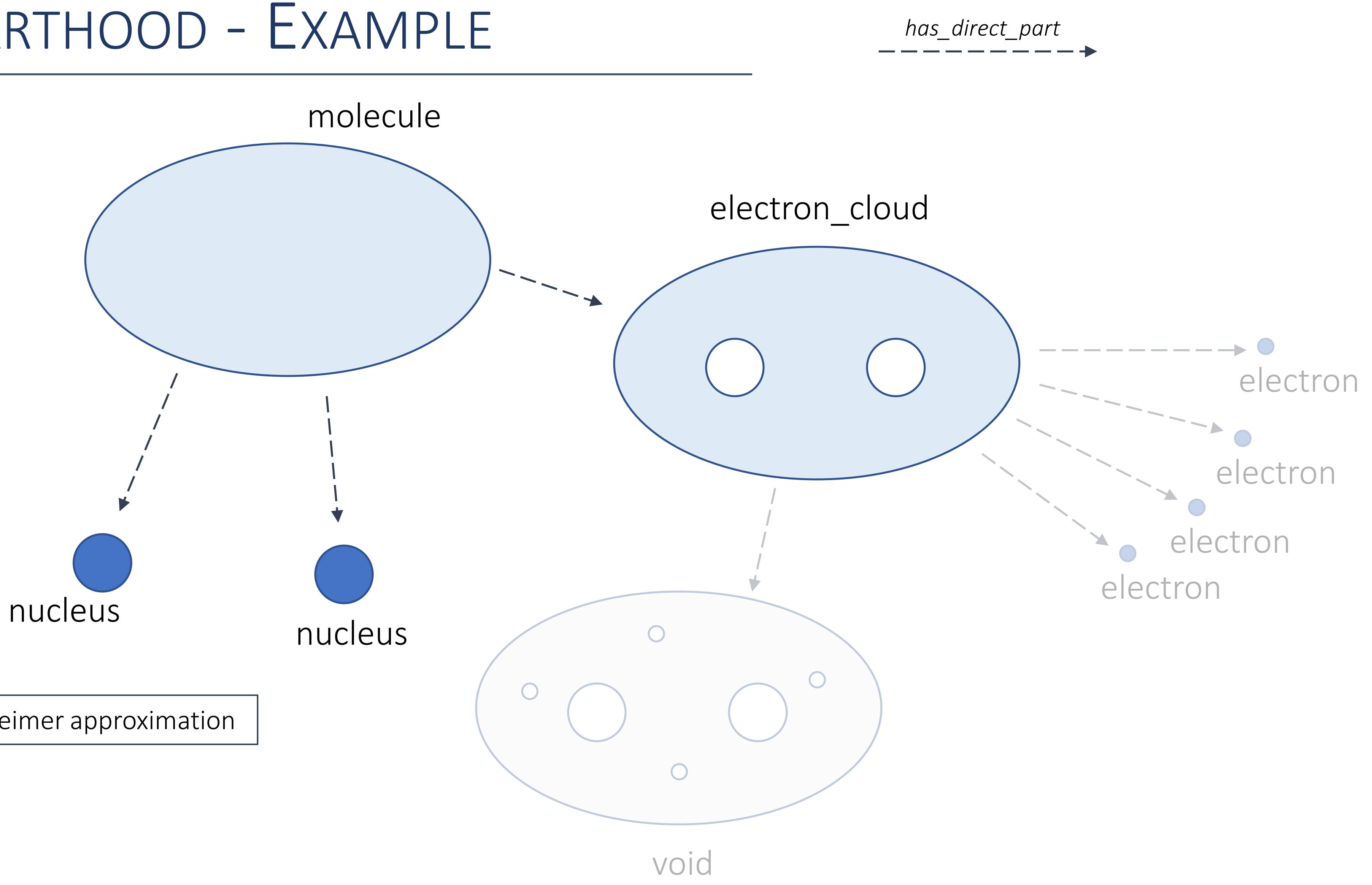
Direct Parthood - Example



Born-Oppenheimer approximation

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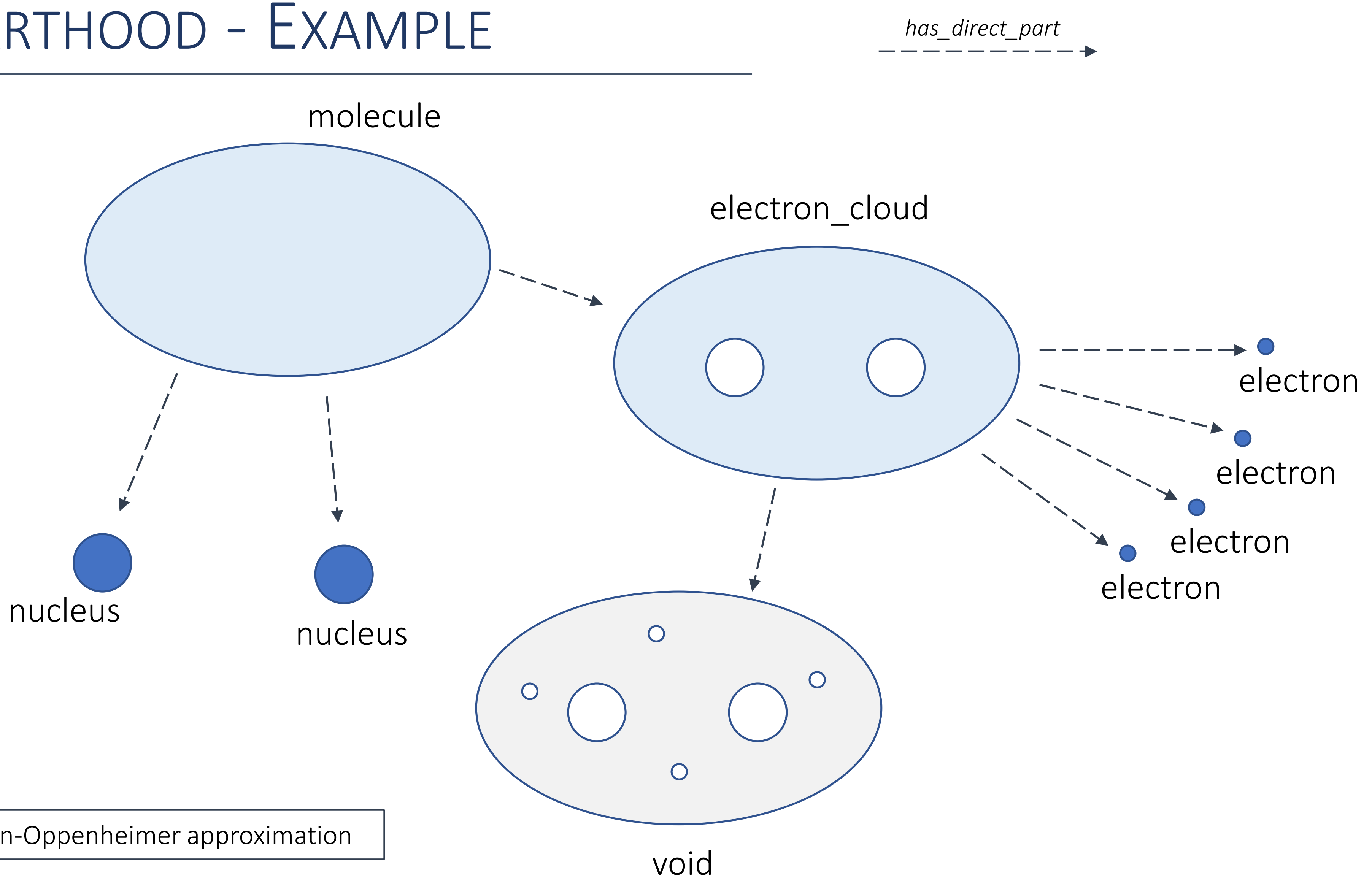
DIRECT PARTHOOD - EXAMPLE



In the Born-Oppenheimer approximation

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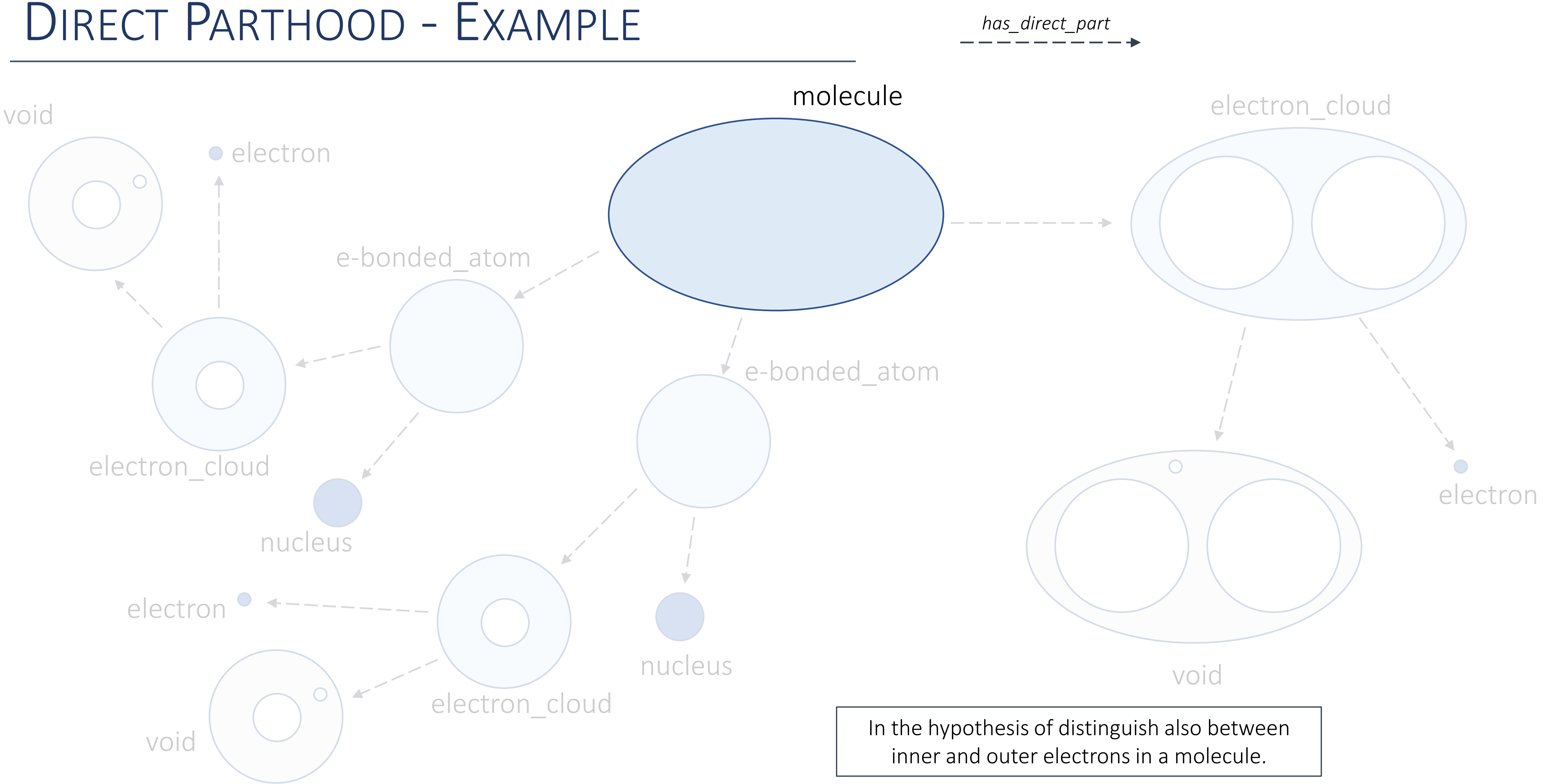
Direct Parthood - Example



In the hypothesis of distinguish also between inner and outer electrons in a molecule.

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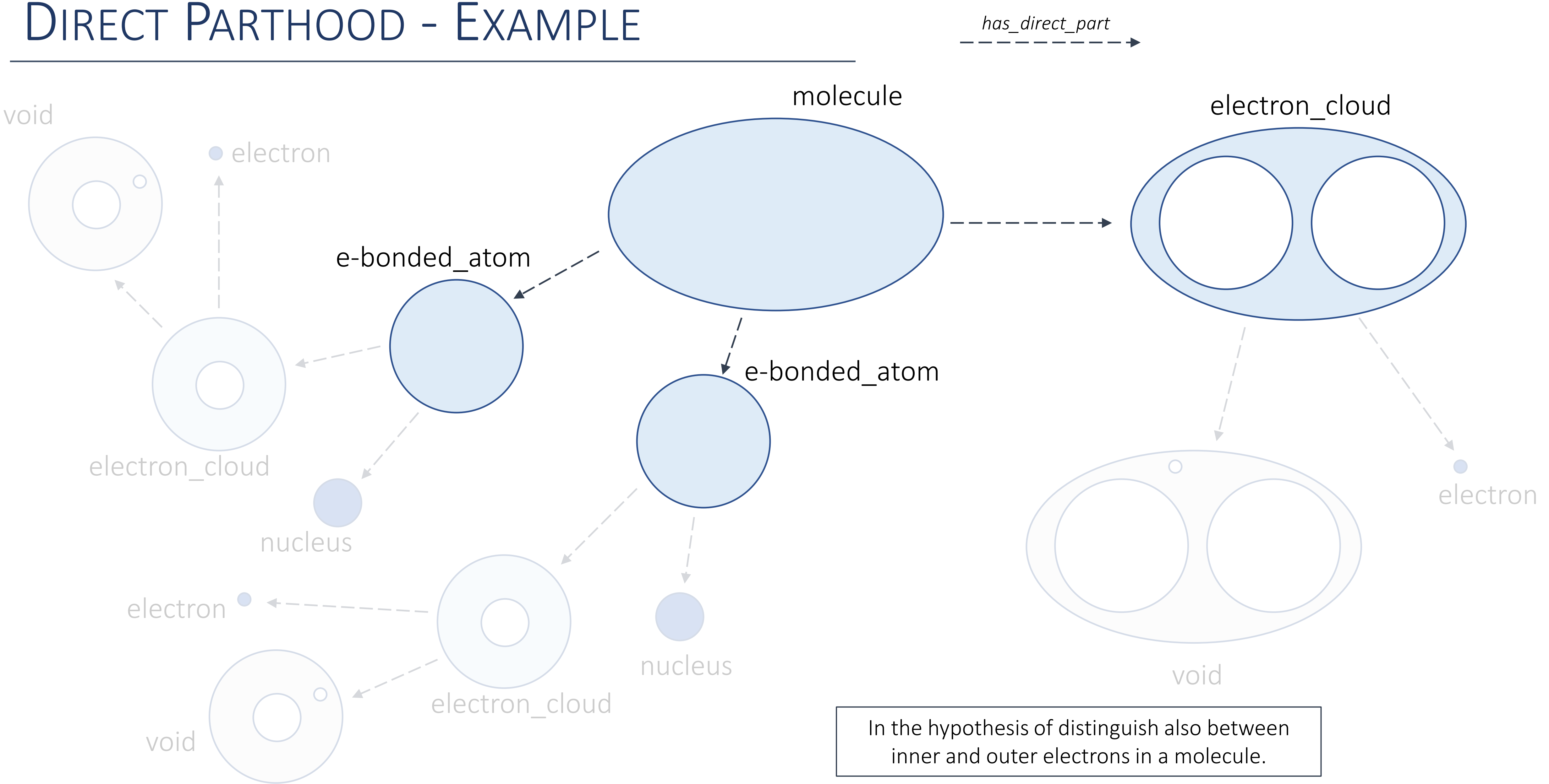
DIRECT PARTHOOD - EXAMPLE



In the hypothesis of distinguish also between inner and outer electrons in a molecule.

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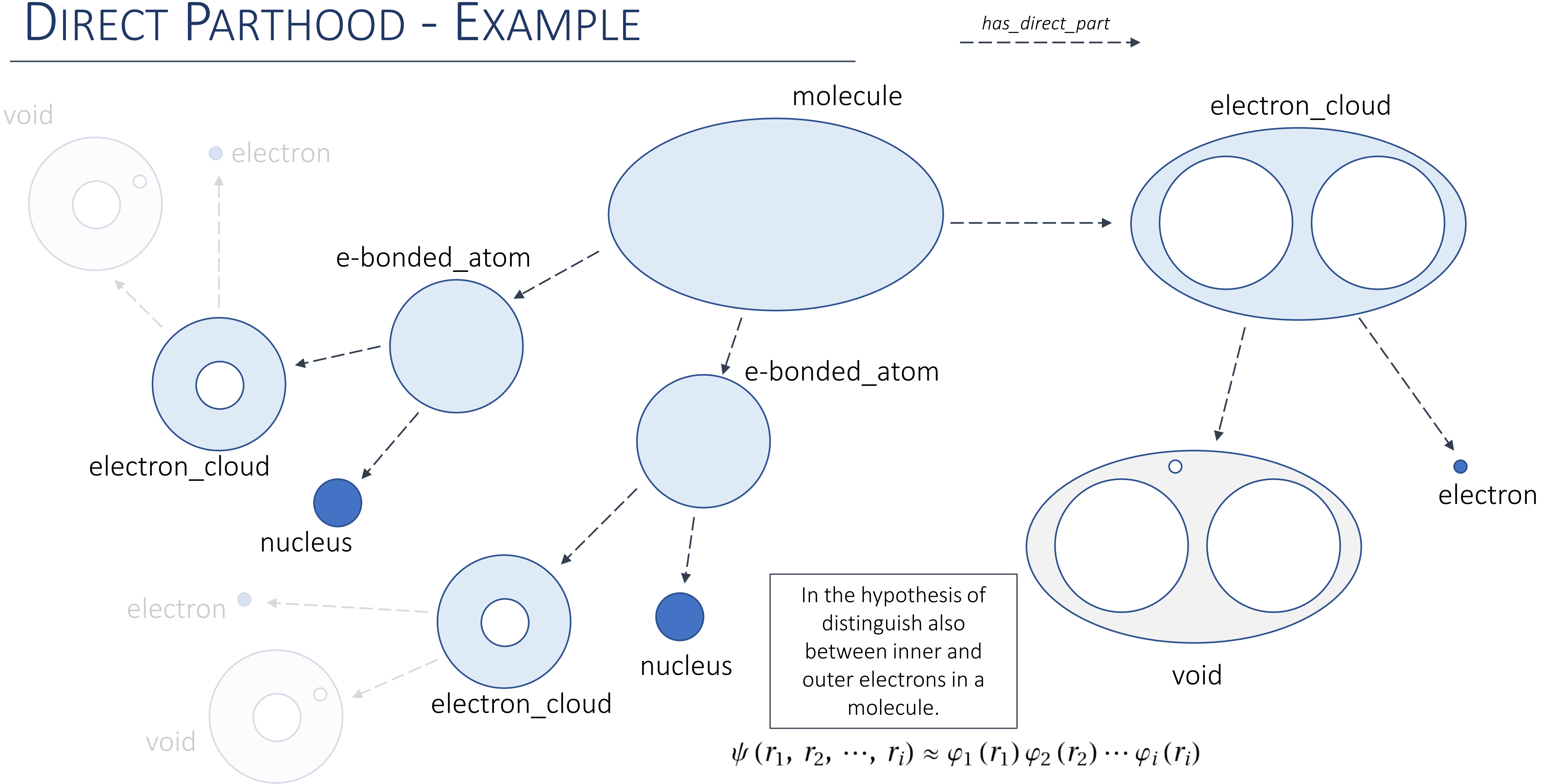
Direct Parthood - Example



In the hypothesis of distinguish also between inner and outer electrons in a molecule.

$$\psi(r_1, r_2, \cdots, r_i) \approx \varphi_1(r_1)\varphi_2(r_2)\cdots\varphi_i(r_i)$$

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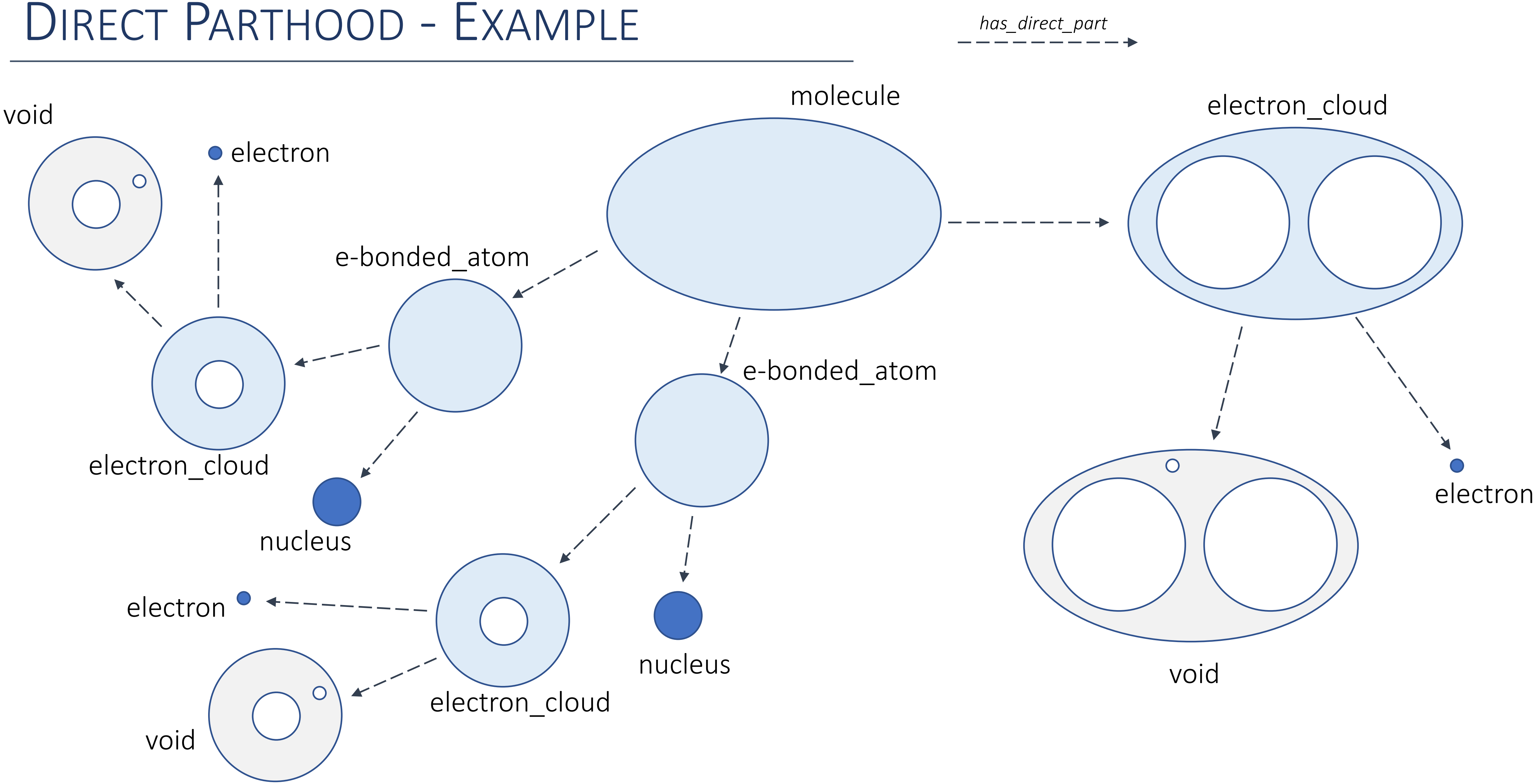
DIRECT PARTHOOD - EXAMPLE



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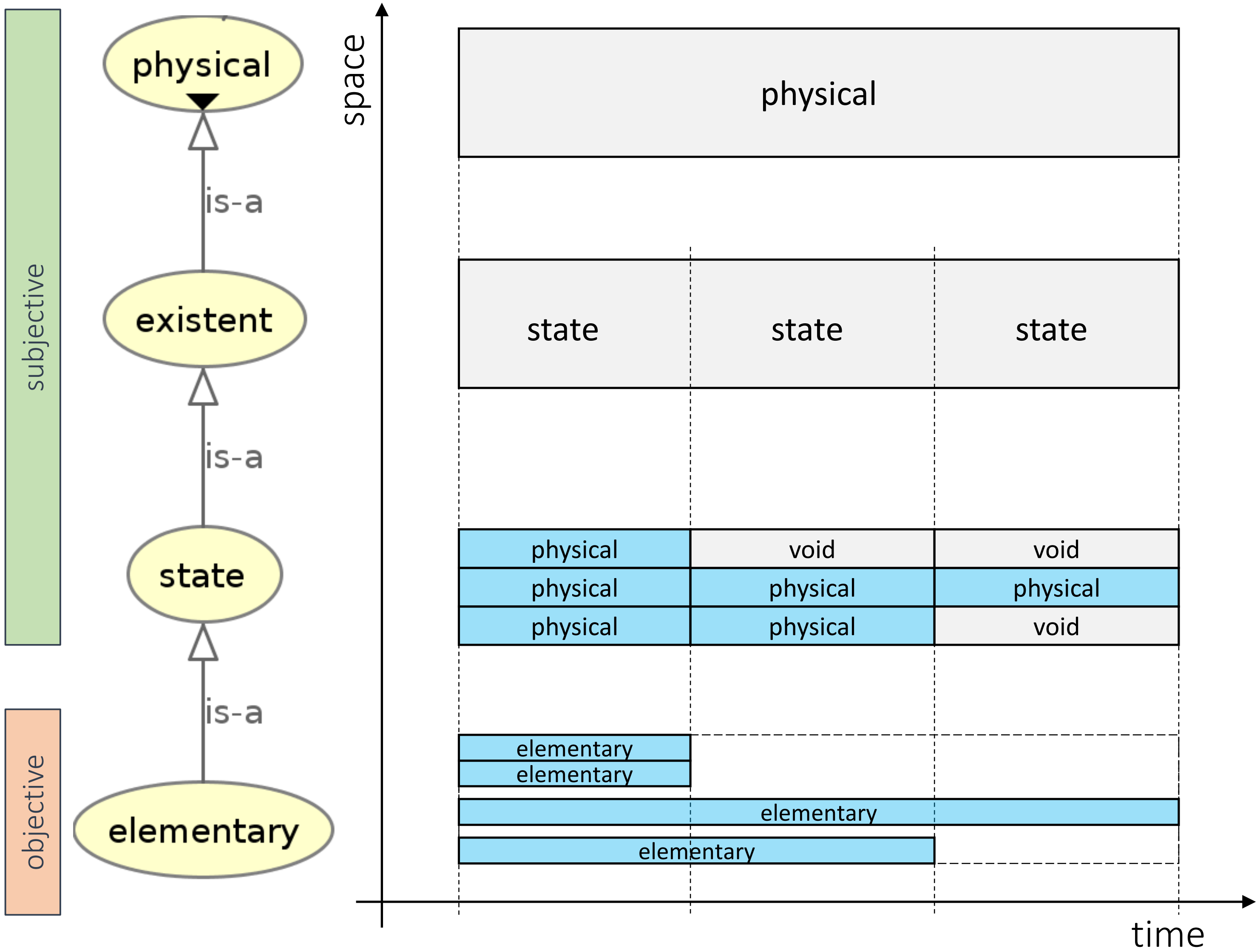
EMMO Core Mereotopology



The **EMMO** identifies a more detailed parthood hierarchy in **physical**s using direct parthood, by introducing the concept of:

- **state** as a **physical** whose parts have a constant cardinality during its life time (similar to endurants)
- **existent** as a succession of **state**s (similar to perdurants)

so that a **physical** entity can be defined using a more strict multiscale perspective.

ex-sistere (latin):
to stay (to persist through time) outside others of the same type (to be distinct from the rest).

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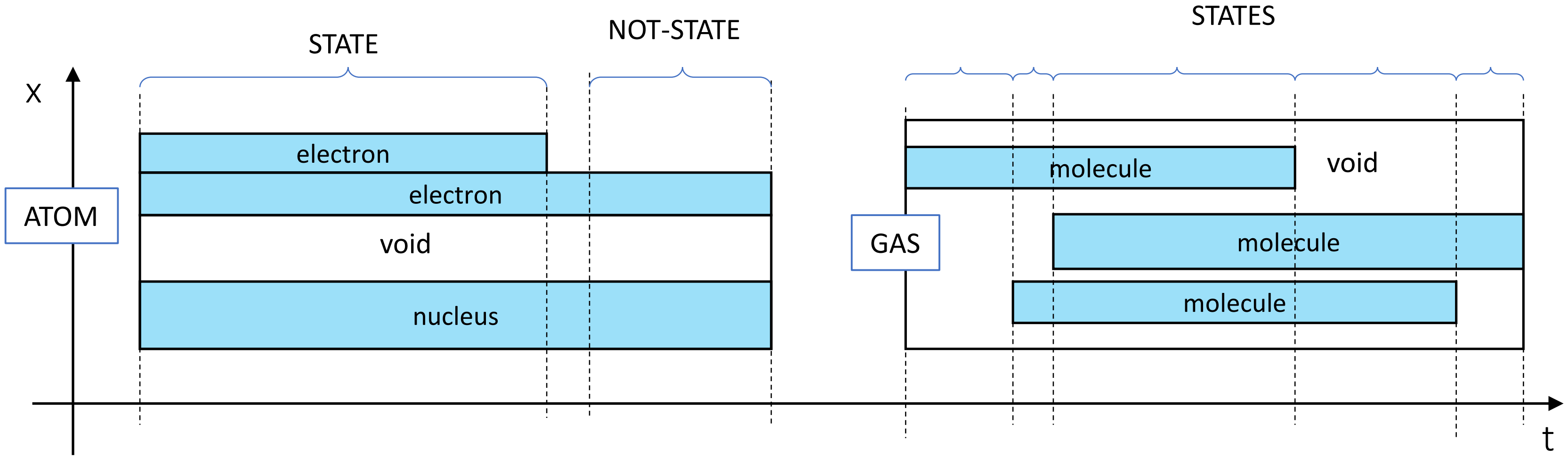
EMMO Material Ontology

State stands for "**physical in a particular configurational state**" and is defined as having spatial direct parts that persists (do not change) throughout the lifetime of the whole: the **state**.
There is no change in granularity or cardinality of parts within a **state**.
The use of spatial direct parthood in **state** definition means that a **state** cannot overlap in space another **state**
A spatial direct part of a **state** can only be **physical** or **vacuum**.
A **state** is like a snapshot of a **physical** in a finite interval.

An **existent** then can be defined as a **physical** that unfolds in time as a succession of **states**
This class is used to represent the whole life of a complex but structured state-changing **physical** entity like e.g. an atom that becomes ionized and then recombines with an electron.



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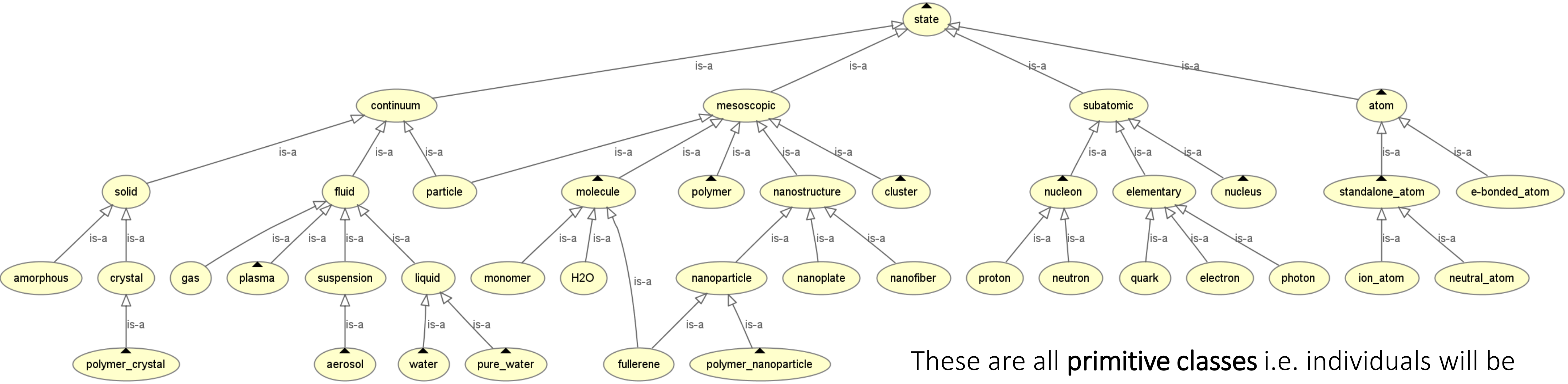
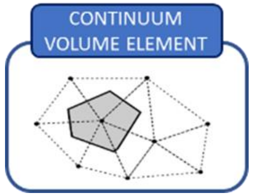
EMMO MATERIAL BRANCH

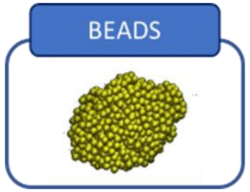
RoMM compliant material description branch

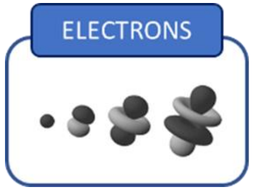
THE **EMMO** MATERIAL DESCRIPTION BRANCH PROVIDES THE 4 DIFFERENT VIEWS PROPOSED BY THE RoMM, DEPENDING ON THE LEVELS OF GRANULARITY ADOPTED

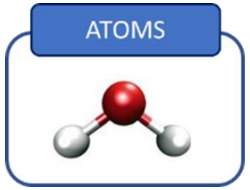


These are all **primitive classes** i.e. individuals will be placed in the classes by user declaration according to the adopted view









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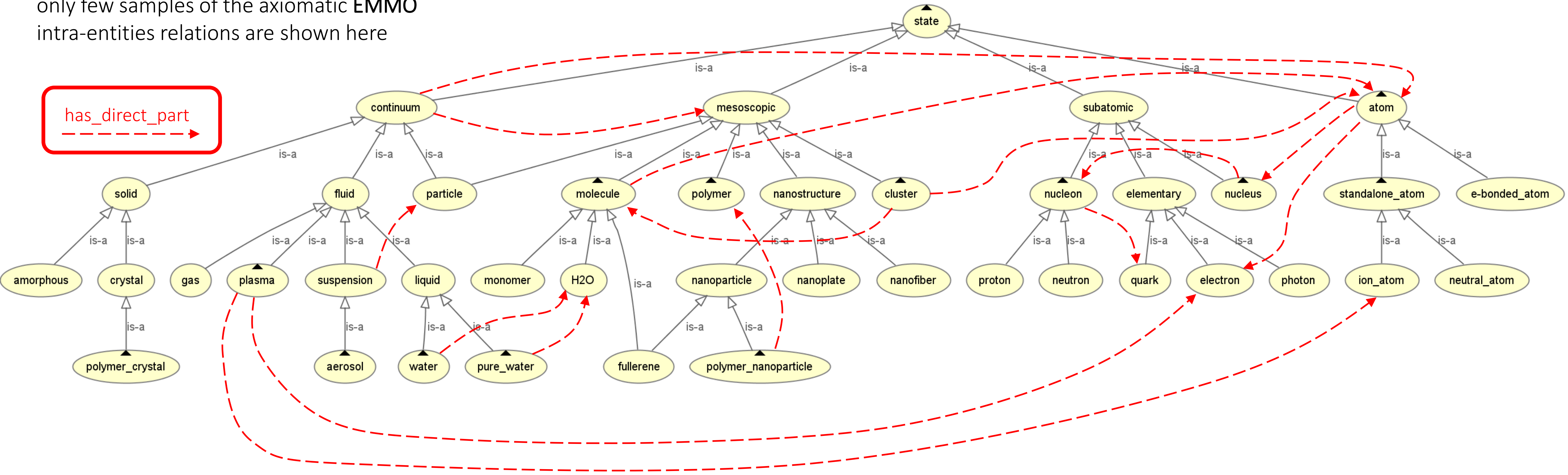
EMMO MATERIAL BRANCH

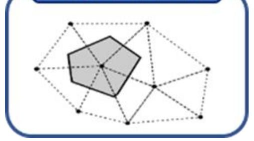
RoMM compliant material description branch

only few samples of the axiomatic **EMMO** intra-entities relations are shown here

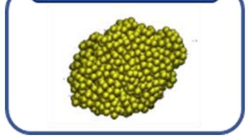
THE **EMMO** MATERIAL DESCRIPTION BRANCH PROVIDES THE 4 DIFFERENT VIEWS PROPOSED BY THE RoMM, DEPENDING ON THE LEVELS OF GRANULARITY ADOPTED



CONTINUUM VOLUME ELEMENT

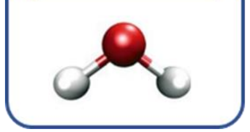


BEADS



ELECTRONS

ATOMS



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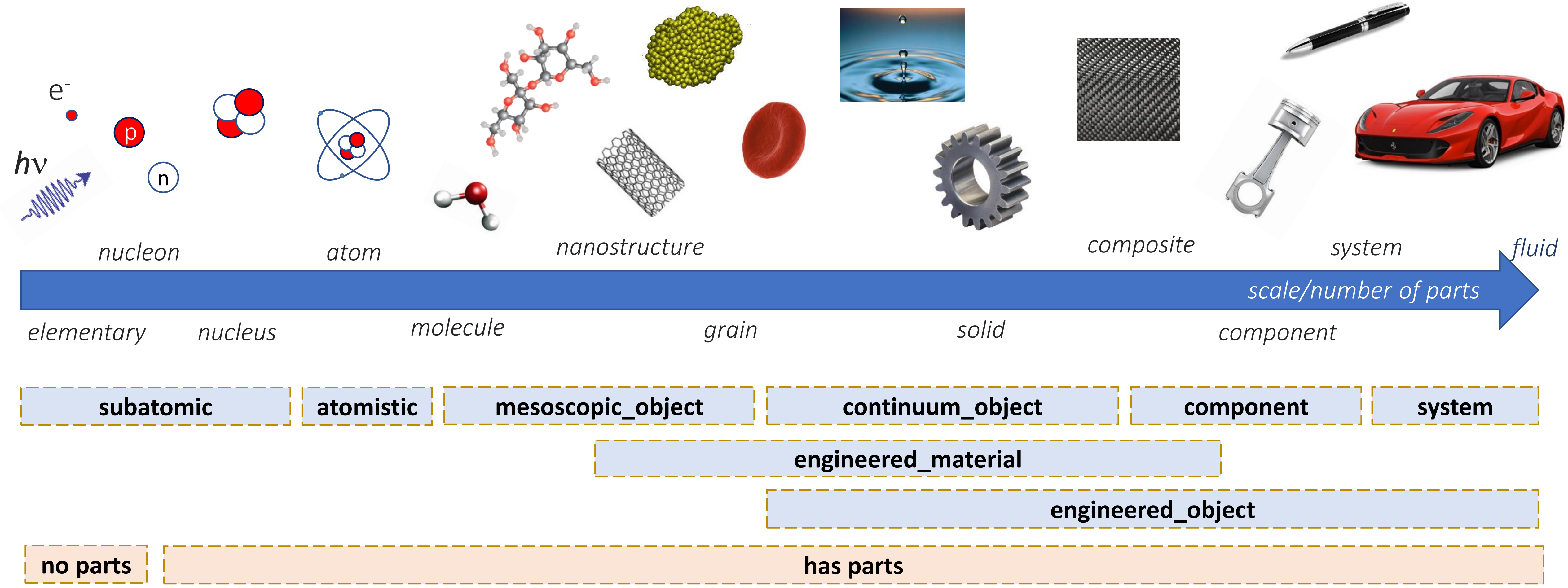
EMMO MATERIAL BRANCH



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EMMO Material Ontology

SPACETIME
the substrate of existence of real things

PHYSICAL
a spacetime that exibits some physical properties

EXISTENT
a physical that is categorized by the ontologist according to its own criteria

STATE
a simple existent that is made of parts that persists through all its lifetime

ELEMENTARY
a physical that has no spatial proper parts

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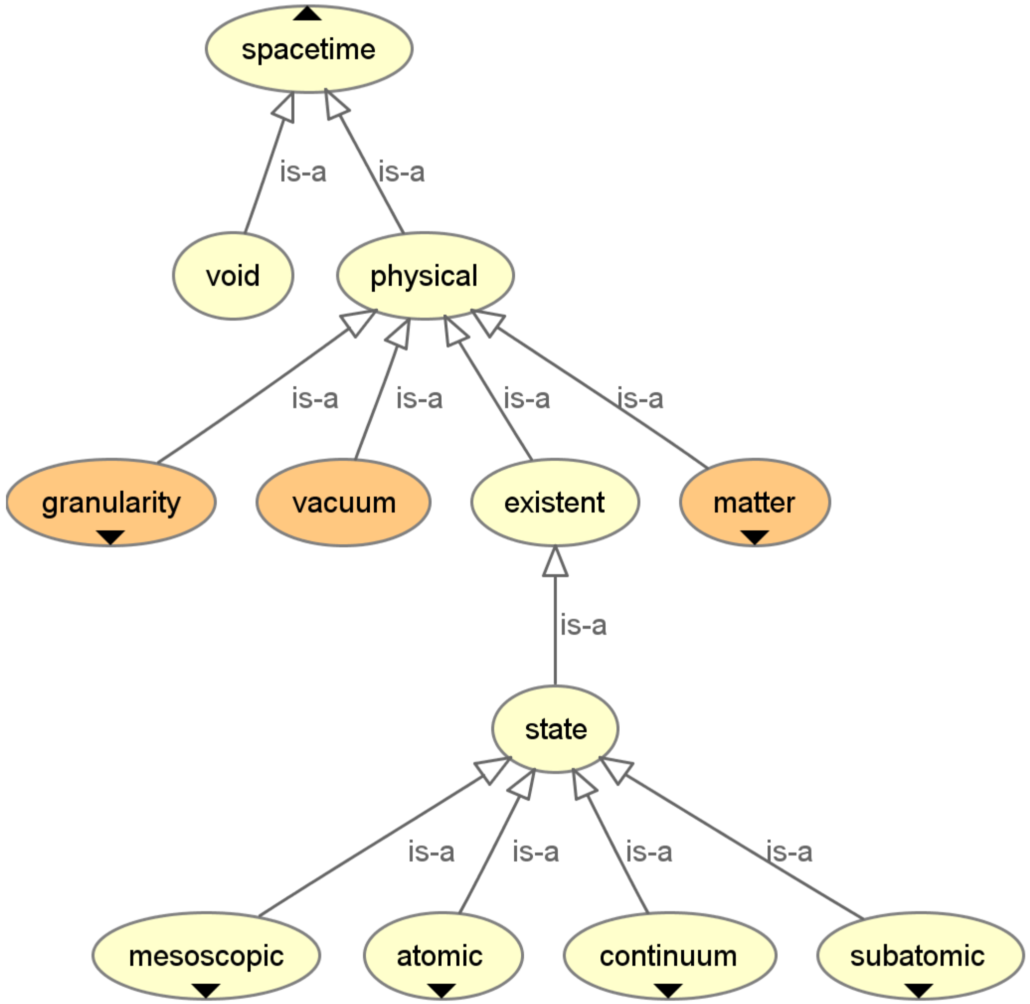
EMMO MATERIAL ONTOLOGY

GRANULARITY

“**Granularity**” stands for “**physical with a particular granularity**” .

Granularity is then defined as a superclass of defined subclasses that are defined as **physical** that is composed of specific types of objects (and vacuum) and whose partitions respect direct parthood criteria.

The **granularity** class (and its inherited classes) is useful since a reasoner can automatically puts the individuals defined by the user under a generic class that expresses clearly the types of its compositional parts.



Since most of physics based modelling tools are designed to describe systems made of a specific base-object (e.g. atoms, fluids, particles) the granularity classes can be directly linked to model types.

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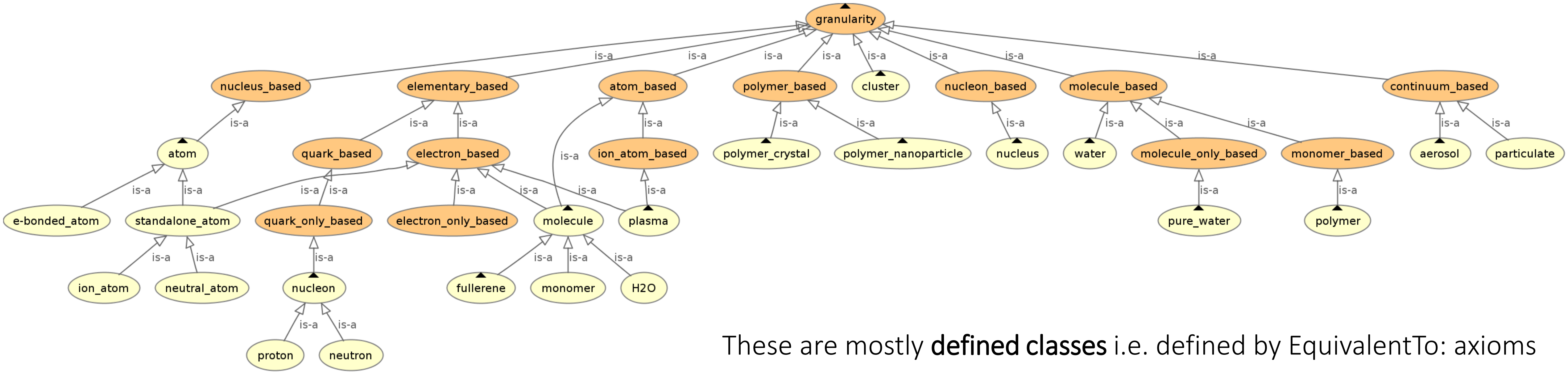
EMMO MATERIAL BRANCH

RoMM compliant material description branch arranged by granularity



These are mostly **defined classes** i.e. defined by EquivalentTo: axioms

This arrangement of the classes greatly helps to **identify the constituents** of the materials.

Placement of individuals is not intended to be provided by the user, but **automatically done by the reasoner** once the granularity chosen by the describer is given.

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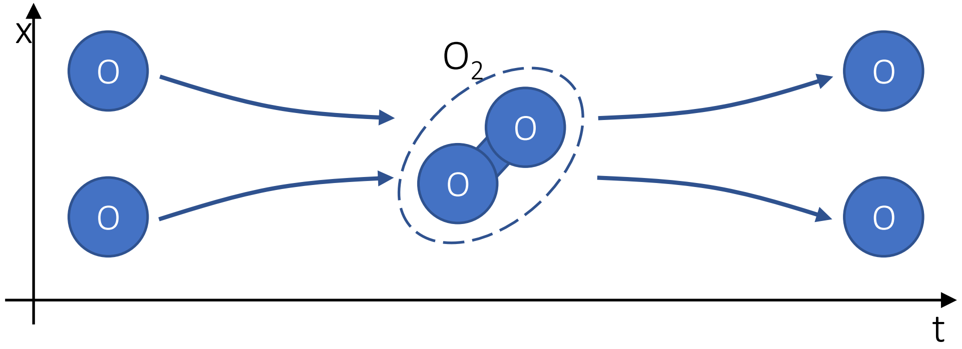
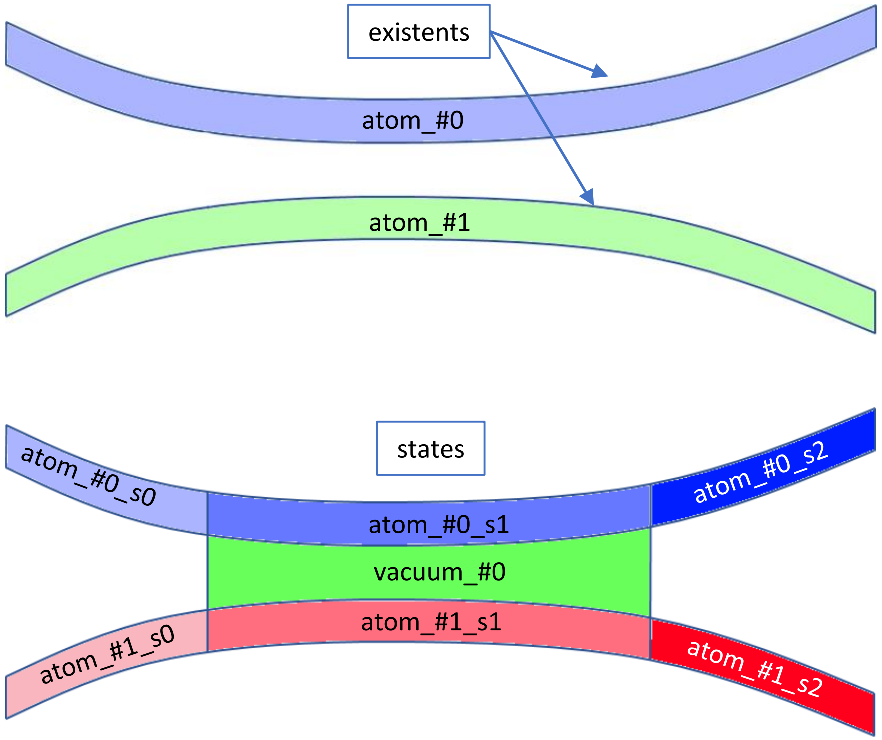
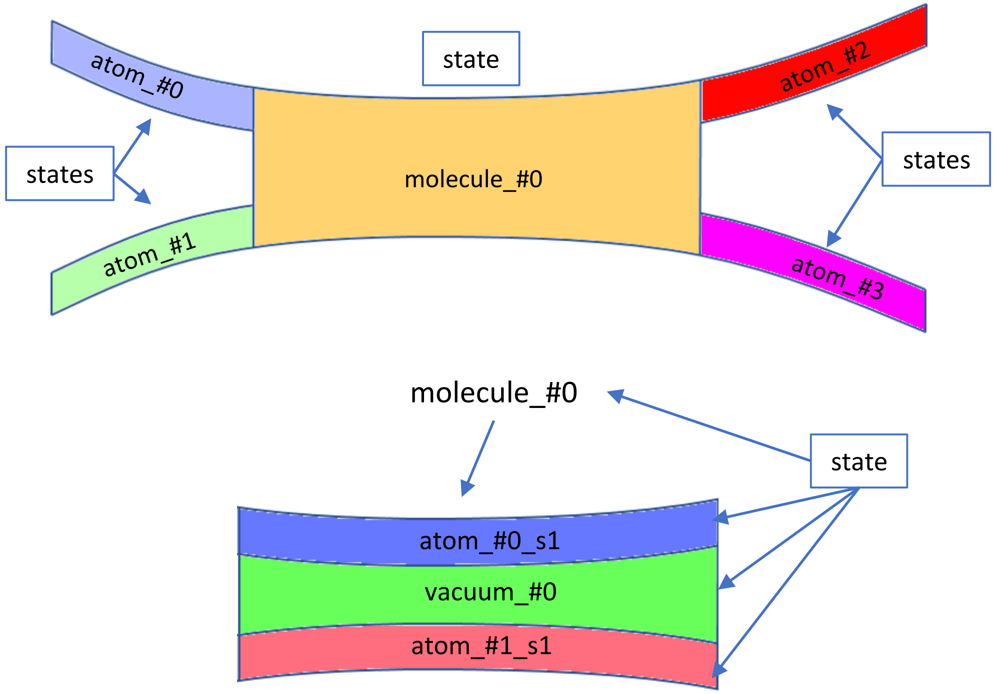
EMMO MOLECULE FORMATION EXAMPLE

EMMO representation of a O_2 molecule formations and dissociation







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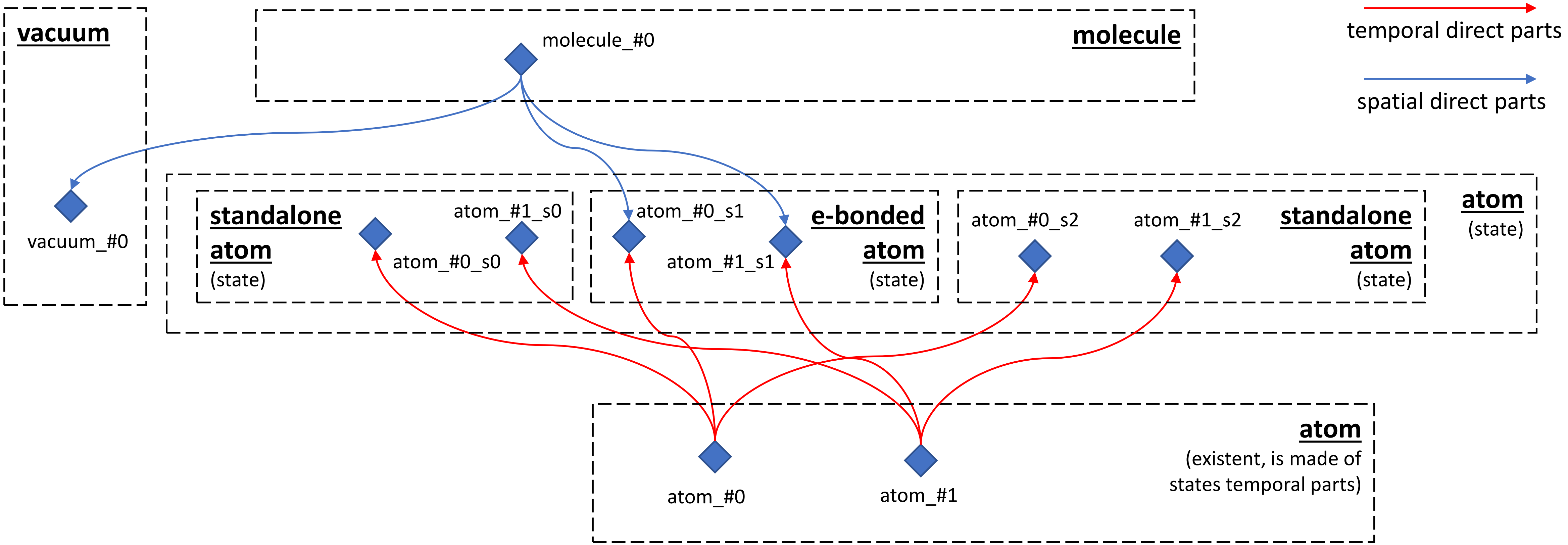
EMMO MOLECULE FORMATION EXAMPLE

Items cannot be **spatial direct part** of more than one whole.
Items cannot be **temporal direct part** of more than one whole.
But an item **can be spatial part** of an item and **temporal part** of another one.



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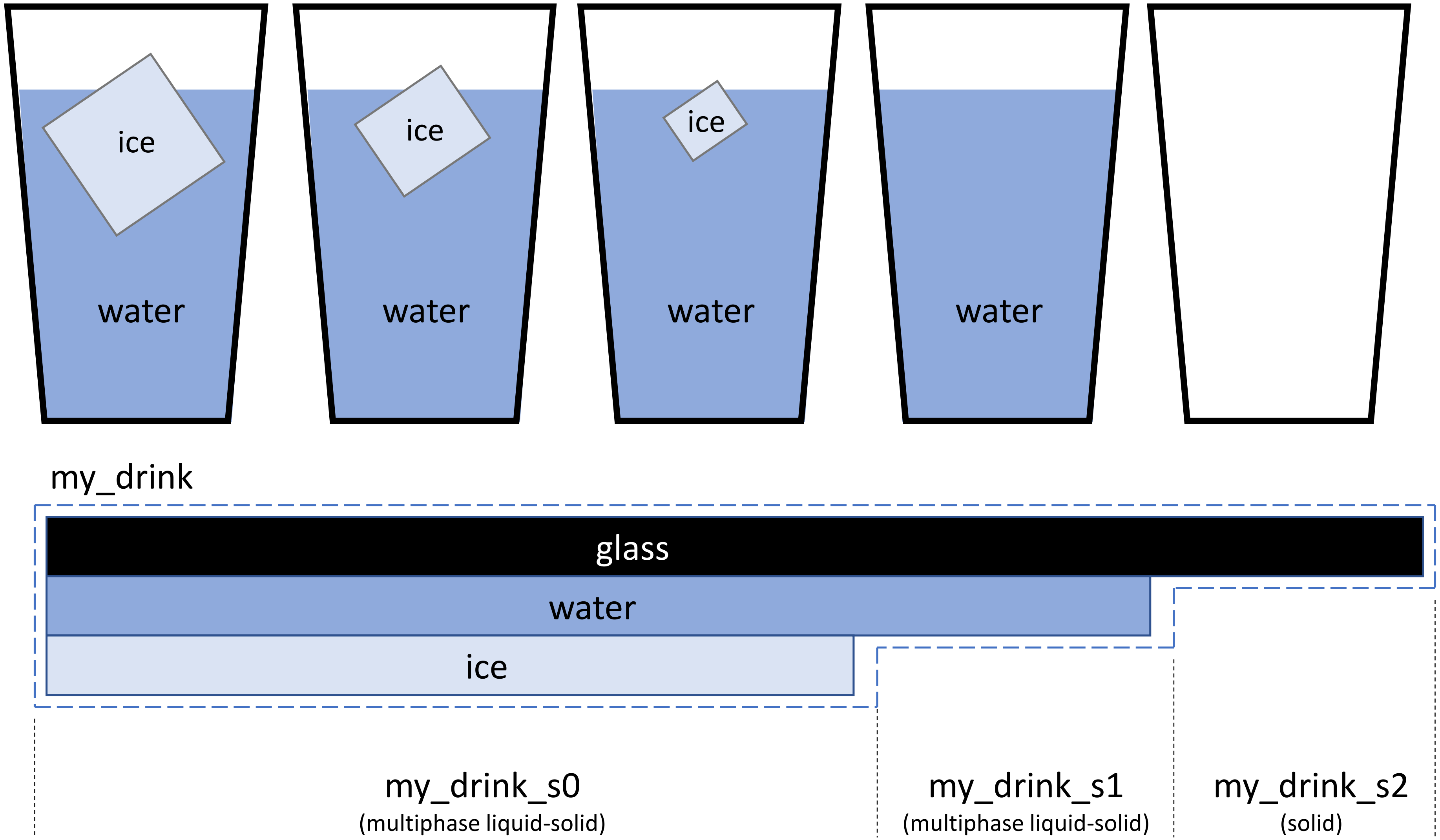
EMMO COLD DRINK EXAMPLE



my_drink is an existent made of three states.

As long as a state (**my_drink_s0**) does not lose direct parts (**ice** or **water** or **glass**), it's still a state.

ice, **water** and **glass** are existents, since the are the sum of several states (their parts number is changing overtime).

ice is losing direct parts (i.e. the H2O molecules that goes from **ice** to **water**) but still is a direct part of **my_drink**.

When **ice** disappears, then **my_drink_s0** stops to exist.

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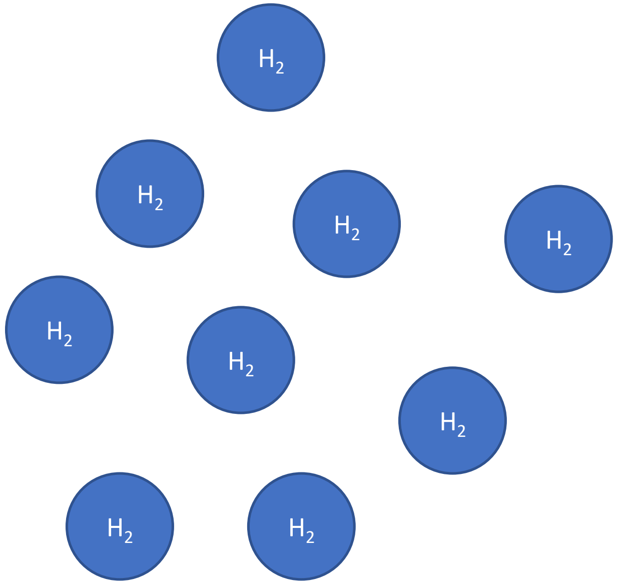
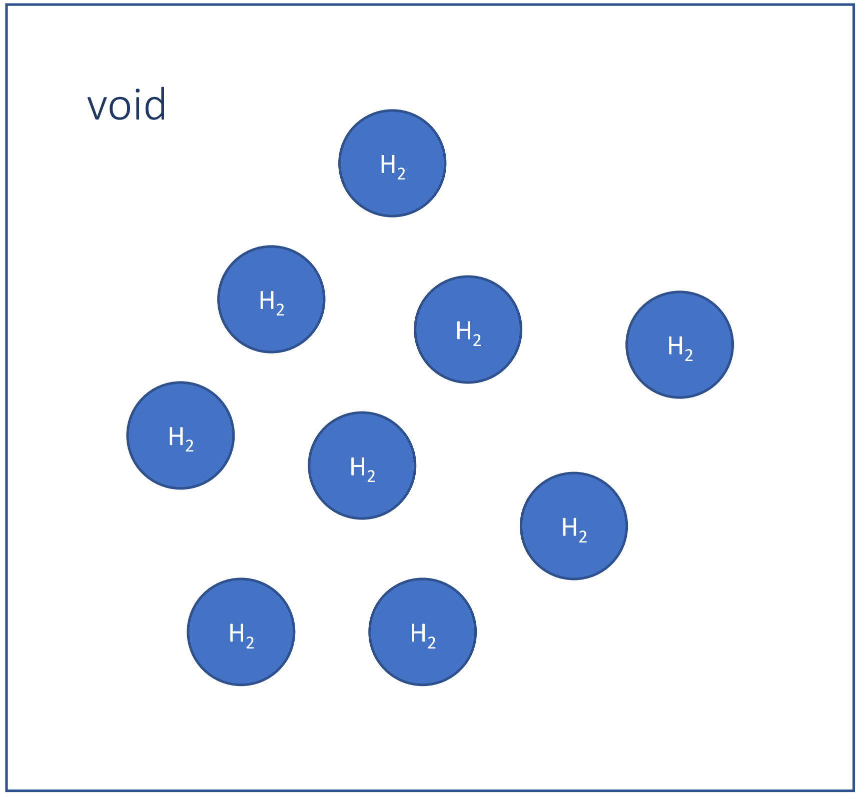
EMMO GAS EXAMPLE

A **set** of H_2 molecules (not a physical)
membership based



A **gas** of H_2 molecules + vacuum (a physical)
parthood based



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EMMO SET OR WHOLE

In **EMMO** the same 'material' or 'product' can have <u>two different representations</u>:

- the **item** representation, in which sub-granular objects are parts
- the **set** representation, in which sub-granular objects are a collection members

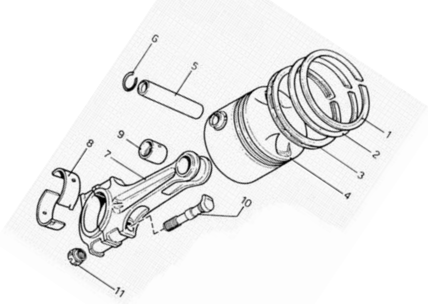
The **set** members can be at different levels of granularity;
e.g. steel ring can be seen as a grain collection, as an atom collection or a nuclei/electrons collection.

However, a physical object is only an **item** in order to maintan causality connection between parts.

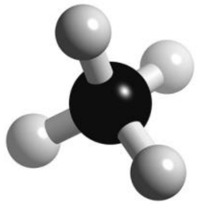
car (whole)

car components set

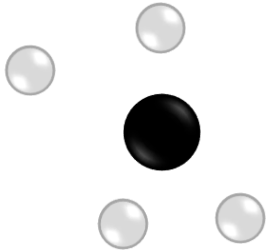
piston (whole)



mechanical parts set

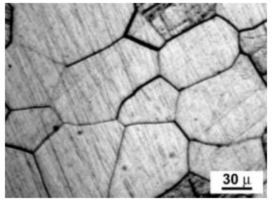


molecule (whole)



atoms set

steel ring (whole)



grain set

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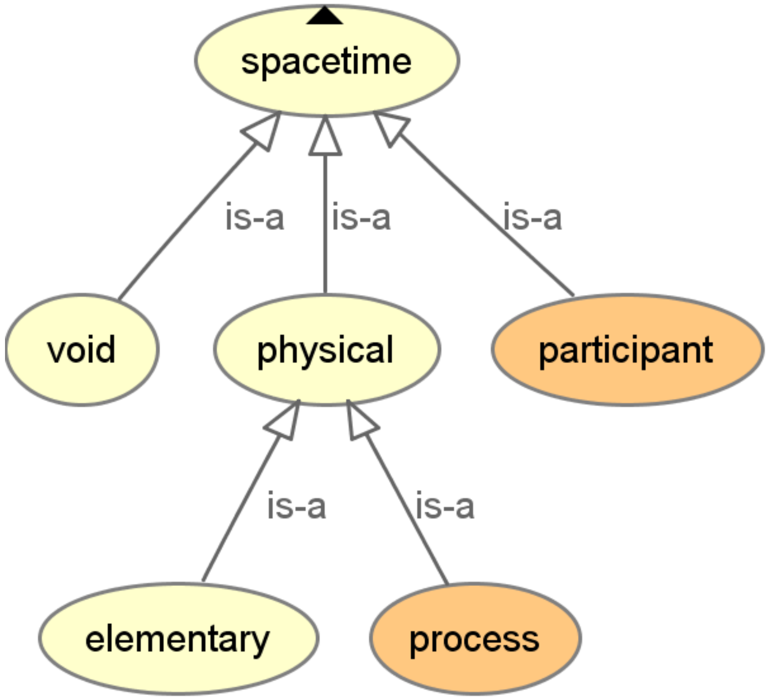
Processes and Participants

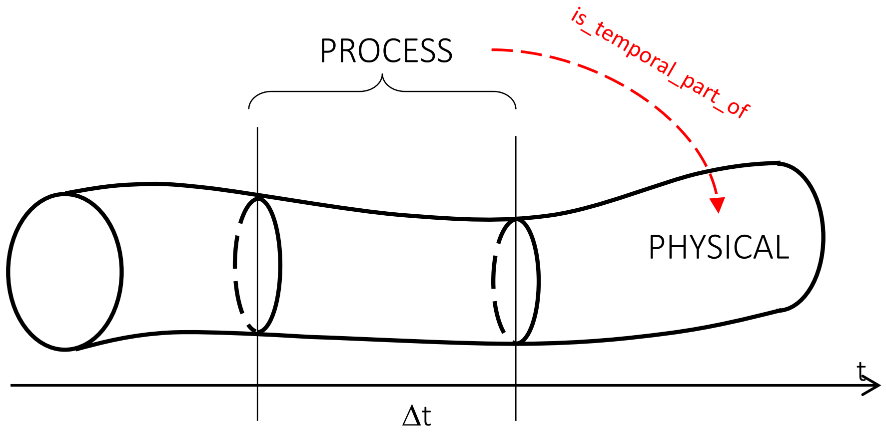
A **process** is easily defined as a temporal part of a **physical** that is categorized in a primitive **process** subclass according to what type of **process** we want to represent.

Strictly speaking, every **physical** is a 'process' since it always has a time dimension, but here we restrict the meaning of 'process' to **physical**s whose evolution in time have a meaning for the material ontologist.

Participants of a process are always parts of that particular **process** (i.e. they are spacetime). It means that **is_participant** relation is subclass of **is_part_of** relation (e.g. you cannot participate to a party if you are not enclosed by the party room)

A **participant** can be both a **physical** or a **void**, since also empty regions of spacetime may play a role in a physical process.





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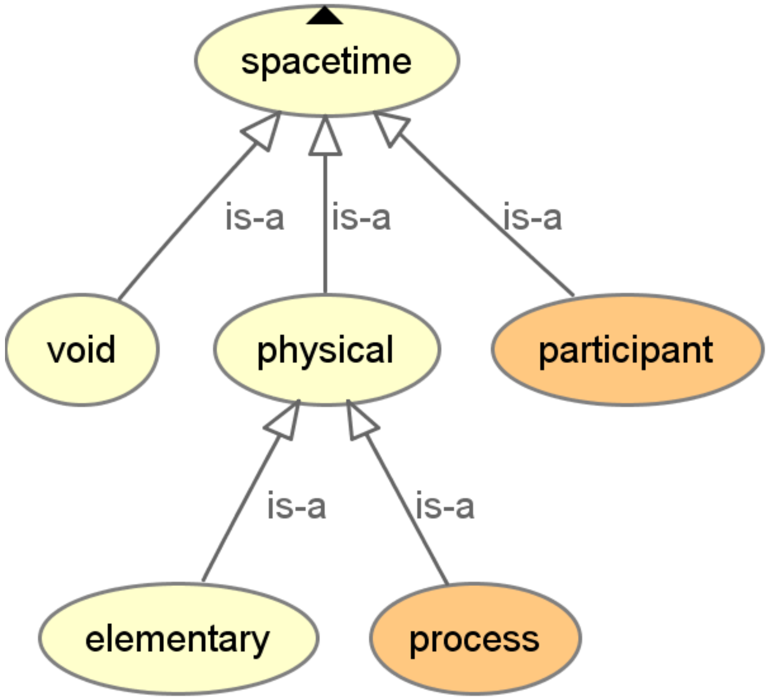
PROCESSES AND PARTICIPANTS

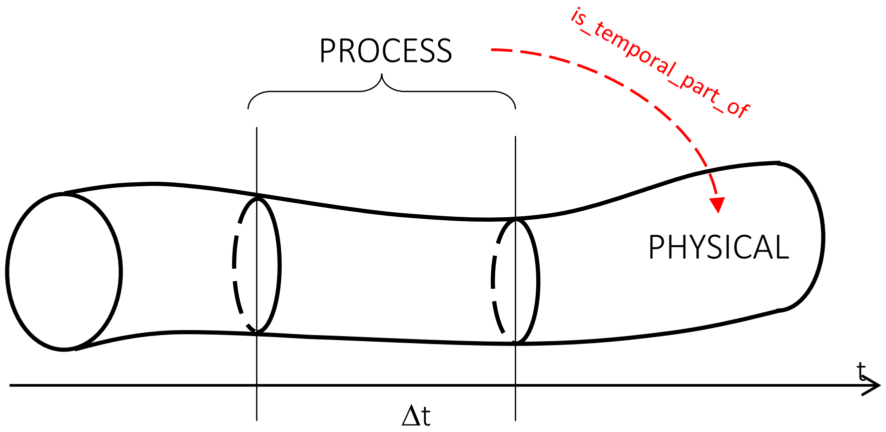
From the above definitions, it comes natural to identify a parthood hierarchy between **process** and **participant** individuals since a **participant** is always a part of some **process**.

The *has_participant* is the OWL-DL relation that specializes the *has_part* relation between **process** and **participant** individuals.

This is a very important result for the EMMO, since:

- the *has_participant* relation is a sub-relation of *has_part*, simplifying the EMMO relation hierarchy towards a vertical classification (i.e. relation inheritance) instead of horizontal classification (i.e. independent relations)
- the participation to a process formally implies a topological connection between the participants (*has_part* is *connected* subrelation), which is a strong reductionistic statement that takes into account the fact that a participant has by definition a causal relation with the process itself (e.g. the process of talking between two persons has participants the persons and the air as the physical mean through which the communication occurs)
- prevents a **set** individual to be also a **process** individual, due to the lack of causal connection between set members.





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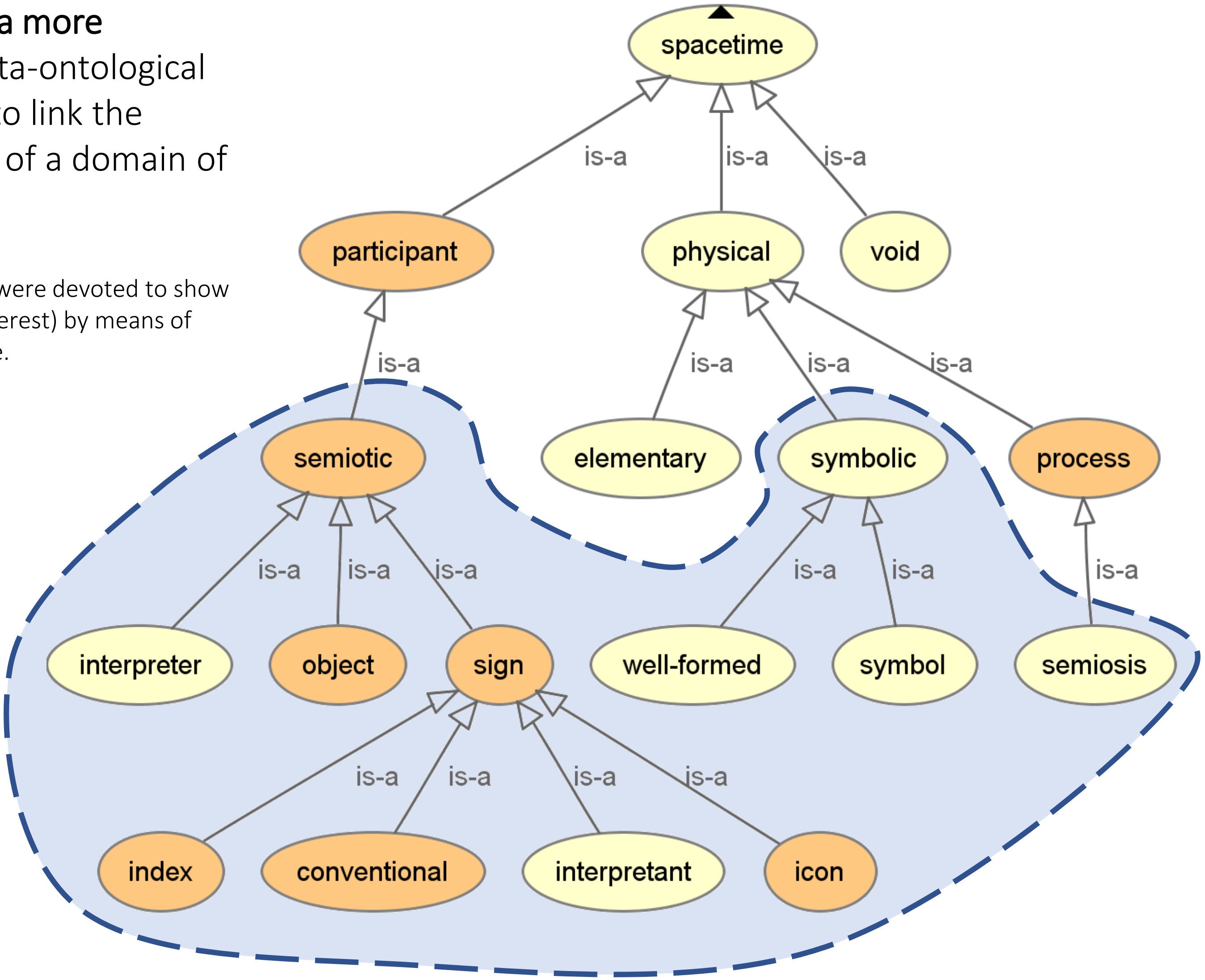
EMMO SEMIOTIC

Within the EMMO semiotic perspective, **an ontology is a part of a more inclusive representational system** that makes use of so called meta-ontological means (e.g. annotations, elucidations) to enable an interpreter to link the ontology entities (i.e. classes, individuals, axioms) to the objects of a domain of interest.

In this paper, we introduced the EMMO OWL-DL as the ontology, while all previous sections were devoted to show to the reader how to link EMMO OWL-DL entities to real world objects (i.e. the domain of interest) by means of meta-ontological concepts, such as e.g. mereotopology, physical theories and common sense.

This semiotic perspective is useful to explain **the mechanisms through which meaning is given to ontology entities within an upper level system**, but it can also be used within the ontology itself to **formalize semiotic processes occurring within the domain of interest**.

This feature is **paramount for the ontologization of interpreter-dependent processes**, i.e. processes whose result depends on the specific interpreter perspective, such as formulation of **physical theories** or **experimental measurements**.



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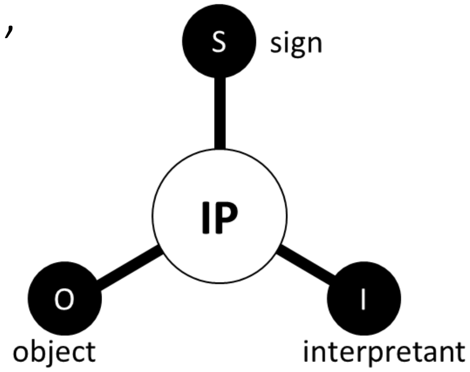
EMMO SEMIOTIC

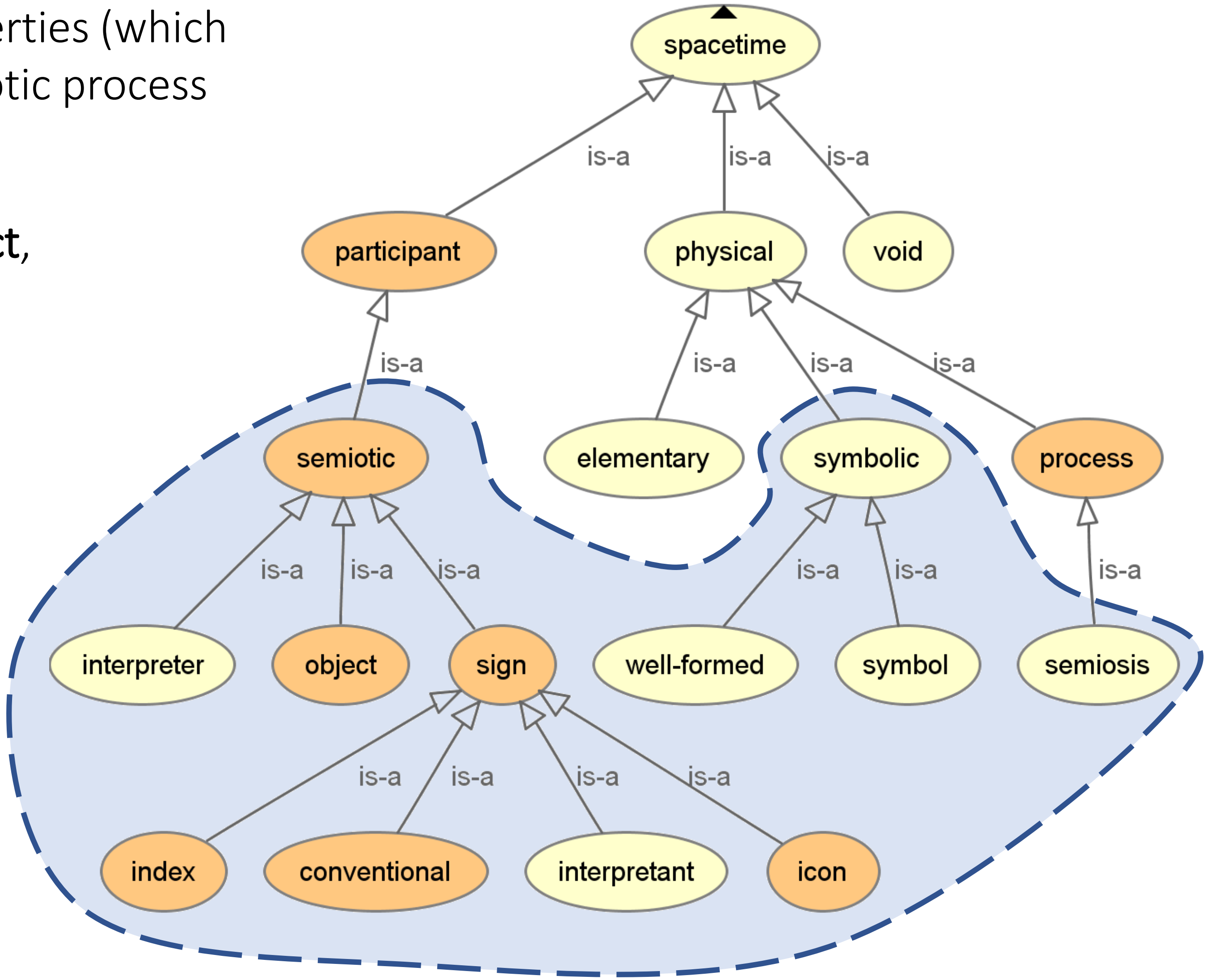
Since the **EMMO** must represent models and properties (which are signs that stand for a physical entity), the semiotic process must be described also within the **EMMO** itself.

The concepts of Peirce semiotics (**interpreter**, **object**, **sign**) are included in the semiotic branch, together with the **semiosis** process.

Besides that, a branch for representing **symbol**s and **symbolic** entities (e.g. characters, numbers, words) has been introduced, based on <u>formal languages</u> approach.

Symbols of a formal language need not be symbols of anything.





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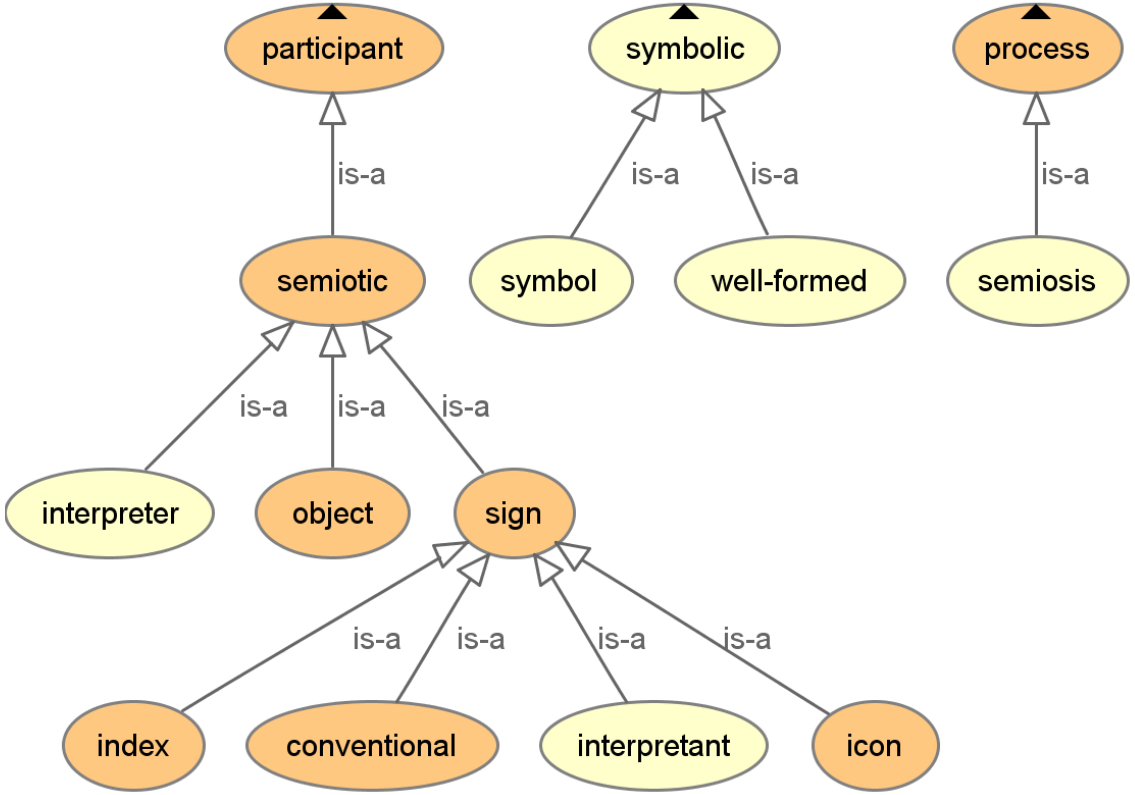
EMMO Semiotic

The **semiotic** class is an OWL-DL class whose individuals stand for semiosis process participants that are categorized under:

- the **sign** class, whose individuals stand for real world objects that stand for other real world objects
- the **object** class, whose individuals stand for the real world objects that have other real world objects standing for them, the latter being represented by **sign** individuals
- the **interpreter** class, whose individuals stand for the real world objects that act as interpreters agent in semiosis processes.
- the **interpretant** class, whose individuals are signs that stand for the interpreters internal representation of the objects (i.e. subparts of the interpreters), and that are determined by interaction of the interpreters with the signs or the objects.



The **semiotic** class is defined as the union of **sign**, **object** and **interpreter**, meaning that a semiotic individual must fall in one of the three subclasses (covering axiom). Moreover, **semiotic** individuals must be participants to a semiotic process.
The **semiosis** class is an OWL-DL class whose individuals stand for a semiosis process. It is required that a **semiosis** individual *has_participant* one individual from each of the **object**, **sign** and **interpreter** classes.

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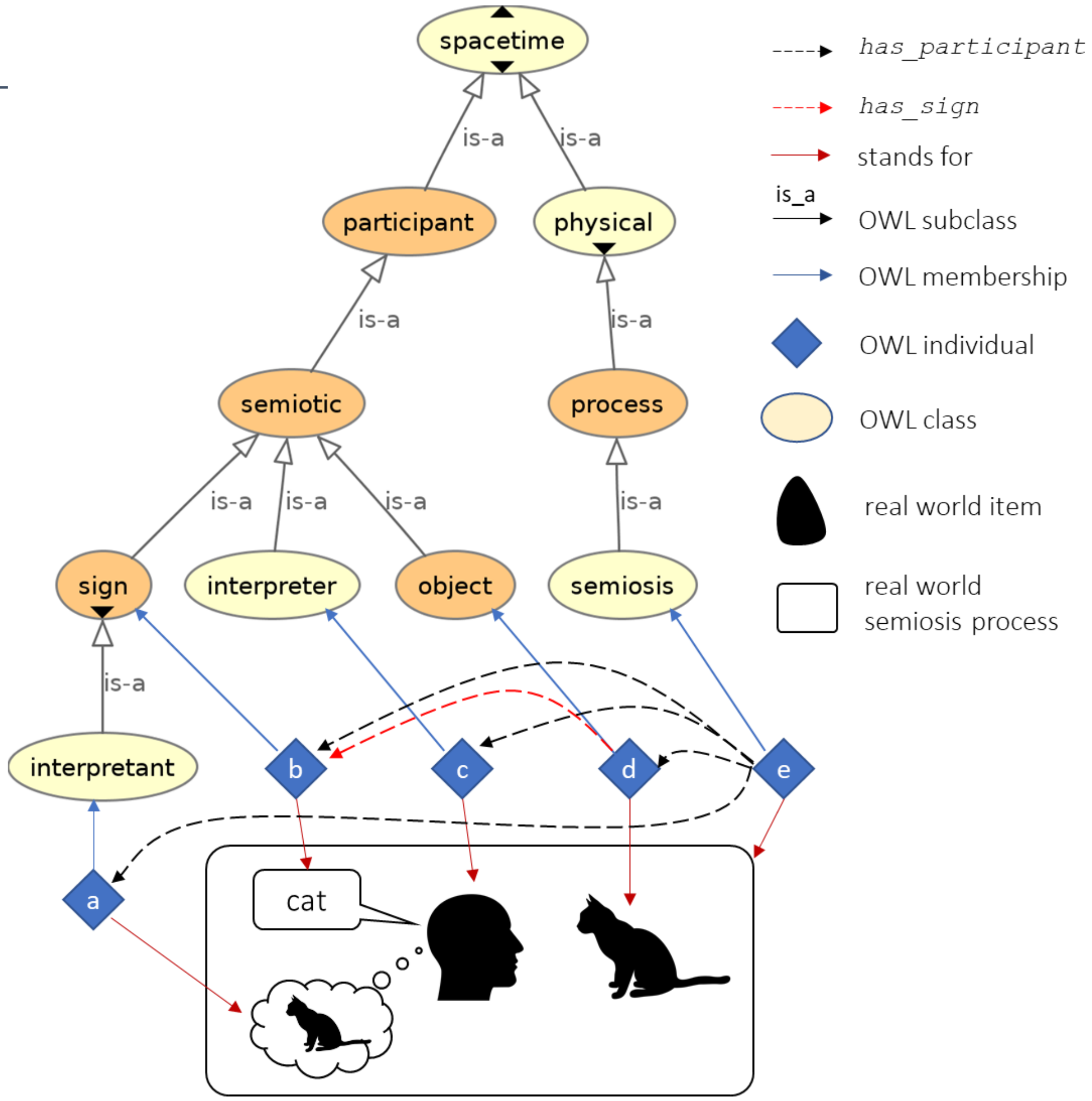
EMMO Semiotic

Individual c stands for the interpreter (a human being), individual d stands for the object (a cat), individual a stands for the interpretant determined by the observation process (the complex neuronal process that represents the cat within the human being brain) and individual b is the sign produced by the interpreter (the word "cat") that stands for the object.

The fusion of real world object, interpreter, interpretant and sign is the semiotic process.

It's important to underline that OWL-DL does not allow for triadic relations, which are the most straightforward way to represent a semiotic process, according to Peirce. However, the fact that a sign is linked to an object for an interpreter (which can be also a class of interpreters) can always be inferred by an OWL-DL reasoner by following the relation path that starts with the sign, its participation to a semiotic process and the interpreter that co-participates to the same semiotic process.



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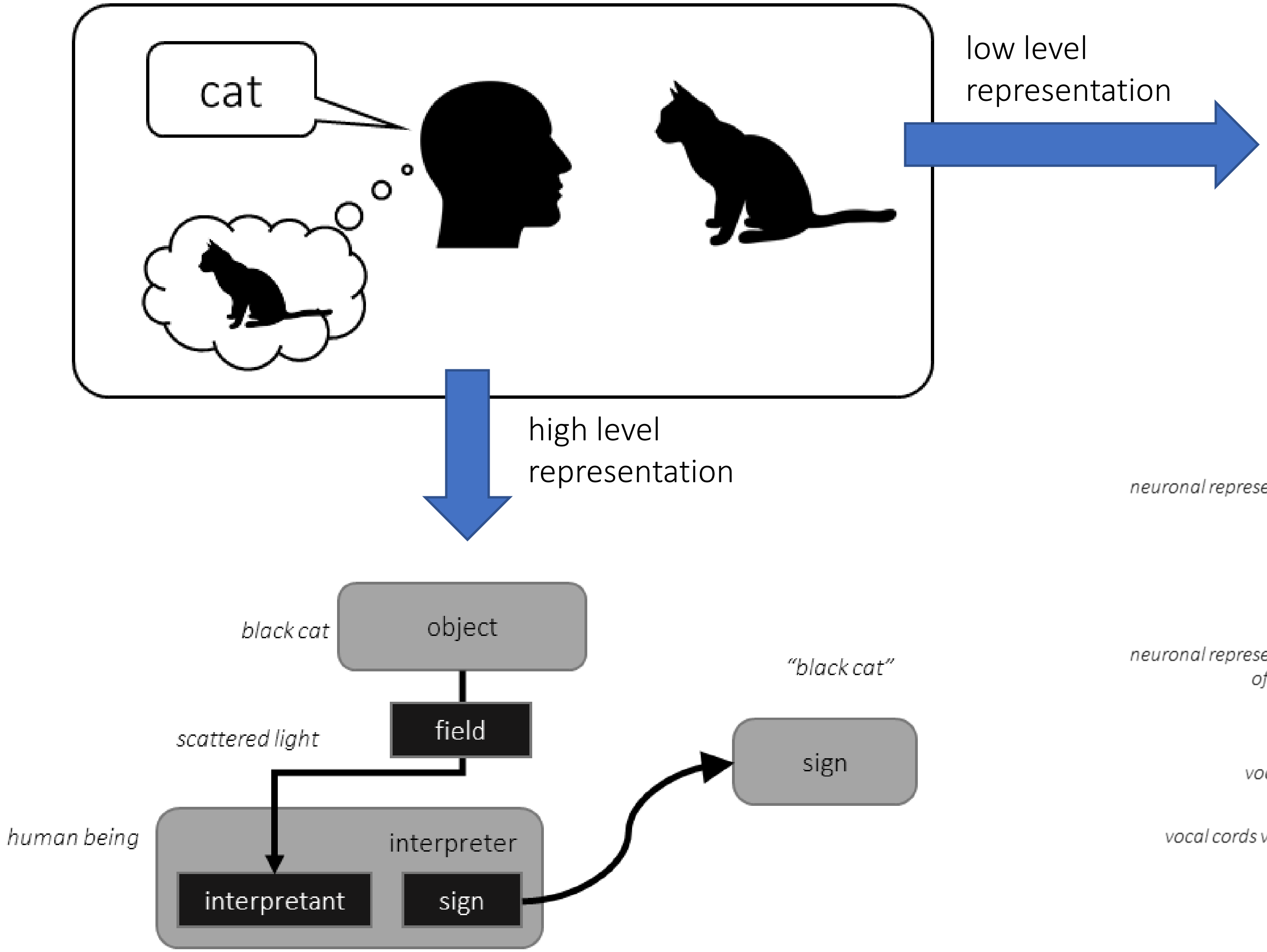
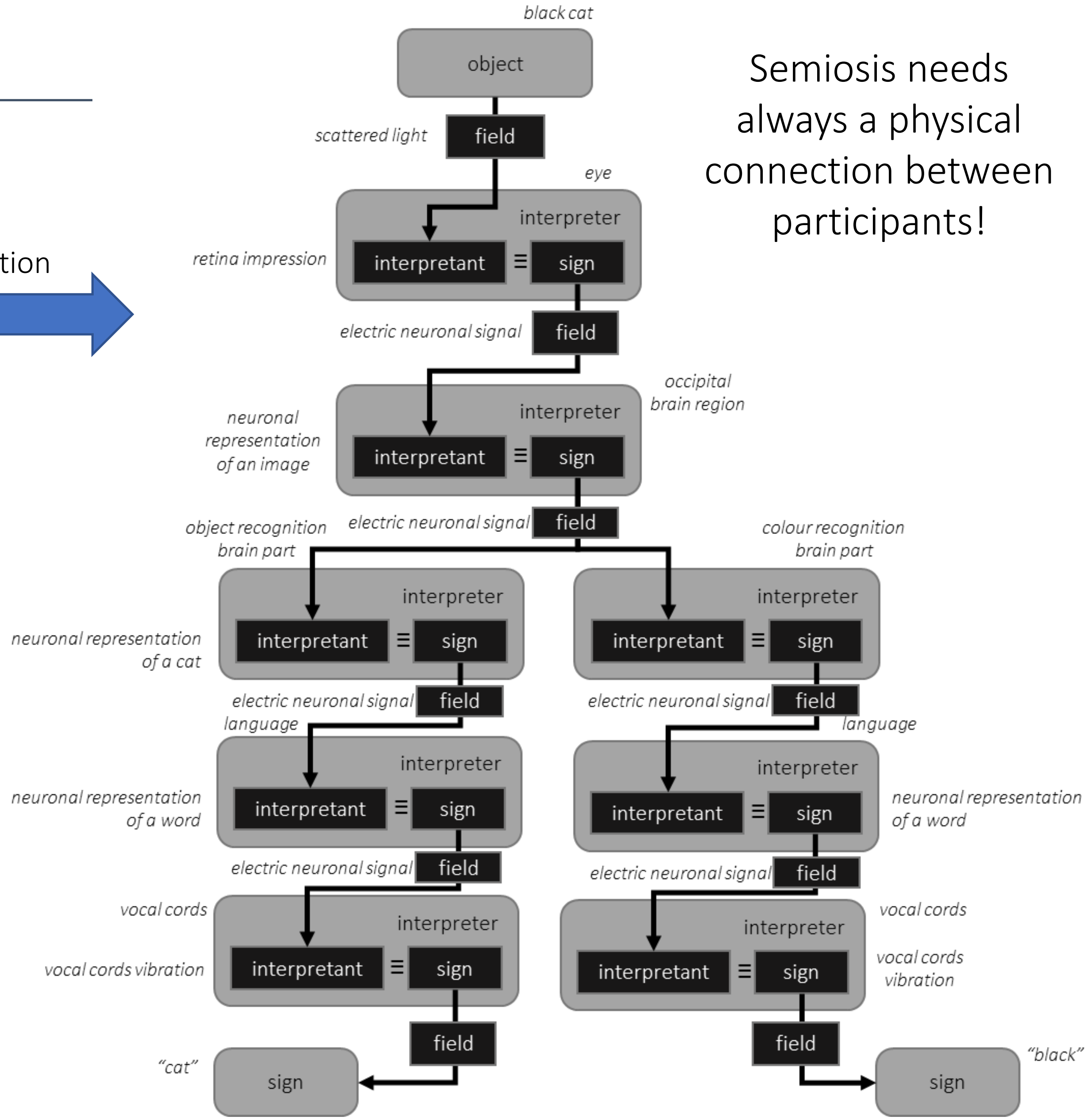
EMMO Semiotic Reductionism





Semiosis needs always a physical connection between participants!

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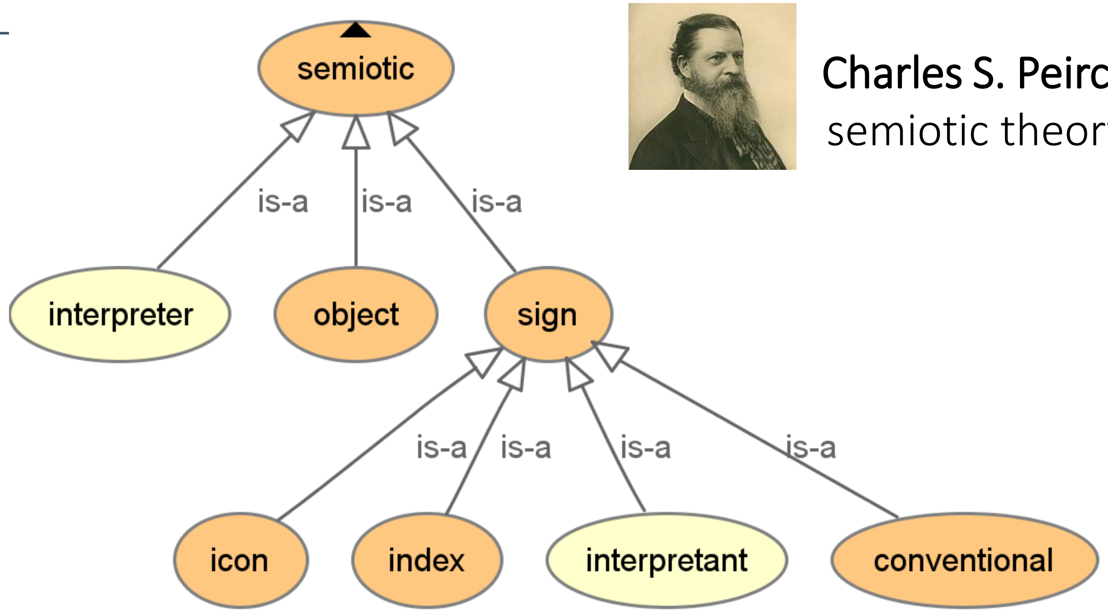
EMMO SEMIOTIC

According to Peirce, a sign can be classified into three principal subcategories:

- symbols, that stand for an object through conventional laws or habit, without any resemblance to it (e.g. words)
- indexes, that stand for an object due to causal contiguity (e.g. smoke is an index for a fire)
- icons, that stand for an object by resembling or imitating it, in shape or by sharing a similar logical structure (e.g. road sign, physical equation).

The **conventional**, **icon** and **index** classes are the OWL-DL representation of such concepts.

The term 'conventional' (meaning a conventional sign) has been used, instead of the most straightforward term 'symbol', because of the different meaning given to the term 'symbol' in semiotics and formal language field (i.e. computer science). While in the first case the term 'symbol' stands for an object that refers to something, in the latter case such a reference is not necessary.



Charles S. Peirce
semiotic theory

These categories are used in the EMMO to classify as signs of different types some fundamental concepts in applied physics (e.g. physics equations, physical properties) and to link these concepts with formal languages tokens used to represent them.

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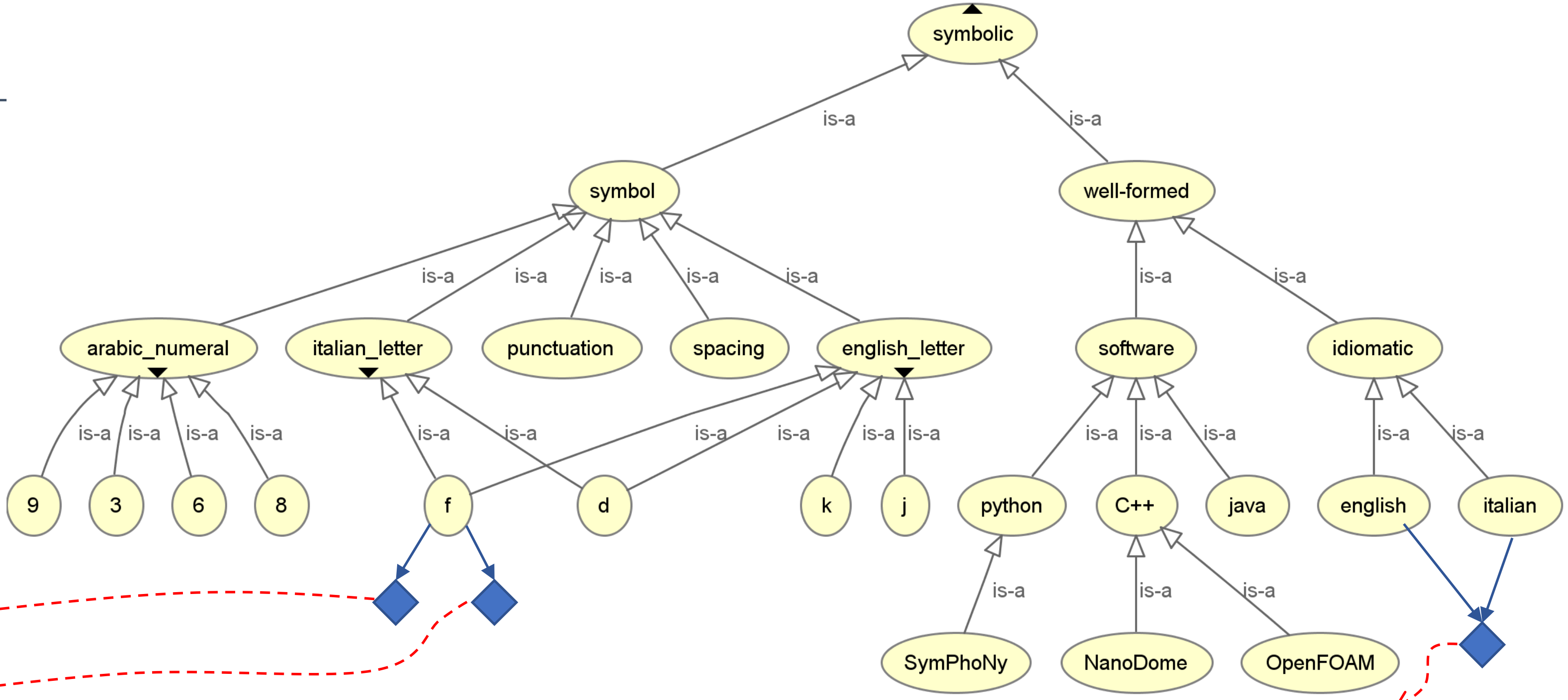
EMMO SEMIOTIC



Since EMMO scope is not only to represent real world objects but also to represent the different ways in which they are analyzed, measured and modelled by applied sciences, the EMMO includes classes for the representation of the objects that are used to exchange information, through the concept of symbol and string of symbols, as defined in formal languages field. An object is a symbol when it can be identified by the interpreter as an elementary mark of a specific symbolic code (or alphabet). The **symbol** class is the EMMO OWL-DL representation of this concept.

Subclasses of **symbol** may specify specific types of symbols, like e.g. math symbols or the single character types within an alphabet. The class is the idea (i.e. type, definition) of a symbol, while the individual of that class stands for a specific mark (or token) of that idea. For example, the class defining the letter 'A' is the symbol intended as an idea, while a letter A (i.e. the physical object) is the mark.

The **well-formed** class individuals stands for a composition of symbols respecting a specific language syntactic rules (i.e. a formal language). It's important to notice that even a well formed string of symbol may refer to nothing (e.g. 'blitiri', 'bu-ba-baff') or refer to something not known by the interpreter (e.g. a word in a foreign language).

The **symbolic** class is the EMMO OWL-DL representation of a symbolic object, and is defined as the union of **symbol** and **well-formed** classes, aimed to contain all individuals that refers to symbols or strings of symbols. An OWL-DL individual member of both **symbolic** and **sign** classes, stands for an object that is an expression of a language and refers to a specific real world object, or classes of objects.

The symbolic branch enables the EMMO to represent raw formatted data as individuals and to transform them in knowledge as soon as semiotic relations with other EMMO individual are declared by the interpreter.

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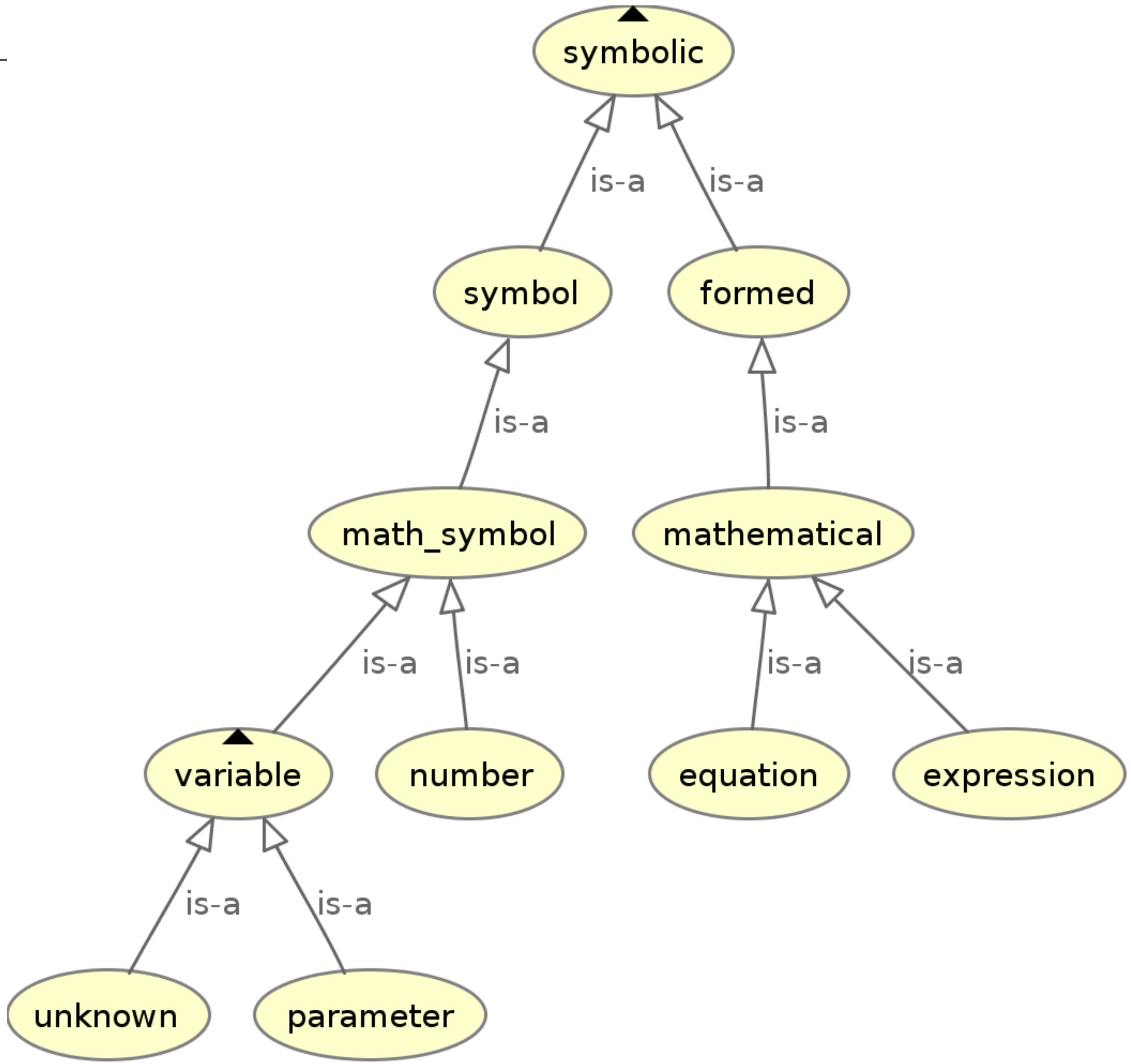
EMMO MATH

The **symbolic** class is the superclass of the math branch, since mathematics is seen in the **EMMO** as a formal language, based on an alphabet of **mathematical symbols**.

Mathematical expressions that have a meaning (i.e. are used to represent physical phenomena) are also **sign**s (e.g. physics equations).

The **formed** class includes formal languages constructs (i.e. list of symbols) that follows the rules of a specific language.



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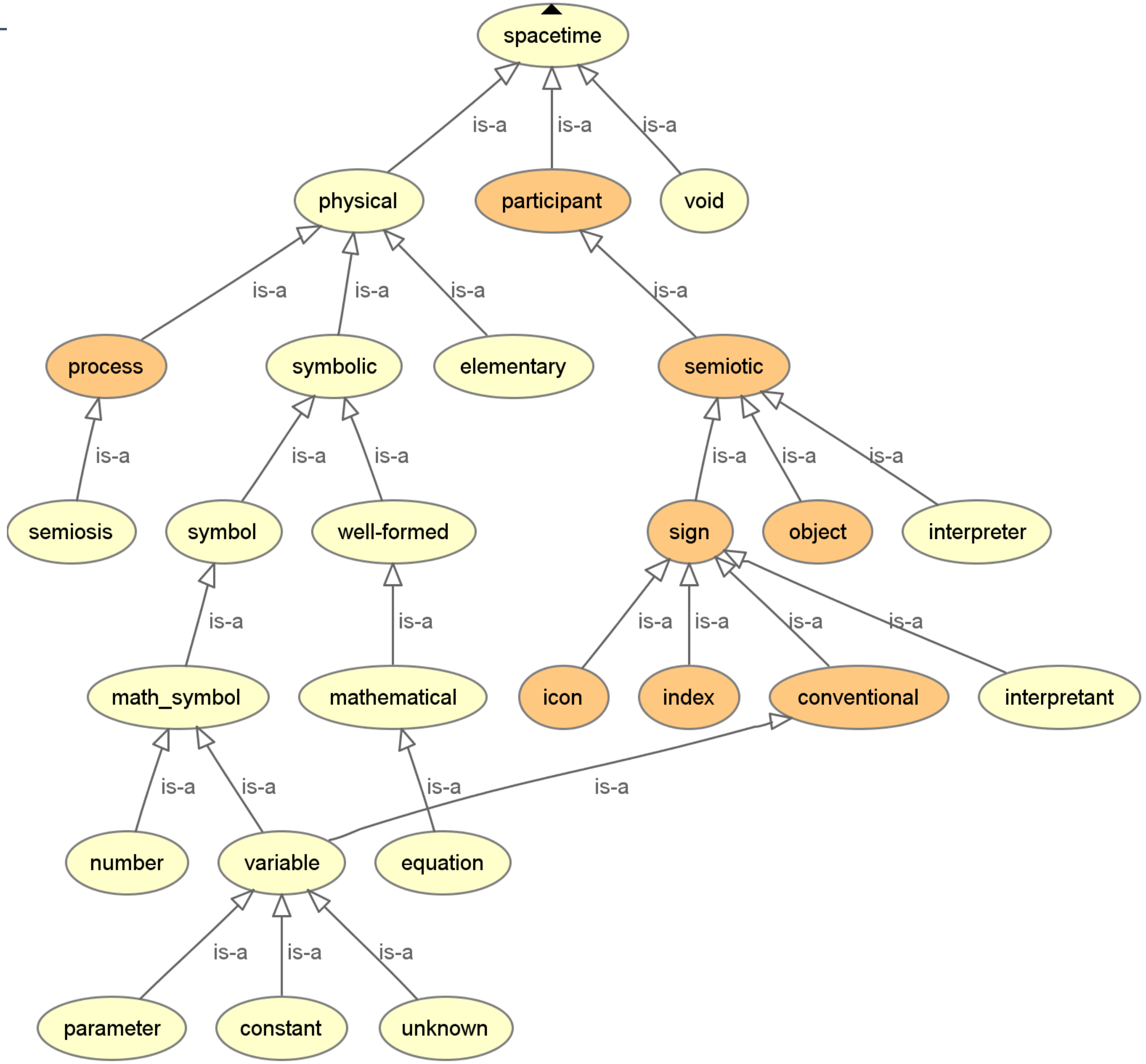

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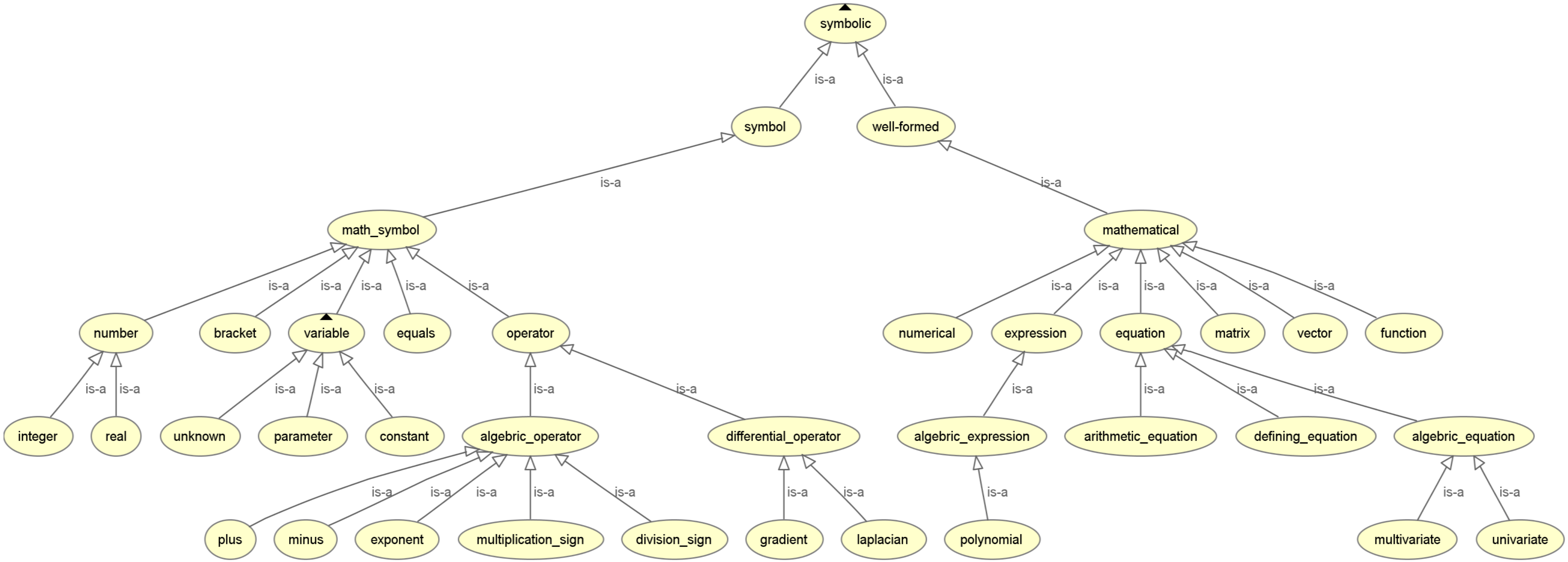
EMMO MATH



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EMMO PROPERTIES

The concept of property (also known as quality or attribute) is a fundamental concept in philosophy and science. Basic scientific activities and results (e.g. scientific theories and models) use property-based statements (e.g. physical equation) to describe the structure and behaviour of real world objects. Properties are usually defined in philosophy as entities that are predicates of things and that things are said to bear or to possess, but the fundamental nature of properties and even their existence has been extensive matter of debate since the beginning of rational thinking.

The EMMO approach on properties is based on the principles previously expressed and represented within the overlying EMMO semiotic framework.

Properties in the EMMO are:

- **real world objects** and not abstract (i.e. nominalism)
- **intrinsically dependent on the observer** (i.e. pluralism)
- categorized according to the **physical phenomena** (i.e. reduction) through which the object-observer interaction happens (i.e. semiotics).

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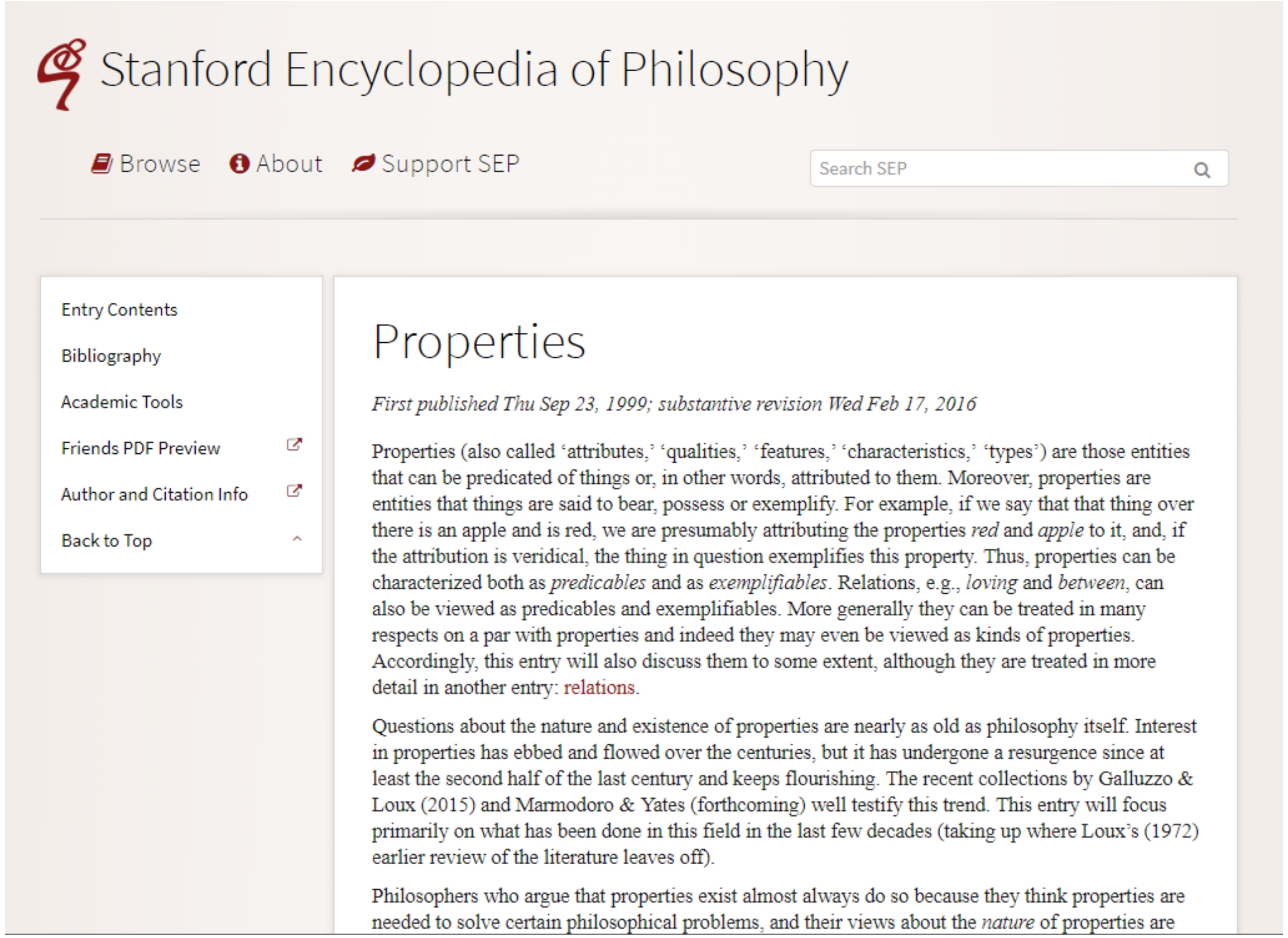
EMMO PROPERTIES

Formally, EMMO properties can be defined as **signs that stand for real world objects** that interpreters perceive through **specific observation processes**.

In other words, a property is a **partial representation of an object**, reflecting object capability to be part of a specific observation process.

As example, ‘redness’ is an abstract concept that cannot exist in the EMMO as individual. It rather expresses the capability of an object to be perceived within a well defined perception channel (e.g. excitation by photon of a red-sensitive sensors) by an observer (e.g. human retina impression, chromatograph).

The result of the observation process is a sign (or an interpretant, if the sign is an internal representation) that the observer uses to represent the fact that the object interacted with him through that specific perception channel (e.g. “It’s red”).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Properties

First published Thu Sep 23, 1999; substantive revision Wed Feb 17, 2016

Properties (also called ‘attributes,’ ‘qualities,’ ‘features,’ ‘characteristics,’ ‘types’) are those entities that can be predicated of things or, in other words, attributed to them. Moreover, properties are entities that things are said to bear, possess or exemplify. For example, if we say that that thing over there is an apple and is red, we are presumably attributing the properties *red* and *apple* to it, and, if the attribution is veridical, the thing in question exemplifies this property. Thus, properties can be characterized both as *predicables* and as *exemplifiables*. Relations, e.g., *loving* and *between*, can also be viewed as predicables and exemplifiables. More generally they can be treated in many respects on a par with properties and indeed they may even be viewed as kinds of properties. Accordingly, this entry will also discuss them to some extent, although they are treated in more detail in another entry: relations.

Questions about the nature and existence of properties are nearly as old as philosophy itself. Interest in properties has ebbed and flowed over the centuries, but it has undergone a resurgence since at least the second half of the last century and keeps flourishing. The recent collections by Galluzzo & Loux (2015) and Marmodoro & Yates (forthcoming) well testify this trend. This entry will focus primarily on what has been done in this field in the last few decades (taking up where Loux’s (1972) earlier review of the literature leaves off).

Philosophers who argue that properties exist almost always do so because they think properties are needed to solve certain philosophical problems, and their views about the *nature* of properties are

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EMMO PROPERTIES

In the **EMMO**, a **property** is a **sign** that stands for an **object** that the **interpreter** perceived through a well defined **observation** process.

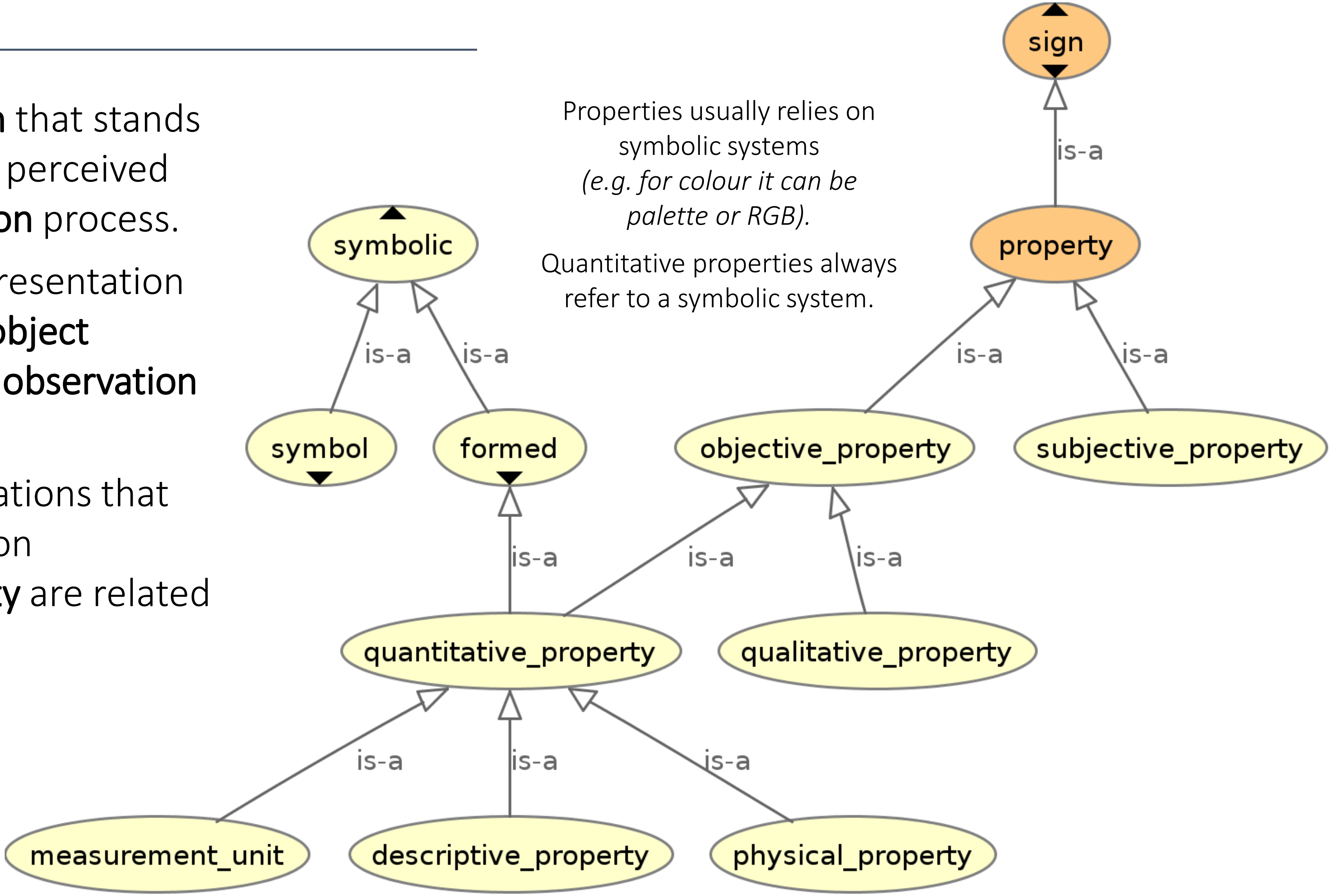
A **property** is always a partial representation of an **object** since it reflects the **object** capability to be part of a specific **observation** process.

Property subclasses are specializations that depend on the type of observation processes. A **quantitative property** are related to an **observation** subclass called **measurement**.

e.g. the property 'colour' is related to a process that involves emission or interaction of photon and an observer who can perceive electromagnetic radiation in the visible frequency range.

Properties usually relies on symbolic systems *(e.g. for colour it can be palette or RGB).*

Quantitative properties always refer to a symbolic system.



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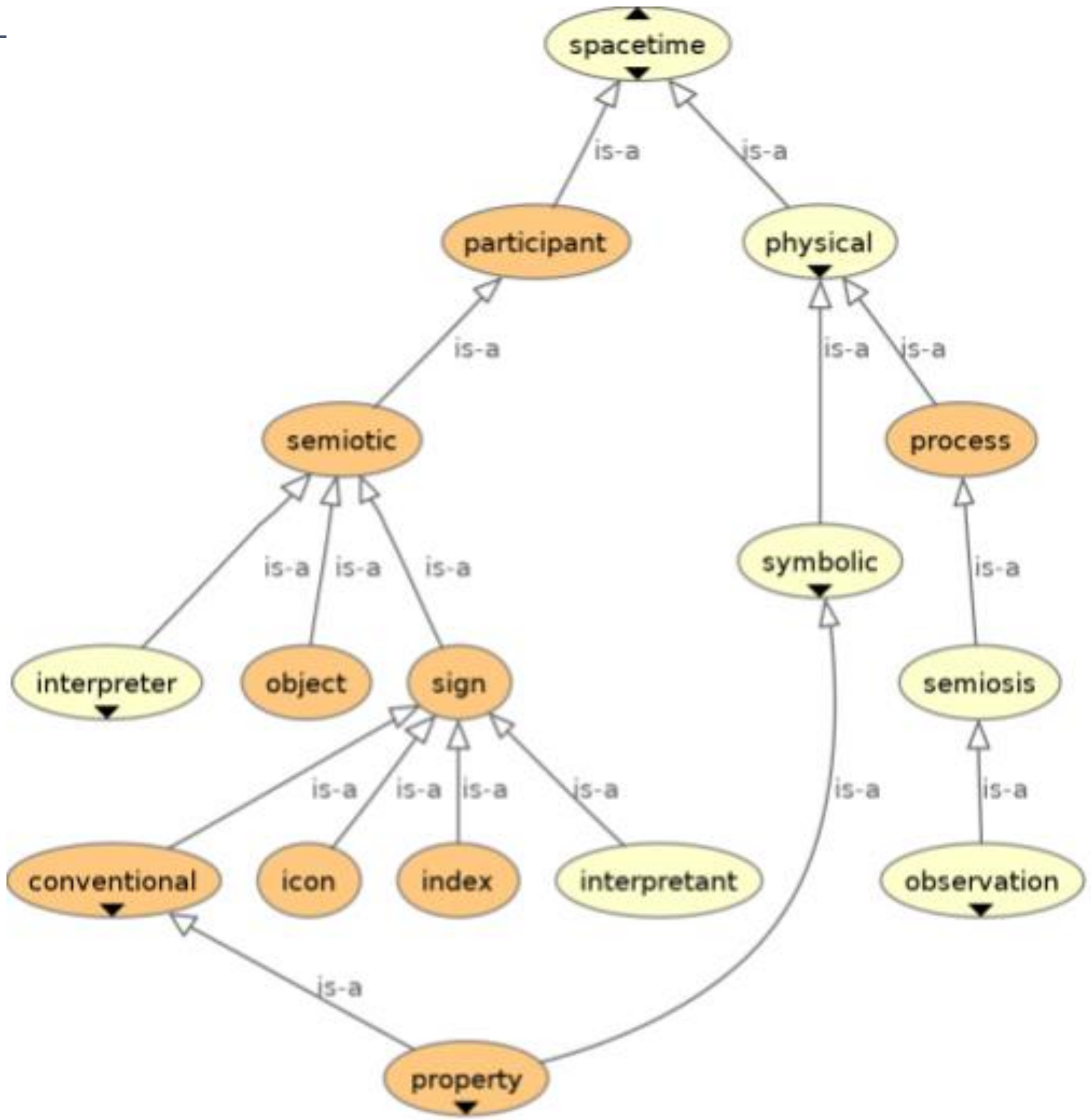
EMMO PROPERTIES

More specifically, a property is represented and shared between interpreters usually according to a **well defined symbolic code**, that is defined by convention according the the results of the of observer-object interaction.

For example, there exist several conventional symbol systems for colors, like the natural language categorization (e.g. red, blue, yellow) or the standardized color spaces (e.g. RGB, CMYK) for a more precise numerical categorization. Another examples are physical properties, for which the International System of Units (SI) is an important standard conventional system.

For this reason properties in the EMMO falls under the category of **conventional signs**, and are always **associated to a symbolic object** that is standardized by convention like common habit or international standard.



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EMMO PROPERTIES

TECHNICAL SPECIFICATION

ISO/TS 10303-1002

First edition
2001-09-01

Industrial automation systems and integration — Product data representation and exchange —

Part 1002:
Application module: Colour

Systèmes d'automatisation industrielle et intégration — Représentation et échange de données de produits —

Partie 1002: Module d'application: Couleur

4.2.1 Colour

A Colour is a name for a property of reflecting light at a particular wavelength.

EXPRESS specification:

```
*)
ENTITY Colour;
  name : STRING;
END_ENTITY;
(*
```

Attribute definitions:

name: The **name** specifies the word or group of words by which the Colour is known.

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EMMO PROPERTIES

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Partie 1002: Module d'application: Couleur

4.2.3 Pre_defined_colour

A Pre_defined_colour is a Colour that has its definition established and maintained in the Colour module.

EXPRESS specification:

```
*)
ENTITY Pre_defined_colour
  SUBTYPE OF (Colour);
WHERE
  WR1: SELF.name IN
        ['red',
         'green',
         'blue',
         'yellow',
         'magenta',
         'cyan',
         'black',
         'white'];
END_ENTITY;
(*
```


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EMMO PROPERTIES

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Partie 1002: Module d'application: Couleur

4.2.4 User_defined_colour

A User_defined_colour is a Colour that has its definition established without referencing any standard.

EXPRESS specification:

```
*)
ENTITY User_defined_colour
  SUBTYPE OF (Colour);
  red   : REAL;
  green : REAL;
  blue  : REAL;
WHERE
  WR1: {0.0 <= red <= 1.0};
  WR2: {0.0 <= green <= 1.0};
  WR3: {0.0 <= blue <= 1.0};
END_ENTITY;

END_SCHEMA;
(*
```

Attribute definitions:

red: the intensity of the red colour component.

green: the intensity of the green colour component.

blue: the intensity of the blue colour component.

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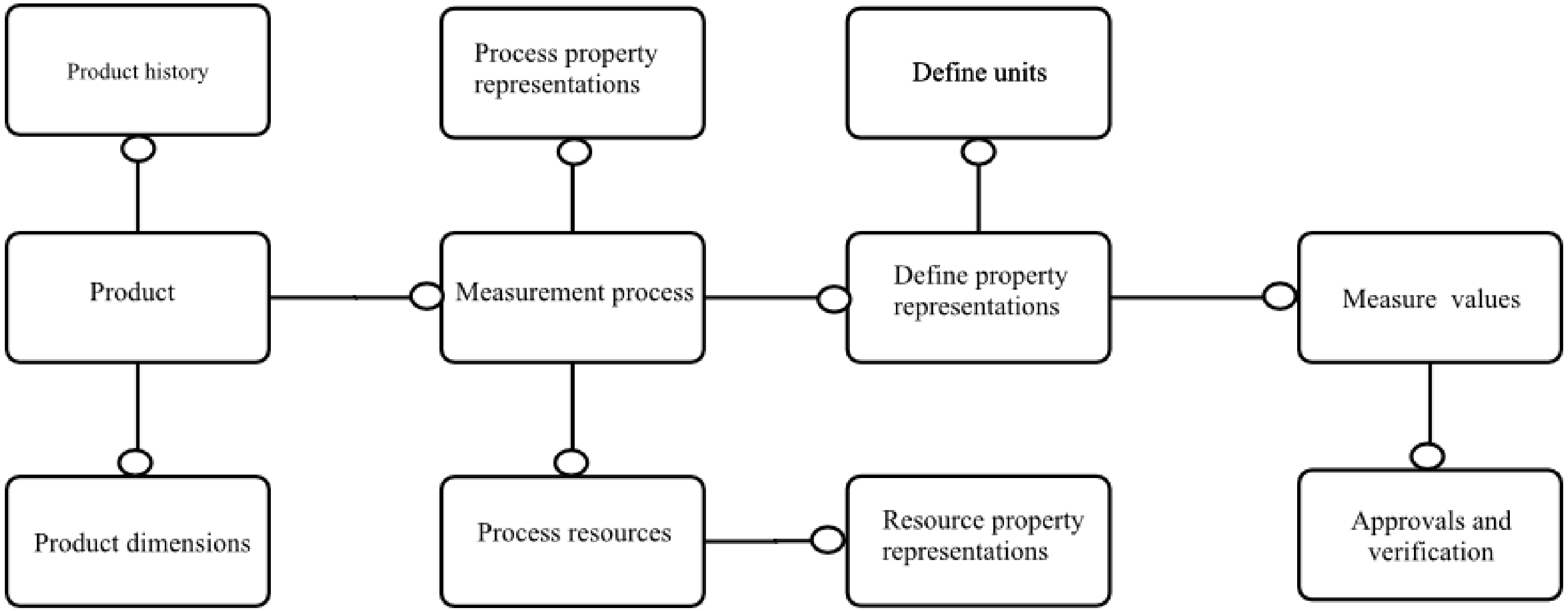
EMMO Properties

ISO 10303-235 is an Application Protocol (AP) from ISO Technical Committee 184 Sub-committee 4 (ISO TC184/SC4) that can represent the measurement of any property of any product measured by any method in a computer processable form that is independent of any proprietary software.

This enables the information to be more easily exchanged between different software systems and archived for long-term data preservation

The principal concepts are:

- Everything is a product, including a 'material'
- **The meaning of a 'property' is defined by the measurement process**
- The magnitude of the property value may be determined by the properties of the process



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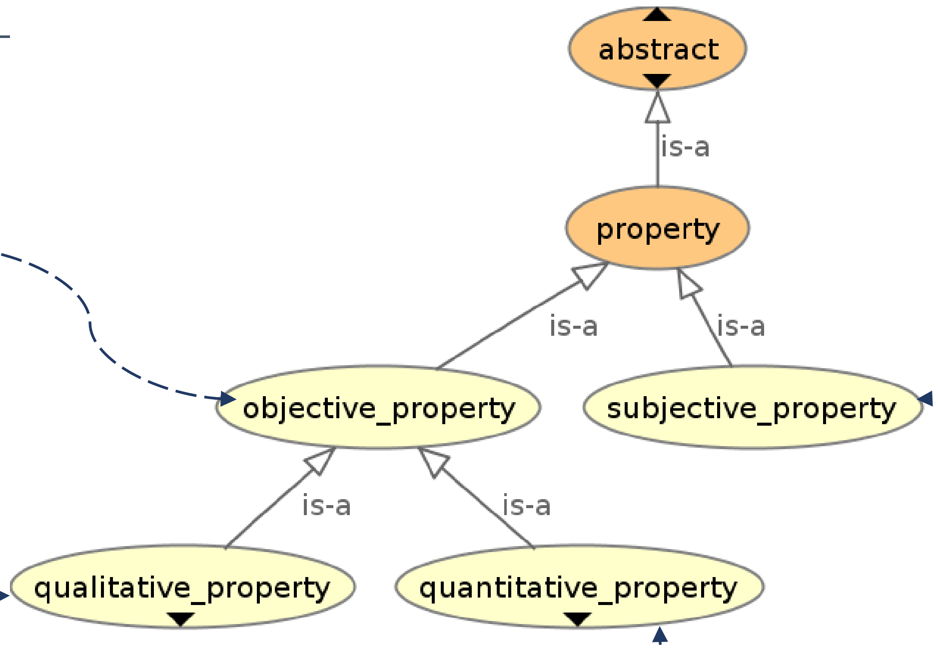
EMMO PROPERTIES

objective_property

A *property* that is univocally <u>measurable</u> by each observer by a <u>measuring process</u>, and that can be used to describe a state of a physical system.



subjective_property

An *property* of a phenomenon, body, or continuum object, that is observer dependent.

qualitative_property

A *objective_property* that is univocally <u>measurable</u> by each observer by a <u>measuring process</u>, but that cannot quantified numerically
(e.g. an SEM image of a nanoparticle)

quantitative_property

An objective_property of a phenomenon, body, or continuum object, that can be <u>quantified</u> with respect to a <u>standardized reference *physical*</u> instance
(e.g. the prototype meter bar, the kg prototype).

Each material object is going to have a specific set of properties by axioms.
e.g. *atom* **has_property** *mass*, *fluid object* **has_property** *viscosity*

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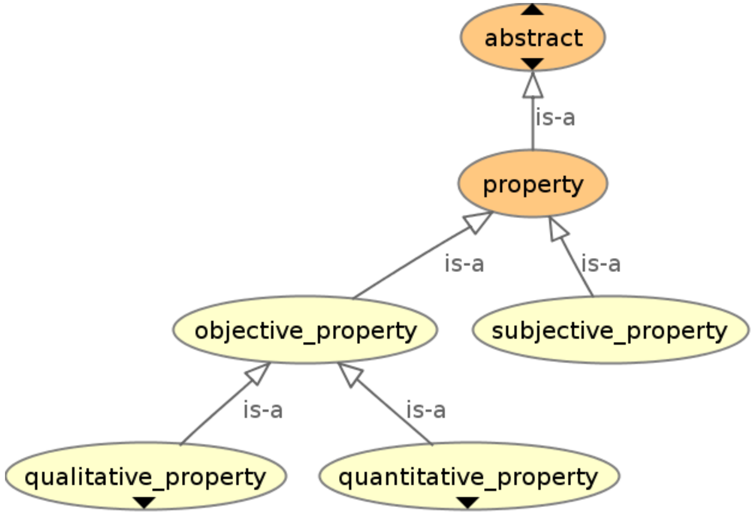
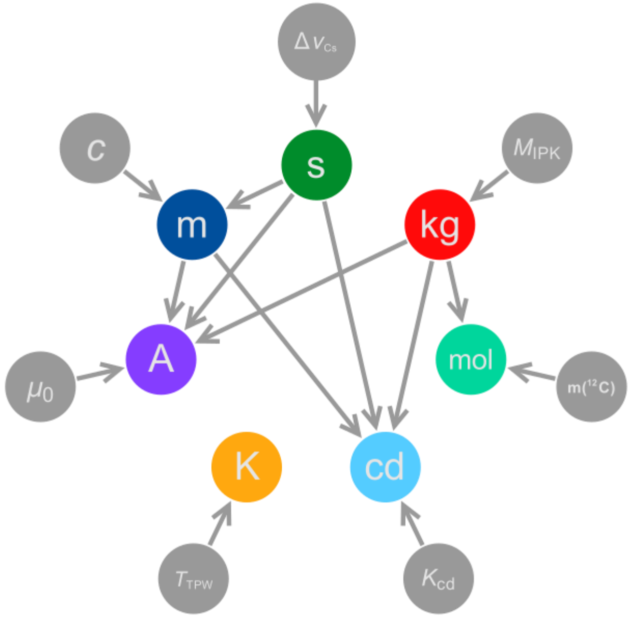
PROPERTIES

Measured and **simulated** physical properties are always defined by a physical law, connected to a physical entity through a **model perspective** and **measurement is done according to the same model**.



Systems of units suggests that this is the correct approach, since except for the fundamental properties (length, time, charge) every physical quantity is **derived by mathematical relations (i.e. physical laws or definitions) between other fundamental quantities (i.e. the SI units)**.



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EMMO PROPERTIES

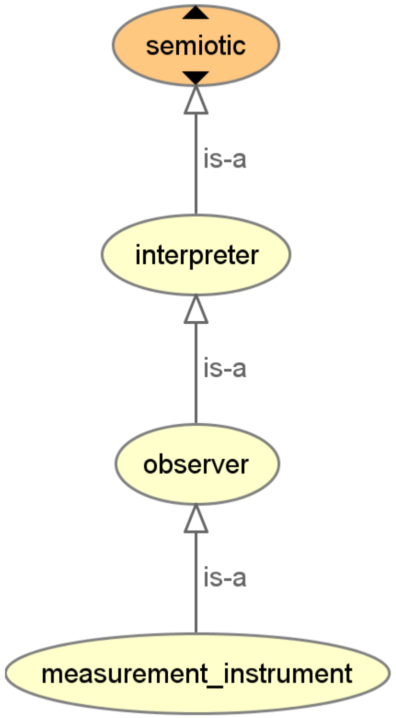
Physical properties always depends on a model for their evaluation. The measurement system is designed according to the specific phenomena and model to quantify the properties.

Thermal conductivity [W/m^2 K] is defined and measured according to some physical laws, e.g. Fourier Law.

$$\vec{q} = k\nabla T$$

Specific heat [J/Kg K] is defined and measured according to the following definition:

$$dh = c_p dT$$



Another example is the distinction between **gravitational and inertial mass**: they are assumed to be equal, but their measurement occurs using two different laws (i.e. gravitation, second law of dynamics)

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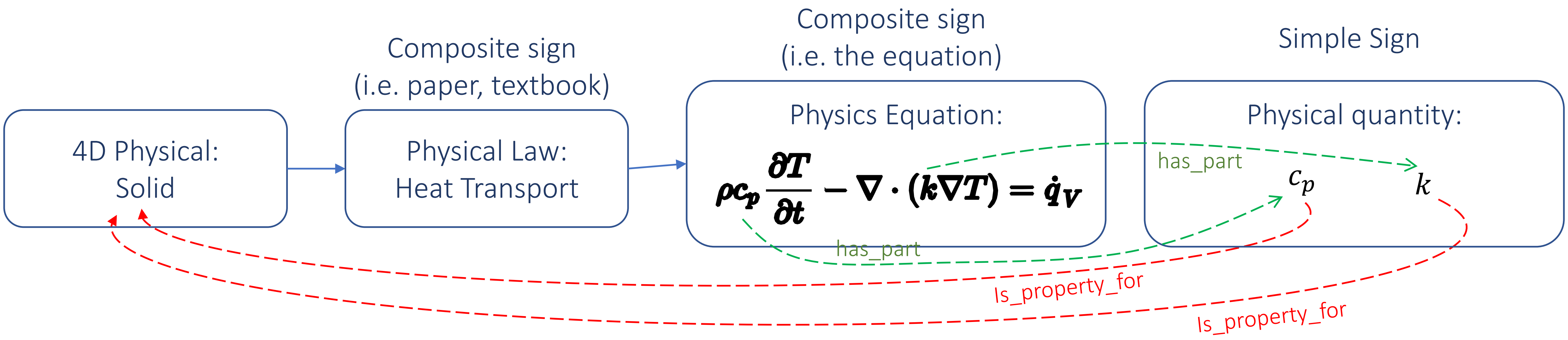

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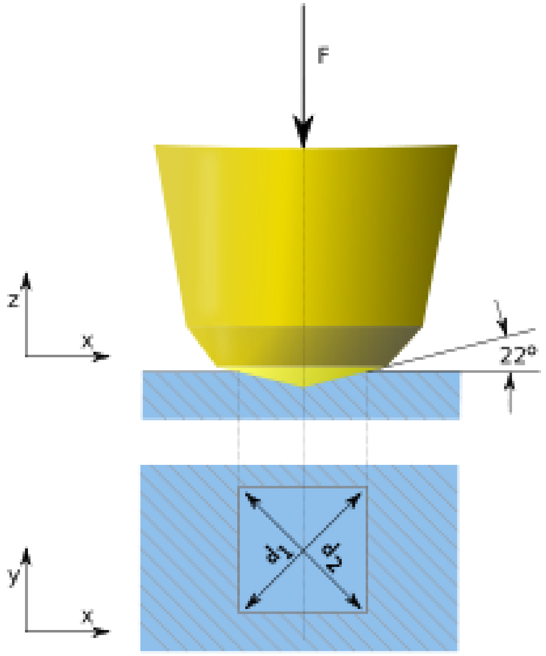
EMMO Properties

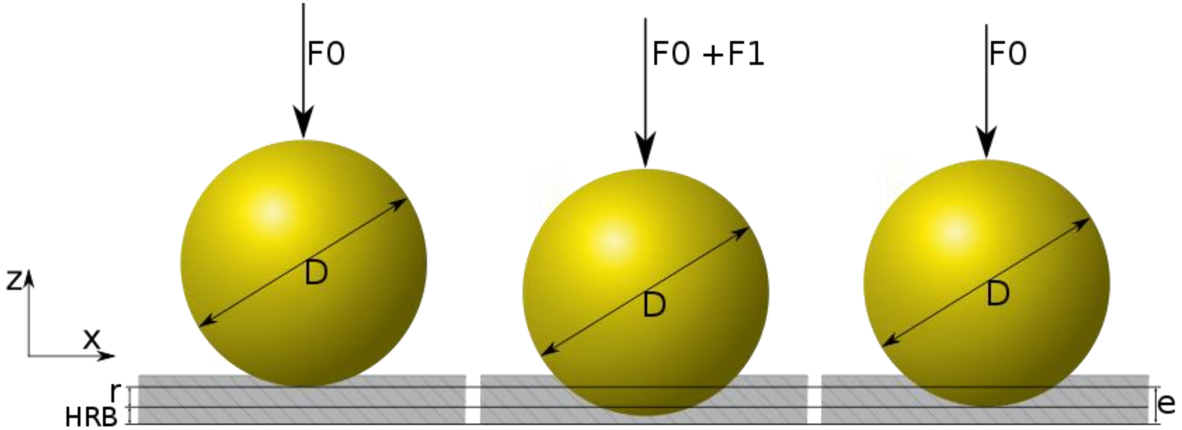
QUANTITATIVE DESCRIPTIVE PROPERTY

Properties such as **Rockwell or Vickers hardness** are different.

They do not stick to a model, but are measurements related to a **specific standardized measurement process** that is <u>not generalizable as a physical law</u>.

Hardness is a **measurement process dependent property** that <u>cannot be used in a physical model build on a physics equation</u>.





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EMMO PROPERTIES

QUALITATIVE PROPERTIES

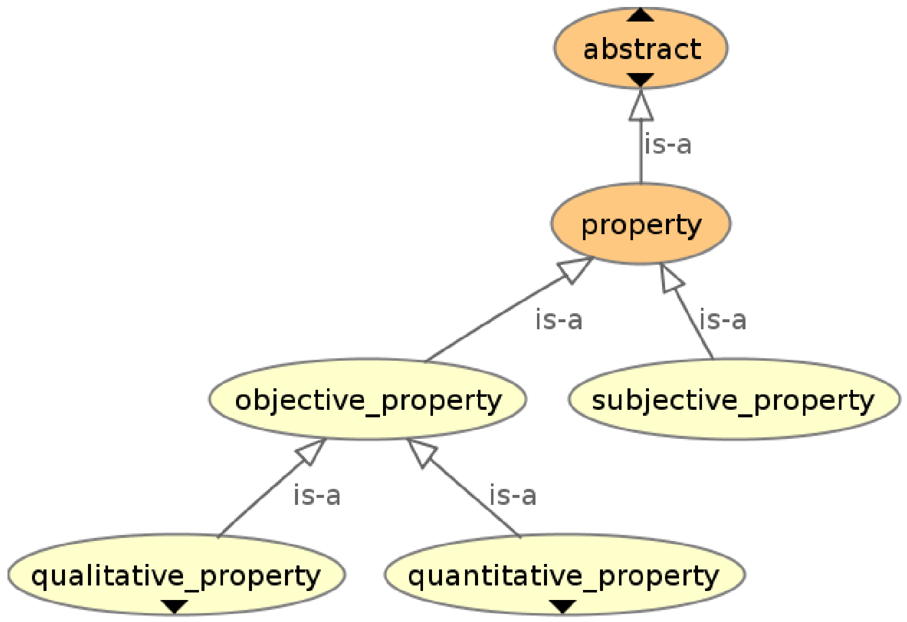
Crystal morphology is strictly speaking not a property: is a **categorization of a physical**.

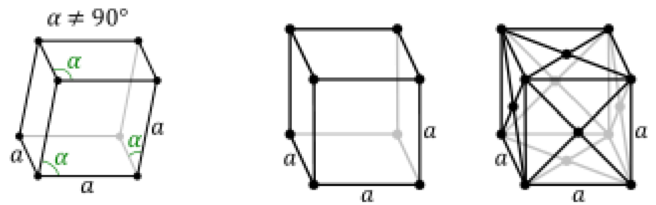
It can be introduced in the EMMO as **subclass of solid**.

The standard crystal systems are a **symbols** that **stands for a material class**. Those symbols are the properties that infrom a user about the morphology of crystalline solid (just like a number for thermal conductivity)

The real structure of a crystalline solid is provided by the arrangement of the subparts which is never so perfect as its representation.

This is an example of **qualitative property**: univocally defined by a standard measurement process, not as number but as class (and represented by a symbol).





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EMMO PROPERTIES

3.4 kg

The semiotic branch paves the way for the inclusion in the **EMMO** of formal languages and **data recognition**.

Change **raw data** into **information** through **interpretation** of the format.

Semantic extraction is represented within the **EMMO** at the same time for several interpreters!

How to represent the 'thing' on the left within the **EMMO**? It depends on the interpreter:

physical: it is a physical object, i.e. the black and white pixels on the screen

existent: its a physical that unfolds in time retaining its meaning (i.e. does not change class)

symbolic: is made of symbols coming from a code (i.e. math and western alphabet) for an interpreter used to this alphabet

sign/property: has a meaning for an interpreter who is skilled in numbers measurement units

physical property: stands for a physical property of another physical entity according to an interpreter who knows a bit of physics

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EMMO MODELS

MODA - modelling data

is a **template** for the **standardised description** of **materials models** (https://emmc.info/moda-workflow-templates/)

The **MODA** is meant to **guide users** towards a complete **high-level documentation** of material models, starting from the **end-user case** to the **computational details**.

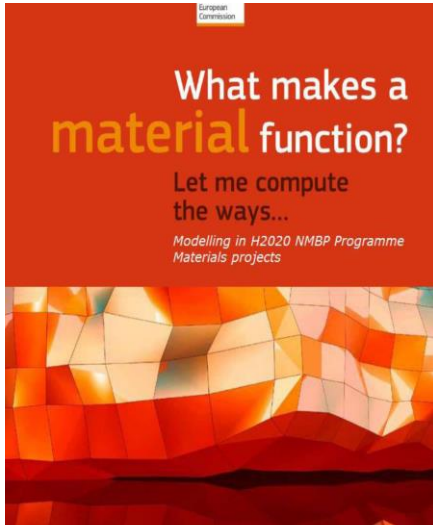
It provides all necessary aspects for: **description, reproducibility, curation** and **interfacing** with other models.

The MODA is based on the **core concepts** of

PHYSICS BASED MODELS

MODEL ENTITY

It includes also information about the **user case**, the **numerical solver** and **model input/output.**



Modelling in
H2020 LEIT-NMBP Programme
Materials and Nanotechnology projects

Review of Materials Modelling VI
RoMM

Vocabulary, classification and metadata for materials modelling (130 FP7 and H2020 projects)

https://bookshop.europa.eu/en/what-makes-a-material-function--pbKI0616197/

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EMMO MODELS

PHYSICS BASED MODEL

PHYSICS EQUATION
PE

Equation based on a **physical/chemical theory** which describes the spatial and temporal evolution of a chosen physics quantities of the entity

PHYSICS QUANTITIES

MATERIAL RELATIONS
MR

Information on the material needed to **close the PE** and to make the system of Governing Equations **solvable**

EXAMPLES

CLASSICAL MOLECULAR DYNAMICS

PE
Newton's equation of motion

$$\frac{dV}{dr} = -m\frac{d^2r}{dt^2}$$

MR
Lennard-Jones potential

$$V_{\mathrm{LJ}} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

FLUID DYNAMICS

Navier Stokes equation

PE $$\frac{\partial}{\partial t}(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}) = -\nabla\cdot p\mathbf{I} + \nabla\cdot\boldsymbol{\tau} + \rho\mathbf{g}$$

Stress tensor for incompressible flows

MR $$\nabla\cdot\boldsymbol{\tau} = 2\mu\nabla\cdot\boldsymbol{\varepsilon} = \mu\nabla\cdot\left(\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathrm{T}}\right) = \mu\nabla^2\mathbf{u}$$

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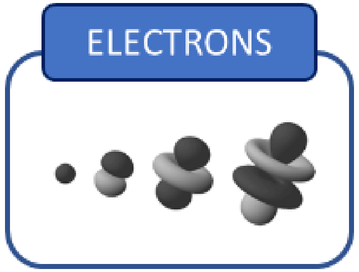
EMMO MODELS



Computational limits

Number of entities:
10 - 100

Length scale:
0.1 - 1 nm

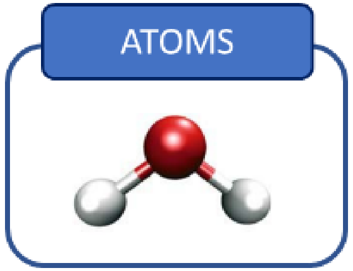
Time scale:
-

ELECTRONIC MODEL

Physics Based Model using a Physics Equation describing the behaviour of electrons quasi particles either as waves, particles or distributions.

1.1 Schrödinger Equation based models
- *Single particle Schrödinger models*
- *Many body Schrödinger models*
- *Quantum mechanical time dependant Schrödinger models*

1.2 Kohn Sham equation Density Functional Theory (electronic DFT)
1.3 Quantum Dynamic Mean Field Theory
1.4 NEGF
1.5 Statistical charge transport model
1.6 Statistical spin transport model



Computational limits

Number of entities:
10^2 - 10^9

Length scale:
0.1 - 100 nm

Time scale:
fs - μs

ATOMISTIC MODELS

Physics Based Model using a Physics Equation and Material Relation describing the behaviour of atoms either as waves, particles or distributions.

2.1 Classical Density Functional Theory and Dynamic DFT
2.2 Newton's equation based models
2.3. Statistical Mechanics atomistic models
2.4 Atomistic spin models
2.5 Statistical transport model at atomistic level
2.6 Atomistic phonon-based models (Boltzmann Transport Equation)

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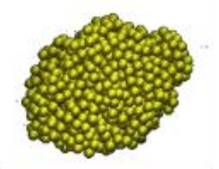
EMMO Models

BEADS



Computational limits

Number of entities:
10^6 - 10^9

Length scale:
0-100 mm

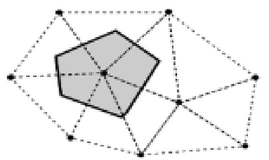
Time scale:
ms - s

Mesoscopic Models

Physics Based Model using a Physics Equation and Material Relation describing the behaviour of Beads either as particles or distributions.

3.1 Mesoscopic Classical Density Functional Theory and Dynamic DFT
3.2. Coarse-Grained Molecular Dynamics and Dissipative Particle Dynamics
3.3 Statistical Mechanics mesoscopic models
3.4 Micromagnetic models
3.5 Mesoscopic phonon models (Boltzmann Transport Equation)

CONTINUUM VOLUME ELEMENT



Computational limits

Number of entities:
-

Length scale:
nm - km

Time scale:
s - ks

Continuum Models

Physics Based Model using a Physics Equation and Material Relation describing the behaviour of Continuum Volume Elements.

4.1 Solid Mechanics
4.2 Fluid Mechanics
4.3 Heat Flow and Thermo-mechanical behaviour
4.4 Continuum Thermodynamics and Phase Field models
4.5 Chemistry reaction (kinetic) models (continuum)
4.6 Electromagnetism (incl optics, magnetics and electrical)
4.7 Application of models to Processes and Devices

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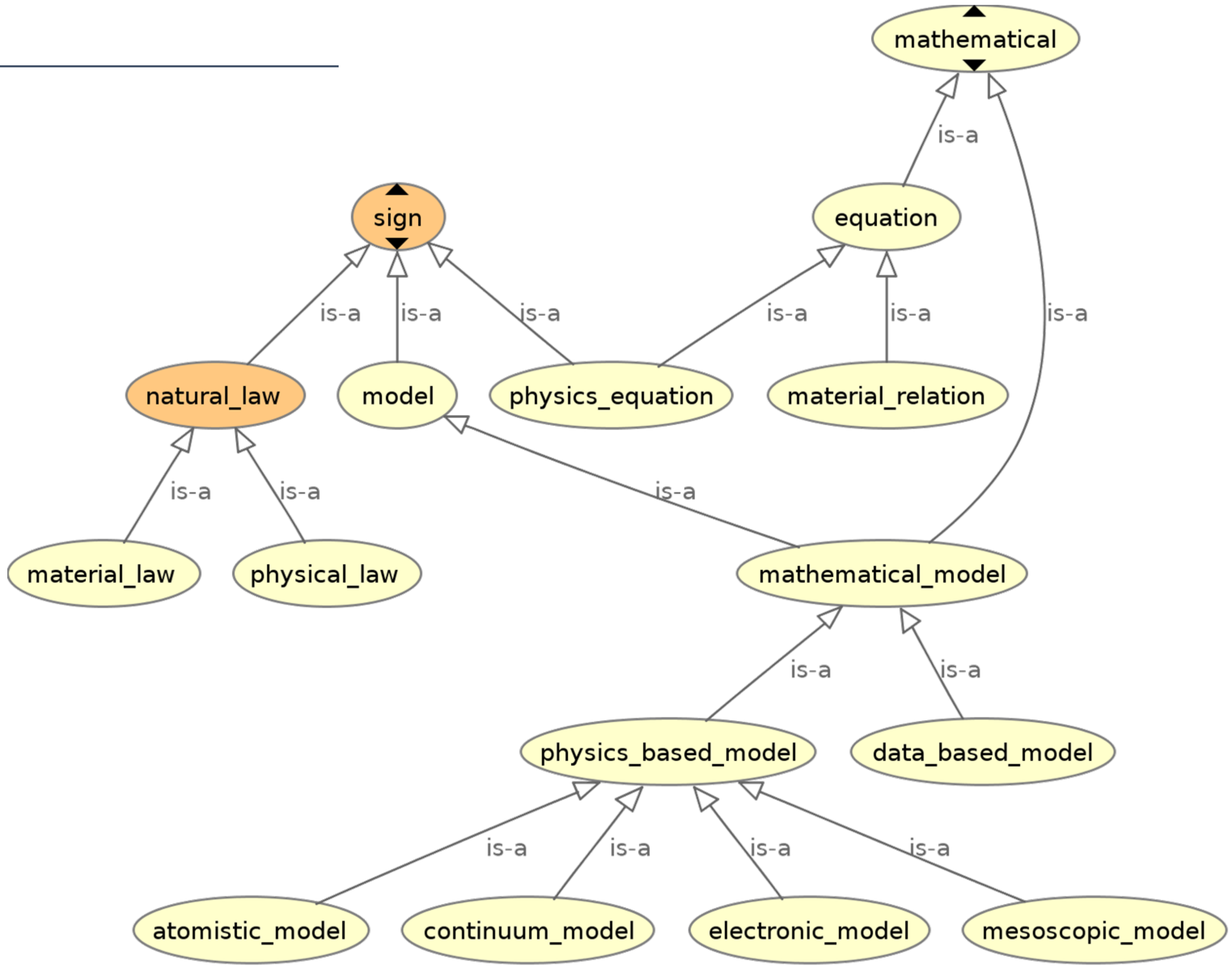
EMMO MODELS

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).



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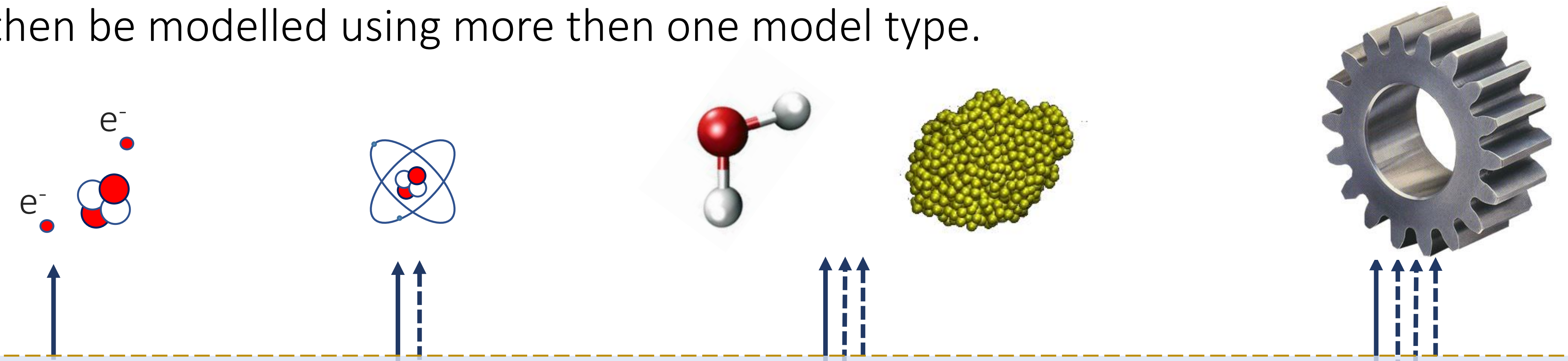
EMMO MODELS

Each 'material' can be observed at different levels of granularity and can then be modelled using more then one model type.



ELECTRONIC OBSERVATIONS AND MODELS

ATOMISTIC OBSERVATIONS AND MODELS

MESOSCOPIC OBSERVATIONS AND MODELS

CONTINUUM OBSERVATIONS AND MODELS

ONE USER CASE:
MULTIPLE OBSERVATION GRANULARITY LEVELS
MULTIPLE MODEL GRANULARITY LEVELS

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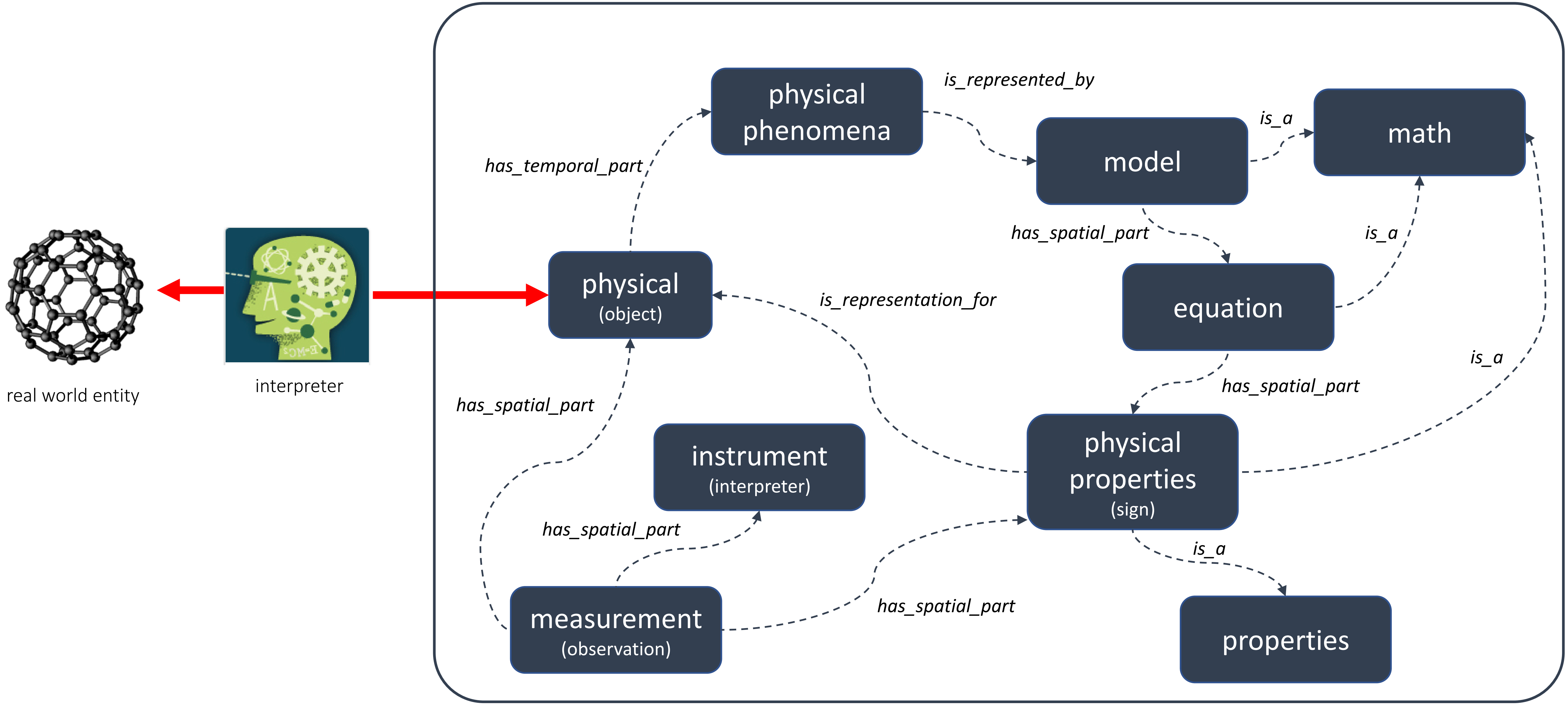
EMMO MODELS



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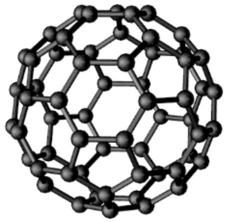
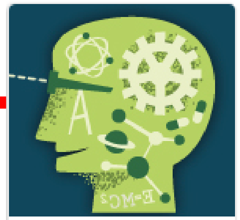
EMMO Models

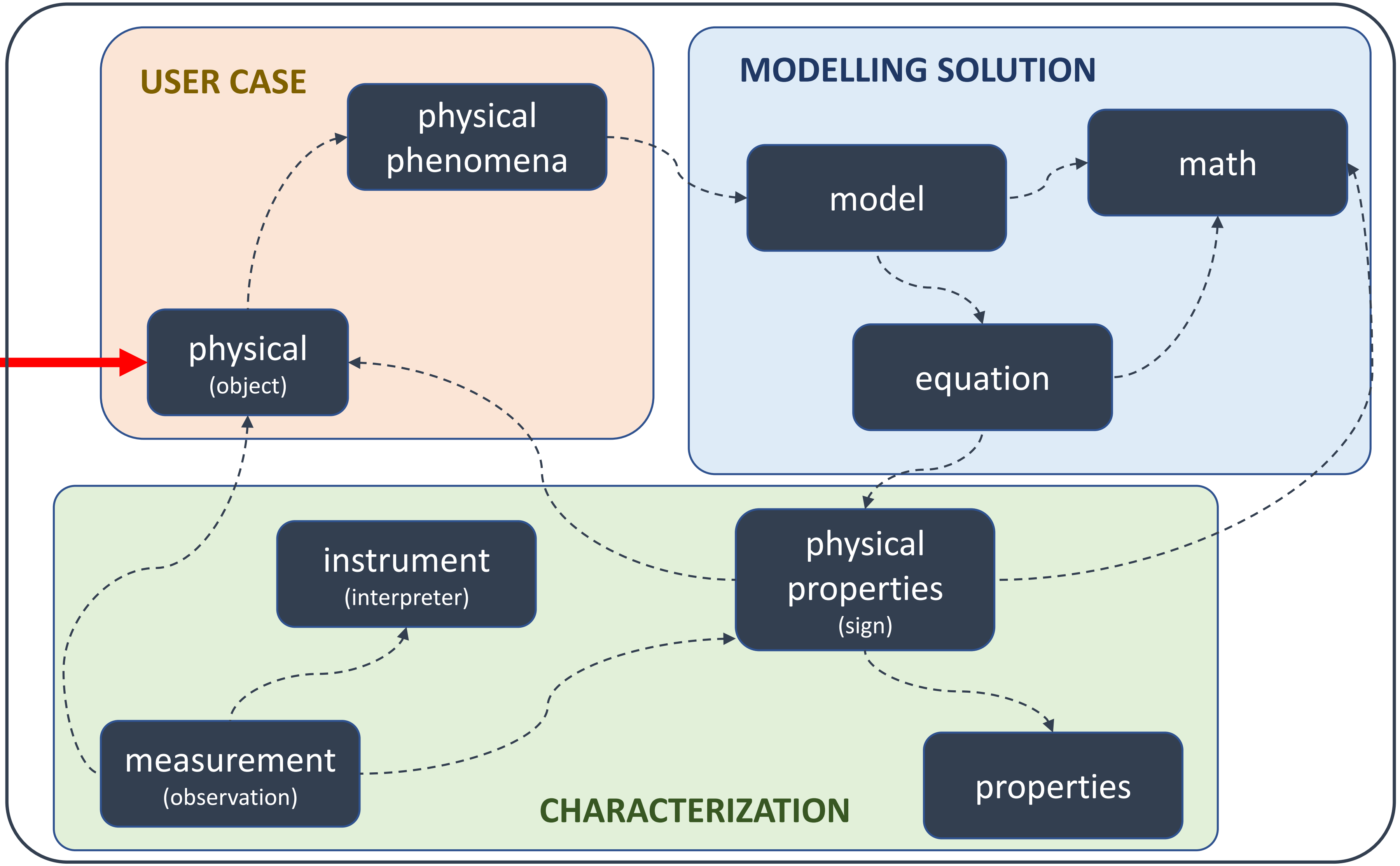
Horizontal interoperability: one user case, multiple modelling solutions.



real world entity



interpreter



Linking between properties database, models and user cases to facilitate **validation** and **data collection**.

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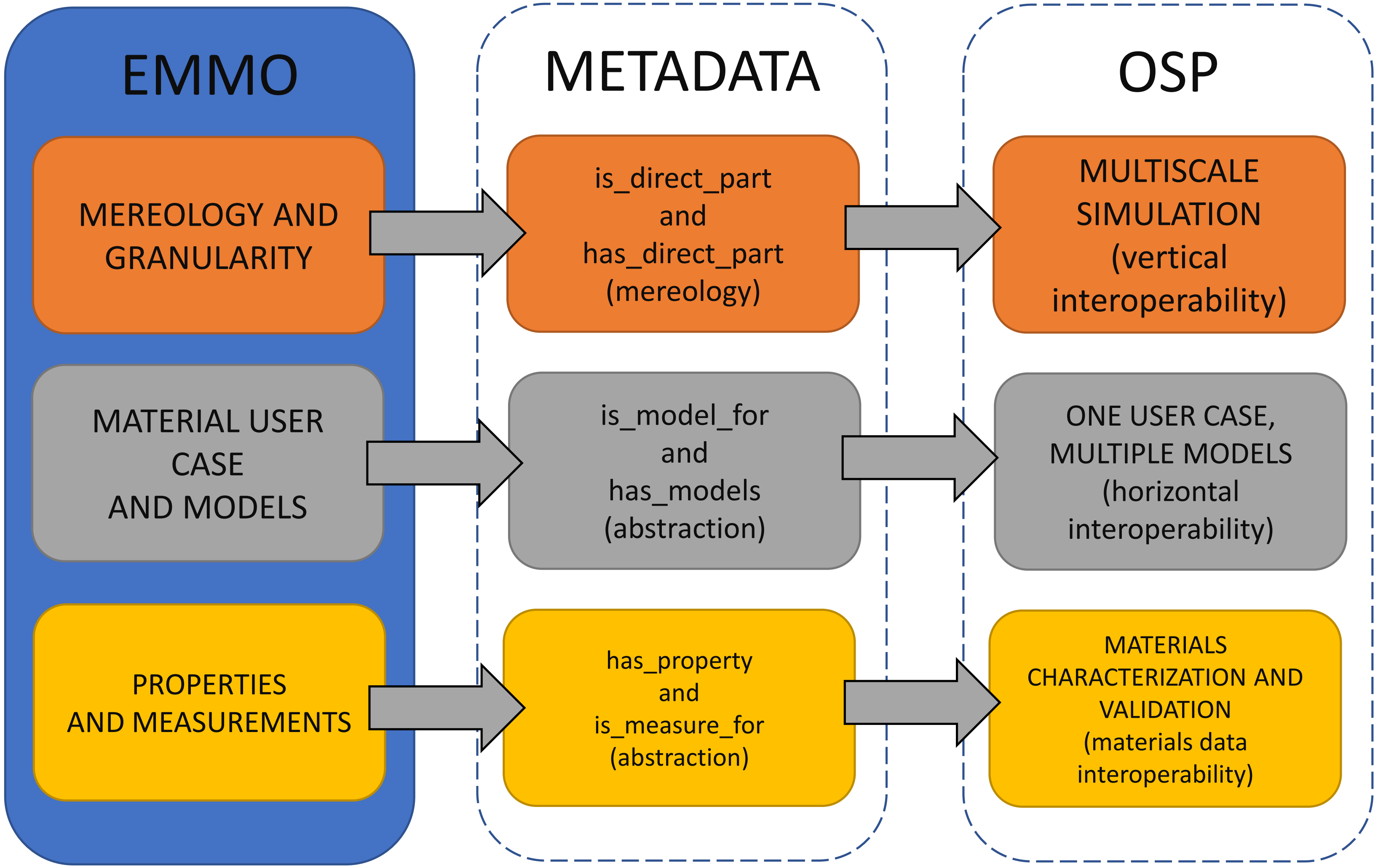
EMMO BASED METADATA ARCHITECTURE

EMMO can be used to define **metadata for each ontological concept** (e.g. material, device, process) that can be used to give a meaning to raw data.

Each **ontological relations** (e.g. has_property, has_part) can be expressed by metadata.

The **translation** from an ontology written in a particolar format (e.g. OWL, FOL) to a metadata schema can be done by automated code generator.



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EMMO RELATIONS

EMMO has very limited and strictly categorized relations, easy to use, understand and maintain. All goes down to **three primitive relations families**:

SET THEORY
Membership

MEREOTOPOLOGY
Parthood and *Slicing*

SEMIOTIC
Representation

Relations such as participation to a process falls under mereology.

e.g. you have to be part of a 4D process in order to participate to it

Mereology is also used to declare symbols that constitute symbolic entities.

e.g. unit of measurement as part of a physical property

EMMO taxonomy is strongly based on reasoning, up to level of expressivity allowed by OWL-DL.

(EMMO concepts would be better expressed in FOL or even Second Order Logic)

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EMMO RELATIONS

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EMMO MAINTAINERS

Who will ensure a constant development and testing of the **EMMO** in the next years?

NMBP-24-2016

Logo	Project	Year	Outcome
EMMC	European Materials Modelling Council - CSA	2019	**EMMO** foundations laid within this CSA project.

DT-NMBP-09-2018

Logo	Project	Year	Outcome
SimDOME	Digital Ontology-based Modelling Environment for Simulation of materials	2022	**EMMO** applications cases and integration within a OSP expected within 2020-2021. Team of philosophers, ICT experts and applied scientists.

NMBP-25-2017

Logo	Project	Year	Outcome
MarketPlace	Materials Modelling Marketplace for Increased Industrial Innovation	2022	**EMMO** applied to larger materials modelling communities and marketplaces infrastructures.
VIMMP	Virtual Materials Market Place	2021	

... more **existing projects** to involve and more to come in the **next DT-NMBP calls** (hopefully)!!!

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Potential Issues

- Insufficient expressivity of OWL-DL to capture the ontological details to be represented
- Reasoning software limitations in terms of number of axioms and complexity
- Incompatible standards that requires redefinition of well known and used concepts (e.g. IUPAC)
- …

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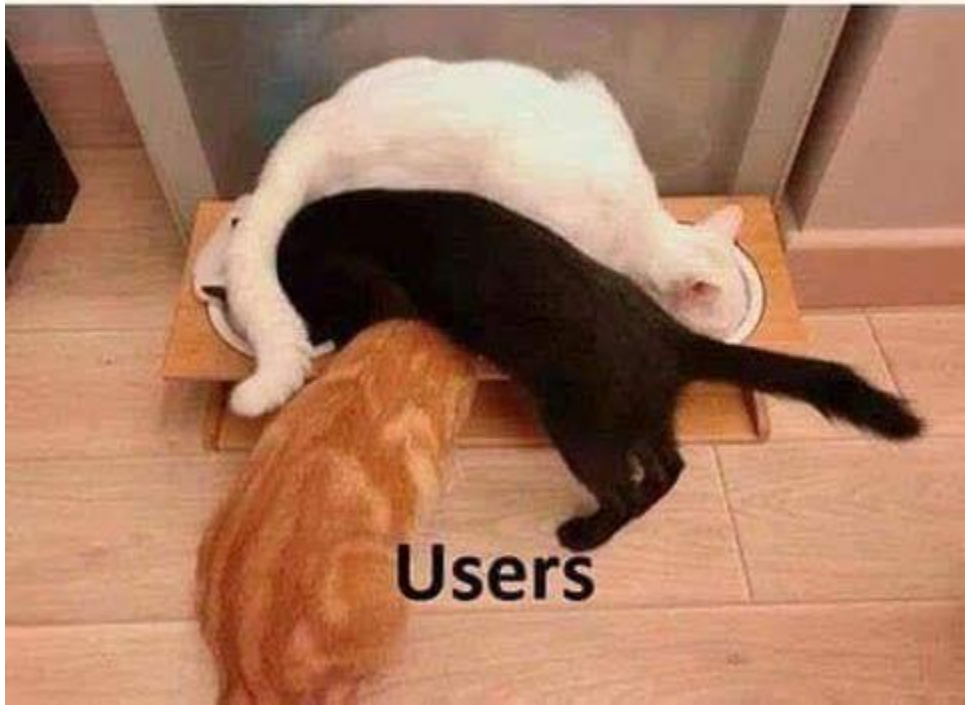
Potential Issues

- Irresponsible use by the users to be prevented by examples and documentation: educate the interpreters



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EMMO NEXT STEPS

OntoKin: An Ontology for Chemical Kinetic Reaction Mechanisms

Feroz Farazi[1], Jethro Akroyd[1,4], Sebastian Mosbach[1,4], Philipp Buerger[1], Daniel Nurkowski[2], Markus Kraft[1,2,4]

released: 18 January 2019

SimDOME

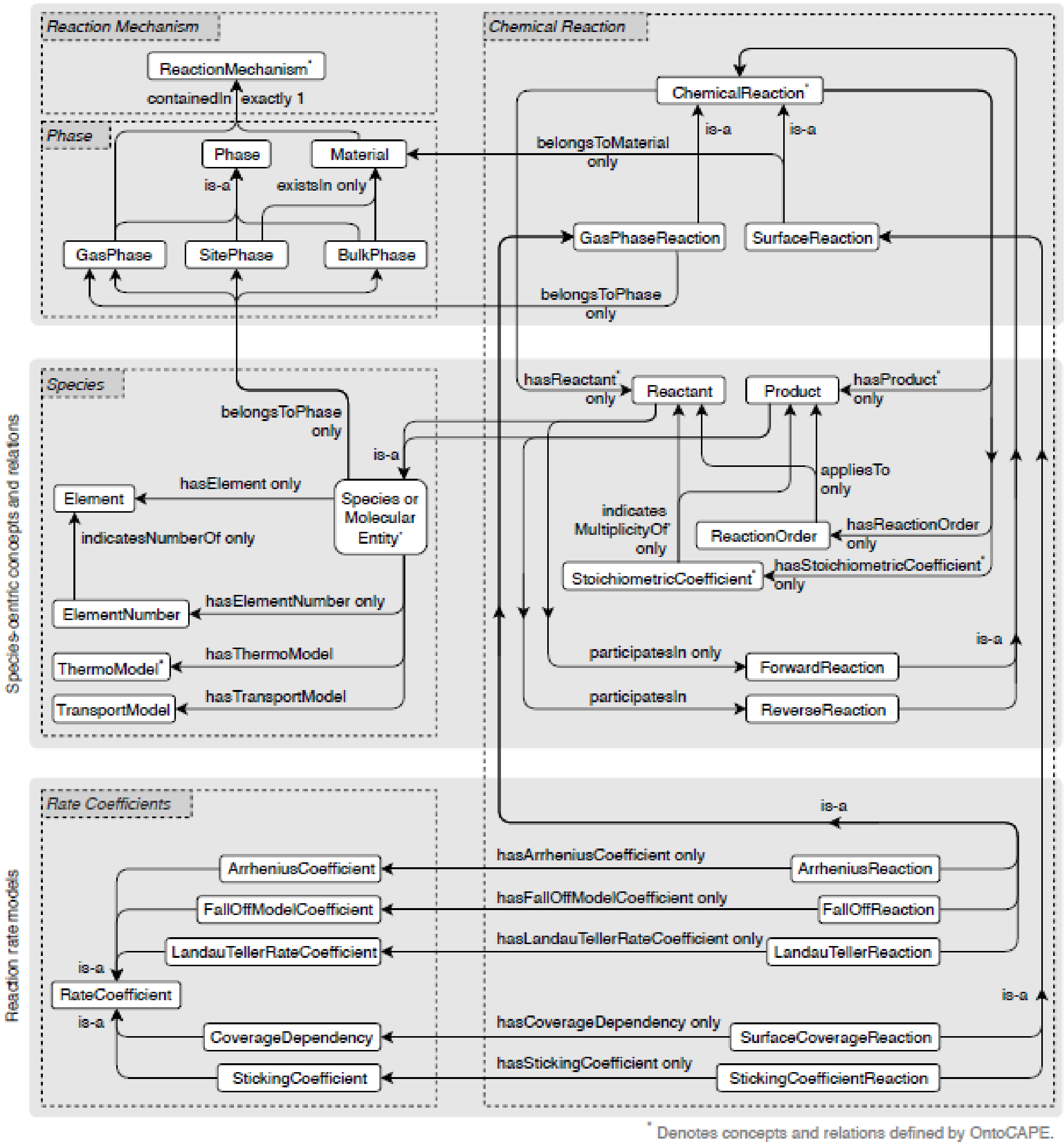

Figure 1: *The core concepts and properties of the OntoKin ontology.*

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EMMO NEXT STEPS (WE ONLY SCRATCHED THE SURFACE)

- Development of modules driven by applications to improve the existent EMMO upper level and extend the mid- and low-level

- Already working on a CHEMKIN-based branch for chemical kinetics

- Development of tools using EMMO, like SimPhoNy

- Populate the property and the math branch with e.g. field like properties and connect properties to material entities

- Populate the modelling branch with physical models

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EMMO NEXT STEPS (WE ONLY SCRATCHED THE SURFACE)

- Widen the EMMO contributors and testers
- Define a governance that should decide long and mid term strategies of EMMO development
- Disseminate EMMO approach over a wide range of communities (e.g. philosophers, ICT)
- Mapping existing ontologies with EMMO

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THANKS FOR YOUR ATTENTION

EMMO authors:

Emanuele Ghedini *(University of Bologna)*
Gerhard Goldbeck *(Goldbeck Consulting)*
Adham Hashibon *(Fraunhofer IWM)*
Georg Schmitz *(ACCESS)*
Jesper Friis *(SINTEF)*

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