EMMO

the EUROPEAN MATERIALS MODELLING ONTOLOGY

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Georg Schmitz *(ACCESS)*

Establishment of the EMMC

On **27th Feb. 2014** in **Brussels** a number of **experts** in the field of material modelling met in Covent-Garden in Brussels to discuss several issues pertaining to the **future of material modelling in Europe**.

The meeting was organized by the **EC Directorate-General for Research and Innovation**, Directorate D - *Key Enabling Technologies*, Unit D.3 - *Advanced Materials and Nanotechnologies*

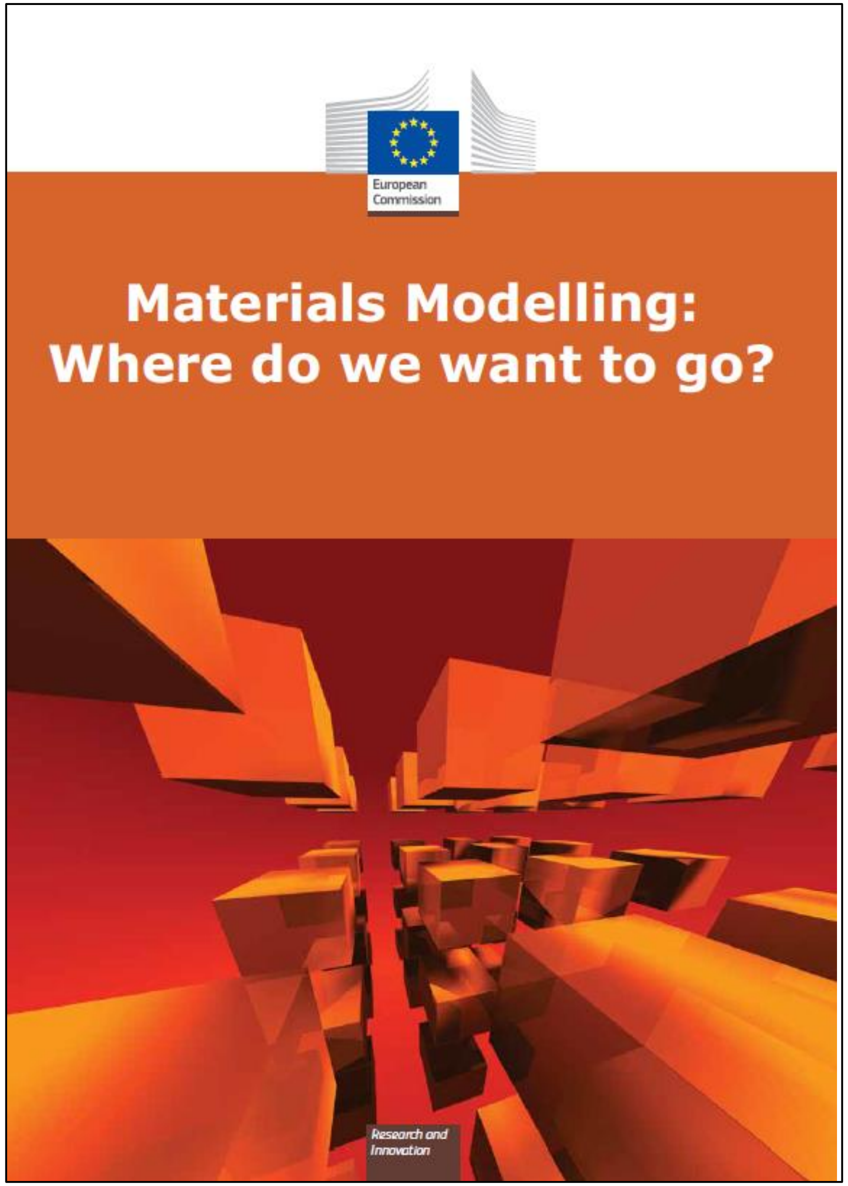
This assembly of scientists and experts formed the initial core of the **European Material Modelling Council (EMMC)**.

Materials modelling has progressed into a **predictive tool** allowing explanation of the **properties and behaviour of materials**.

Materials models fall into **four categories**: electronic, atomistic, mesoscopic and continuum models.

The ability to **integrate** and **communicate** between these model types is a **key factor** for the prediction of materials properties and behaviour in operation.

Experimental and computational data are needed to **validate** codes, to **data-mine** for high throughput approaches, and for **model development**.



EMMC SCOPE

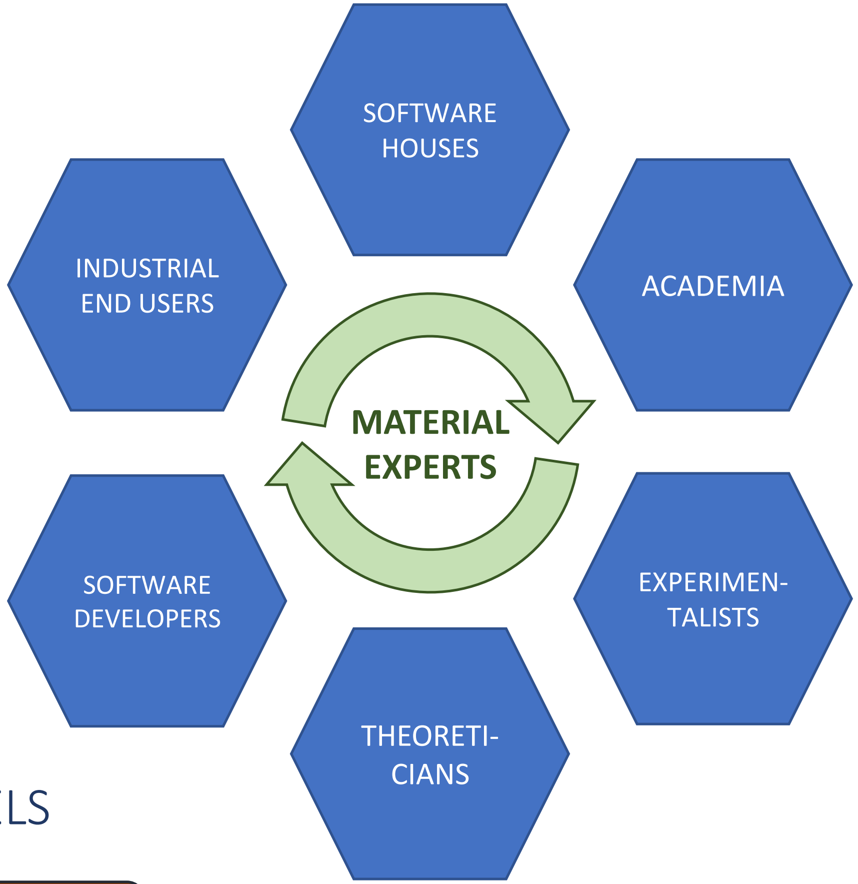
INTERACTIONS BETWEEN MATERIALS MODELLING **STAKEHOLDERS** IS OFTEN **THWARTED BY COMPLEXITY**.

OFTEN THE MODELLING APPROACH IS ONLY **PARTIALLY DESCRIBED**, MENTIONING ONLY:

- PHENOMENA (e.g. microkinetics)
- SCALE (e.g. atomic, mesoscale)
- SOFTWARE (e.g. LAMMPS, OpenFOAM)
- SOLVER (e.g. FEM, CV)

EACH COMMUNITY **HAS ITS OWN TERMINOLOGY**

MULTI-SCALE MATERIALS MODELLING REQUIRES **MULTIDISCIPLINARITY** AND **INTERACTIONS** BETWEEN DIFFERENT MODELS

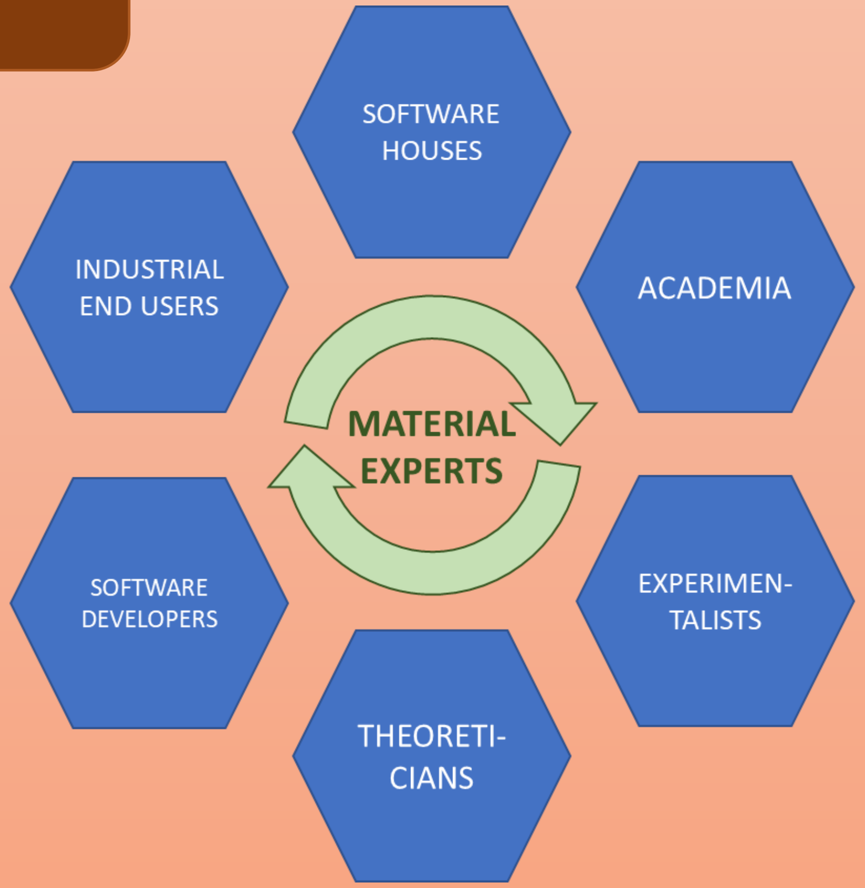


SOLUTION

ESTABLISH A **COMMON TERMINOLOGY** (DEFINITION OF **CONCEPTS** AND **VOCABULARY**) IN **MATERIALS MODELLING**
WHICH WILL LEAD TO
GREATLY **SIMPLIFIED** AND MUCH MORE **EFFICIENT COMMUNICATION**

THE EU CAN CLAIM GLOBAL LEADERSHIP IN MODELLING.

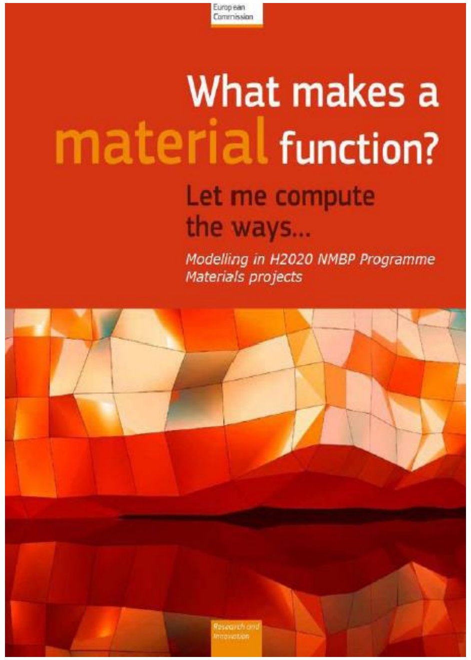
This can only be exploited if **complete materials model systems** are created and when these are complemented by **highly skilled actors** who **translate industrial problems into cases to be simulated with materials models.**



RoMM

Review of Materials Modelling VI

Anne de Baas, EC



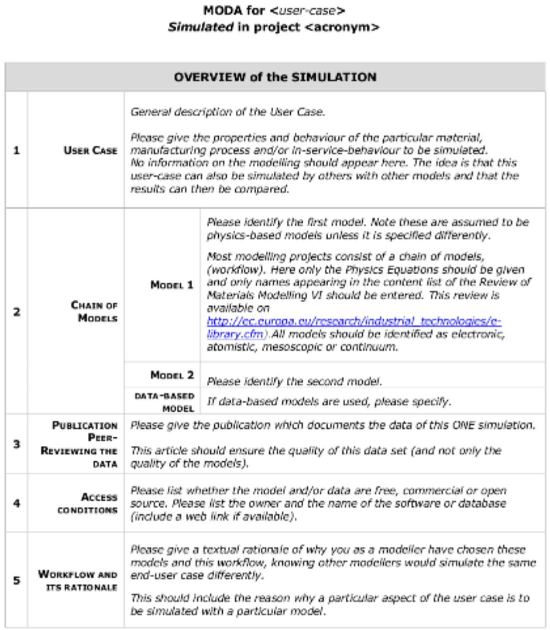
CEN Workshop Agreement

Endorsed by >15 EU organisation

CEN/WS MODA

Materials modelling - terminology, classification and metadata

MODA template

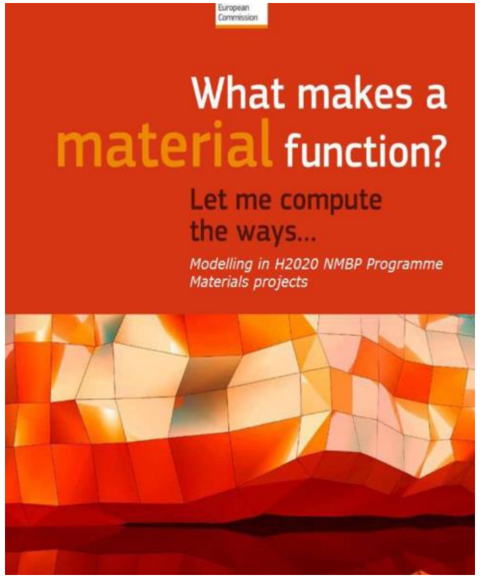


MODA for <*user-case*>
***Simulated* in project <acronym>**

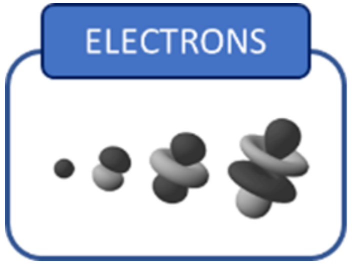
OVERVIEW of the SIMULATION			
1	USER CASE		*General description of the User Case.* *Please give the properties and behaviour of the particular material, manufacturing process and/or in-service-behaviour to be simulated. No information on the modelling should appear here. The idea is that this user-case can also be simulated by others with other models and that the results can then be compared.*
2	CHAIN OF MODELS	MODEL 1	*Please identify the first model. Note these are assumed to be physics-based models unless it is specified differently.* *Most modelling projects consist of a chain of models, (workflow). Here only the Physics Equations should be given and only names appearing in the content list of the Review of Materials Modelling VI should be entered. This review is available on http://ec.europa.eu/research/industrial_technologies/e-library.cfm).All models should be identified as electronic, atomistic, mesoscopic or continuum.*
		MODEL 2	*Please identify the second model.*
		DATA-BASED MODEL	*If data-based models are used, please specify.*
3	PUBLICATION PEER-REVIEWING THE DATA		*Please give the publication which documents the data of this ONE simulation.* *This article should ensure the quality of this data set (and not only the quality of the models).*
4	ACCESS CONDITIONS		*Please list whether the model and/or data are free, commercial or open source. Please list the owner and the name of the software or database (include a web link if available).*
5	WORKFLOW AND ITS RATIONALE		*Please give a textual rationale of why you as a modeller have chosen these models and this workflow, knowing other modellers would simulate the same end-user case differently.* *This should include the reason why a particular aspect of the user case is to be simulated with a particular model.*

EMMC MODEL TYPES

RoMM VI

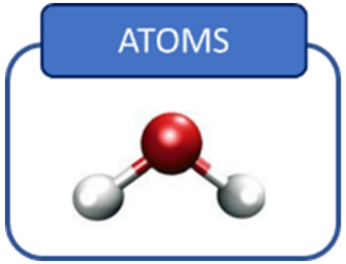


Modelling in H2020 LEIT-NMBP Programme Materials and Nanotechnology projects



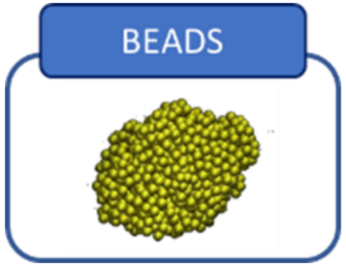
Electronic Model

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



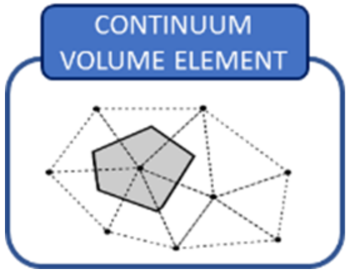
Atomistic Models

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



Mesoscopic Models

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



Continuum Models

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

MODA are tables that take the modeller by the hand and ask the relevant questions step for step.

MODA for <*user-case*>
Simulated in project <acronym>

OVERVIEW of the SIMULATION			
1	User Case		*General description of the User Case.* *Please give the properties and behaviour of the particular material, manufacturing process and/or in-service-behaviour to be simulated.* *No information on the modelling should appear here. The idea is that this user-case can also be simulated by others with other models and that the results can then be compared.*
2	Chain of Models	Model 1	*Please identify the first model. Note these are assumed to be physics-based models unless it is specified differently.* *Most modelling projects consist of a chain of models, (workflow). Here only the Physics Equations should be given and only names appearing in the content list of the Review of Materials Modelling VI should be entered. This review is available on* *http://ec.europa.eu/research/industrial_technologies/e-library.cfm). All models should be identified as electronic, atomistic, mesoscopic or continuum.*
		Model 2	*Please identify the second model.*
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3	Publication Peer-reviewing the data		*Please give the publication which documents the data of this ONE simulation.* *This article should ensure the quality of this data set (and not only the quality of the models).*
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5	Workflow and its rationale		*Please give a textual rationale of why you as a modeller have chosen these models and this workflow, knowing other modellers would simulate the same end-user case differently.* *This should include the reason why a particular aspect of the user case is to be simulated with a particular model.*

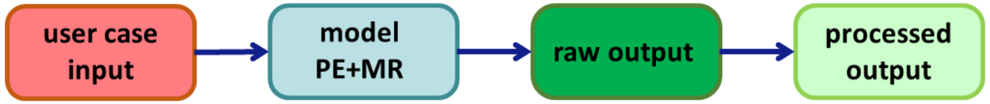
1	Aspect of the User Case / System to be Simulated	
1.1	Aspect of the User Case to be simulated	*Describe the aspects of the User Case textually.* *No modelling information should appear in this box. This case could also be simulated by other models in a benchmarking operation!* *The information in this chapter can be end-user information, measured data, library data etc. It will appear in the pink circle of your workflow picture.* *Simulated input which is calculated by another model should not be included (but this input is listed in chapter 2.4)* *Also the result of pre-processing necessary to translate the user case specifications to values for the physics variables of the entities can be documented here.*
1.2	Material	*Chemical composition, ...*
1.3	Geometry	*Size, form, picture of the system (if applicable)* *Note that computational choices like simulation boxes are to be documented in chapter 3.*
1.4	Time Lapse	*Duration of the User Case to be simulated.* *This is the duration of the situation to be simulated. This is not the same as the computational times to be given in chapter 3.*
1.5	Manufacturing process or in-service conditions	*If relevant, please list the conditions to be simulated (if applicable).* *E.g. heated walls, external pressures and bending forces.* *Please note that these might appear as terms in the PE or as boundary and initial conditions, and this will be documented in the relevant chapters.*
1.6	Publication on this data	*Publication documenting the simulation with this single model and its data (if available and if not already included in the overall publication).*

2	Generic Physics Of The Model Equation		
2.0	Model type and name		*Model type and name* ***chosen from RoMM content list*** *(the PE).* *This PE and only this will appear in the blue circle of your workflow picture. Please do not insert any other text although an indication of the MR is allowed.*
2.1	Model entity		*The entity in this materials model is <finite volumes, grains, atoms, or electrons>*
2.2	Model Physics/ Chemistry equation PE	Equation	*Name, description and mathematical form of the PE* *In case of tightly coupled PEs set up as one matrix which is solved in one go, more than one PE can appear.*
		Physical quantities	*Please name the physics quantities in the PE, these are parameters (constants, matrices) and variables that appear in the PE, like wave function, Hamiltonian, spin, velocity, external force.*
2.3	Materials relations	Relation	*Please, give the name of the Material Relation and which PE it completes.*
		Physical quantities / descriptors for each MR	*Please give the name of the physics quantities, parameters (constants, matrices) and variables that appear in the MR(s)*
2.4	Simulated input		*Please document the simulated input and with which model it is calculated.* *This box documents the interoperability of the models in case of sequential or iterative model workflows. Simulated output of the one model is input for the next model. Thus what you enter here in 2.4 will also appear in 4.1 of the model that calculated this input.* *If you do simulations in isolation, then this box will remain empty.* *Note that all measured input is documented in chapter 1 "User Case".*

Workflows are representation of the simulation as modelling chain and flow of data. Its components are explained in RoMM.

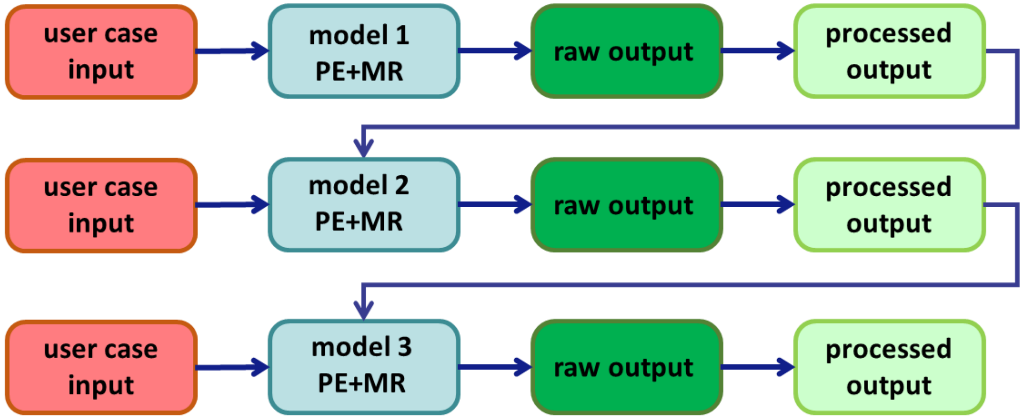
(examples of workflows on www.emmc.info)

workflow for a **standalone model**



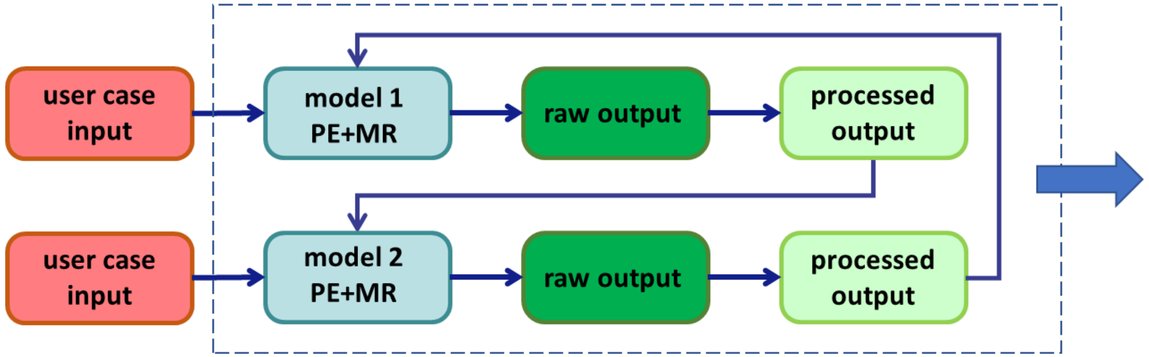
workflow for a chain of **linked models**

equations solved sequentially
(i.e. one-way dependency)



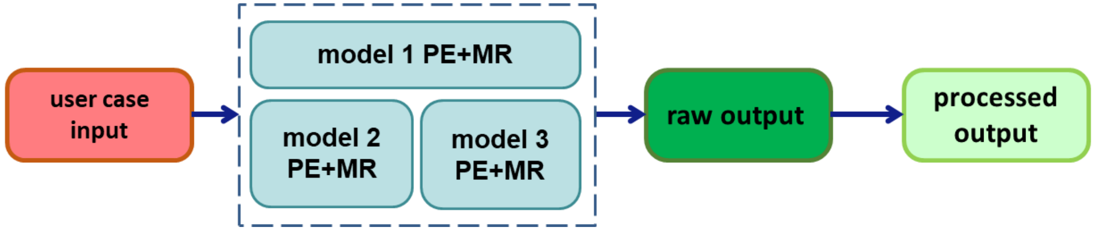
workflow for a chain of **coupled models**

Iterative solution of segregated equations



workflow for **tightly coupled models**

equations solved together
(running different models for the same entity concurrently by solving one matrix)



European Committee for Standardization

CEN Workshop Agreement

"Materials modelling - terminology, classification and metadata"

EMMC has coordinated the organisation of a CEN Workshop. The end result is the adoption of a CEN Workshop Agreement (CWA), a best practices document for further standardisation efforts.

published by CEN in May 2018:

https://www.cen.eu/News/Workshops/Pages/WS-2017-012.aspx

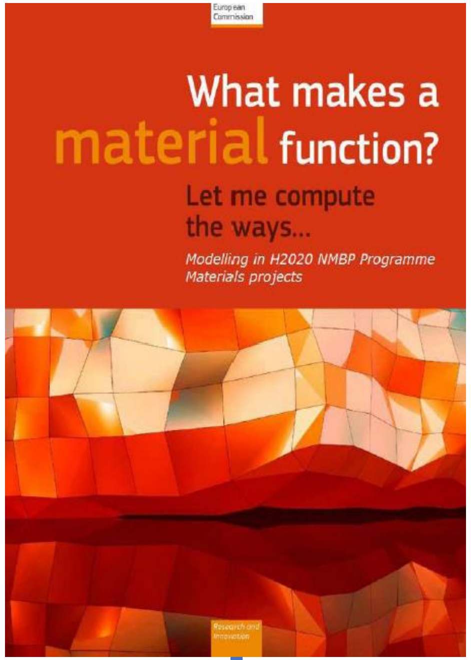
Endorsed by >15 EU organisation

- Definitions of fundamental terms.
- Classification of materials models.
- Systematic description and documentation of simulations.

RoMM

Review of Materials Modelling VI

Anne de Baas, EC



CEN Workshop Agreement

Endorsed by >15 EU organisation

CEN/WS MODA

Materials modelling - terminology, classification and metadata

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access

Fraunhofer

GOLDBECK CONSULTING

SINTEF

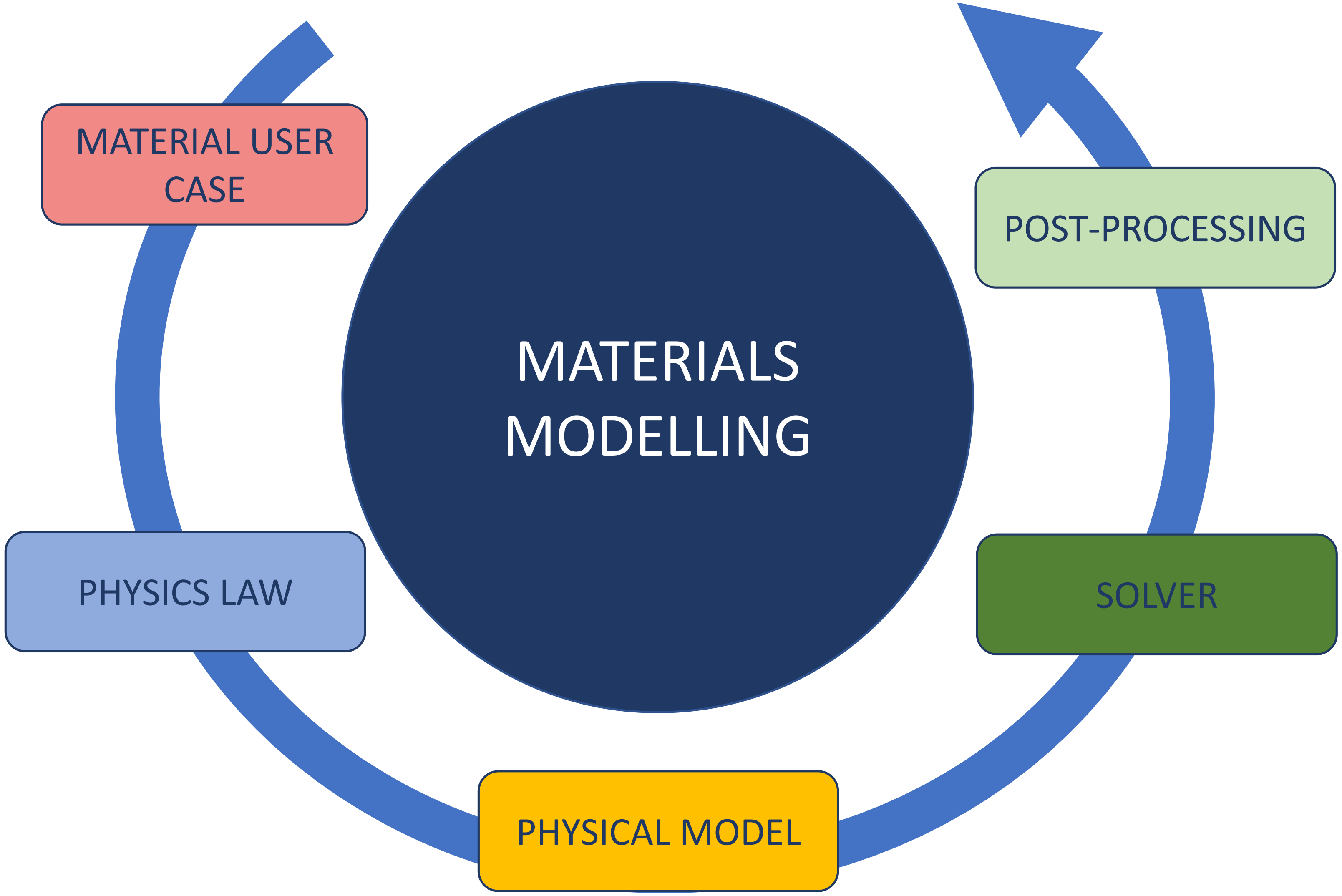
EMMO

EUROPEAN MATERIALS MODELLING ONTOLOGY

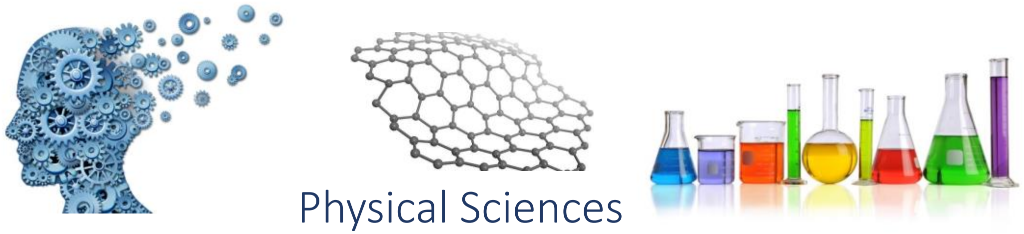
EMMO Scope

EMMO MUST COVER ALL THE ASPECTS OF MATERIALS MODELLING:

- THE **MATERIAL** ITSELF THAT MUST BE DESCRIBED IN A RIGOROUS (ONTOLOGICAL) WAY
- THE **PHYSICS LAW** THAT DESCRIBES THE MATERIAL BEHAVIOUR
- THE **PHYSICAL MODEL** WHICH IS AN APPROXIMATION OF PHYSICS LAWS
- THE **SOLVER** INCLUDING THE **NUMERICAL DISCRETIZATION** METHOD THAT LEADS TO A SOLVABLE MATHEMATICAL REPRESENTATION UNDER CERTAIN SIMPLIFYING ASSUMPTIONS
- THE **NUMERICAL SOLVER** WHO PERFORMS THE CALCULATIONS
- THE **POST PROCESSING** OF DATA

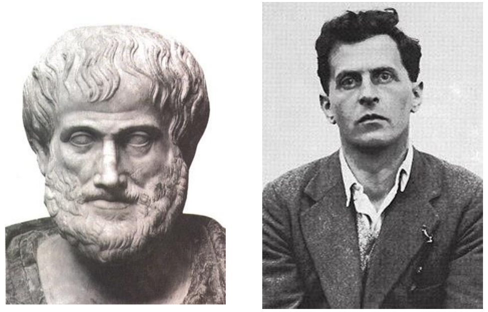


THE **EMMO** IS A <u>MULTIDISCLIPLINARY EFFORTS</u> WITHIN THE **EMMC** AIMED TO THE DEVELOPMENT OF A **<u>STANDARD REPRESENTATIONAL FRAMEWORK</u>** (THE ONTOLOGY) BASED ON CURRENT MATERIALS MODELLING KNOWLEDGE.



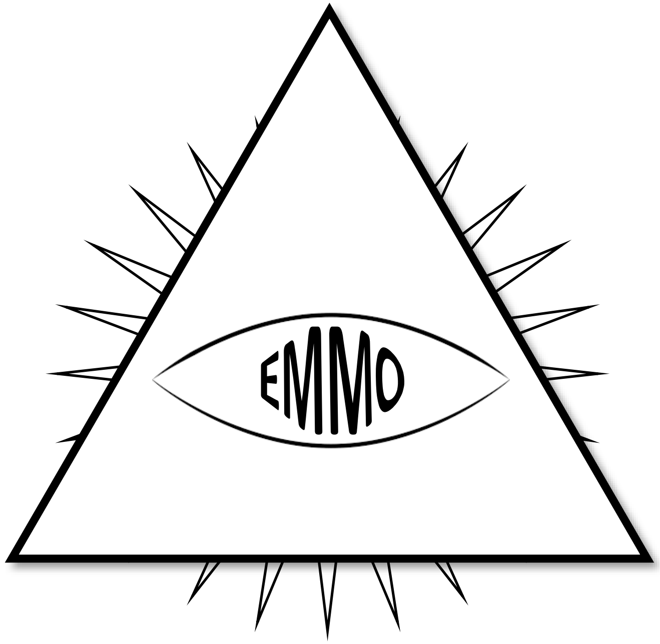
Physical Sciences

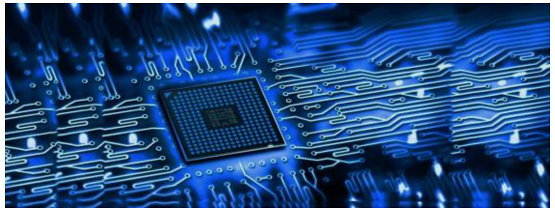
(e.g. physics, chemistry, material science, engineering)



Analytical Philosophy

(e.g. mereotopology, semiotics, logic)





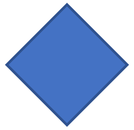
Information and Communication Technologies

(e.g. reasoners, platforms, formats)

EMMO PROVIDES A FRAMEWORK FOR THE REPRESENTATION (BY SIGNS) OF PHYSICAL WORLD ENTITIES

SIGN (or *semeion*)

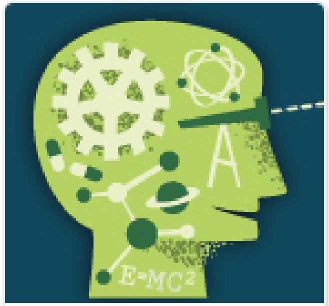
a physical entity that conventionally stands for another physical entity



ONTOLOGY WORLD

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 representation created/determined by a sign or an object (interpreter dependent)

OBJECT

any physical entity

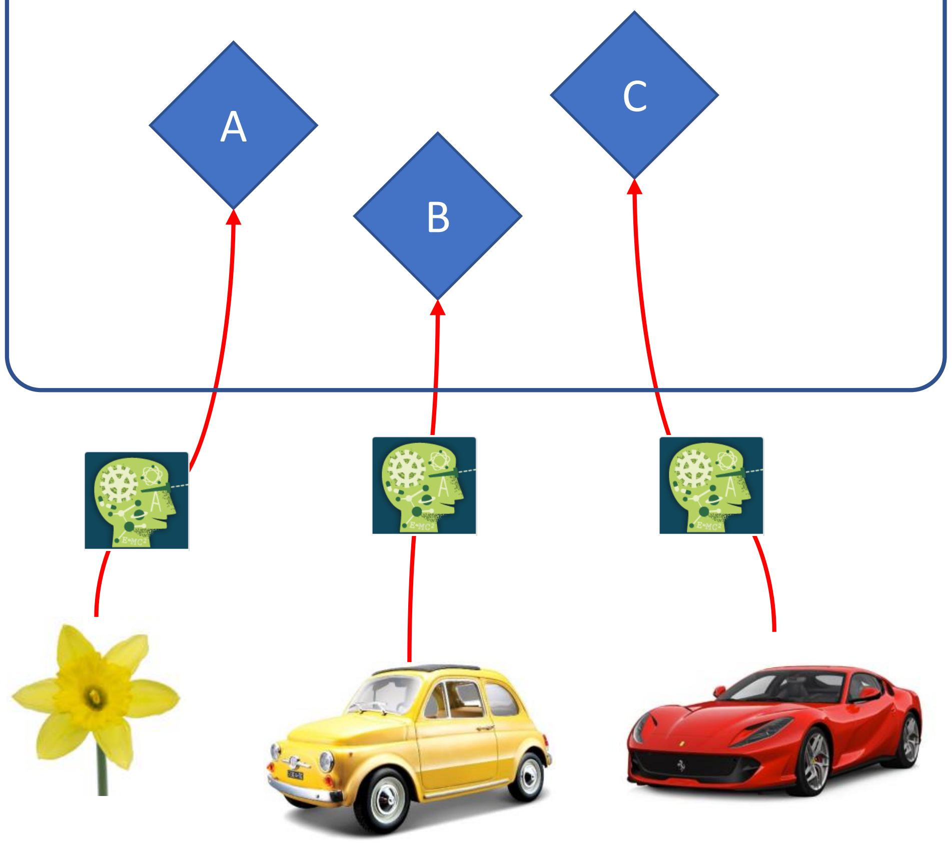
PHYSICAL WORLD

Strong multidisciplinary intesection with **Peirce's theory of semiotics**

EMMO PRIMITIVE ELEMENTS

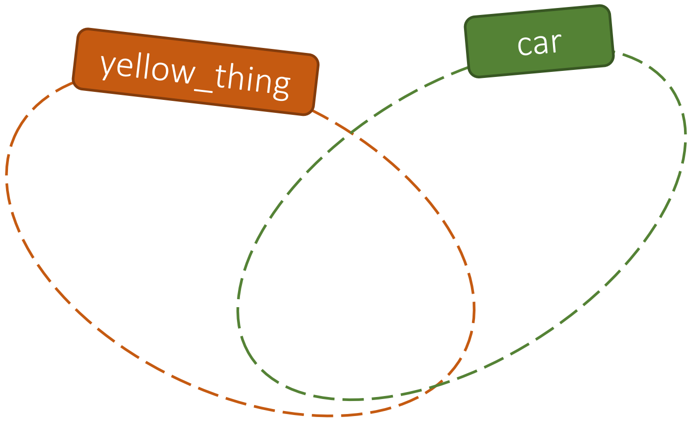
Individuals

(or signs, semeion, simulacra, picture)



Classes

(or collections, sets)

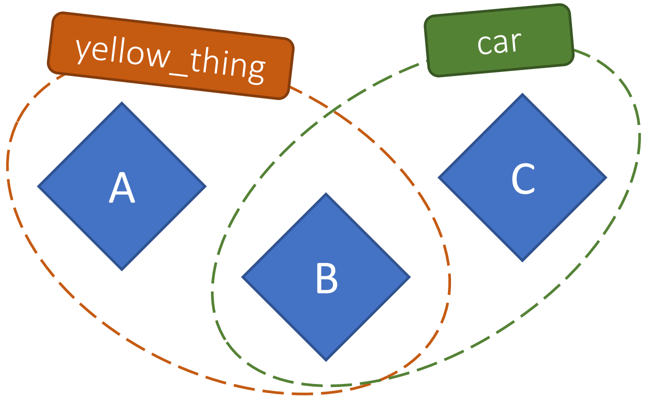


Axioms

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".

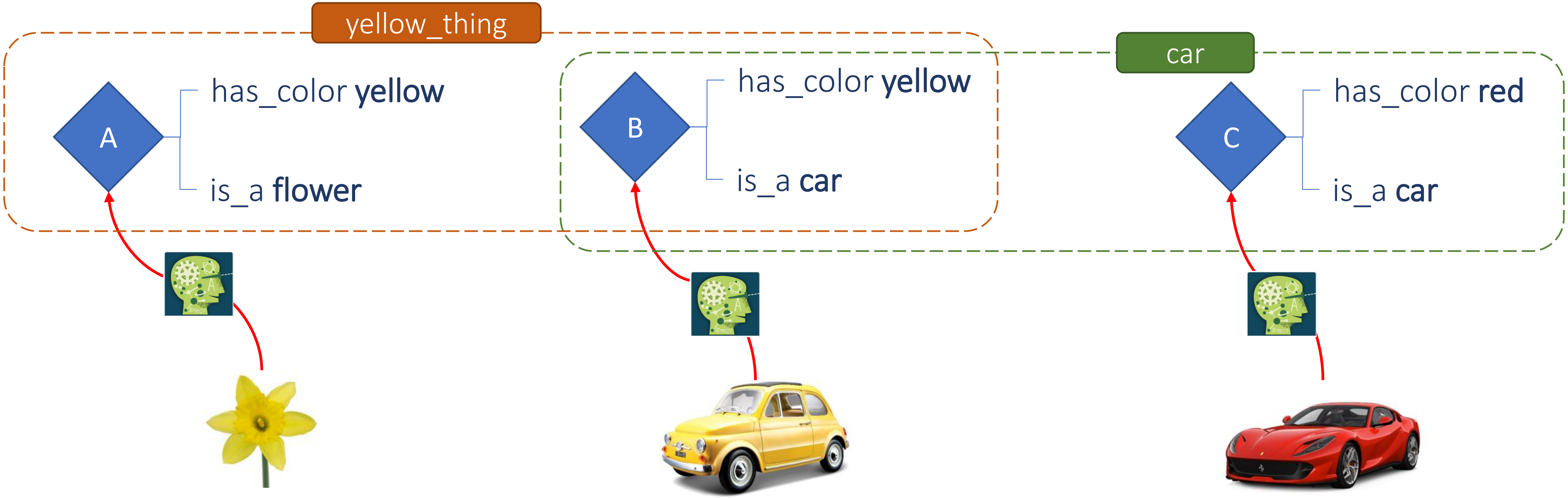
"2.1 We picture facts to ourselves"
cit. **Ludwig Wittgenstein**, *Tractatus Logico-Philosophicus*, 1921

Strong multidisciplinary intesection with **analytical philosophy** (ontological perspectives and logic) and with ICTs (digital implementation and reasoning)

Individuals are not simple, but possess attributes in form of **axioms** that are defined by the user (interpreter) upon declaration

The **axioms** are used to categorize **individuals** in **classes**

Individuals in an ontology are a logical picture of the real world entity.



EMMO GENERAL USAGE

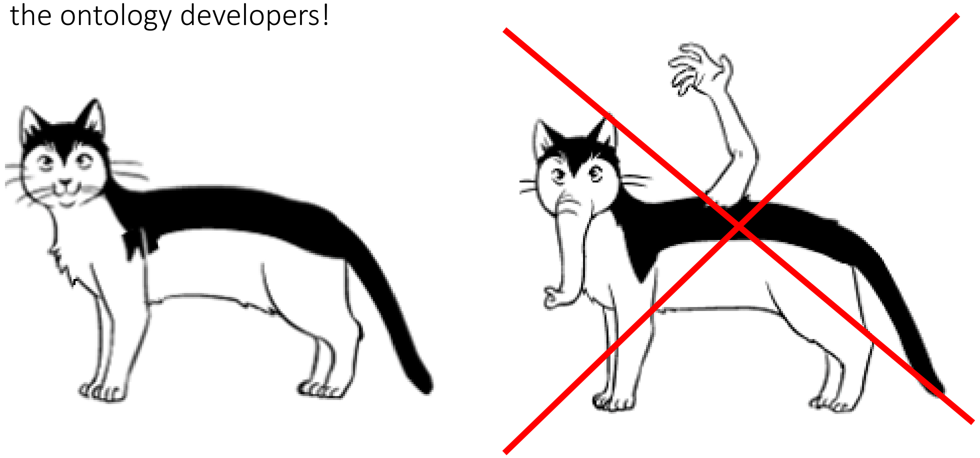
CONFIDENTIAL

EMMO DEFINITION

The **EMMO** is a representational framework of predefined classes and axioms (ontology) provided by experts (EMMC) that enables end users (industry, research, academy) to represent real life physical entities (materials, devices), models and properties using ontological signs (individuals) in a standard way to facilitate interactions and exchanges (data, software, knowledge) between all involved material modelling and characterization communities and stakeholders.

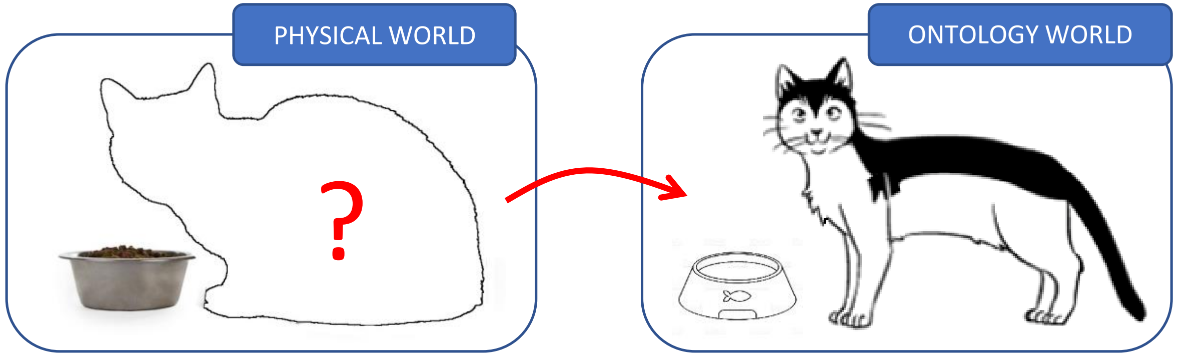
The EMMO does provide the consistency of the symbolic representation.

i.e. you cannot say everything in EMMO, but only what is realistic according the ontology developers!



The EMMO does not guarantee that the representation is a sign for an actually existing physical entity.

i.e. you can use symbolic representation to express something that is realistic in the EMMO but that does not exist (a realistic lie or a novel)

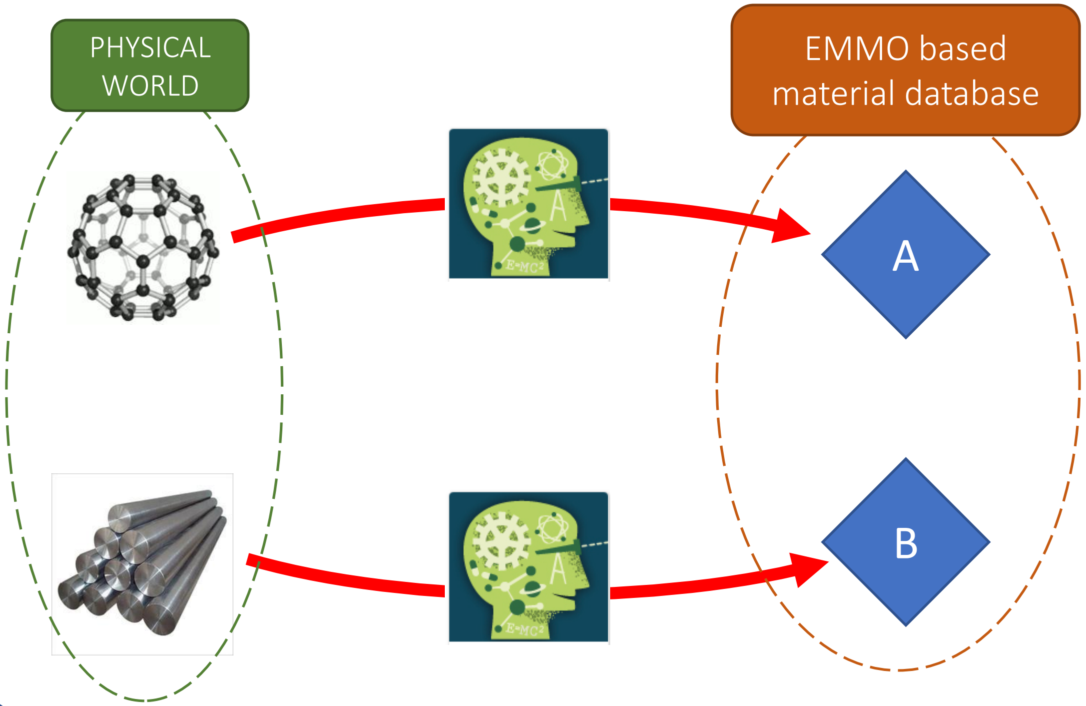


EMMO GENERAL USAGE EXAMPLES

DEFINITION: A **<u>lie</u>** something that can possibly exists in a defined space and time in the real world, but does not actually exists!

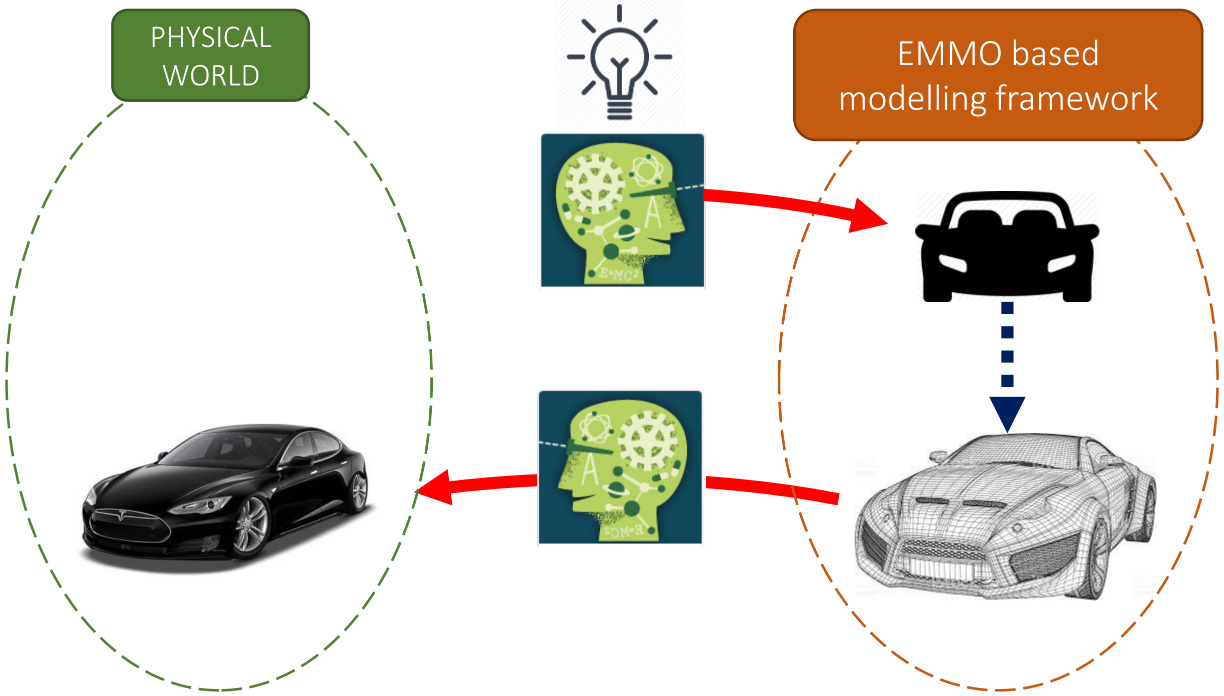
MATERIALS CHARACTERIZATION

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 <u>used in order to lie</u>. 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!

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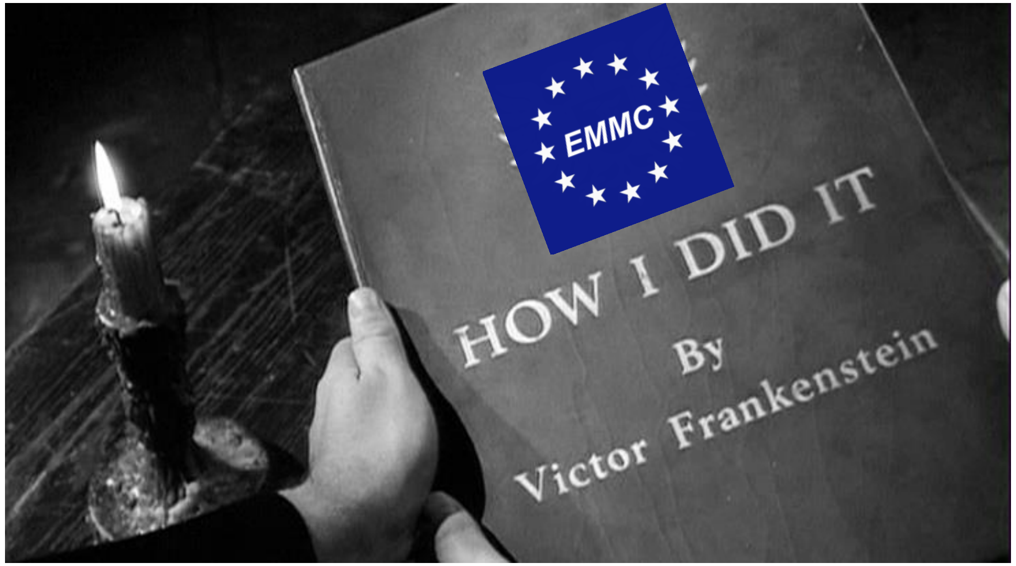
EMMO MAIN OBJECTIVES:

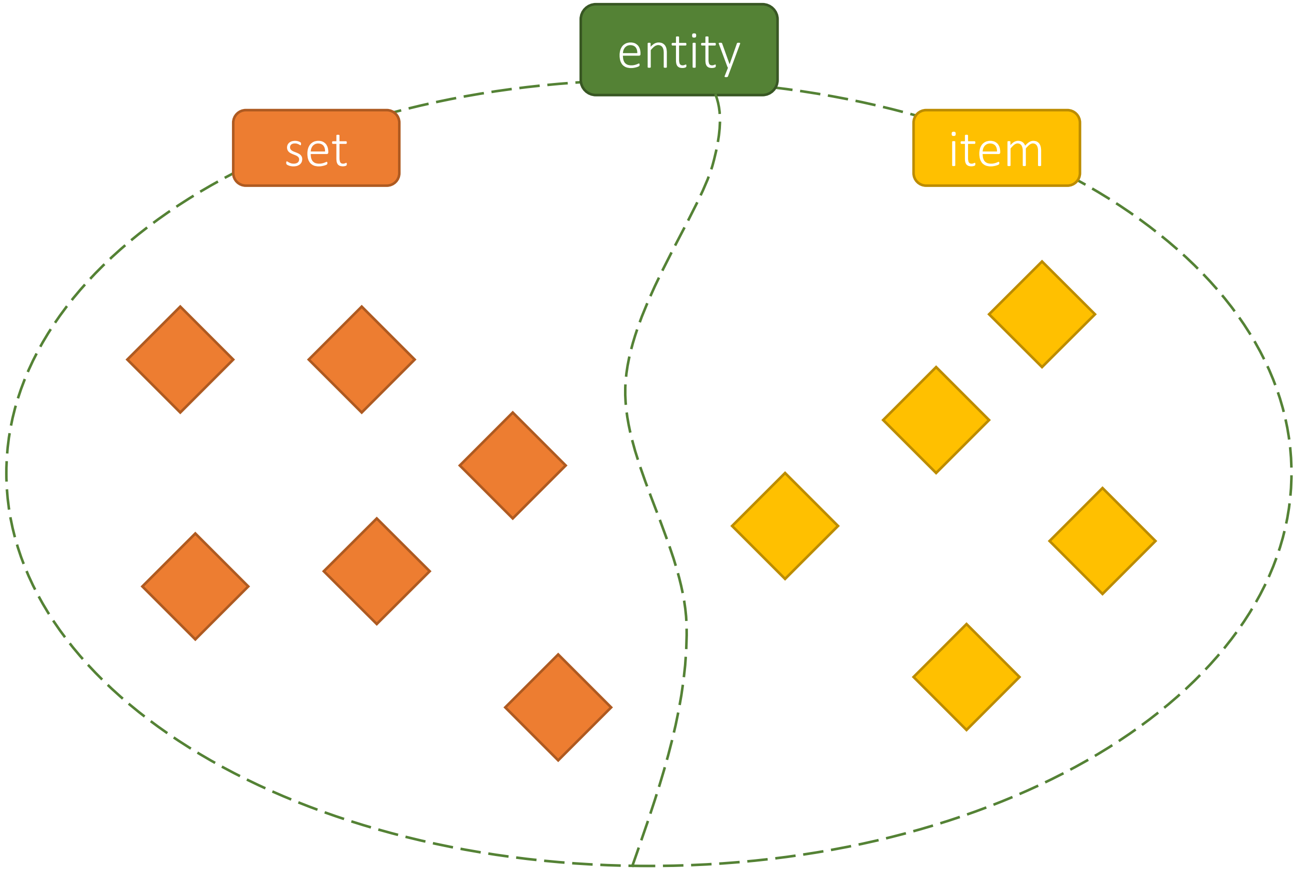


- PROVIDE A BASIC FRAMEWORK FOR THE DESCRIPTION OF MATERIALS FOLLOWING MATERIAL SCIENCE APPROACH AND TERMINOLOGY
- PROVIDE EFFICIENT REPRESENTATION OF PHYSICAL ENTITIES BY USING GRANULARITY LEVELS TO FACILITATE MULTISCALE MATERIALS MODELLING AND CHARACTERIZATION

  POLYMER -> MONOMER -> ATOM -> NUCLEUS -> ...

- INCLUDE PHYSICAL MODELS AND THEIR RELATIONS WITH MATERIAL ENTITIES
- CATEGORIZE MATERIAL PROPERTIES TO FACILITATE THE STANDARDIZATION OF MATERIAL CHARACTERIZATION AND MODEL VALIDATION
- PROVIDE AN INTEROPERABILITY FRAMEWORK FOR A MATERIALS PROPERTIES DATABASE

EMMO FUNDAMENTAL LEVELS



DisjointUnion(:entity :set :item)

entity

Is a class representing the collection of all the individuals (signs) that are used in the ontology. Individuals are declared by the EMMO users when they wants to apply the EMMO to represent the world.

set

Is the class representing the collection of all the individuals (signs) that represents a collection of **item**s

(**item**s and not **entitiy**-s, in order to avoid Russels paradox)

item

Is the class that collects all the individuals that are member of a **set** (it's the most comprehensive **set** individual)

The **item** class is an individual of **set**: it's the **set** individual that contains all **item** individuals.

Subclasses of **item** are other, less generic, individuals of **set**

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

set theory

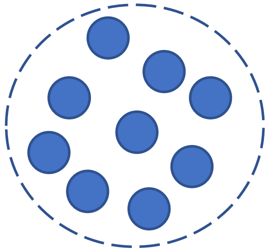
SET

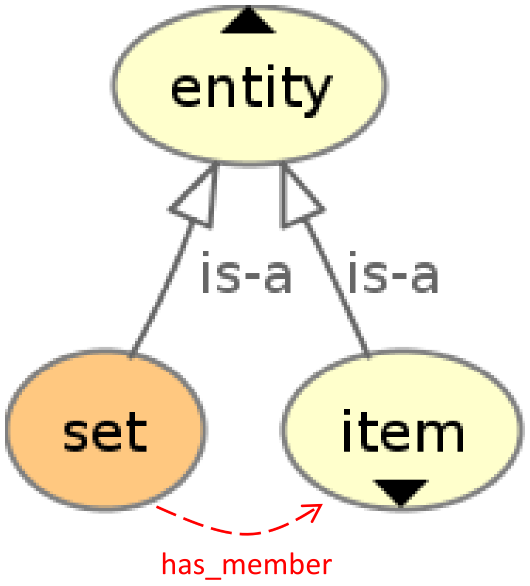
–declared using **has_member** primitive relation

–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 (i.e. Russel's theory of types)

–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

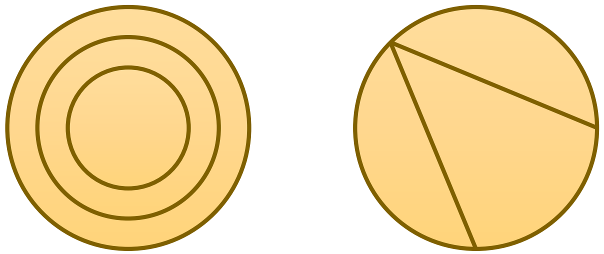
FUSION

–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



THE **FUNDAMENTAL LEVEL** OF THE ONTOLOGY IS BASED ON THE **ZERMELO–FRAENKEL SET THEORY** AXIOMS THAT DISTINGUISH A **SET** FROM AN **ITEM**.

see General Formal Ontology
http://www.onto-med.de/ontologies/gfo/

THE FIRST THREE AXIOMS ARE:

Axiom of extensionality

$$\forall x \forall y [\forall z (z \in x \Leftrightarrow z \in y) \Rightarrow x = y].$$

Two sets are equal (are the same set) if they have the same elements.

Axiom of regularity

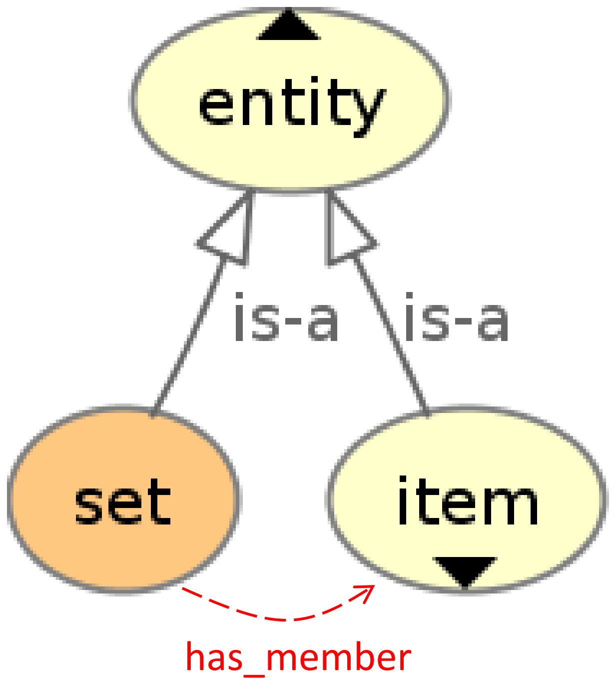
$$\forall x [\exists a (a \in x) \Rightarrow \exists y (y \in x \land \neg \exists z (z \in y \land z \in x))].$$

Every non-empty set x contains a member y such that x and y are disjoint sets.

Axiom of specification

$$\forall z \forall w_1 \forall w_2 \ldots \forall w_n \exists y \forall x [x \in y \Leftrightarrow (x \in z \land \phi)].$$

A set cannot contain itself (avoid Russel paradox). It means that **item** and **set** are disjoint.



EMMO item branch is build upon a hierarchy of mereological relations and axioms:

antisymmetric
transitive
reflexive

is_part_of

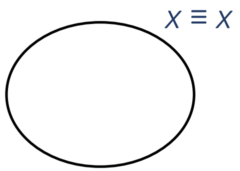
↑

transitive
proper parthood

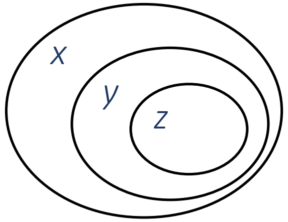
is_proper_part_of

axioms

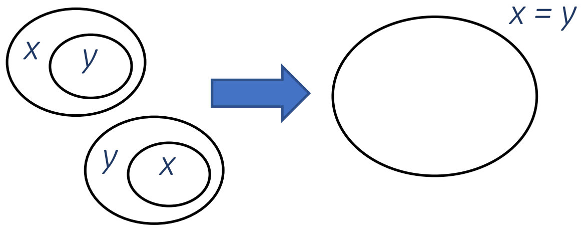
reflexive Pxx



transitive $(Pxy \wedge Pyz) \longrightarrow Pxz$



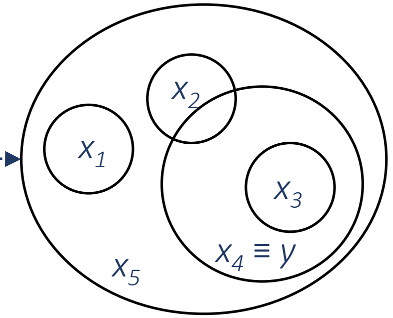
antisymmetric $(Pxy \wedge Pyx) \longrightarrow x = y$



definition

proper parthood $PPxy =_{df} Pxy \wedge \neg x = y$

only x_3 is proper part of y



overlap $Oxy \Leftrightarrow \exists z(Pzx \wedge Pzy)$

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

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

EMMO TOPOLOGY IS ALSO USED TO DEFINE PROPERTIES OF SPACETIME

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

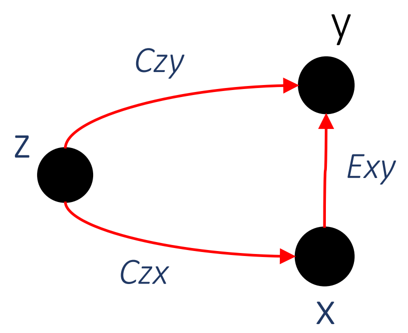
Primitive concept of **connection** between two entities: Cxy *x* is connected with *y*

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*

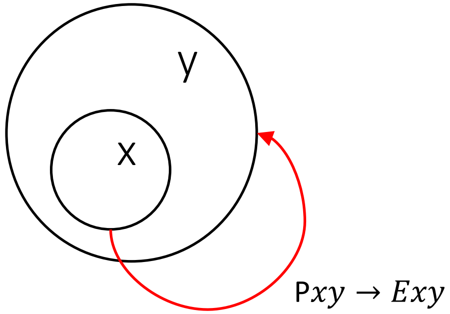


(C.3) $(Exa \Leftrightarrow Exb) \Leftrightarrow a = b$ Extensionality axiom

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

(C.4) $\mathrm{P}xy \rightarrow Exy$ if *x* is part of *y* then *y* encloses *x* (monotonicity)

Theorem: $Oxy \rightarrow Cxy$



EMMO Mereotopology Definitions

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

$ECxy \Leftrightarrow Cxy \wedge \neg Oxy$ — *External Connection*

$TPxy \Leftrightarrow Pxy \wedge \neg IPxy$ — *Tangential part*

$IOxy \Leftrightarrow \exists z(IPzx \wedge IPzy)$ — *Internal Overlap*

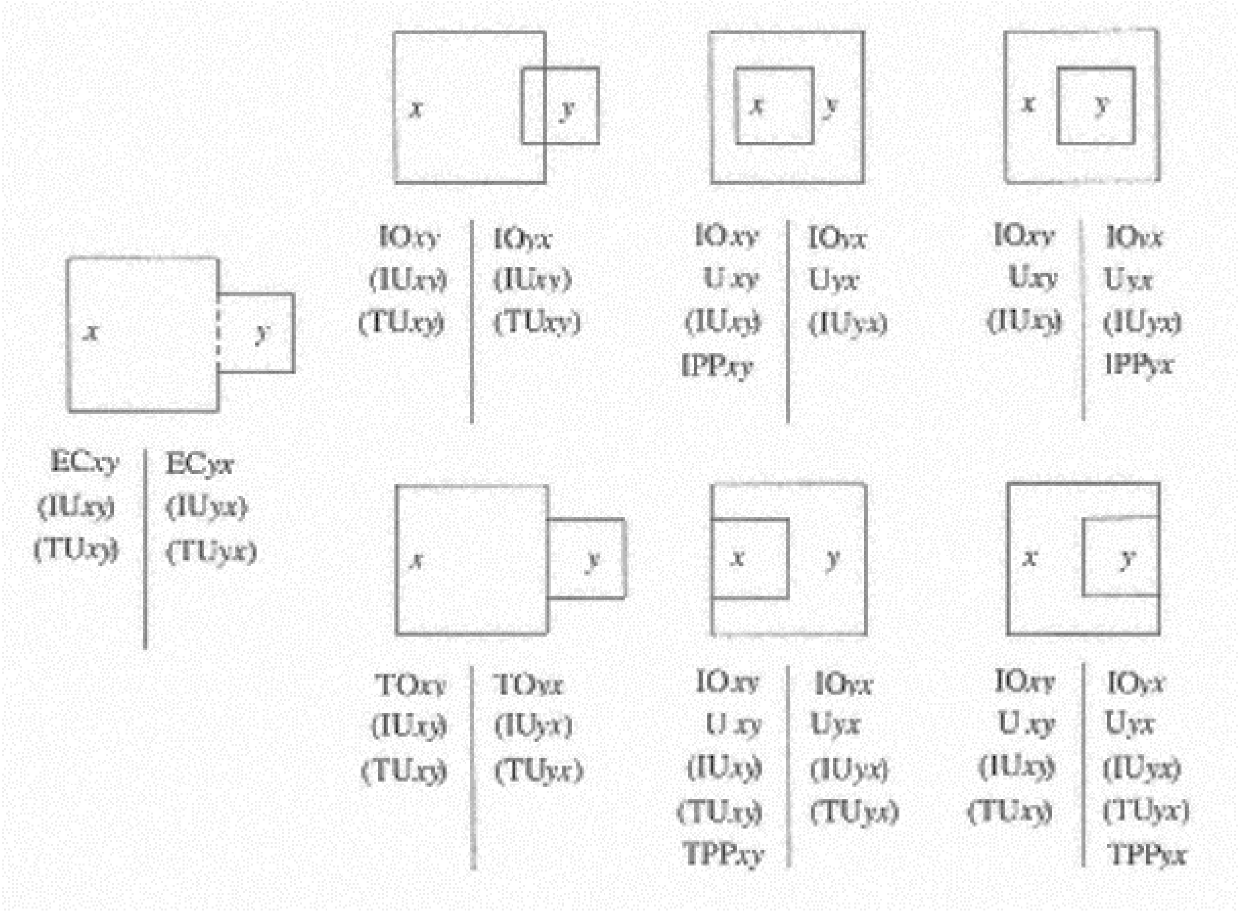
$TOxy \Leftrightarrow Oxy \wedge \neg IOxy$ — *Tangential Overlap*

$IUxy \Leftrightarrow \exists z(IPzx \wedge IPyz)$ — *Internal Underlap*

$IPxy \Leftrightarrow Pxy \wedge \forall z(Czx \rightarrow Ozy)$ — *Internal Part*

$IPPxy \Leftrightarrow IPxy \wedge \neg IPyx$ — *Internal Proper Part*

$TUxy \Leftrightarrow Uxy \wedge \neg IUxy$ — *Tangential Underlap*



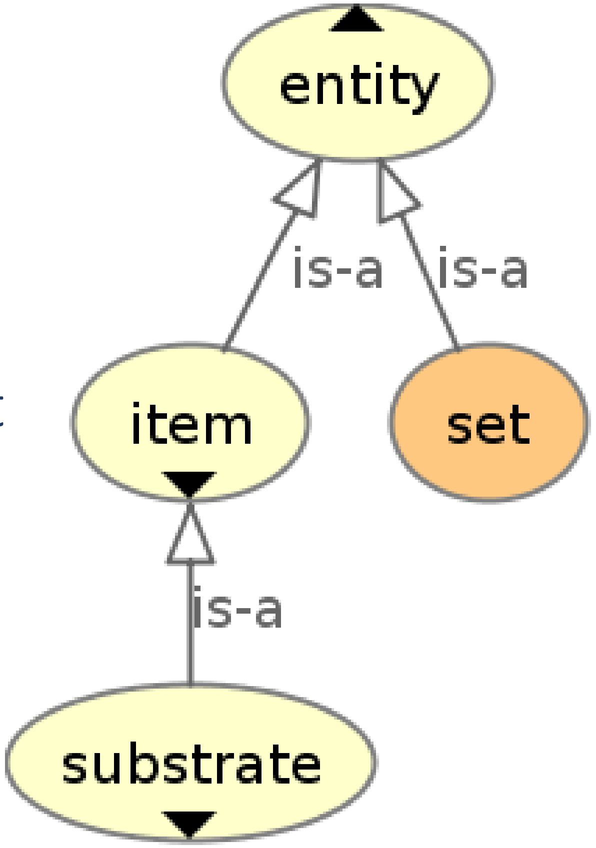
SUBSTRATE

It represents the place (in general sense) in which every real world item exists.

A substrate provides the dimensions of existence for real world entities. It follows the fact that everything that exists is placed somewhere and space and time coordinates can be used to identify it

Substrate is a mereotopological entity.

Substrates are always topologically connected spaces (a topological space X is said to be disconnected if it is the union of two disjoint nonempty open sets. Otherwise, X is said to be connected)



Following Kant, space and time are a priori forms of intuition i.e. they are the substrate upon which we place our intuitions, assigning space and time coordinates to them.

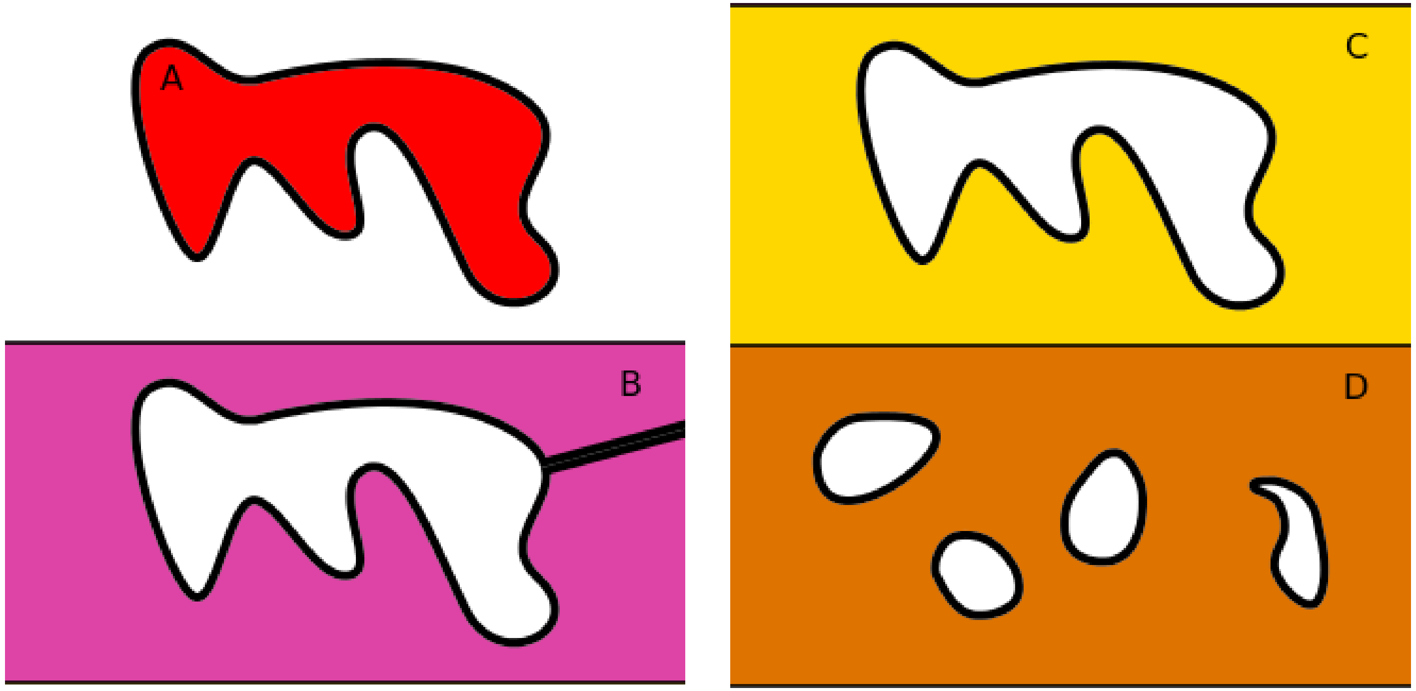
EMMO Item Subclasses

Substrates in the EMMO are always <u>topologically connected space</u>

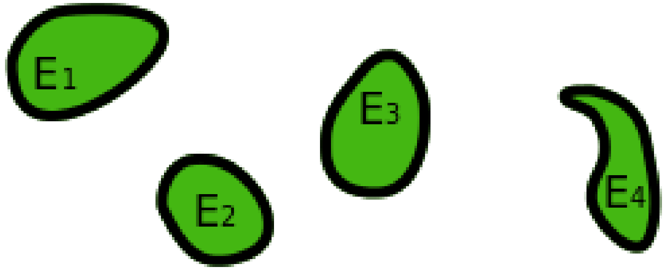
Wikipedia Connected Space examples:

From top to bottom: red space *A*, pink space *B*, yellow space *C* and orange space *D* are all **connected**, whereas green space *E* (made of subsets E1, E2, E3, and E4) is **not connected**.

Furthermore, *A* and *B* are also simply connected (genus 0),
while *C* and *D* are not: *C* has genus 1 and *D* has genus 4.

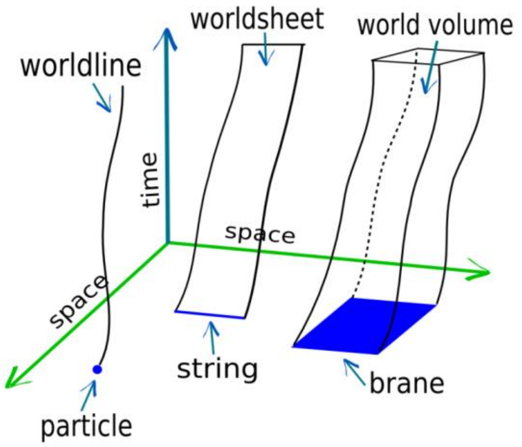


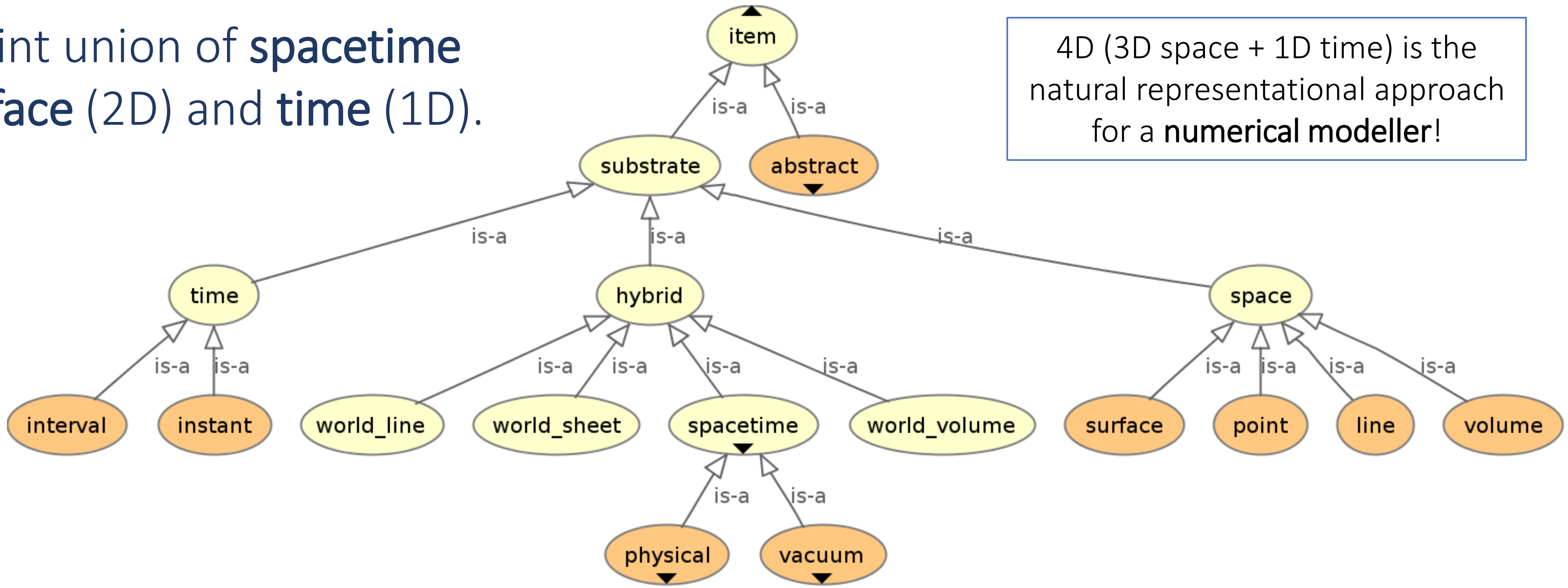
The user can define always define an arbitrary collection of connected spaces by declaring an individual of the **set** class.



ITEM SUBCLASSES

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





4D (3D space + 1D time) is the natural representational approach for a **numerical modeller**!

Each branch of **item** can only have parts of the <u>same type</u>.

It means that parthood is only between substrates of the <u>same dimension</u> (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.

ITEM SUBCLASSES

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

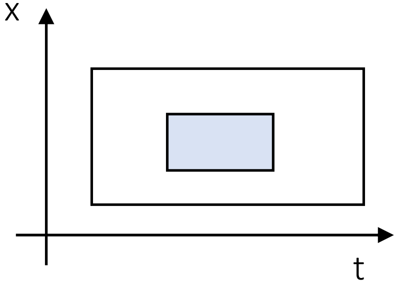
It means that parthood is only between substrates of the same dimension (e.g. a **spacetime** has no **space** parts).

This restriction in the mereological relations is done in order to overcome a typical misuse of the partitioning procedure, that occurs when the user wants to stretch the *is_part_of* relation beyond its applicability limit.

e.g. you can slice a 3D+1D cake in 3D+1D thin parts (3 spatial + 1 temporal dimension), but **it's impossible to slice the cake in infinitely thin 2D+1D slices** (2 spatial + 1 temporal dimension). The relation of parthood applied to material entities cannot reduce spatial dimensions for a material object, since a 2D+1D material object does not exist!

Slicing a 3D+1D entity in a 2D+1D entity can still be done, but **within the substrate level (the topological level)** using the *is_slice_of* relation working on geometrical concepts and not actual materials.

EMMO Mereotopology Relations

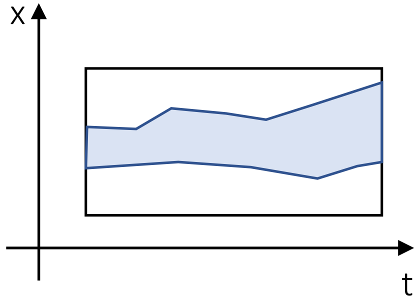


encloses (mereotopology)

has_part (4D mereology)

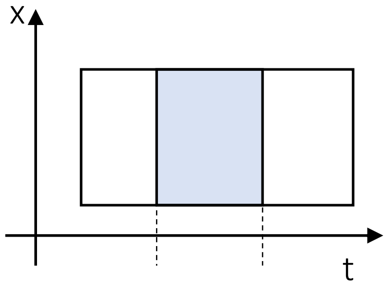
has_subdimensional_space (topology)

has_spatial_part



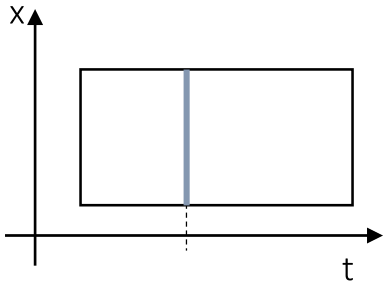
Same dimensionality of the whole.
Extended through all lifetime of the item.
Can be:
has_spatial_proper_part
has_spatial_direct_part

has_temporal_part



Same dimensionality of the whole. Extended through all spatial extension of the item. The left and right boundary must express <u>simultaneity</u> in a specified reference frame.
Can be:
has_temporal_proper_part
has_temporal_direct_part

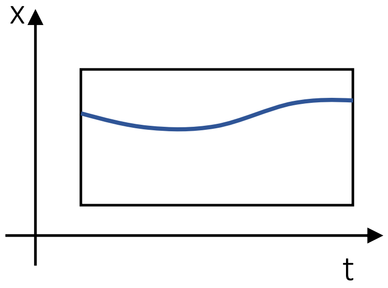
has_time_slice



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

Instantaneous in time. Must express <u>simultaneity</u> in a specified reference frame.

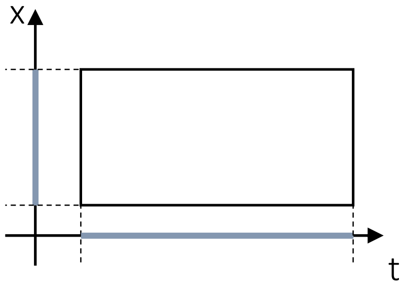
has_space_slice



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

EMMO Mereological Composition

The EMMO basic assumption is that the real world (the world outside us) manifests itself as a one **spacetime** entity, the Universe.

Some mereological parts (regions) of the Universe express peculiar properties that can be perceived by (they interact with) an interpreter/ontologist. These mereological parts can be categorized in **matter** spacetimes or **field** spacetimes individuals.

matter is the subclass of **spacetime** that expresses some mass property.

field is the subclass of **spacetime** that can be perceived by the ontologist, but expresses no mass property.

The EMMO represents real world entities as subclass of **spacetime**.

In that sense a real world entity is a **spacetime entity**

EMMO Mereological Composition

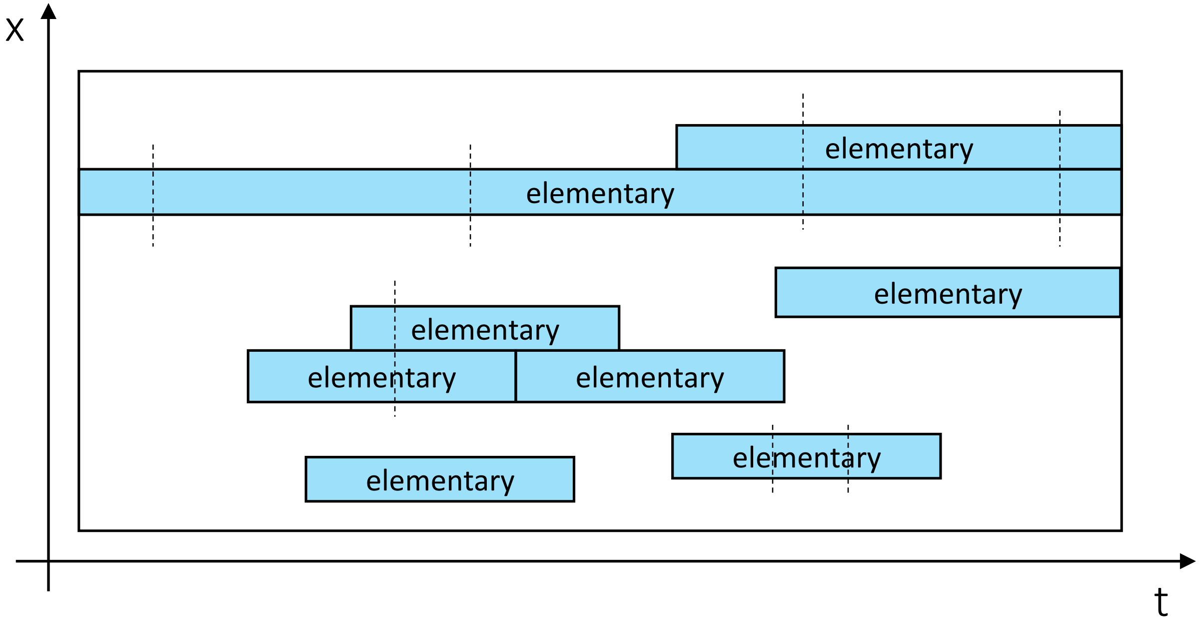
The EMMO basic mereological decomposition assumption is that the most basic manifestation of **matter** is represented by a subclass of **spacetime** called **elementary** whose proper parts can be only temporal parts.

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 'atomic level' in EMMO is defined by the **elementary** class.

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

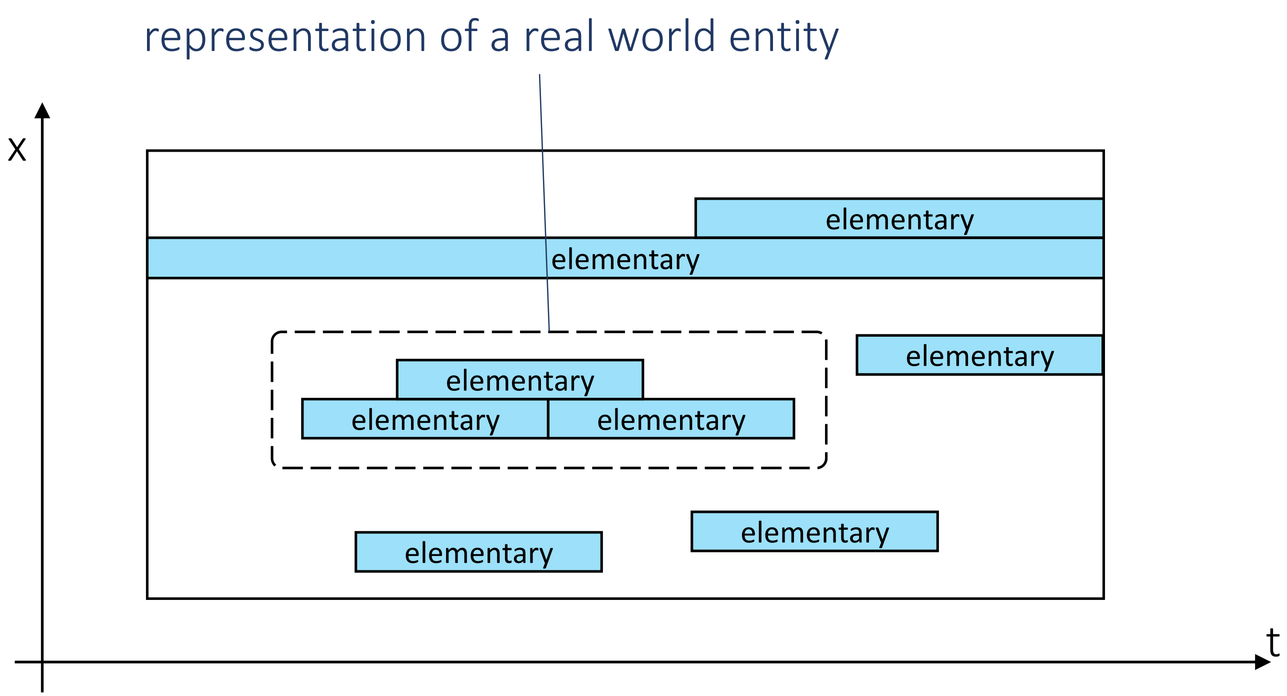
An **elementary** can still be decomposed in temporal parts, that are themselves **elementary**.

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)

Macro-entities are defined by the way we see the world (e.g. car, humans, planet), but the physical laws of these macro-entities are simply the consequences of a complex superimposition of the more fundamental laws that rule **elementary**.

However, a description of materials based on **elementary** is not always practical nor acceptable.



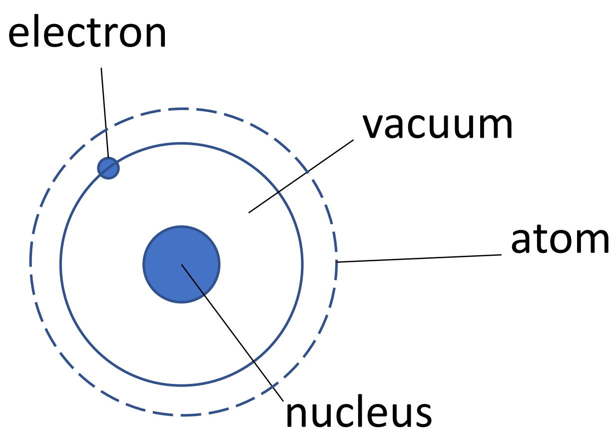
We need to find a way to categorize **matter** entities as a hierarchical composition of **elementary**-es in order to represent with the EMMO the real world macro-entities following a human perspective.

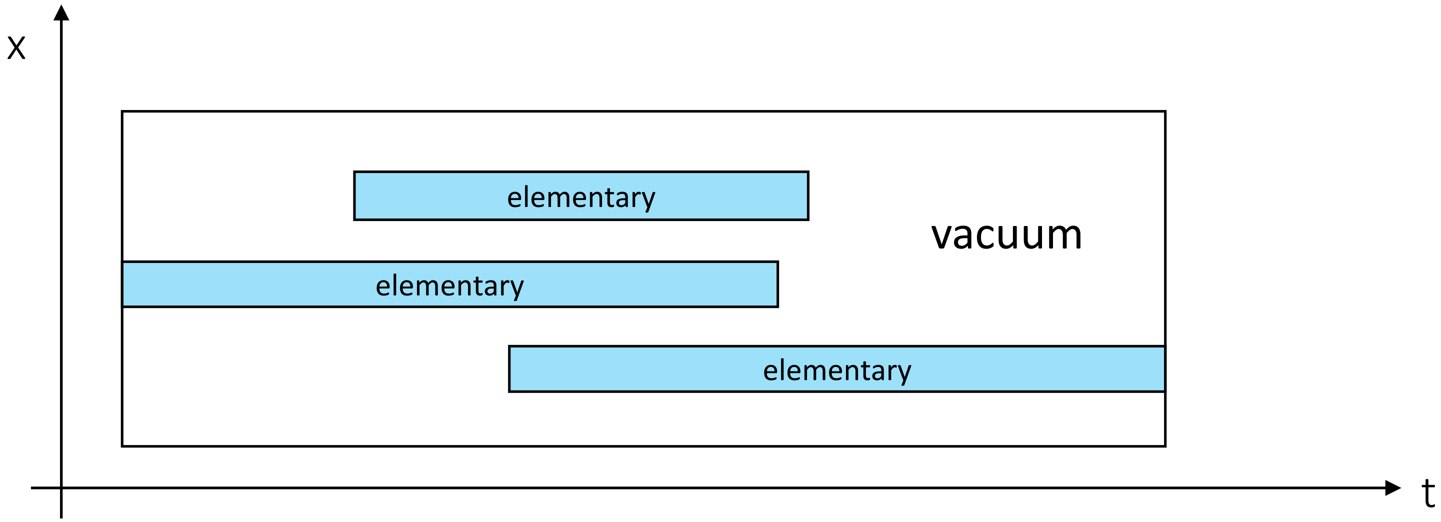
Need for new parthood relations that lead to composition rules for entities forming macro-entities.

EMMO The Vacuum Issue

We must also take into account the presence of **vacuum** between **elementary** that composes a <u>higher granularity level entity</u>.

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





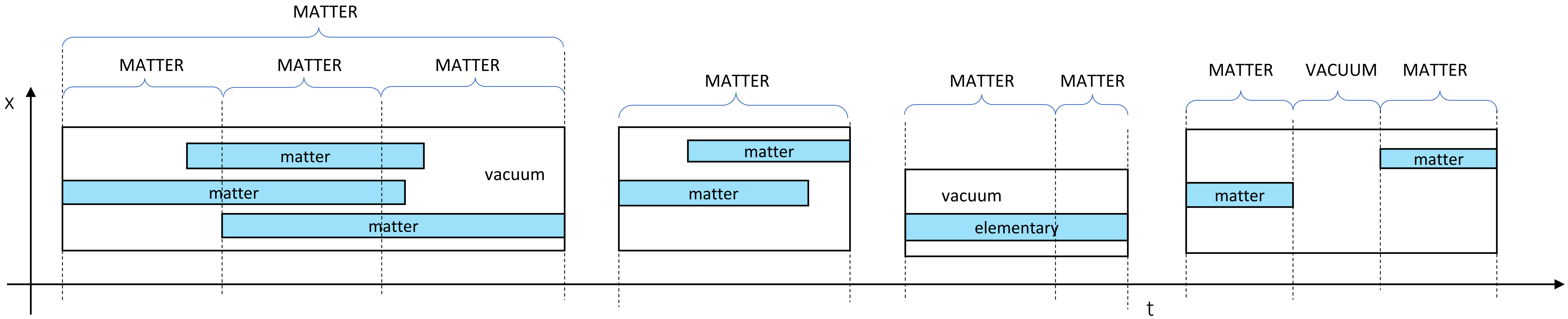
VACUUM

A **spacetime** that has no **elementary** parts.

vacuum is defined as *EquivalentTo:* spacetime and not has_part some elementary

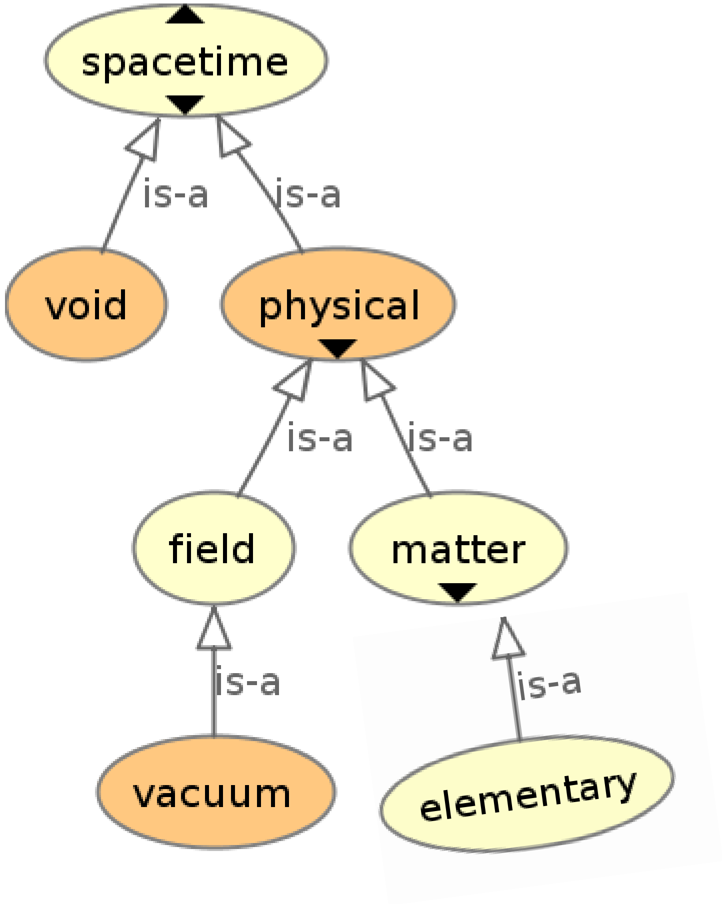
MATTER and ELEMENTARY relation

- **Matter** is a way to represent a group of **elementary** in an enclosing **spacetime**
- All possible temporal parts of a **matter** must have some **elementary** or **matter** as proper parts themselves
- All temporal parts of **matter** are **matter**
- **Elementary** are **matter**
- A **matter** can be decomposed in **matter** parts up to **elementary** level
- A **matter** can have **vacuum** parts: **matter** is porous



A **matter** is an **elementary** or a composition of other **matter** and **vacuum**.

ACCORDING DEFINITIONS ON PREVIOUS SLIDES, THE FOLLOWING IS A POSSIBLE HIERARCHY FOR SPACETIMES:



To retain the mereotopology relations for both physical objects and substrates we need to declare a physical object as a spacetime that manifests some properties of **matter** or **field**.

MATTER
A **spacetime** that manifests the properties of matter (has mass)

FIELD
A **spacetime** that manifests the properties of a field (energy without mass) i.e. electromagnetic, gravitational, …

VACUUM
A **spacetime** that has no **matter** parts (but still can be a **field**)

VOID
A **vacuum** that has no **field** parts

PHYSICAL
Is declared to be *EquivalentTo:* **field** or **matter**. A **spacetime** can be a **field**, a **matter** or both.

A fundamental difference between EMMO and other ontologies is the fact that a material entity (**matter**) is a **spacetime**.

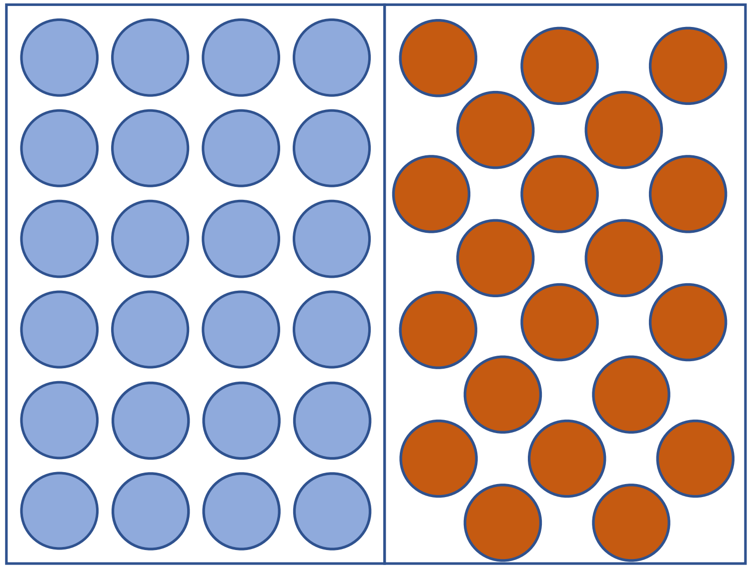
By defining matter as a particular subclass of spacetime we can apply mereotopology directly to material entities.

Doing so we avoid the complexity (and unnecessity) of relations such as occupies_spacetime or exists_in_spacetime.

Matter is always 4D!!! There is no 3D representation of matter.

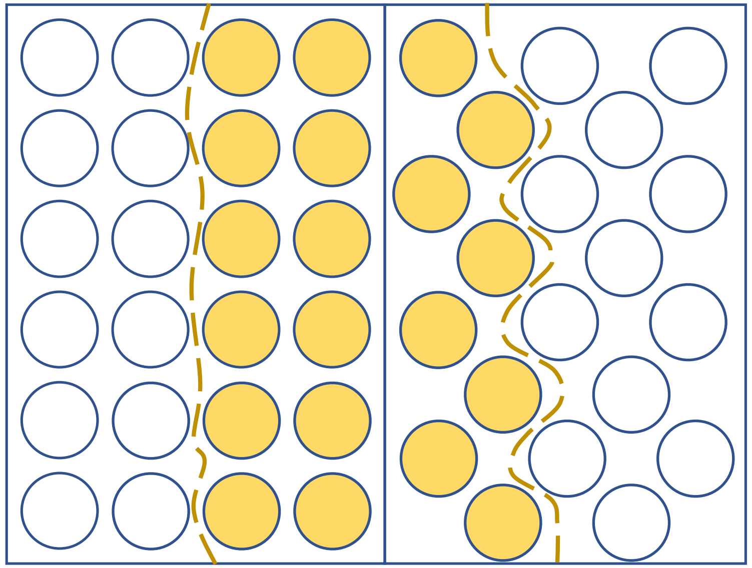
There can be a 3D slice of a matter but is no more matter:

it's simply a 3D spatial region.

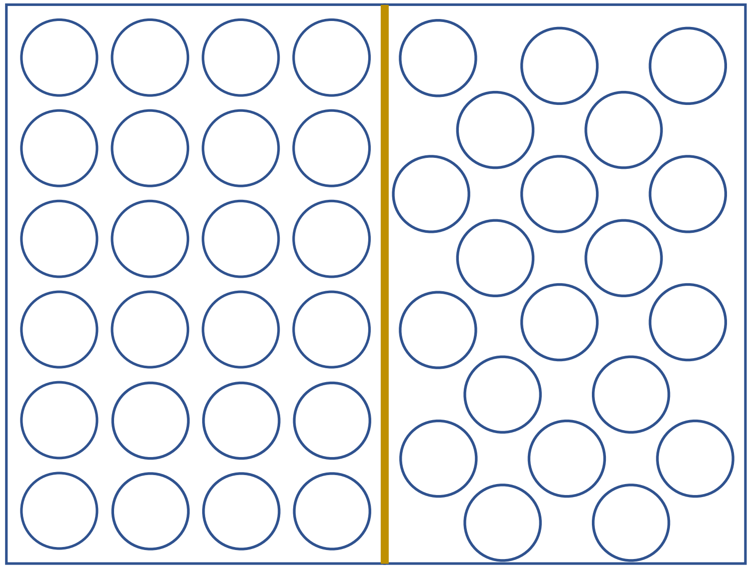


matter **a**
(3D + 1D)

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



boundary (matter)
(3D + 1D)



interface (world_volume)
(2D + 1D)

BOUNDARIES
VS
INTERFACES

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

The boundary is a 3D+1D entity.

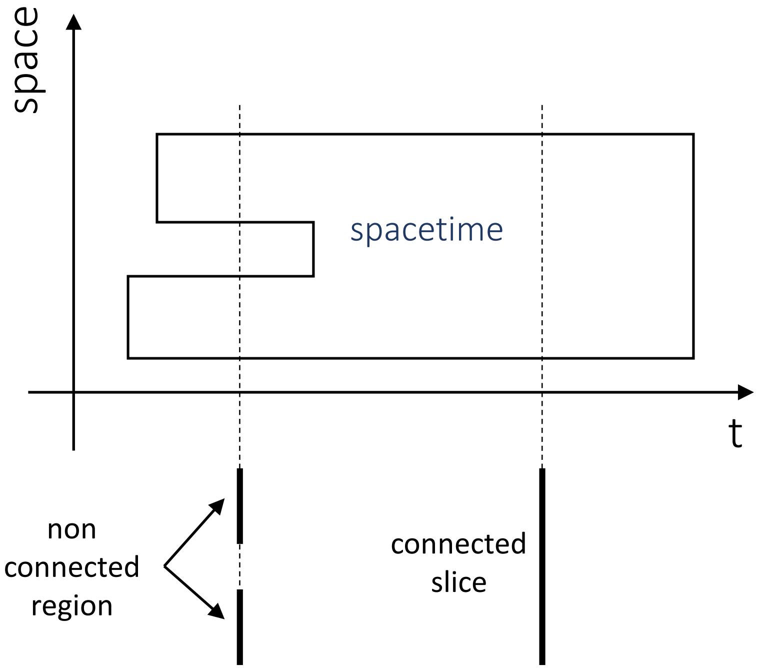
The interface between **a** and **b** can be defined by space slicing **a** or **b** and is e.g. a 2D + 1D entity (a **world_volume**), intended as a **substrate** entity but not a **matter**.

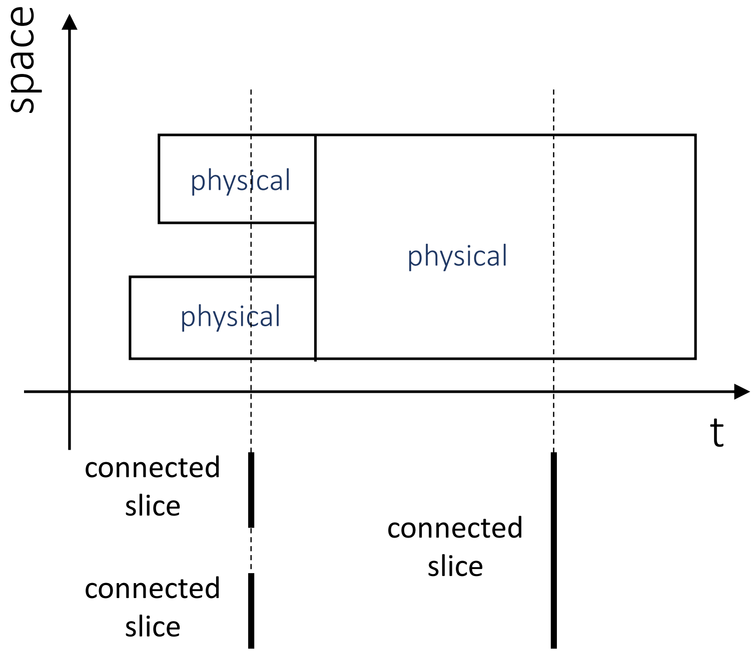
PHYSICAL

A **physical** is something that can be perceived i.e. a **matter** or a **field** or both. In order to be perceived it must hold some physical properties.

Another requirement of a **physical** as a **spacetime** entity is that it has to be sliced only in a single connected **volume**.

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

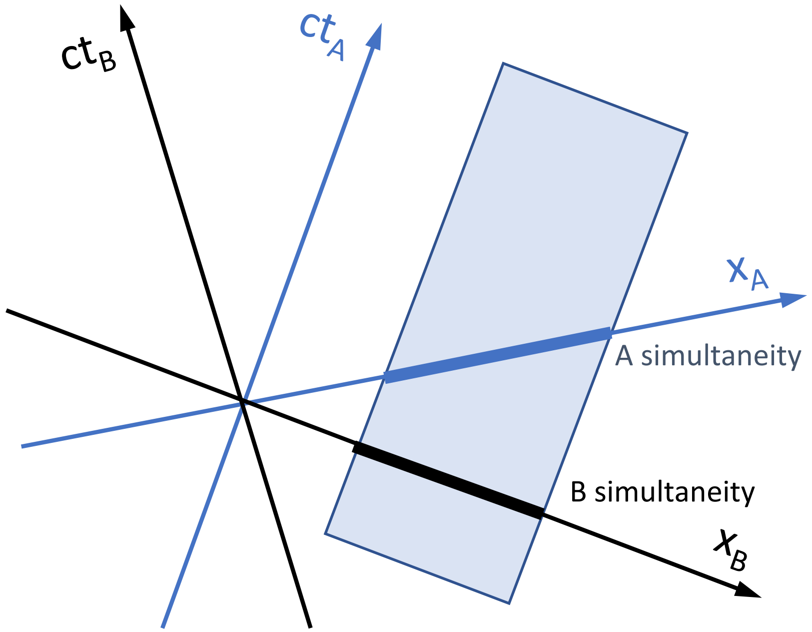




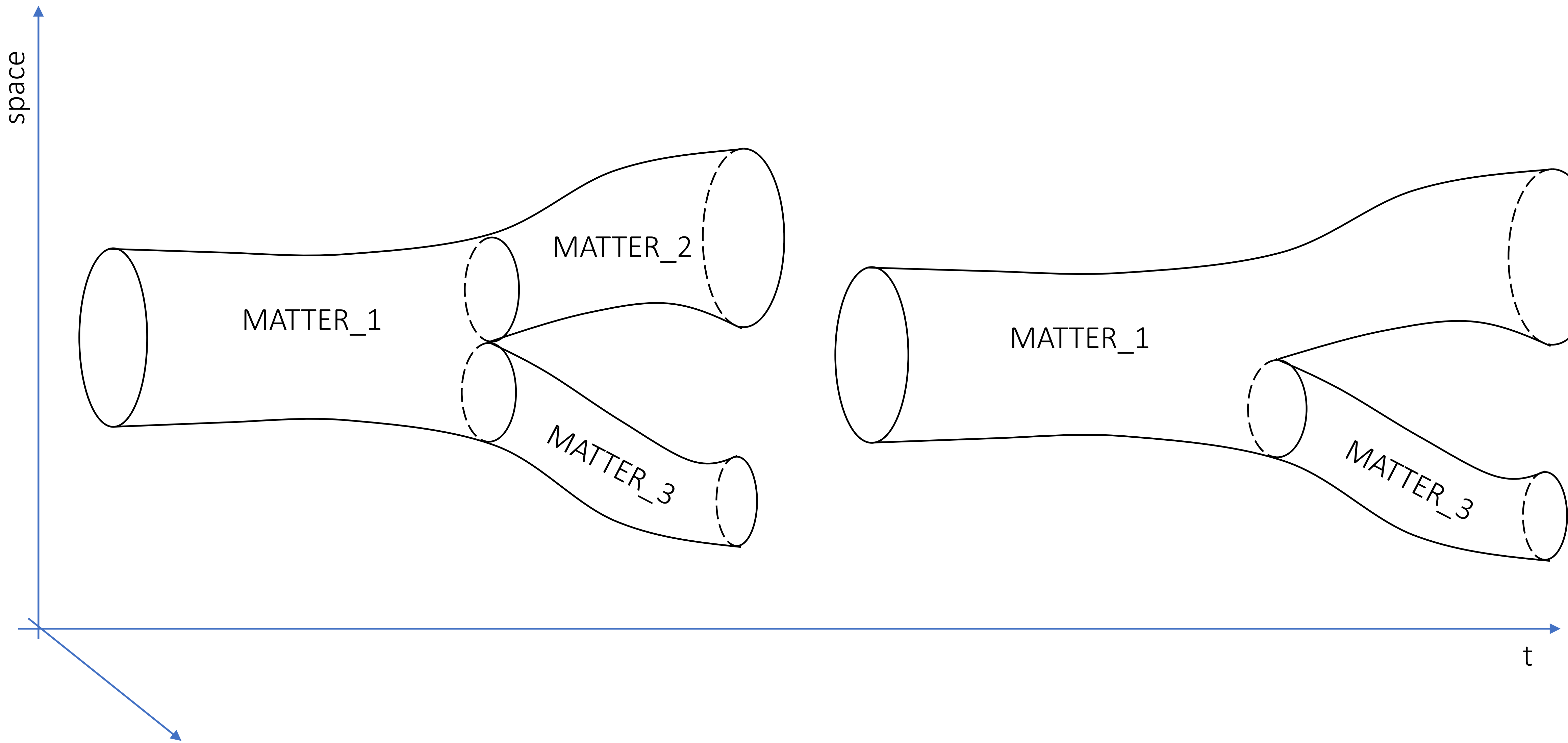
EMMO is compatible with relativity.

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.



3D Representation of two possible decompositions of a time changing physical



Up to now, no compositional rules are declared for a **matter**.

There is total freedom in defining a **matter** as part or made of other **matter**, as long as:

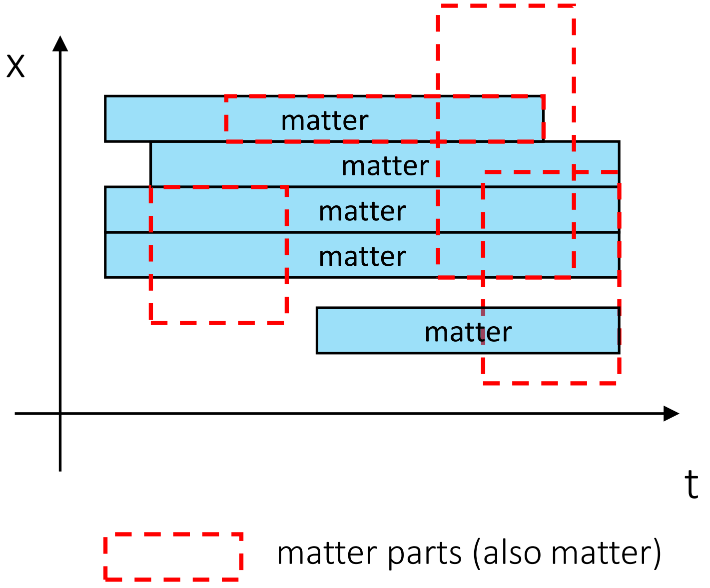
1. it coincides with an elementary OR
2. has part matter and no vacuum temporal parts

<u>Matter entities can overlap each other</u>, and this hampers defining univocal entities.

Matter is <u>very flexible</u> as one can define arbitrary parts of **spacetime** (that includes other **matter**) to be a **matter**.

However, <u>no particular structure or granularity is easily representable except for **elementary**</u>.

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



direct parthood relation

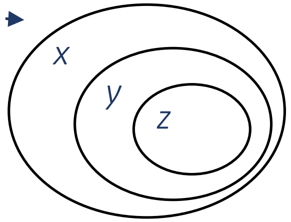
EMMO Mereology of Direct Parts

transitive proper parthood **is_proper_part_of**

↑

proper parthood **is_direct_part_of**

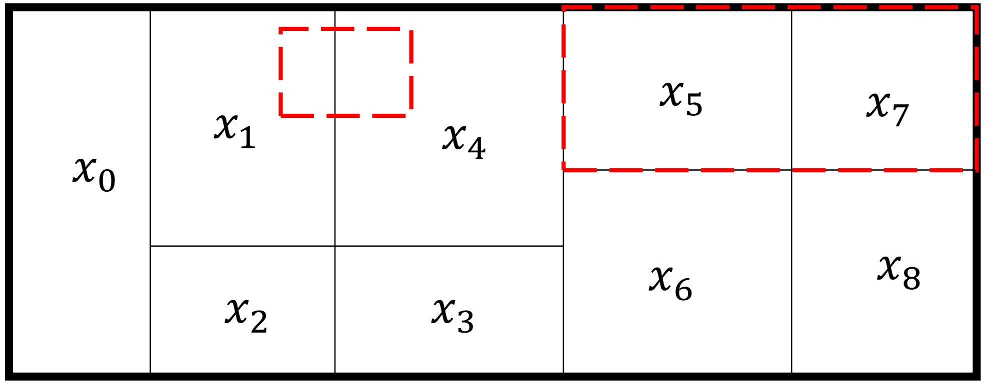
- By dropping transitivity **is_direct_part_of** identifies the entity proper parts that are at the very next lower granularity level.
- Direct parthood requires also the existence of a non overlapping partitioning.
- Direct parthood is functional.



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

z is not direct part of x

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



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**

EMMO Mereology of Direct Parts

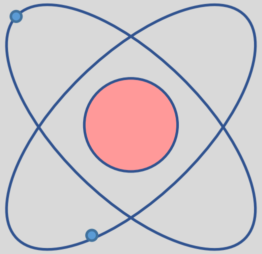
$DPxy \Rightarrow PPxy$	direct part is a **proper part**	A direct part is always “less” than the whole, making it useful for a hierarchy definition.
$DPxy \Rightarrow \forall z\,(DPzy \Rightarrow \neg Oxz)$	direct parts do not **overlap**	Direct parts are a partitioning of a whole with distinct parts.
$DPxy \Rightarrow \forall z\big(\neg(DPyz \wedge DPxz)\big)$	direct part is **non transitive**	Direct parts define single steps in granularity, identifying the lower the upper level of composition of a whole.
$DPxy \wedge DPxz \Rightarrow \mathrm{y} = \mathrm{z}$	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.

EMMO Mereology of Direct Parts Example

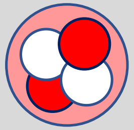
AXIOMS

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

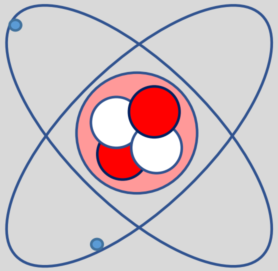


$n = 4$

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

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 all levels of granularity (granularity is flattened).

Atom inheres the nucleus proper parthood relations due to transitivity.

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 the lack of transitivity.

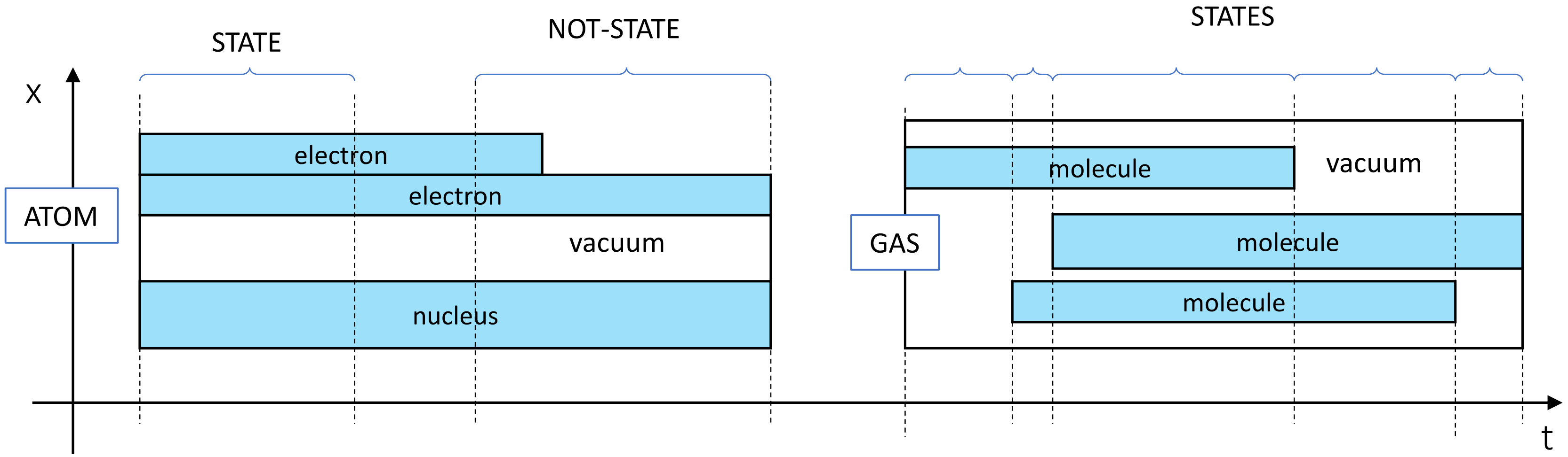
STATE

- ”state” stands for “**matter 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 **matter** or **vacuum**.

A **state** is like a snapshot of a **physical** in a finite interval.

It is similar to the concept of *endurant* (or *continuant)* in other ontologies.

The idea of slicing into a 0D time (instant) is not achievable to real things: it’s an unrealistic mental assumption. You always have an ‘aperture’ time for the observation of a physical e.g. like exposure time in a photo.



EXISTENT

An **existent** then can be defined as a **matter** that <u>unfolds in time as a succession of **states**</u>

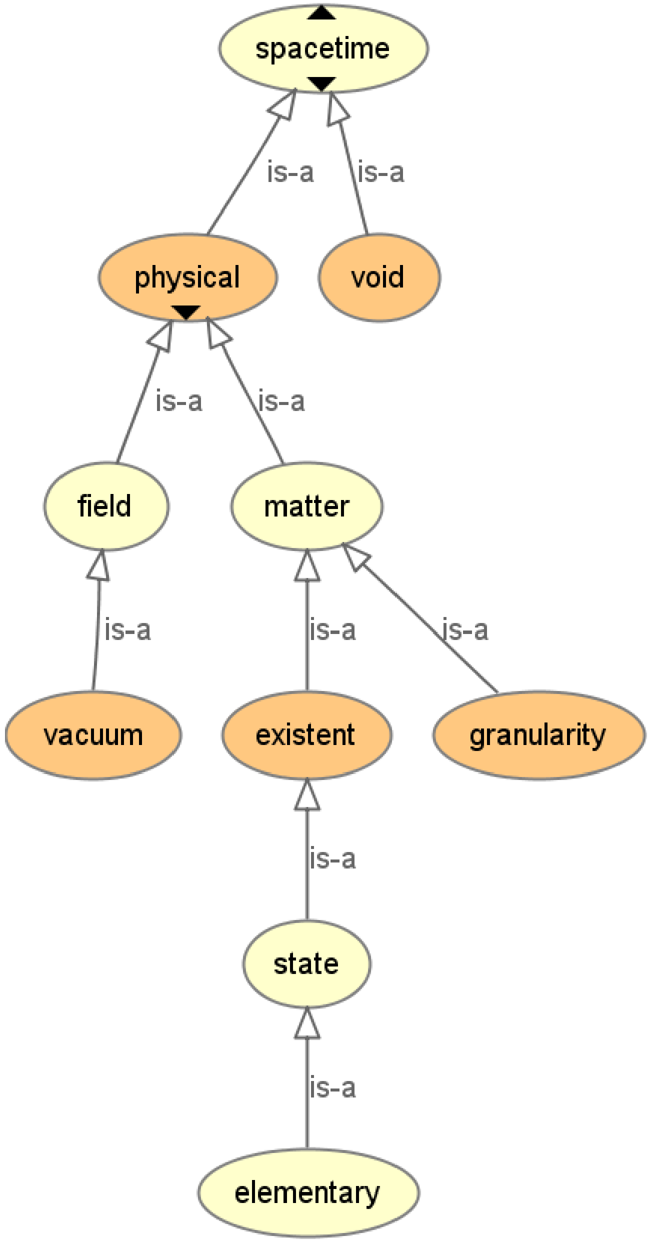
This class is used to represent the whole life of a complex but structured state-changing **matter** entity like e.g. an atom that becomes ionized and then recombines with an electron.

Ex-sistere (latin): to stay (to persist through time) outside others of the same type (it's **matter** that can be distinct from the rest).

On the contrary, a **matter** **and** **not(existent)** entity is something "amorphous", randomly collected and not classifiable by common terms or definitions, i.e. an heterogeneous heap of **elementary**, appearing and disappearing in time.

(we cannot do examples, because we should use a name and implicitly use a definition!)

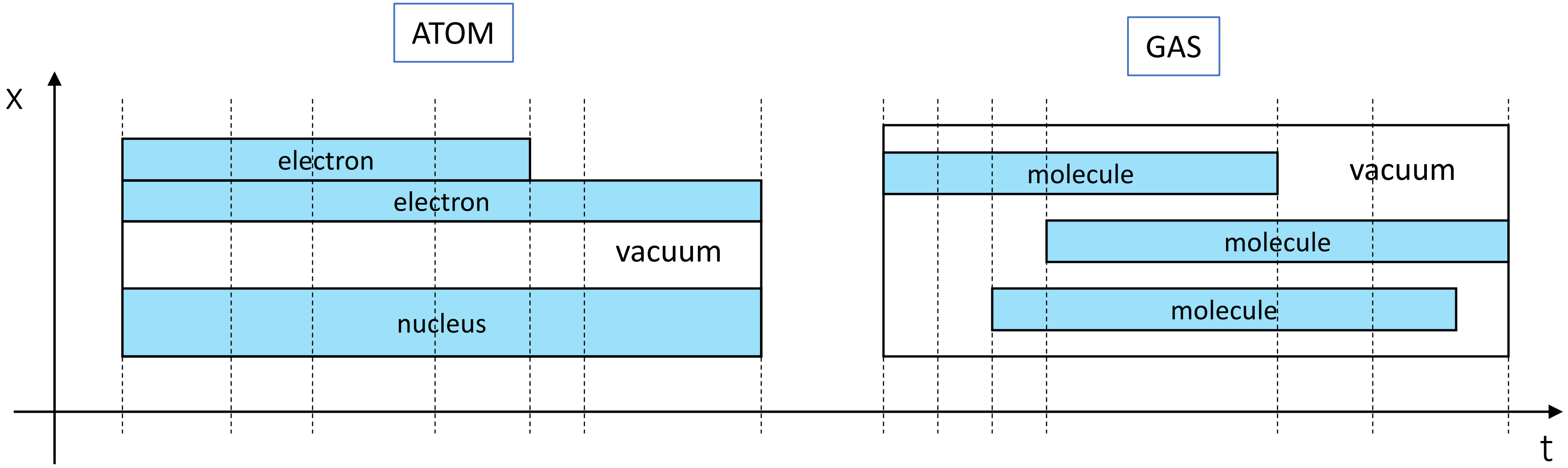
It's similar to what other ontologies call *perdurant* (or *occurrent*).



How to relate STATE and MATTER? We can propose the following axiom:

matter *SubClassOf:* **has_direct_temporal_part some state**

It means that you can always direct partition in time a **matter** as a series of **states**. As axiom, there exists always an interval in which a **matter** has a defined granularity.



The usefulness of **state** is that it makes it possible to describe the evolution in time of an **existent** in terms of series of states that can take into account the disappearance or appearance of parts within an **entity**. A **state** is a recognizable granularity level of **matter**, in the sense that its direct parts do not appear or disappear within its lifetime as it can be for a generic **existent**.

The different specific granularities will help us to create a categorization of **state**s in terms of objects (primitive classes) or generic granularity types (defined classes)

state and **matter** are related and defined using spatial and temporal direct parthood.

spacetime

elementary

matter

has_part
(reflexivity, transitivity, antisymmetry)

has_spatial_part
(reflexivity, transitivity, antisymmetry)

has_temporal_part
(reflexivity, transitivity, antisymmetry)

has_proper_part
(irreflexive, transitivity, antisymmetry)

has_spatial_proper_part
(reflexivity, transitivity, antisymmetry)

has_temporal_proper_part
(reflexivity, transitivity, antisymmetry)

has_spacetime_direct_part
(irreflexive, non-transitivity, antisymmetry, functional)

has_spatial_direct_part
(irreflexive, non-transitivity, antisymmetry, functional)

has_temporal_direct_part
(irreflexive, non-transitivity, antisymmetry, functional)

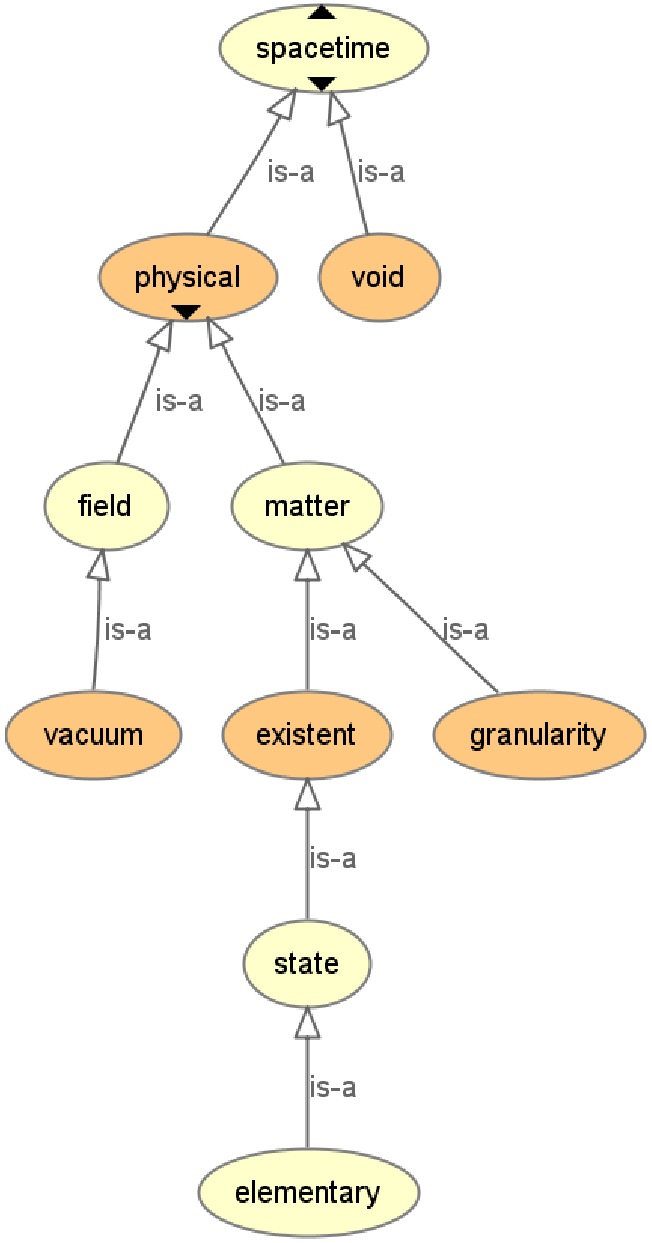
GRANULARITY

"**Granularity**" stands for "**matter with a particular granularity**" .

Granularity is then defined as a superclass of defined subclasses that are defined as **matter** 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.



SPACETIME
the substrate of existence of real things

PHYSICAL
a spacetime that exibits some physical properties

MATTER
a physical that has property mass and is made at least of one elementary

EXISTENT
a matter 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

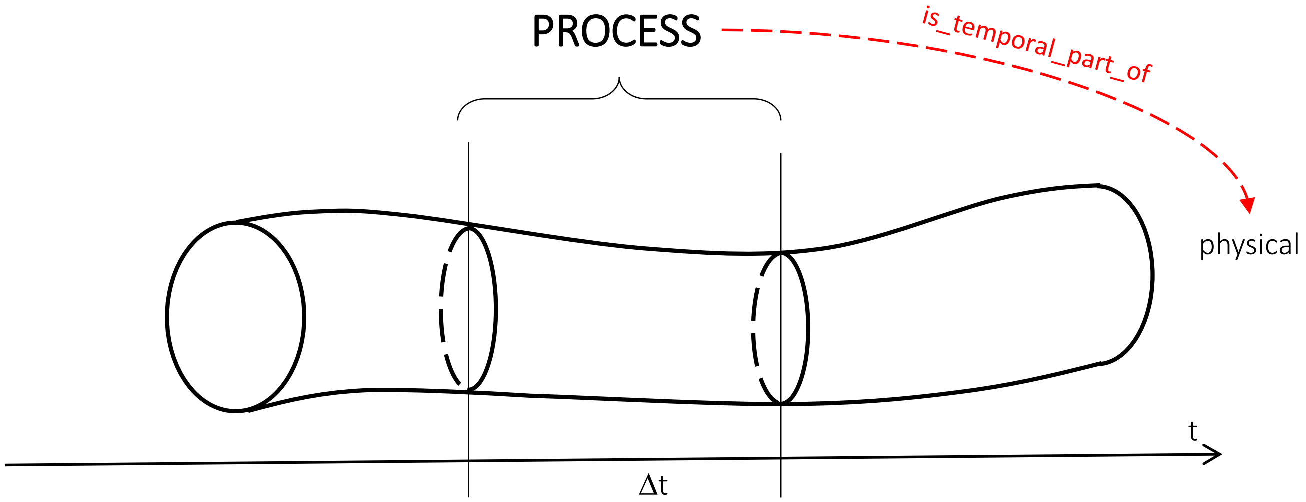
ELEMENTARY
a physical that has no spatial proper parts

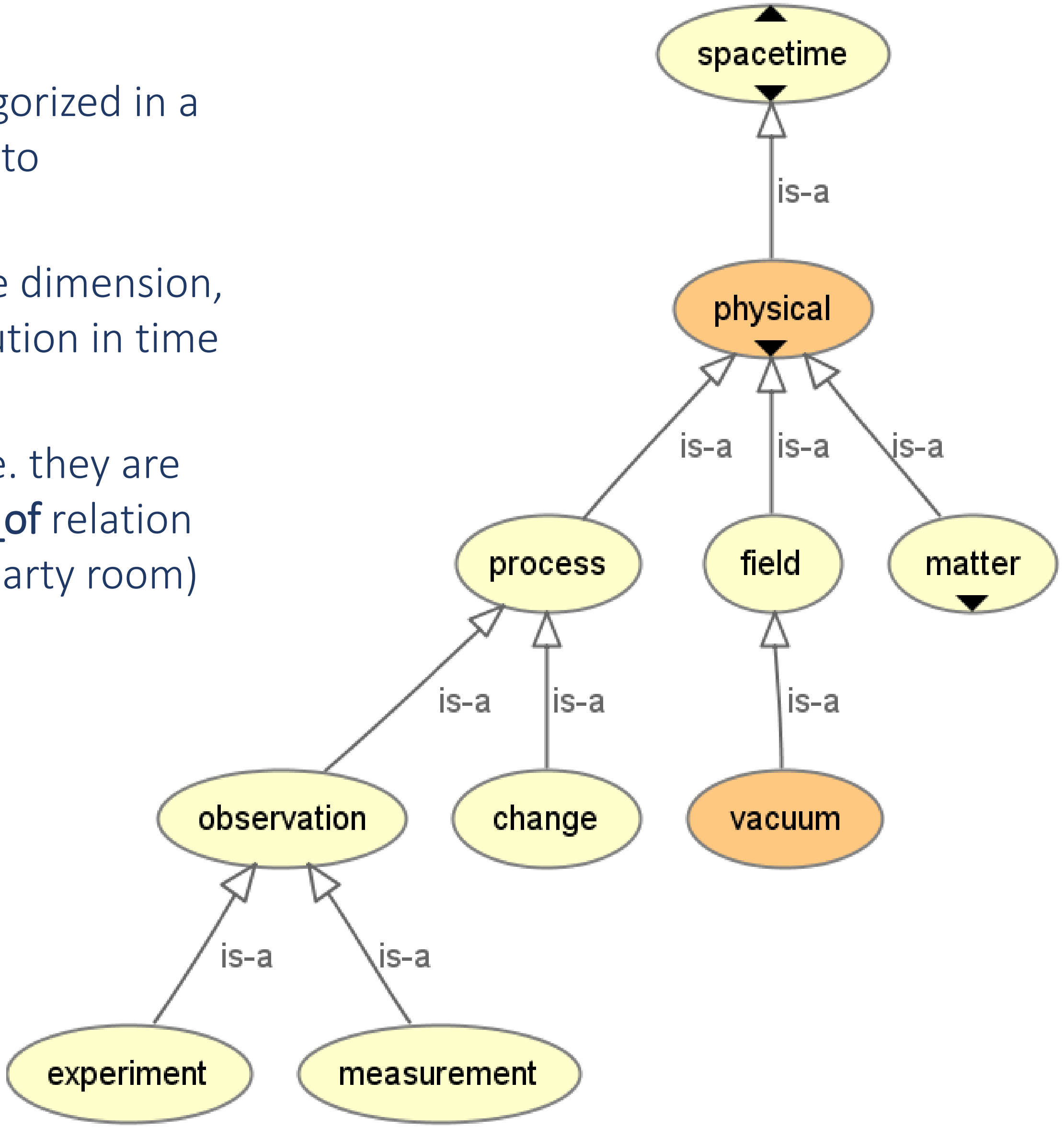
PROCESS

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)





PROCESS

Examples of possible process subclasses:

CHANGE

A process that include the transition of a physical from a state to another (i.e. a discontinuity of parts)

OBSERVATION

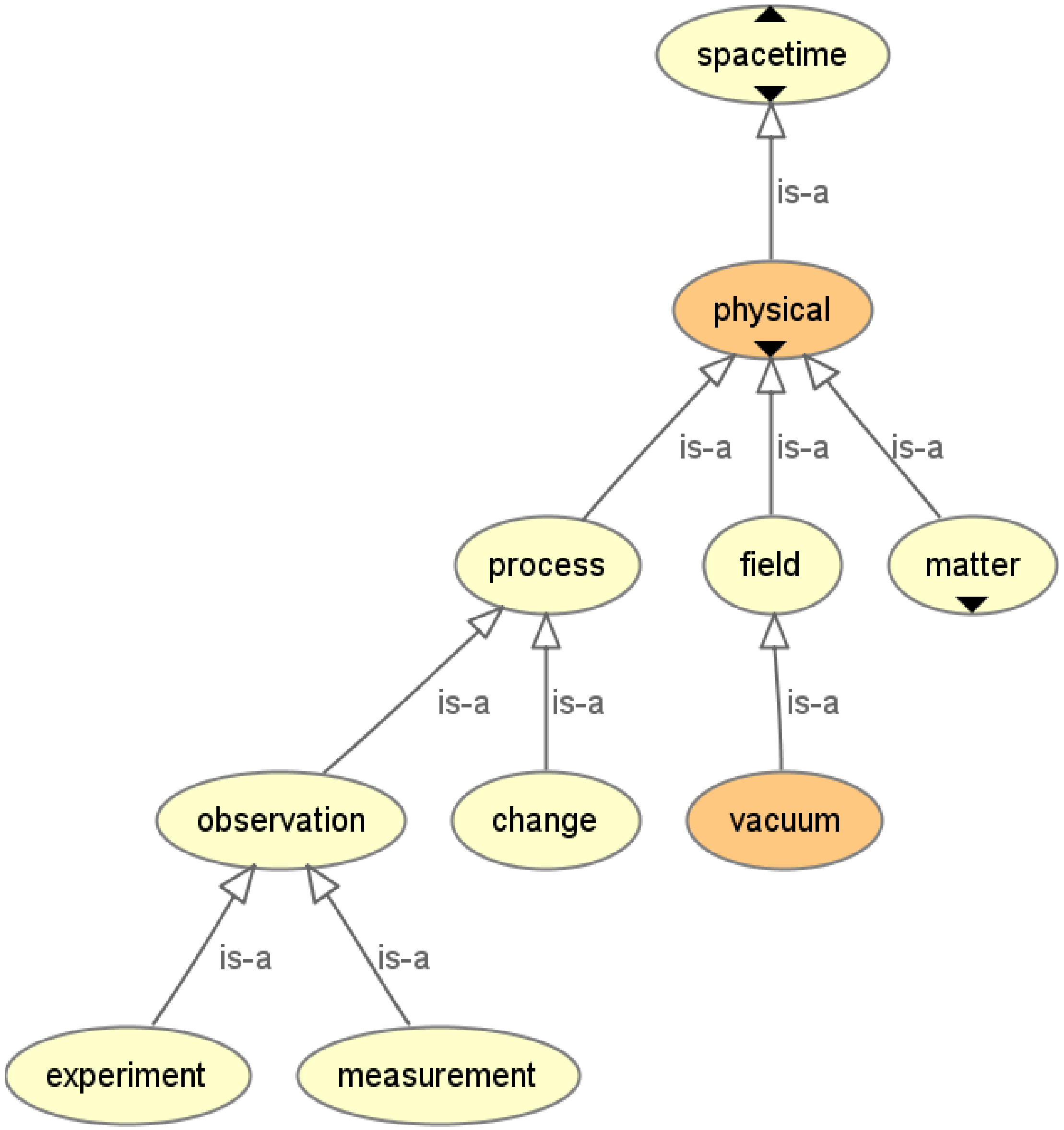
A process that involves an observer that perceives other physicals by interacting with them and track instants or intervals of their evolutions in time.

MEASUREMENT

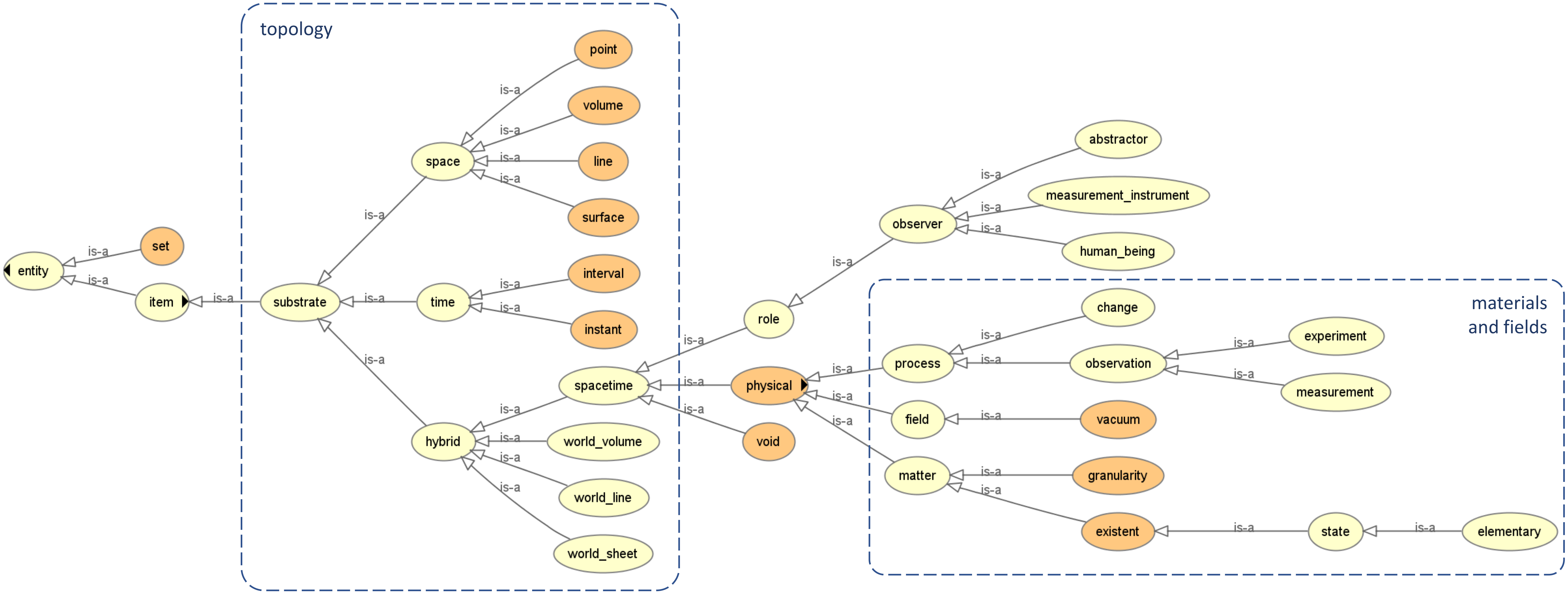
An observation that results in a quantitative comparison of a physical property with a standard reference.

EXPERIMENT

A process that is aimed to replicate a physical phenomena in a controlled environment.



EMMO
material ontology basic branch

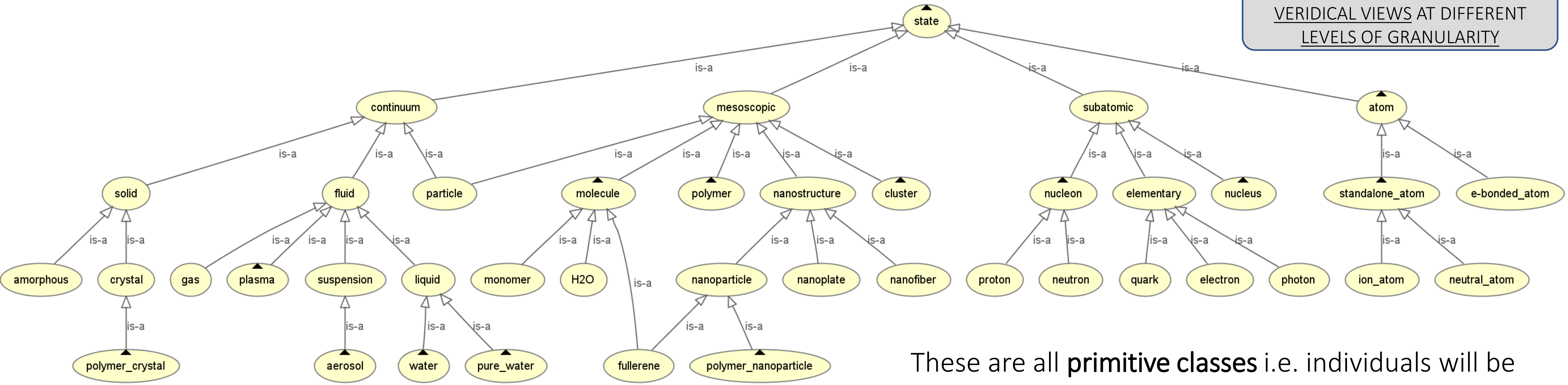


EMMO

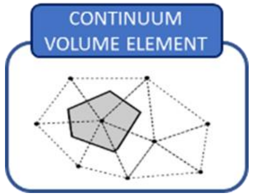
RoMM compliant material description branch

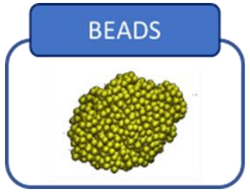
THE **EMMO** MATERIAL DESCRIPTION BRANCH PROVIDES THE 4 DIFFERENT VIEWS PROPOSED BY THE RoMM, DEPENDING ON THE LEVELS OF GRANULARITY ADOPTED

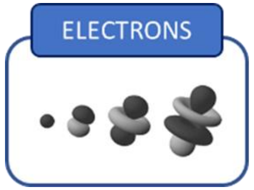
ONE REALITY WITH FOUR VERIDICAL VIEWS AT DIFFERENT LEVELS OF GRANULARITY

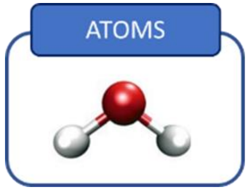


These are all **primitive classes** i.e. individuals will be placed in the classes by user declaration according to the adopted view









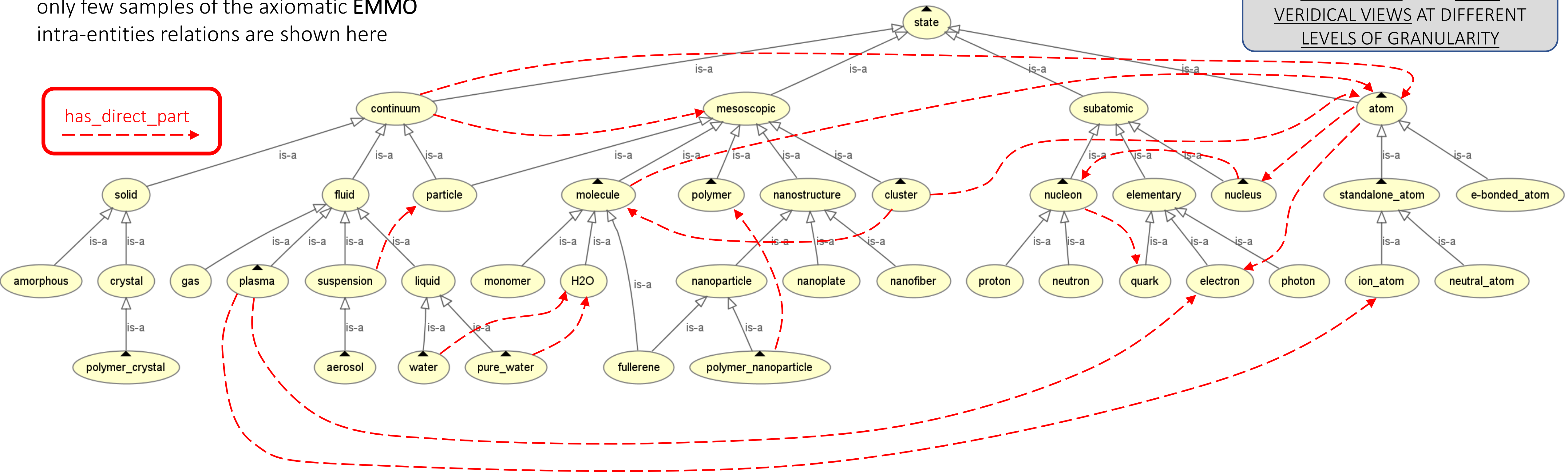
EMMO

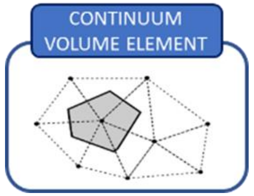
RoMM compliant material description branch

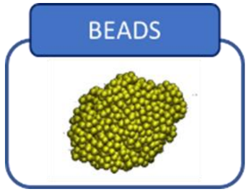
THE **EMMO** MATERIAL DESCRIPTION BRANCH PROVIDES THE 4 DIFFERENT VIEWS PROPOSED BY THE RoMM, DEPENDING ON THE LEVELS OF GRANULARITY ADOPTED

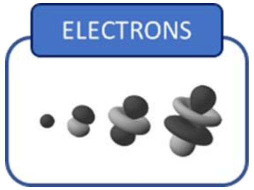
only few samples of the axiomatic **EMMO** intra-entities relations are shown here

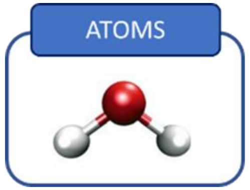
ONE REALITY WITH FOUR VERIDICAL VIEWS AT DIFFERENT LEVELS OF GRANULARITY







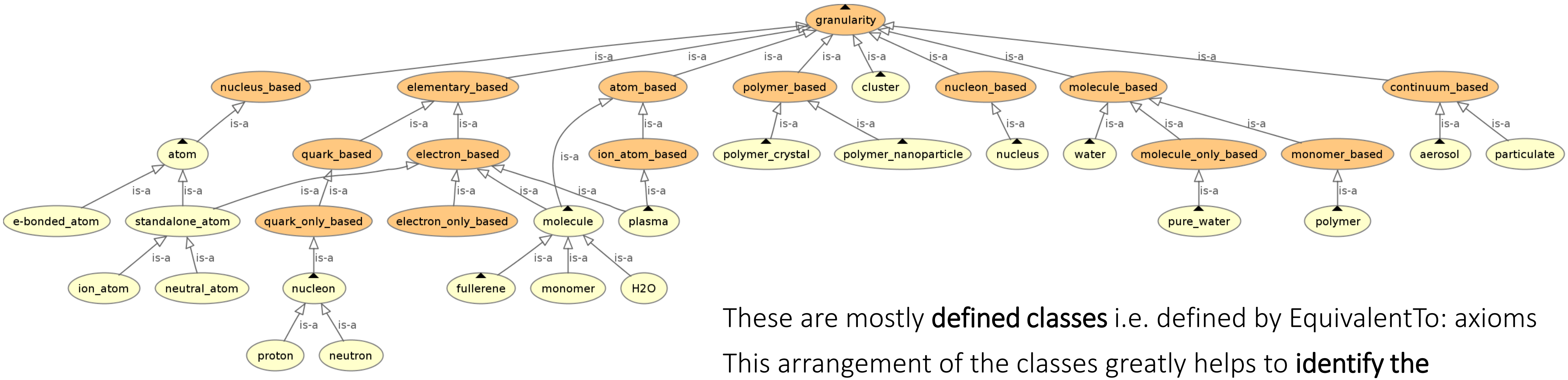




EMMO

RoMM compliant material branch

arranged by granularity



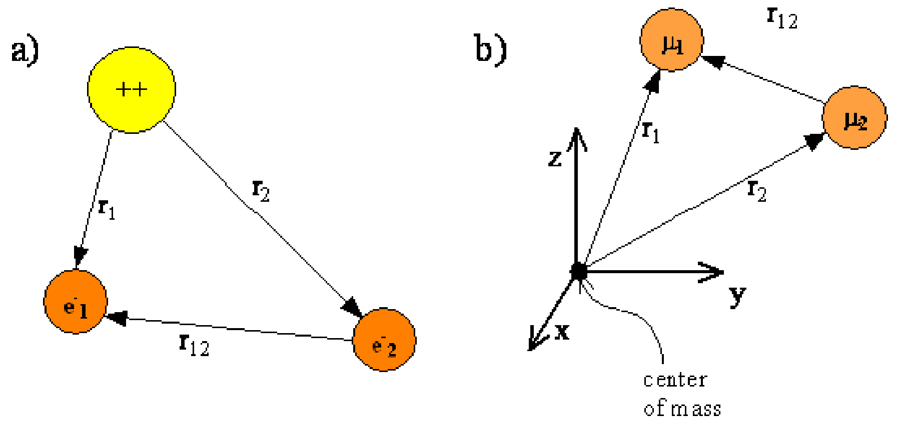
These are mostly **defined classes** i.e. defined by EquivalentTo: axioms

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

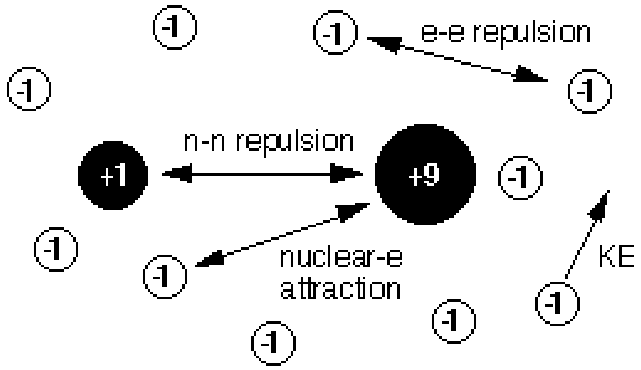
Placement of individuals is not intended to be provided by the user, but **automatically done by the reasoner** once the granularity chosen by the describer is given.

Electronic level representation of atoms and molecules

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 electroning 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

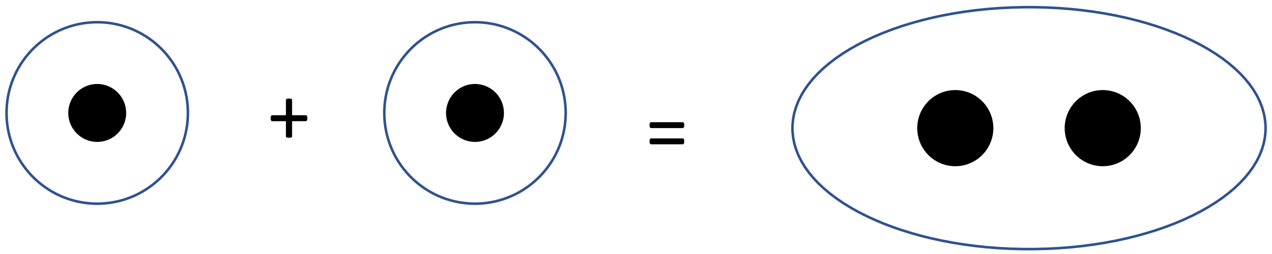
$$\psi(r_1, r_2, \cdots, r_i) \approx \varphi_1(r_1)\varphi_2(r_2)\cdots\varphi_i(r_i)$$

Need for better definitions

IUPAC GOLDBOOK

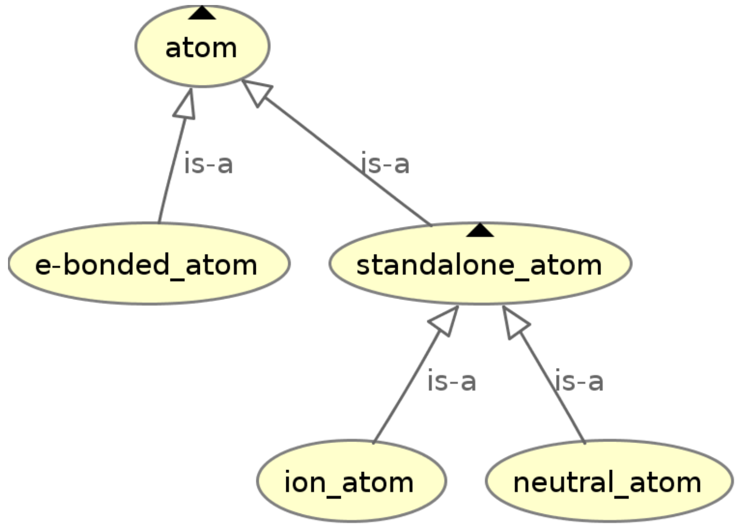
atom
Smallest particle still characterizing a chemical element. It consists of a nucleus of a positive charge (Z is the proton number and e the elementary charge) carrying almost all its mass (more than 99.9%) and Z electrons determining its size.

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 in a strict logical formalism)

EMMO material branch to overcome IUPAC definition inconsistency.



EMMO Material Entities are defined by a
<u>hierarchy of parthood relations,</u>
combining the concepts of direct parthood and object

With **EMMO** we create a representation of the <u>real world granularity</u> of *material entities* that follows physics and materials science perspectives.

A ‘material’ in the user case can be <u>described univocally</u> by declaring *entitie*s under **EMMO** hierarchy.

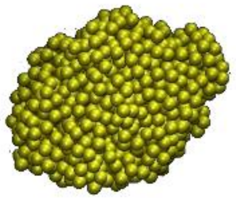
The basic idea is that <u>the ‘material’ can be represented at different levels of granularity,</u> depending on **perspective**.

Every material entity in the EMMO is **placed on a granularity level** and the ontology gives information about the **direct upper and the direct lower levels types**.

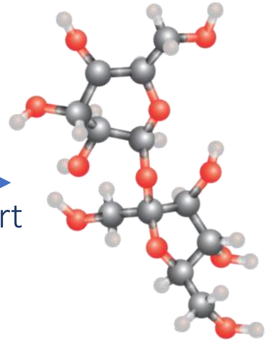
has_part

has_part

has_part

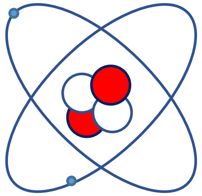


has_part

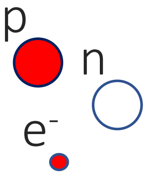


has_part

has_part



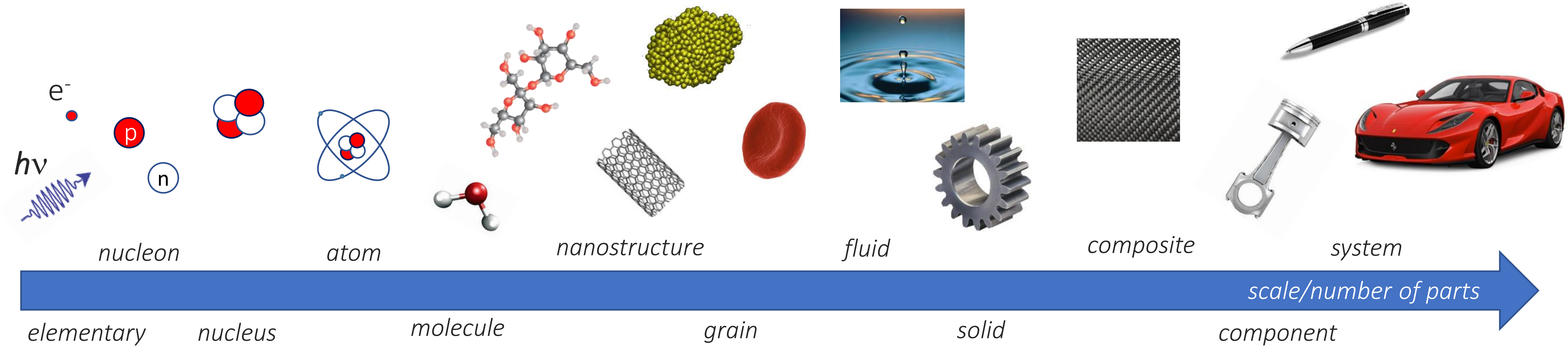
has_part



EMMO Mereological Basis

CONFIDENTIAL

THE **EMMO** MATERIAL CLASSES AMBITION IS TO COVER ALL THE PHYSICS AND MATERIAL SCIENCE SCALES.



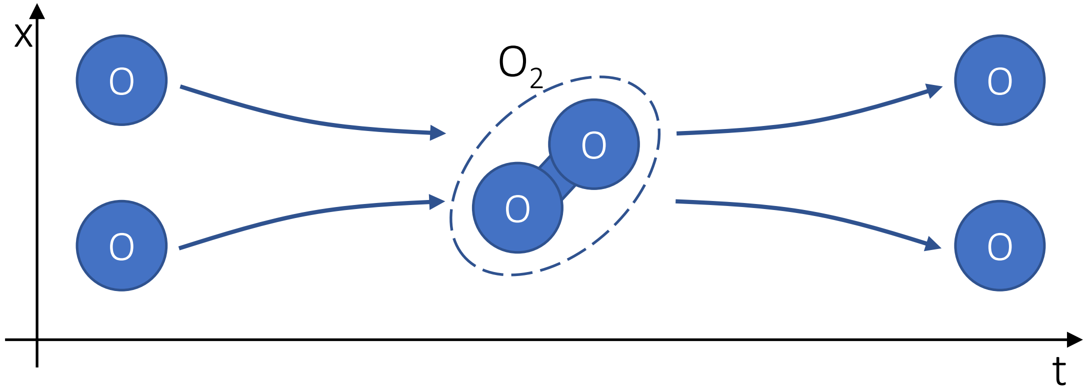
subatomic | **atomistic** | **mesoscopic_object** | **continuum_object** | **component** | **system**

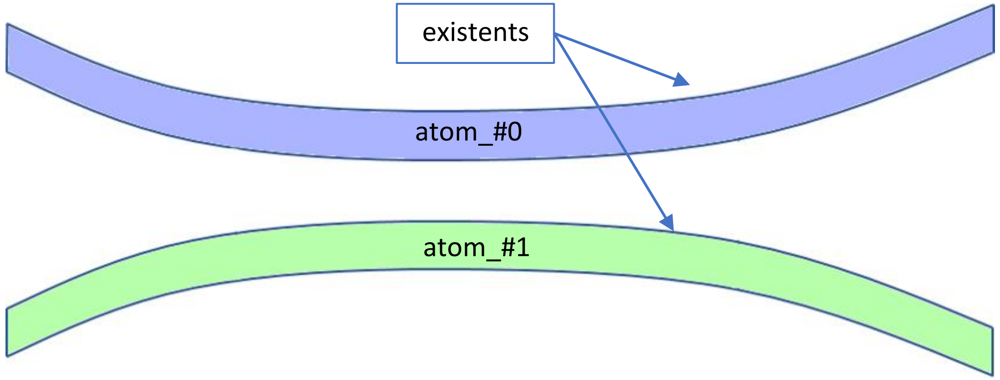
engineered_material

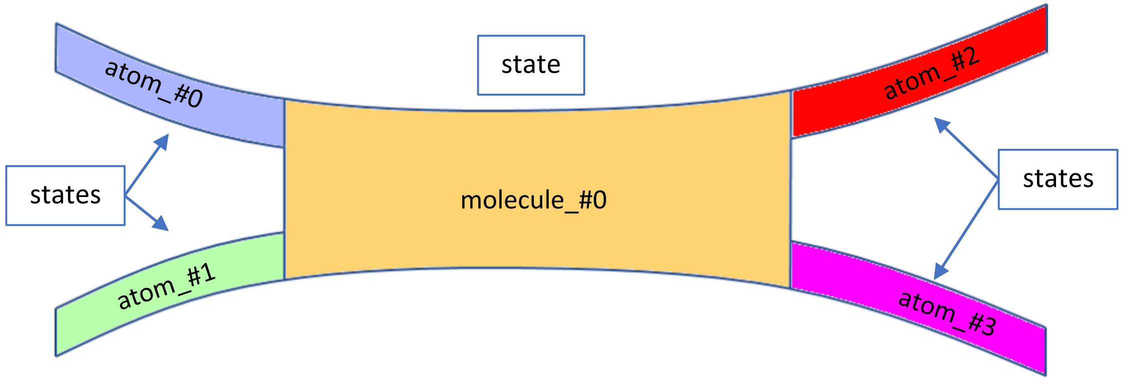
engineered_object

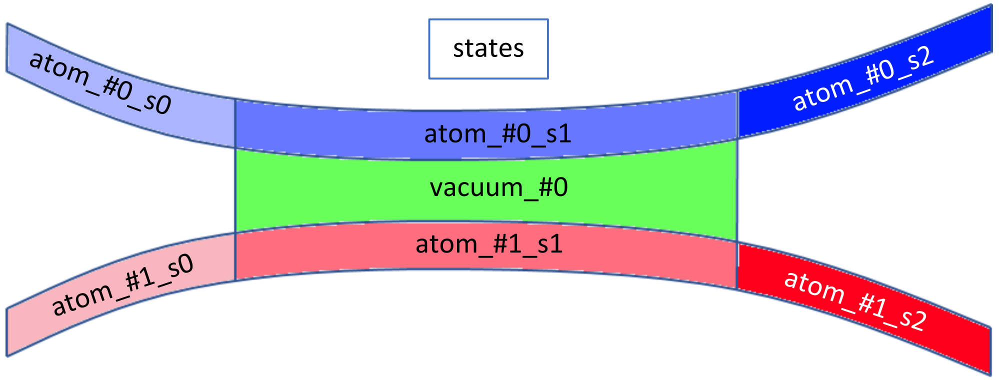
no parts | **has parts**

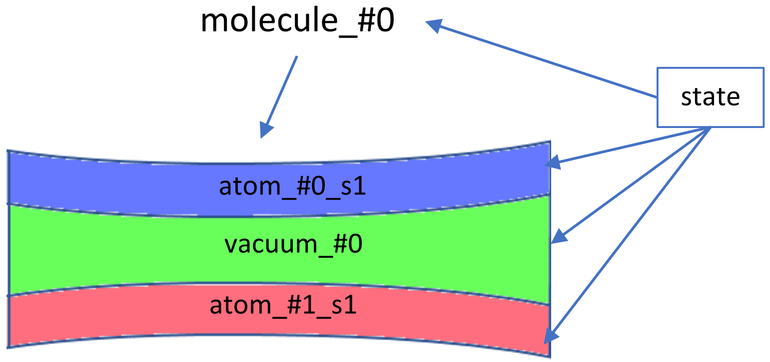
EMMO representation of a O_2 molecule formations and dissociation



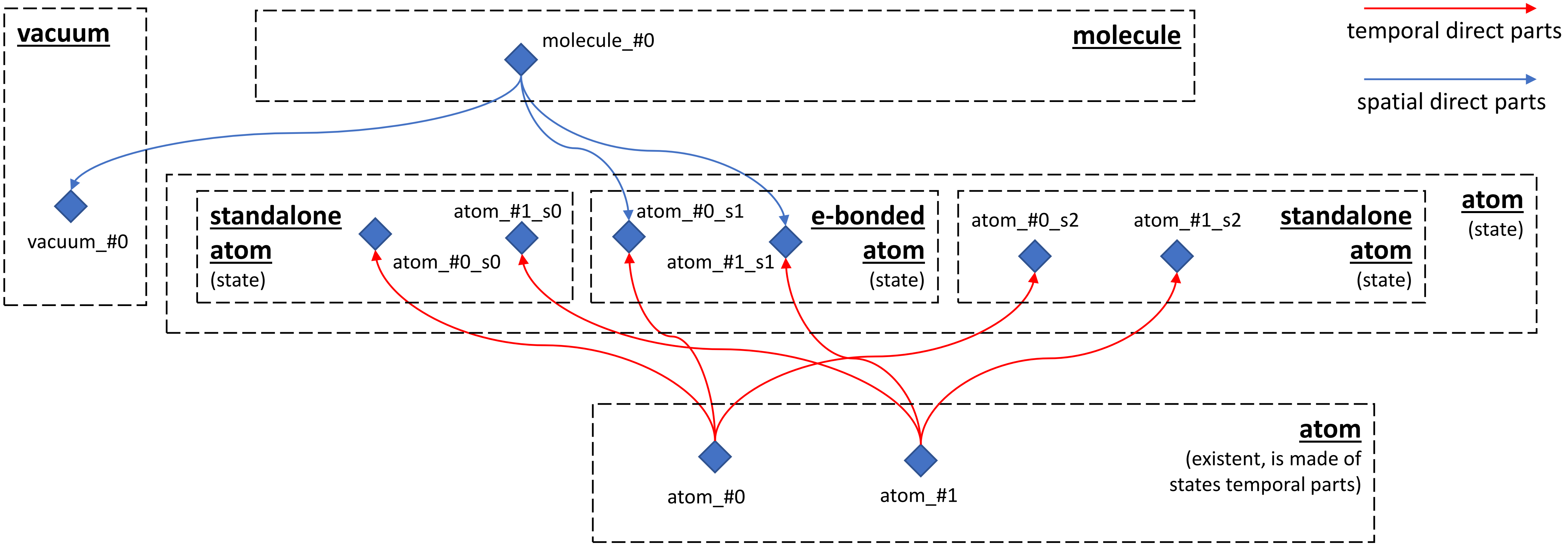


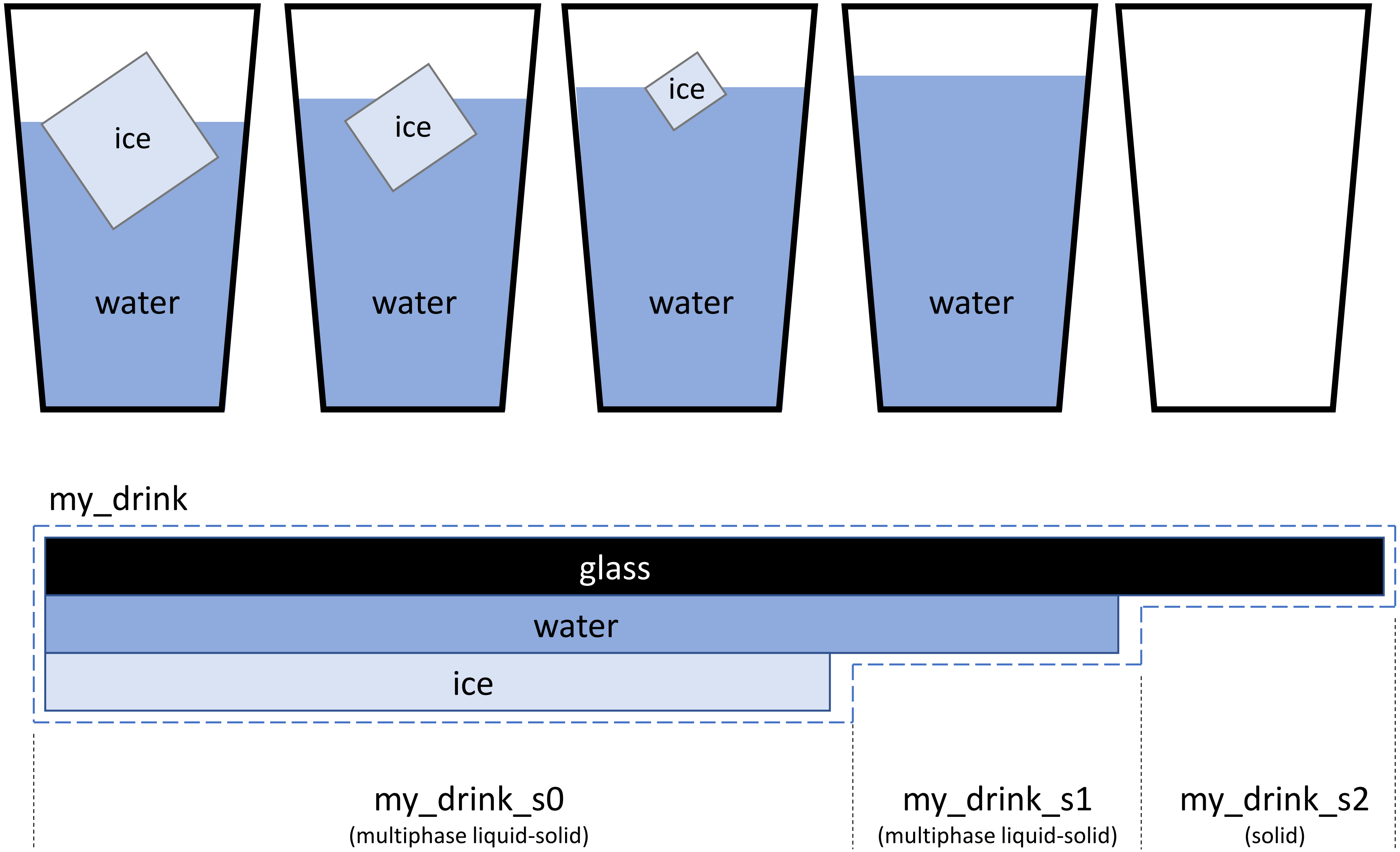






Items cannot be **spatial direct part** of more than one whole.
Items cannot be **temporal direct part** of more than one whole.
But an item **can be spatial part** of an item and **temporal part** of another one.





my_drink is an existent made of three states.

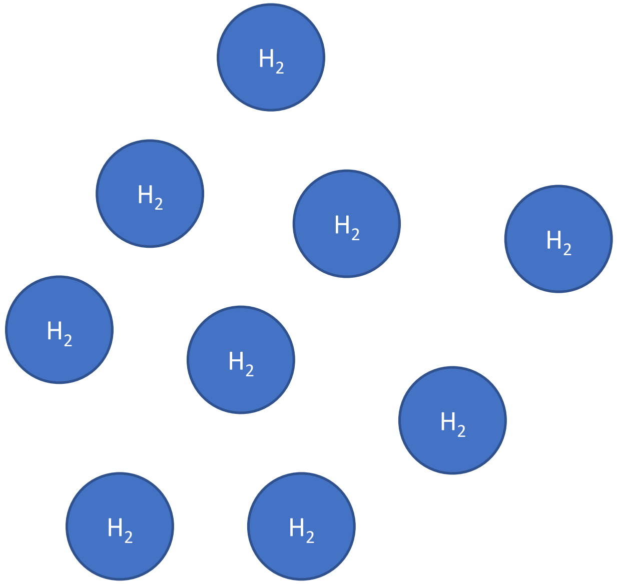
As long as a state (**my_drink_s0**) does not lose direct parts (**ice** or **water** or **glass**), it's still a state.

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

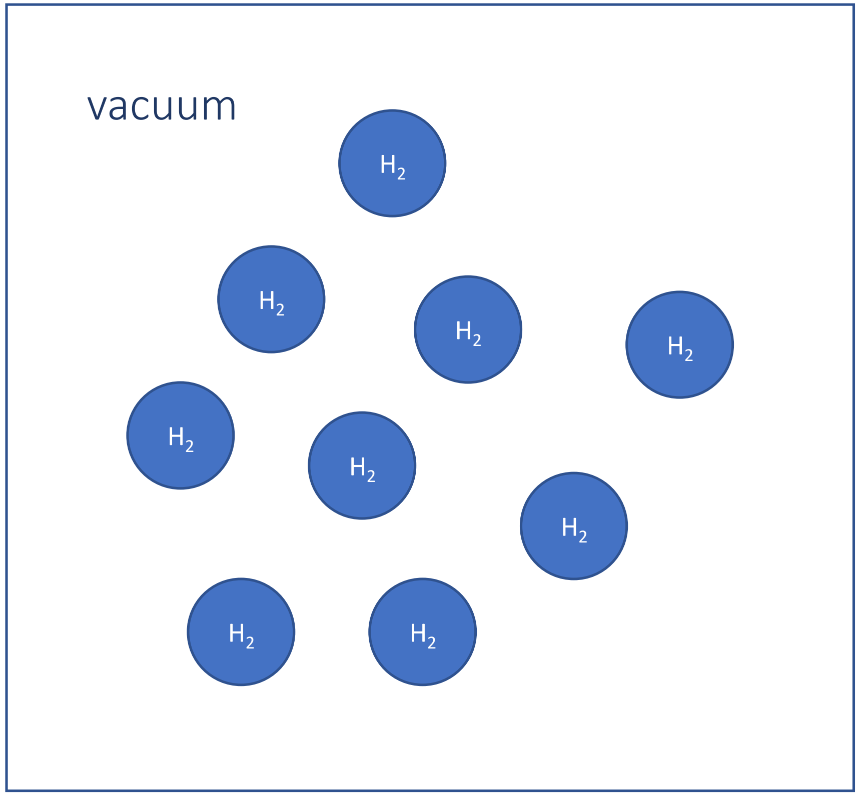
ice is losing direct parts (i.e. the H2O molecules that goes from **ice** to **water**) but still is a direct part of **my_drink**.

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

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



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



EMMO SET OR WHOLE

In **EMMO** the same 'material' or 'product' can have two different *material entity* representations:

- the *whole* representation, in which sub-granular entities are parts
- the *set* representation, in which subgranular parts are a collection members

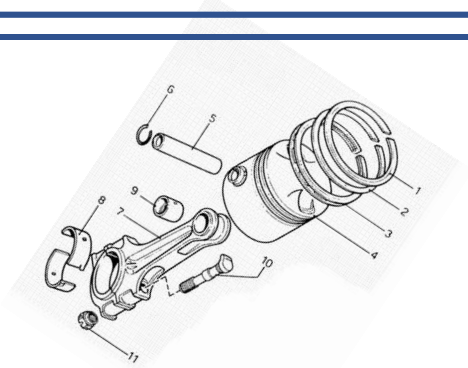
The *set* members can be at different levels of granularity;

e.g. steel ring can be seen as a grain collection, as an atom collection or a nuclei/electrons collection.

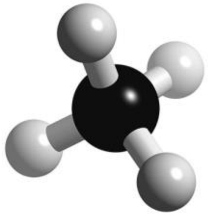
car (whole)

car components set

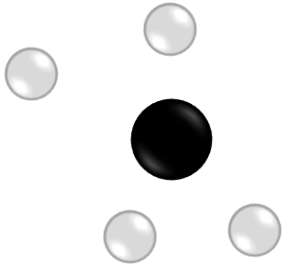
piston (whole)



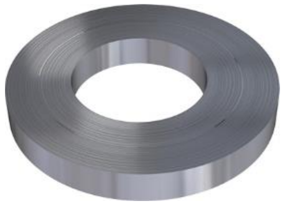
mechanical parts set



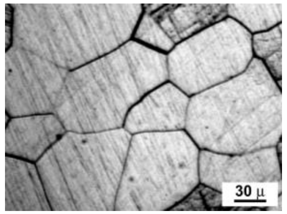
molecule (whole)



atoms set

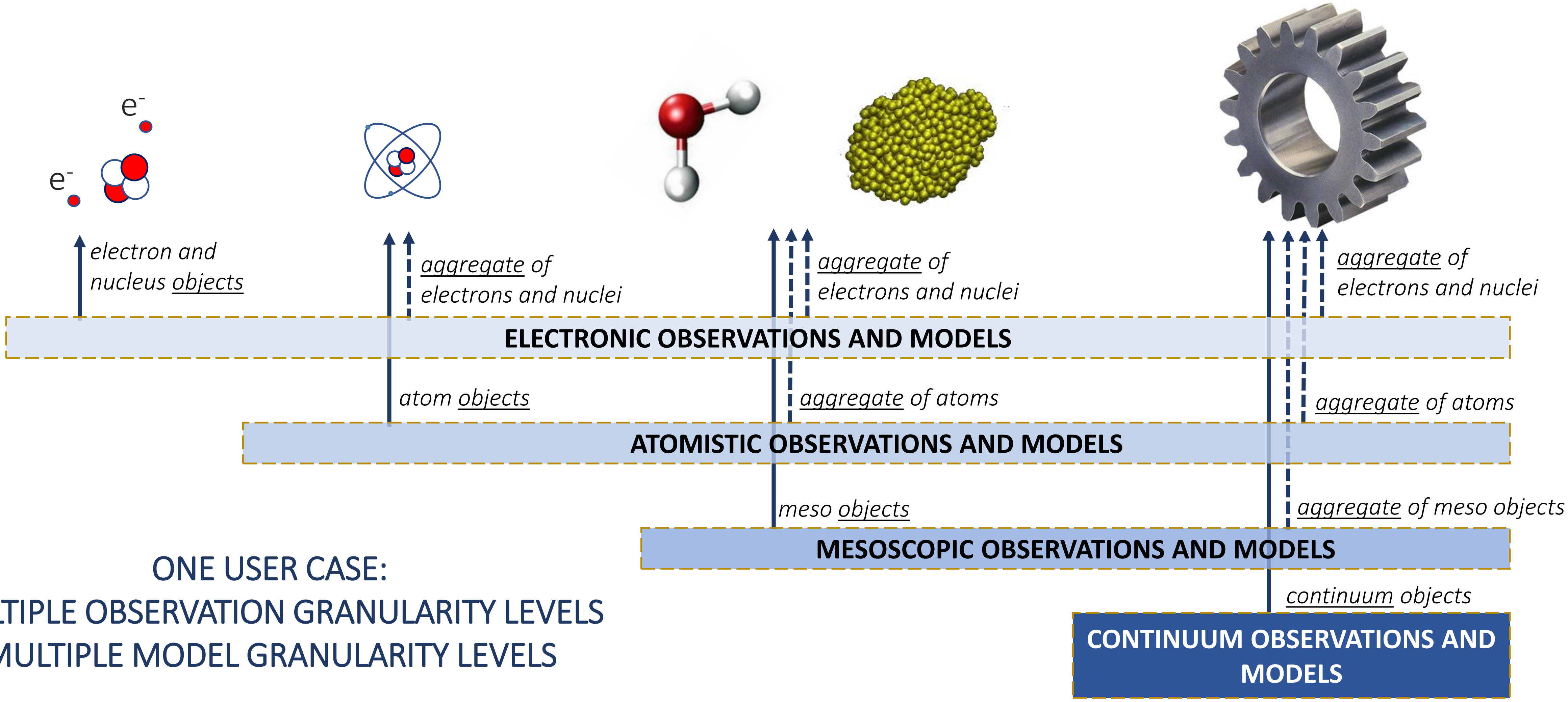


steel ring (whole)



grain set

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



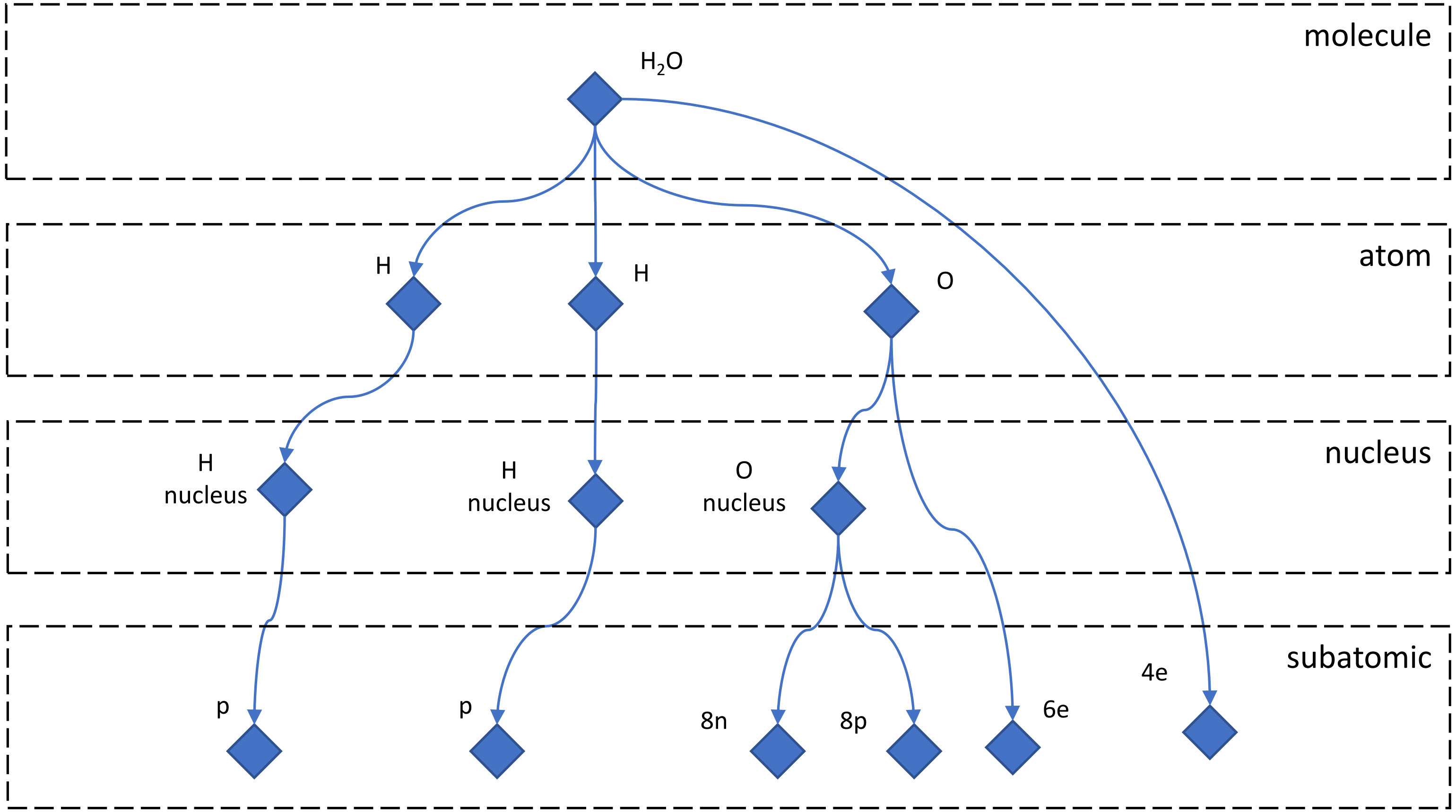
ONE USER CASE:
MULTIPLE OBSERVATION GRANULARITY LEVELS
MULTIPLE MODEL GRANULARITY LEVELS

EMMO COMPOSITIONAL TREE

The individuals are forming a **directed rooted tree**: this is paramount for cross scale interoperability.

This comes from the **«functional»** requirement on direct parthood.

Example of a water molecule represented by means of direct parthood from atomistic to the subnuclear granularity level



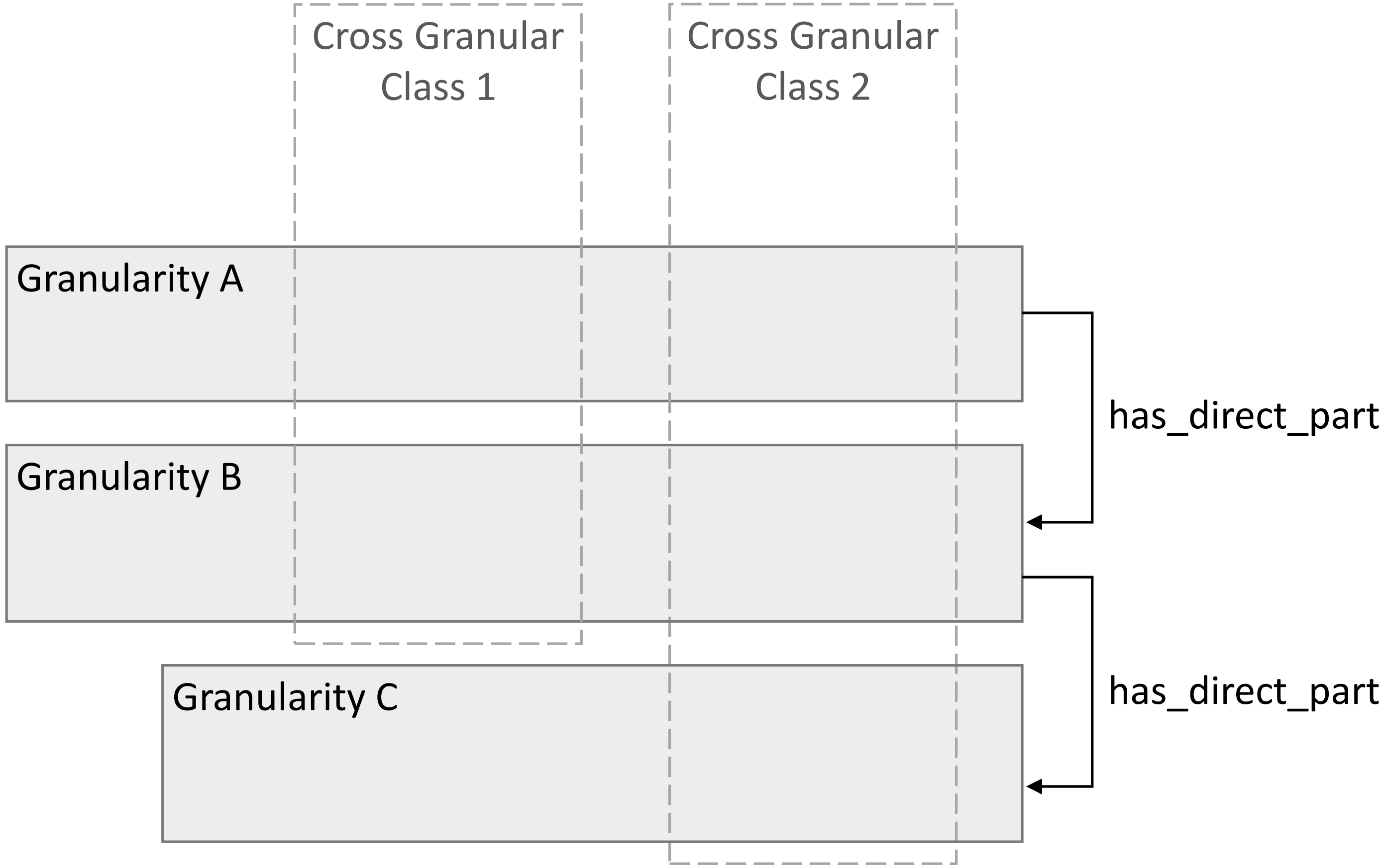
In the **EMMO** material description branch classes can be:

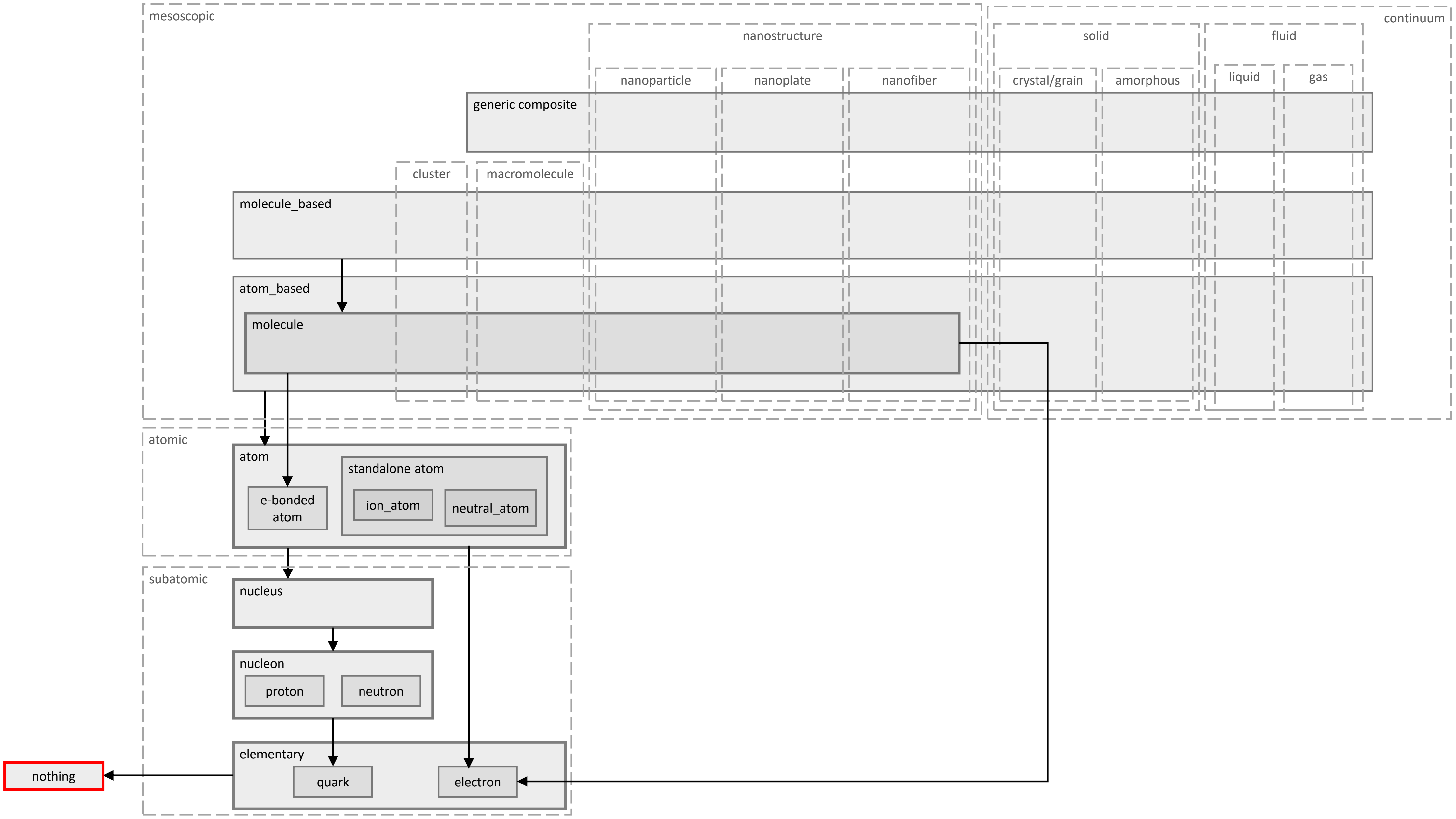
- **Granularity classes**, i.e. materials with specific granularity are described by means of hierarchies of direct parthood relations

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

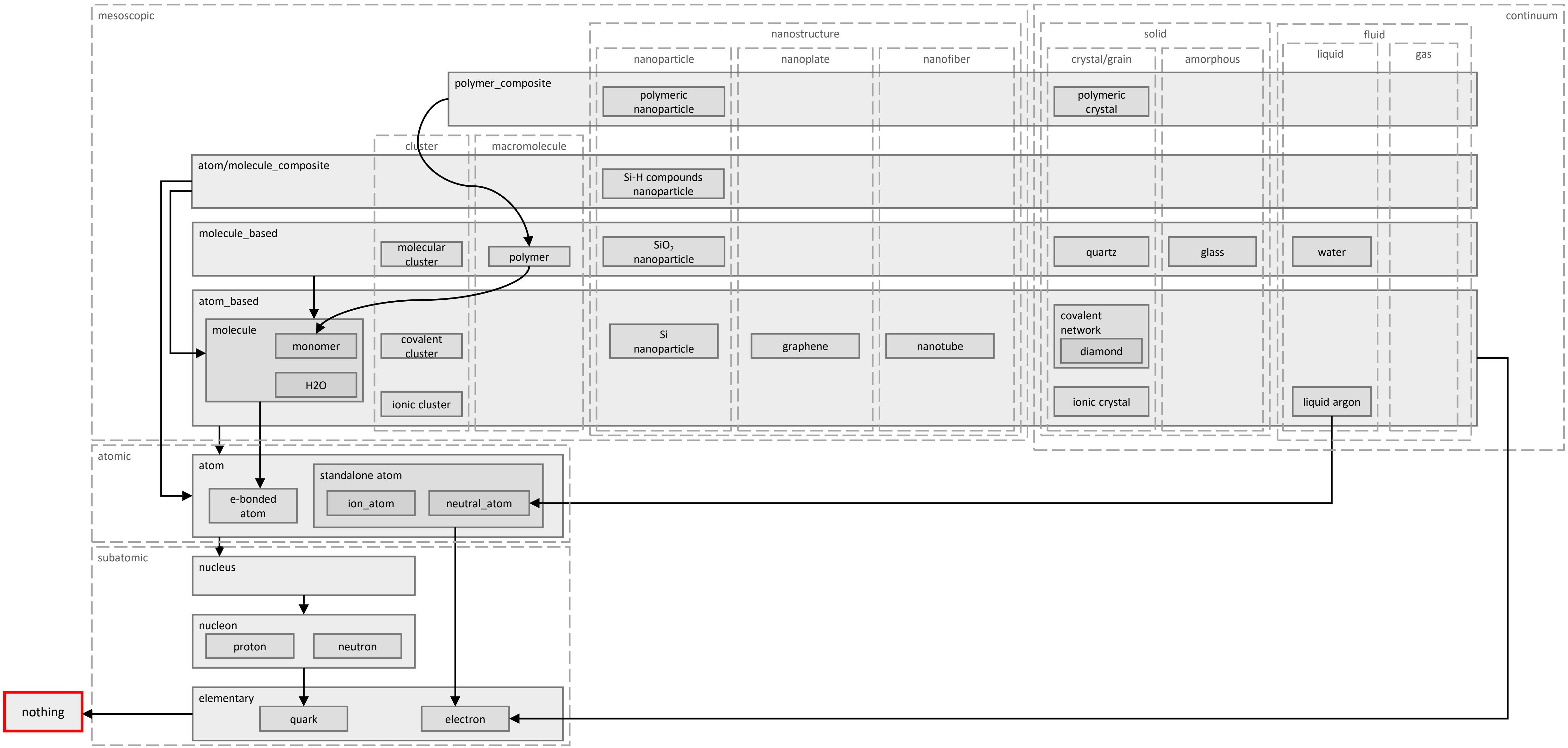
- **Cross-granular classes**, i.e. are declared by means of properties of the individual other than composition

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



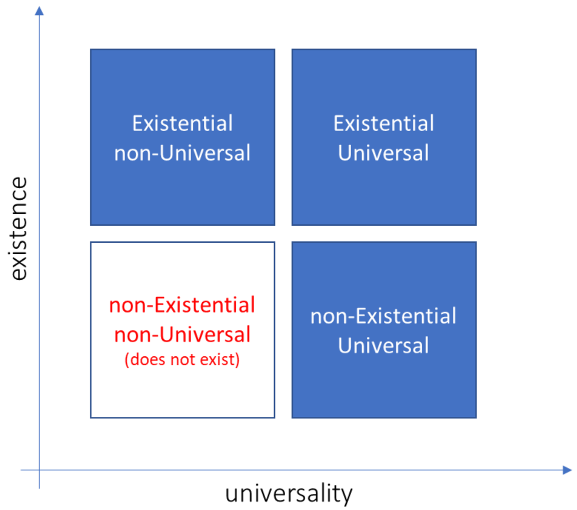

mesoscopic
nanostructure
nanoparticle
nanoplate
nanofiber
continuum
solid
crystal/grain
amorphous
fluid
liquid
gas
generic composite
cluster
macromolecule
molecule_based
atom_based
molecule
atomic
atom
e-bonded atom
standalone atom
ion_atom
neutral_atom
subatomic
nucleus
nucleon
proton
neutron
elementary
quark
electron
nothing

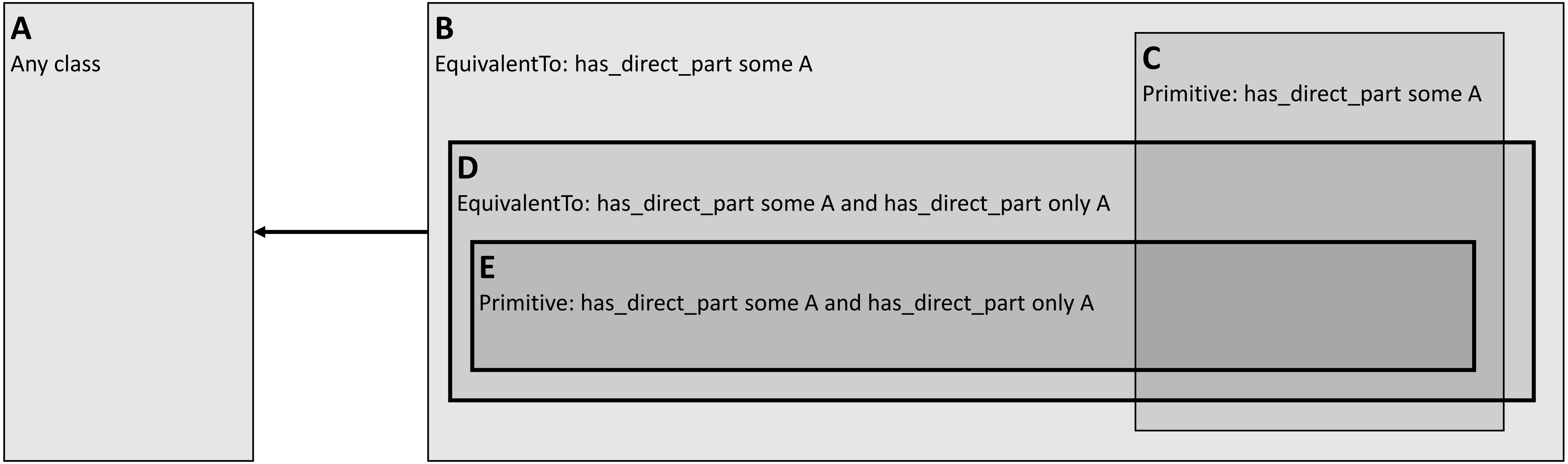
EMMO MATERIAL ONTOLOGY



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):





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.

ABSTRACT

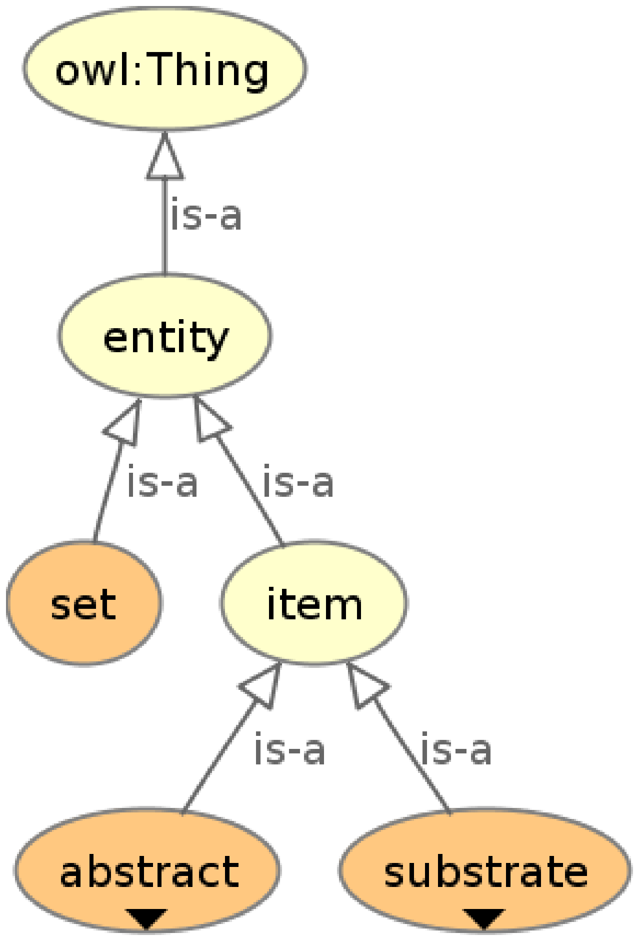
Items that are not substrates.

This branch is an **ontology of signs** i.e. individuals that are signs of other signs that appear in the item branch. They can be categorized as:

- **simple signs**, e.g. character, number
- **composite signs**, e.g. equation, picture

A mereology of abstracts can be introduced e.g. a variable *is_part_of* and equation in terms of symbolic representation

They are entities that exists only in the ontological dimension and depend on an abstractor (e.g. a human being or a set of human beings), and connect an entity (or a set of entities) to another entity (its representation or *semeion*).



This is an expression of strict nominalism: universals do not exist *sub specie aeterni* but are signs that summarize a collection of experiences (e.g. processes).

Abstracts do not exist in time because they are outside time, as ontological representation, and can be expressed by semeion at time t as long as a material representation of them exists at the same time t e.g. a book, a picture, a thought.

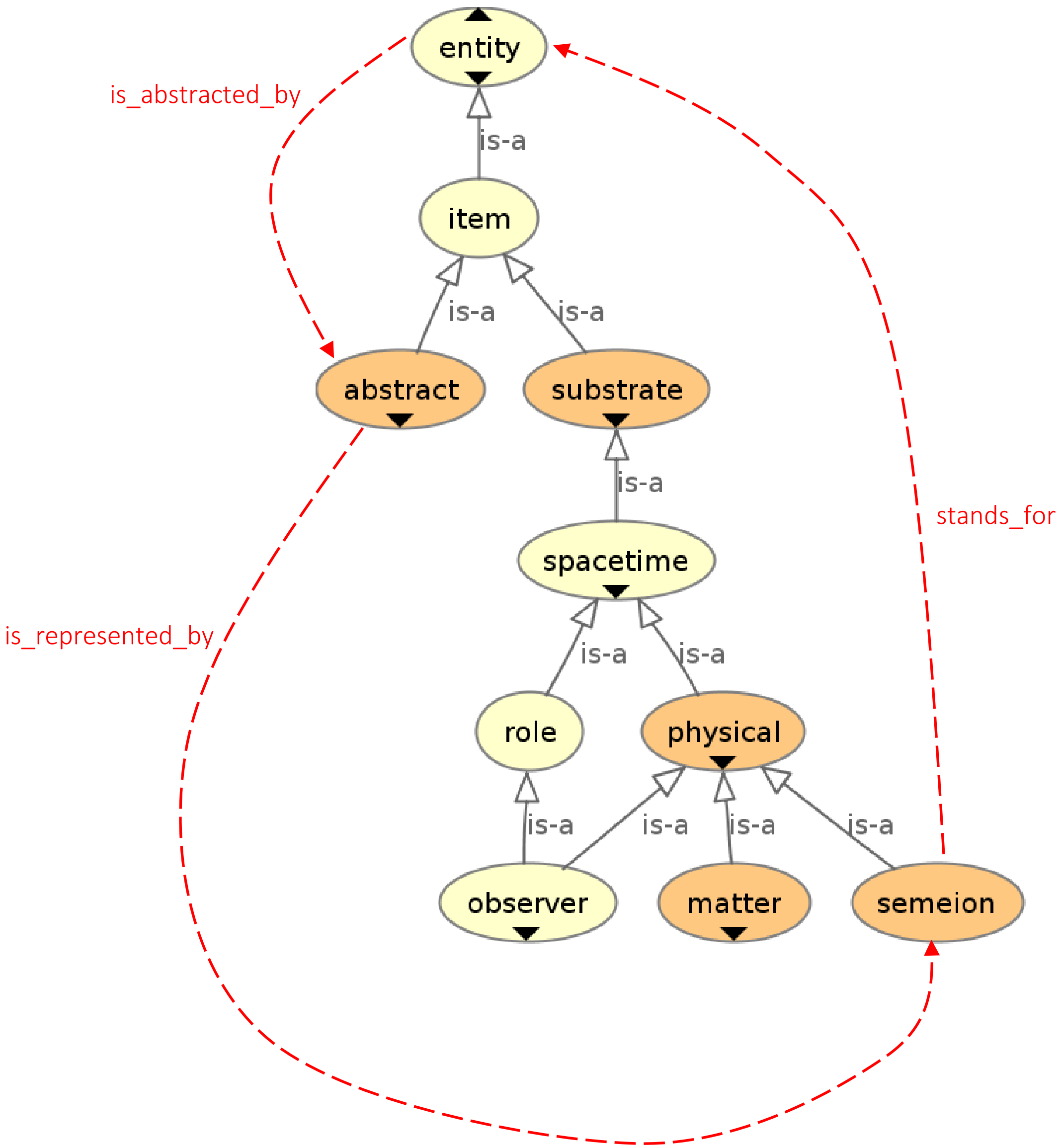
An abstract is an abstraction provided by an **observer**, and are observer dependent. An abstraction can come from a **single being** or from a **group of being** seen as a single entity.

e.g. **my_democracy** is the abstraction of democracy that I have. **chinese_democracy** is the idea of democracy that Chinese people have.

Abstract individuals must be represented by at least one physical entity. A physical entity that represents an abstract object is call **semeion** (i.e. symbol). A **semeion** S "stands" for the **entity** E that has been abstracted by the **abstract** A by an **abstractor** AB (this is related to the discipline of semiotics)

More than one abstract can refer to the same entity depending on the abstractor.

A semiotic approach to ontology.



MATHEMATICAL ENTITY

A class that collects other subclasses that represents the fundamental elements of **mathematical expressions**:

number: an abstraction of sets of specific cardinality (e.g. 2 is an abstraction of two members sets, assuming that the cardinality distinctions between classes and their ordering is a primitive concept).

variable: A variable is a symbol that denotes a mathematical object which could be a e.g. number, a vector, a matrix.

unknown: a variable whose value is not known

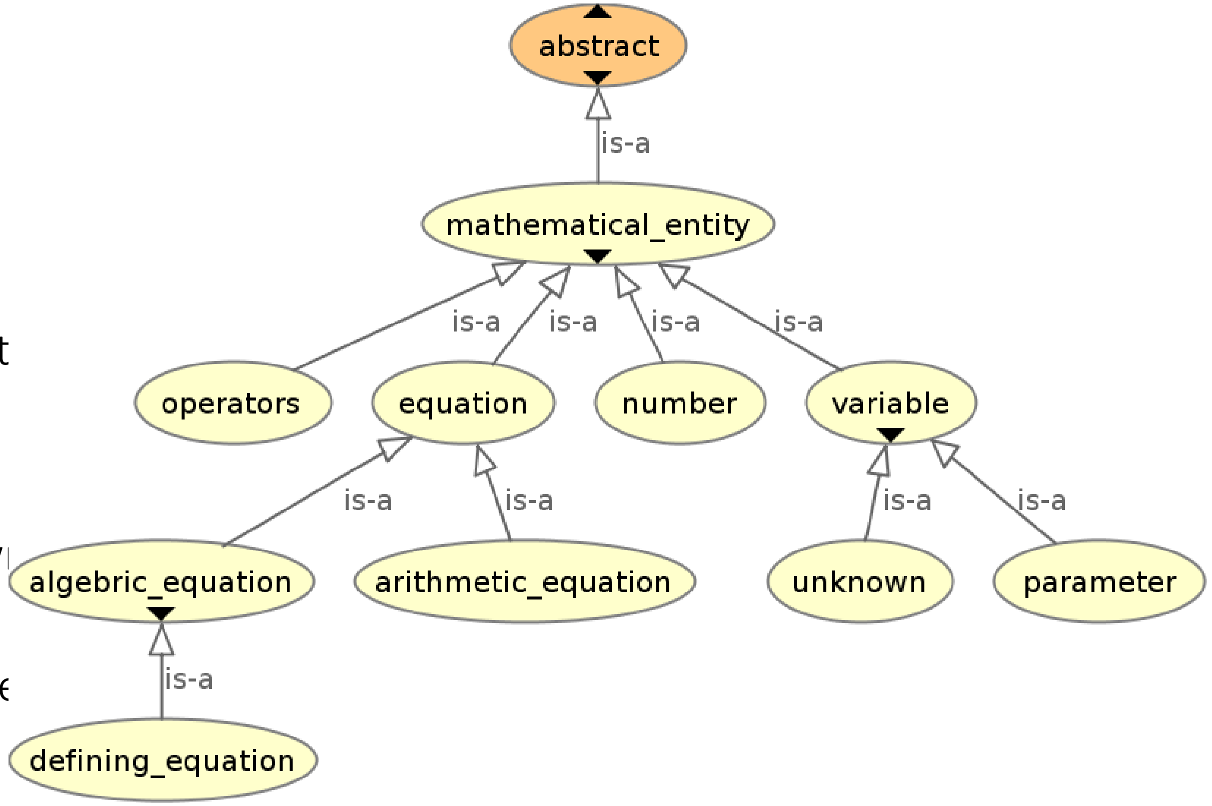
parameter: a variable whose value is know or assumed to be known

equation: a mathematical expression that puts in relation some **number**s or **variable**s by means of operators and that can always be represented as

f(v0, v1, ..., vn) = 0

where f is the expression and v0, v1, ..., vn are the variables.

defining_equation: an equation that defines a new variable in terms of other base variables.



NATURAL LAW

A **natural law** is an abstraction for a series of experiments (process, physical) that tries to define a common cause and effect relations between participants evolution in time. A natural law is a pre-mathematic entity (by definition).

is_abstraction_for some experiment

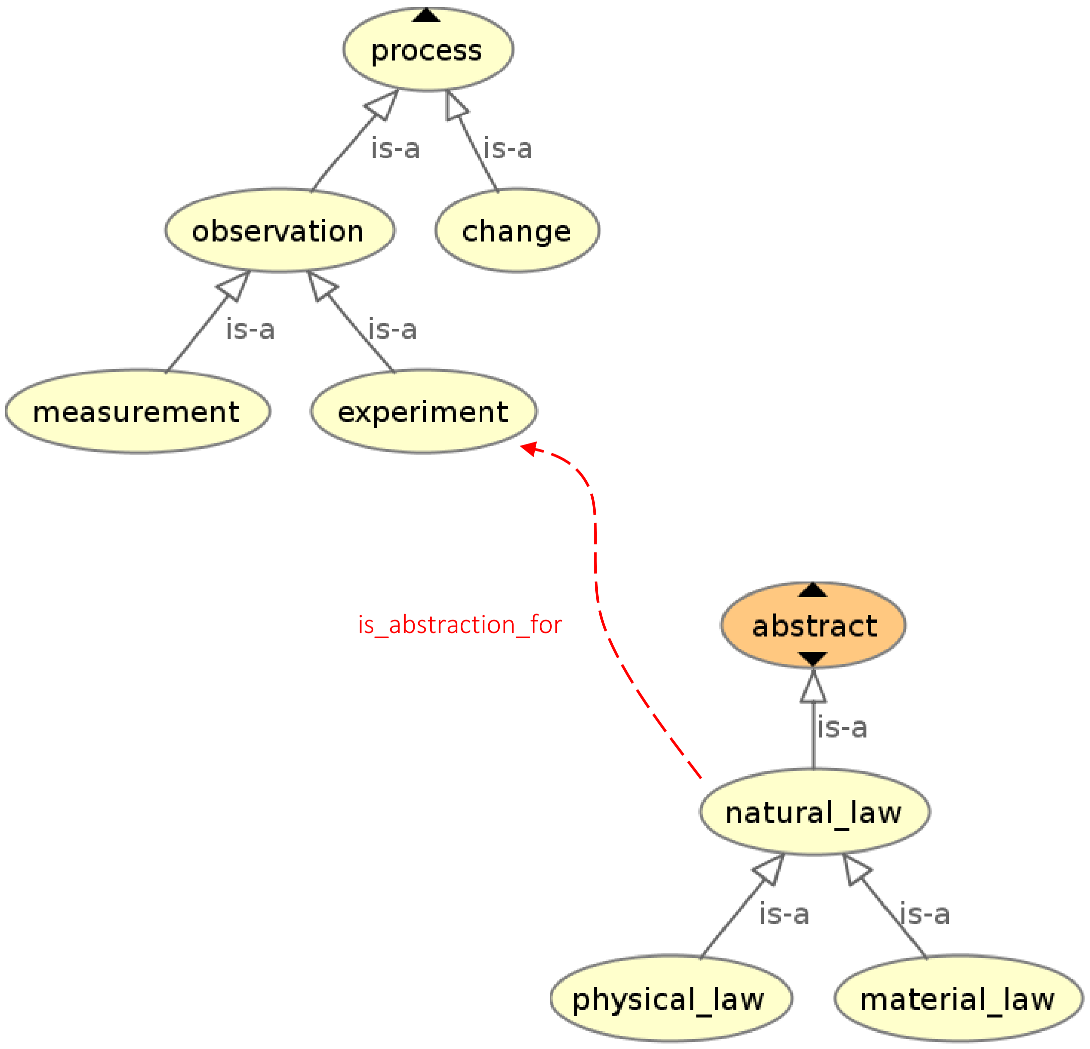
It can be represented e.g. as a thought in the mind of the experimenter, a sketch and textual description in a book of science.

physical law and **material law** are the laws behind physical equations and material relations, respectively, according to the RoMM-CWA.

e.g.:

physical laws: Newton's law of motion, relativity principle, gravitational law, …

material laws: hook's law, drag, deformation of solids, …



PROPERTY

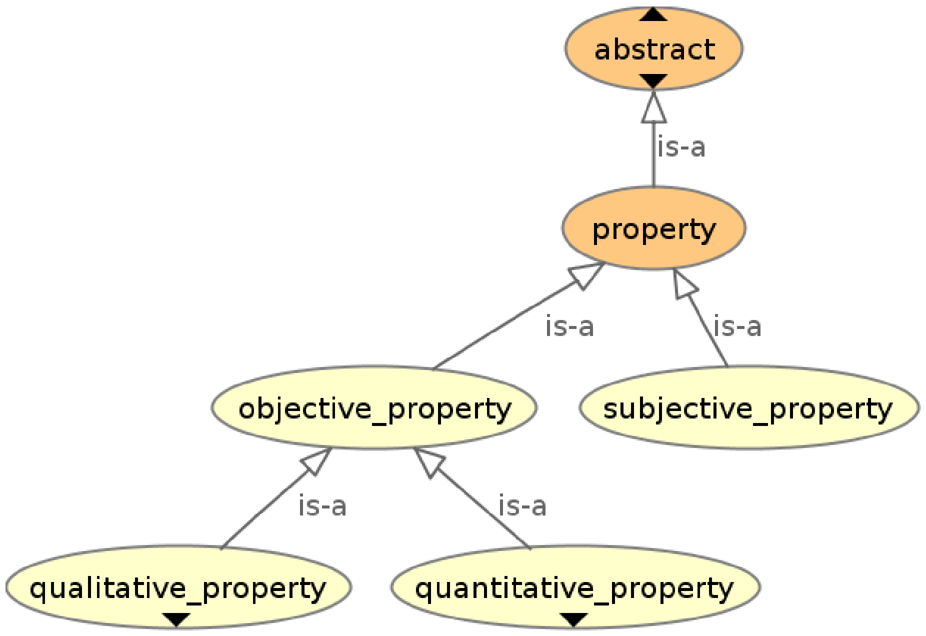
Properties are abstracts that are related to a specific material entity with the relation **has_property**, but that depends on a specific observation process, participated by a specific observer, who catch the physical entity behaviour that is abstracted as property.

It means that **color** is not an intrinsic quality of a physical, but only an abstraction of observation processes that involve photons coming from physicals.

The class **color**, under property, can be a restriction based on the observations that are made by means of a photon sensitive observer (e,g, an eye).

Subclasses of color can be declared depending on e.g. observer type (e.g. an eye, a spectrometer). Individuals of **color** refer to specific measurements processes and observers.

This approach enables to connect a measured property to the measurement process and the measurement instrument (Material Characterization).

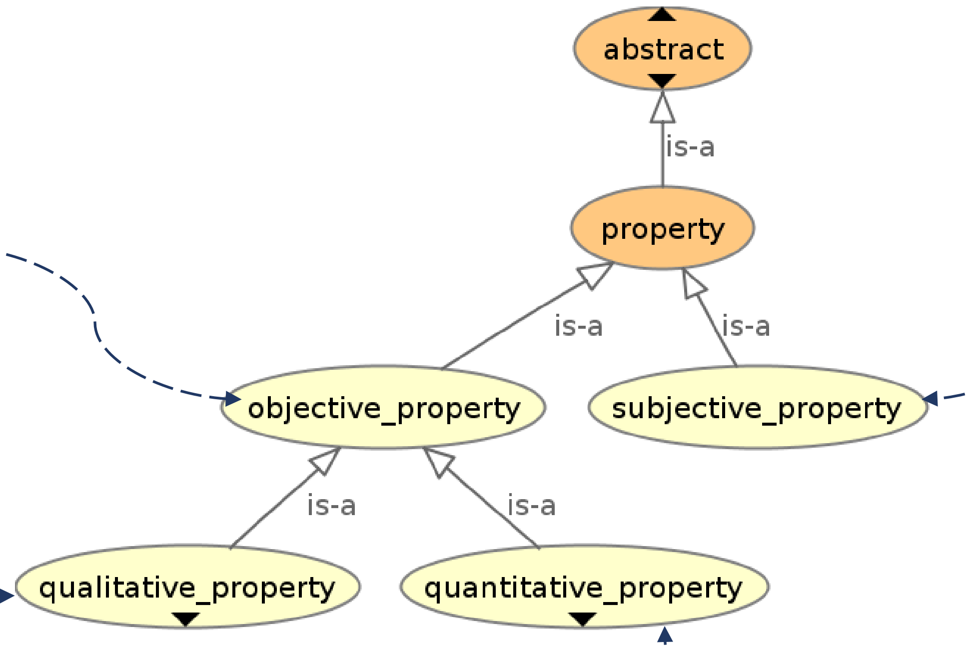


The **has_property** relation is a connection between a **physical** and an **abstract** entity that results from an **observation process**.

has_property states the possibility for a physical to be part of a specific observation process

e.g. a **copper_wire has_property electrical_conductivity** means that my individual wire of copper can be part of a measurement process.

PROPERTIES



objective_property

A *property* that is univocally measurable by each observer by a measuring process, 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.

quaitative_property

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

quantitative_property

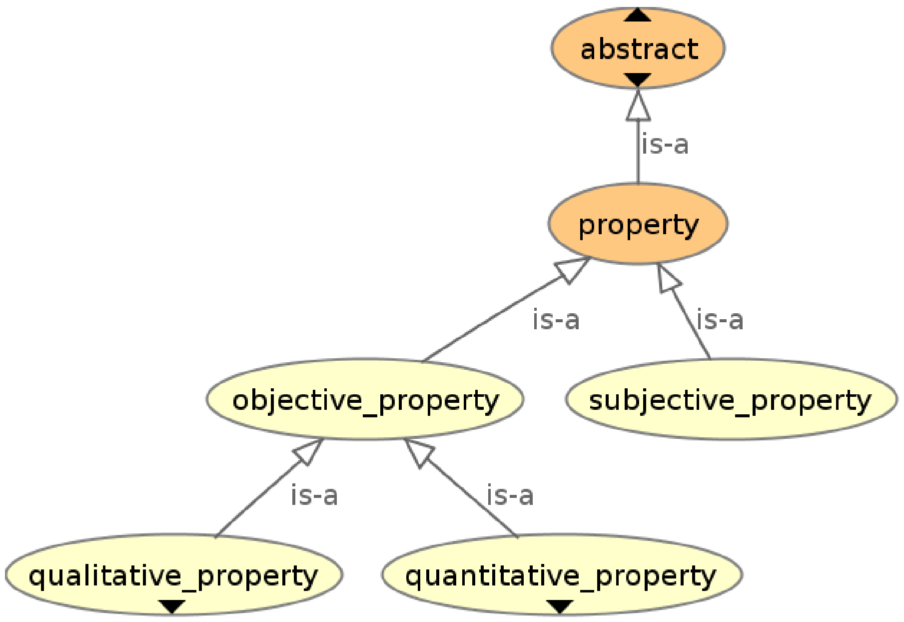
An objective_property of a phenomenon, body, or continuum object, that can be quantified with respect to a standardized reference *physical* instance
(e.g. the prototype meter bar, the kg prototype).

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*

QUANTITATIVE PHYSICAL PROPERTY

Measured and simulated quantitative 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) everything else is derived by mathematical relations i.e. physical laws or definitions.



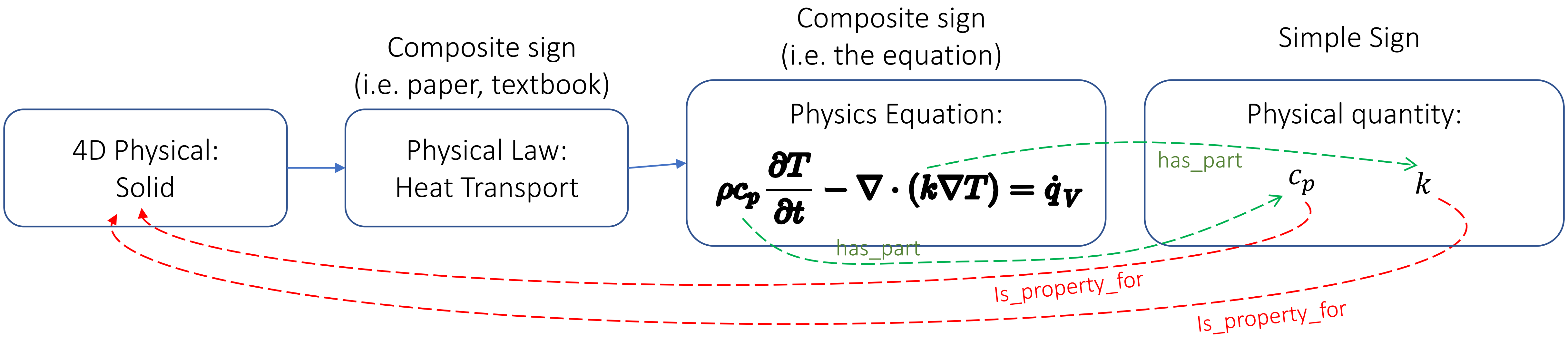
PROPERTIES

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:

$$dh = c_p dT$$



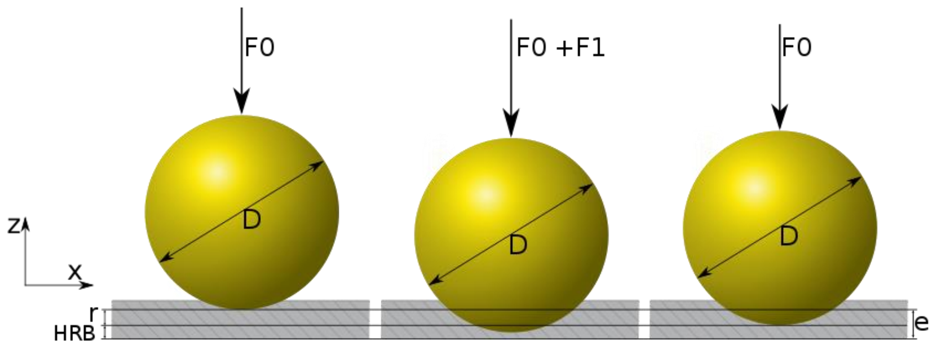
Another example is the distinction between gravitational and inertial mass: they are assumed to be equal, but their measurement occurs using two different laws (i.e. gravitation, second law of dynamics)

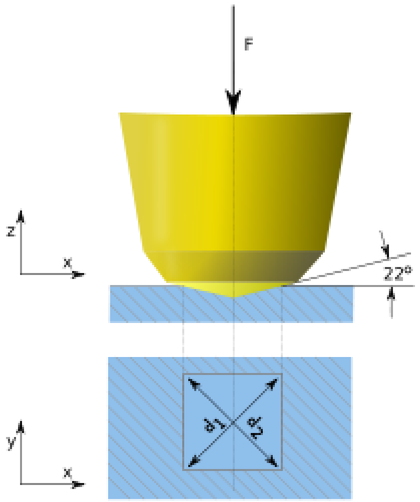
QUANTITATIVE DESCRIPTIVE PROPERTY

Properties such as Rockwell or Vickers hardness are different.

They do not stick to a model, but are measurements related to a specific measurement process that is not generalizable as a physical law.

Hardness is a process_dependent property that cannot be used in a physical model build on a physics equation.





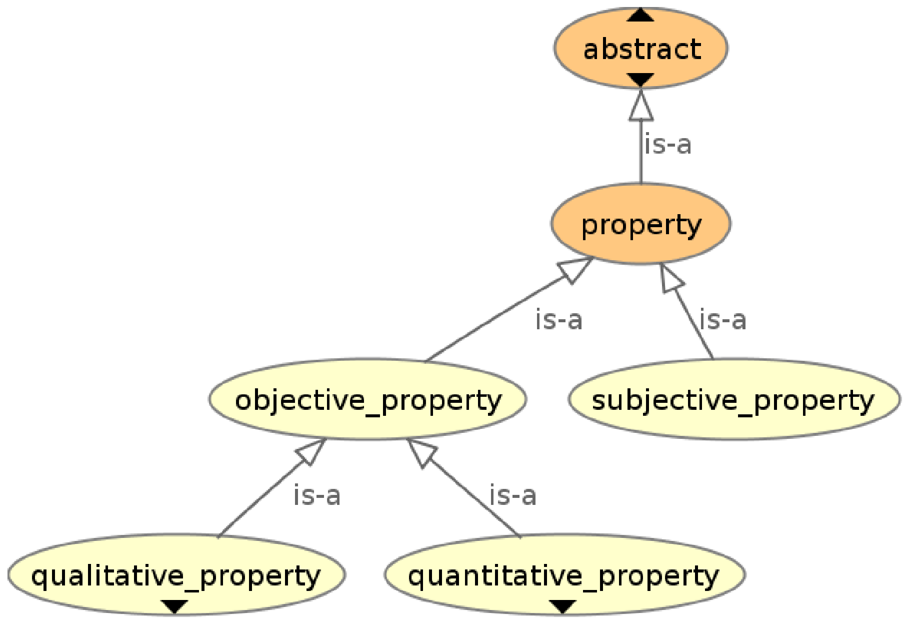
QUALITATIVE PROPERTIES

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.

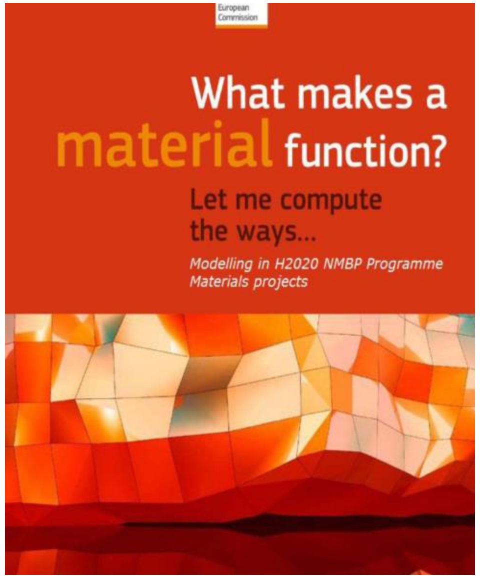
The standard crystal systems are a symbols that stays for a material class.

The real structure of a crystalline solid is provided by the arrangement of the subparts.



RoMM Model Types

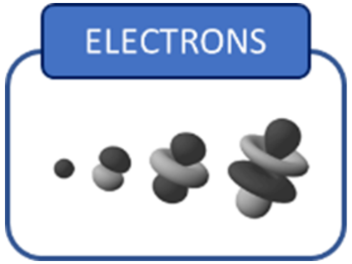
RoMM VI



Modelling in H2020 LEIT-NMBP Programme Materials and Nanotechnology projects

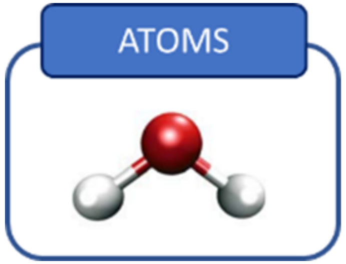
One reality with four veridical views each at a different level of granularity.

This is true for observations and for simulations.



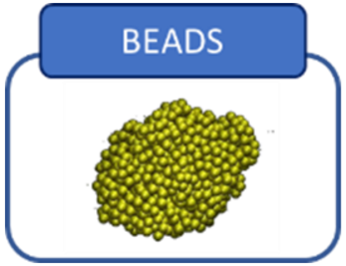
ELECTRONIC MODEL

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



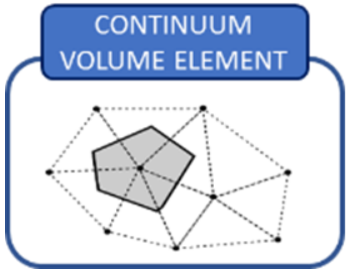
ATOMISTIC MODELS

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



MESOSCOPIC MODELS

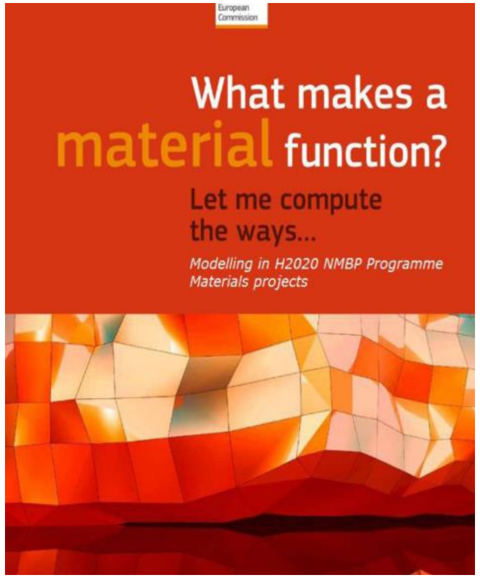
Physics Based Model using a Physics Equation and Material Relation describing the behaviour of Beads either as particles or distributions.



CONTINUUM MODELS

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

RoMM VI



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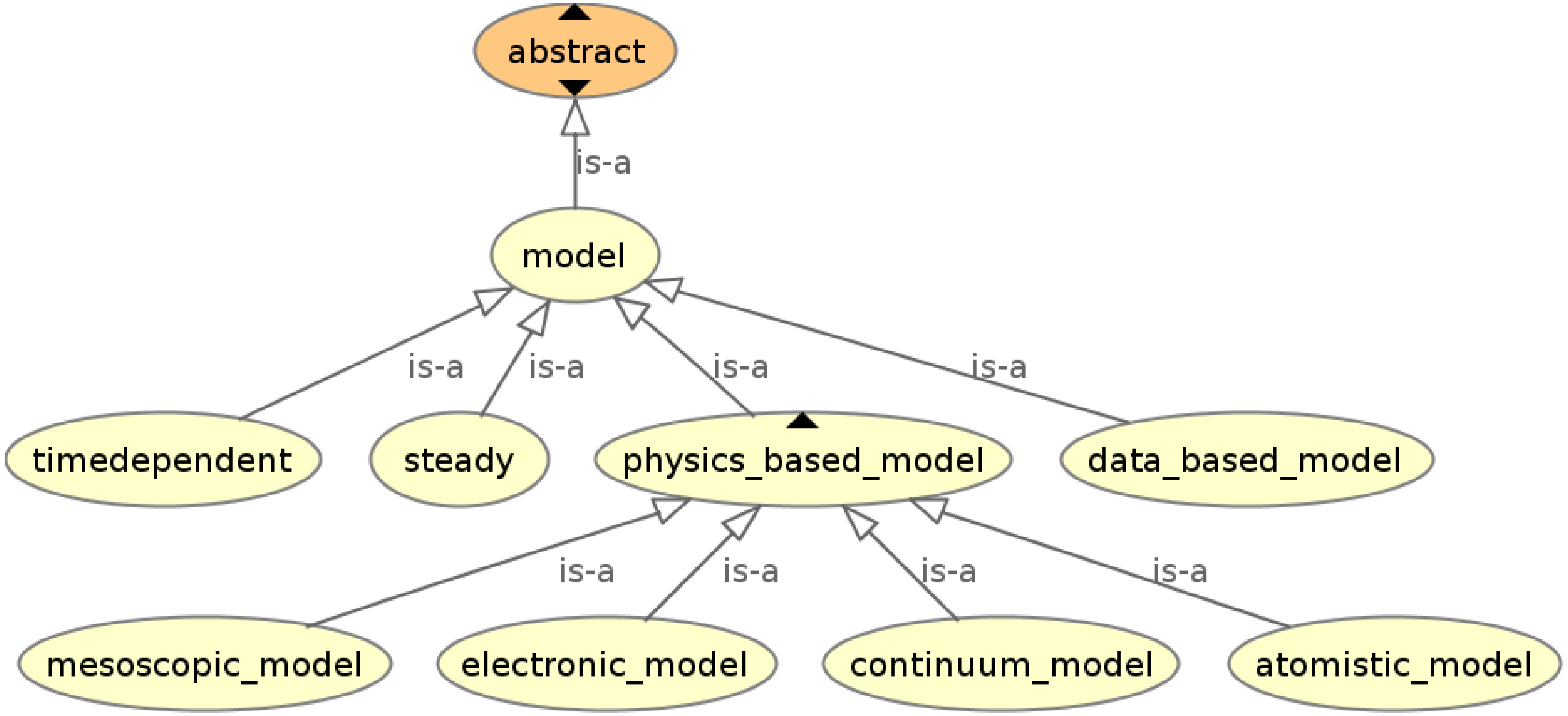
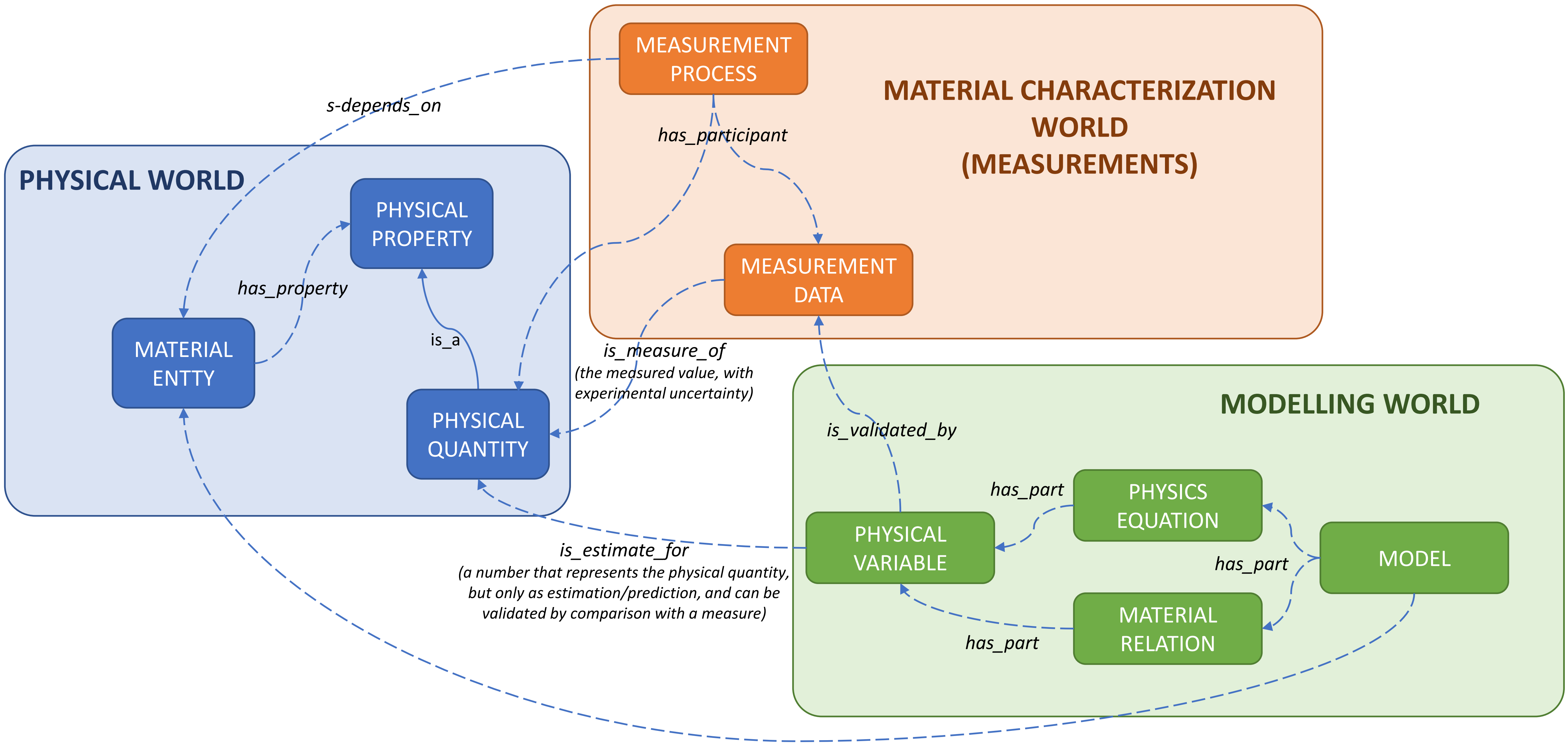
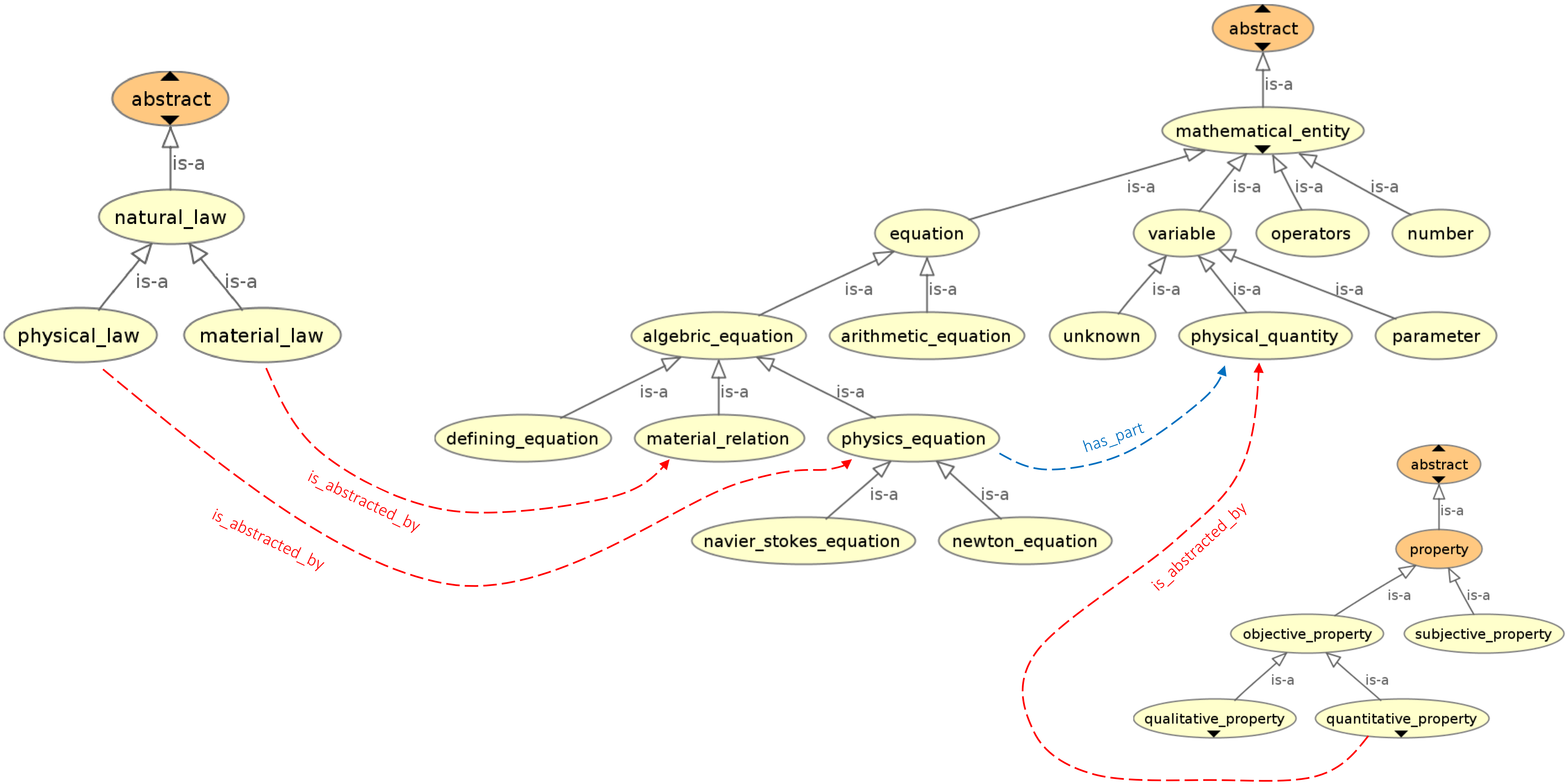


EMMO
abstract branch

EMMO – THE THREE WORLDS



EMMO EQUATION AND PHYSICAL QUANTITY



RELATION BRANCHES

EMMO has very limited and strictly categorized relations, easy to use, understand and maintain:

SET THEORY

is_member_of, distinguish between items and sets

MEREOTOPOLOGY

(mereology + topology)

is_part_of, defines fusions, parts are of the same type and dimensionality of the whole

has_subdimensional_space (slicing) reduction of dimensionality of a physical or substrate

ABSTRACTION/REPRESENTATION

is_abstraction_for, subsumption of a set of things in an abstract by a being (abstractor) that must have at least one physical representation (semeion)

CONCLUSIONS AND FUTURE ACTIVITIES

- Better define properties and their relation with material entities and models (i.e. define the properties peculiar to each material type)
- Introduce data/values and their connection with measurements and mathematical entities in order to enable EMMO as tool for data interoperability
- Finalize a fully commented version 1.0 of EMMO using OWL-DL comments
- Improve logical consistency of the EMMO
- Optimize axioms to reduce reasoner computational costs when individuals are defined
- Start a First Order Logic version of the EMMO
- Provide examples of EMMO applied to simulations
- Test the integration of EMMO with existing ontologies (cross linking/mapping)

But most important:

- <u>How to "give EMMO life"</u>

  (i.e. use it in AI, dynamic interfacing with software, ...)