EMMO

the European Materials Modelling Ontology

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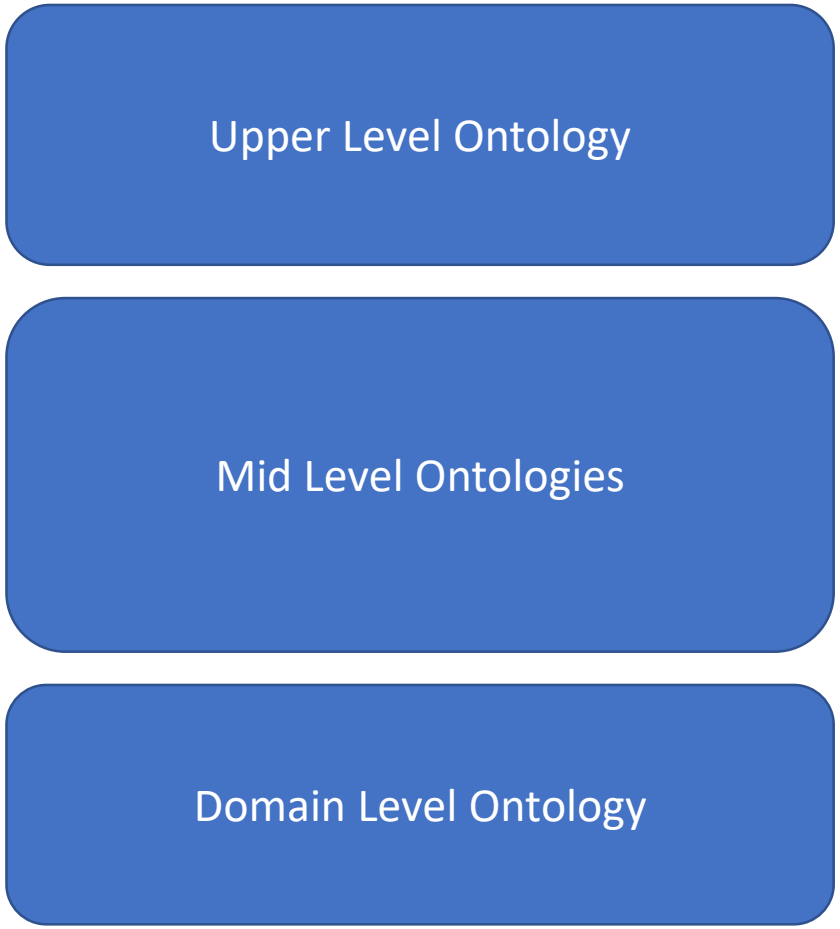
Building Ontologies

- Core concepts
  - Upper and mid level
- Axioms
- Taxonomies
- Domain axioms
- Relations

Ontology levels

- Express fundamental concepts of physics and materials science
- Models, Properties, Processes, Materials (and their structure/granularity), Measurements etc
- Specific taxonomies and ontologies



What are the core concepts?

- MatOnto:
  - Material, Property, Family, Process, Structure, Measurement
- Ashino:
  - Substance, Process, Property, Environment
- PreMap:
  - Material (Composition, Phase, Property, Structure, Morphology, State, Form), Process, Product
- EMMO:
  - Substrate: Spacetime – Physical (Field, Matter, Process etc)
  - Abstract: Property, Natural Law, Model, Mathematical Entity

What are the axioms?

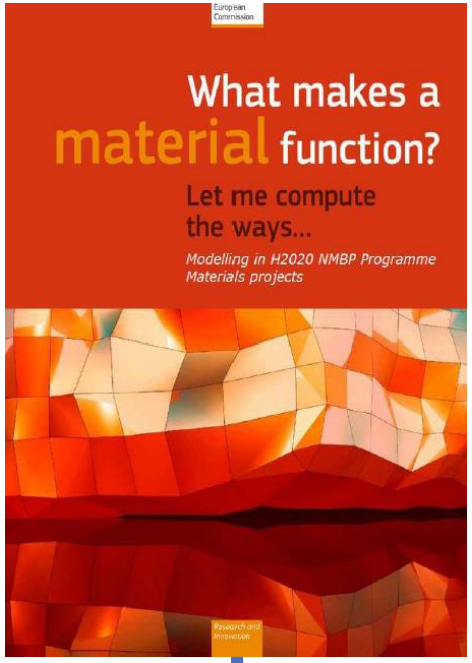
- The foundation of inference, axioms are usually classified as two kinds:
  - Axiom schemata (e.g., disjoint of two concepts, cardinalities of a relation)
    - Set Theory
    - Mereotopology
  - Domain axioms to express the domain-specific semantics
- Axioms inform the relations of an ontology

X. Zhang et al. / Computers in Industry 73 (2015) 8–22

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.*

EMMO

European Materials Modelling Ontology

ALMA MATER STUDIORUM UNIVERSITÀ DI BOLOGNA

GOLDBECK CONSULTING

access

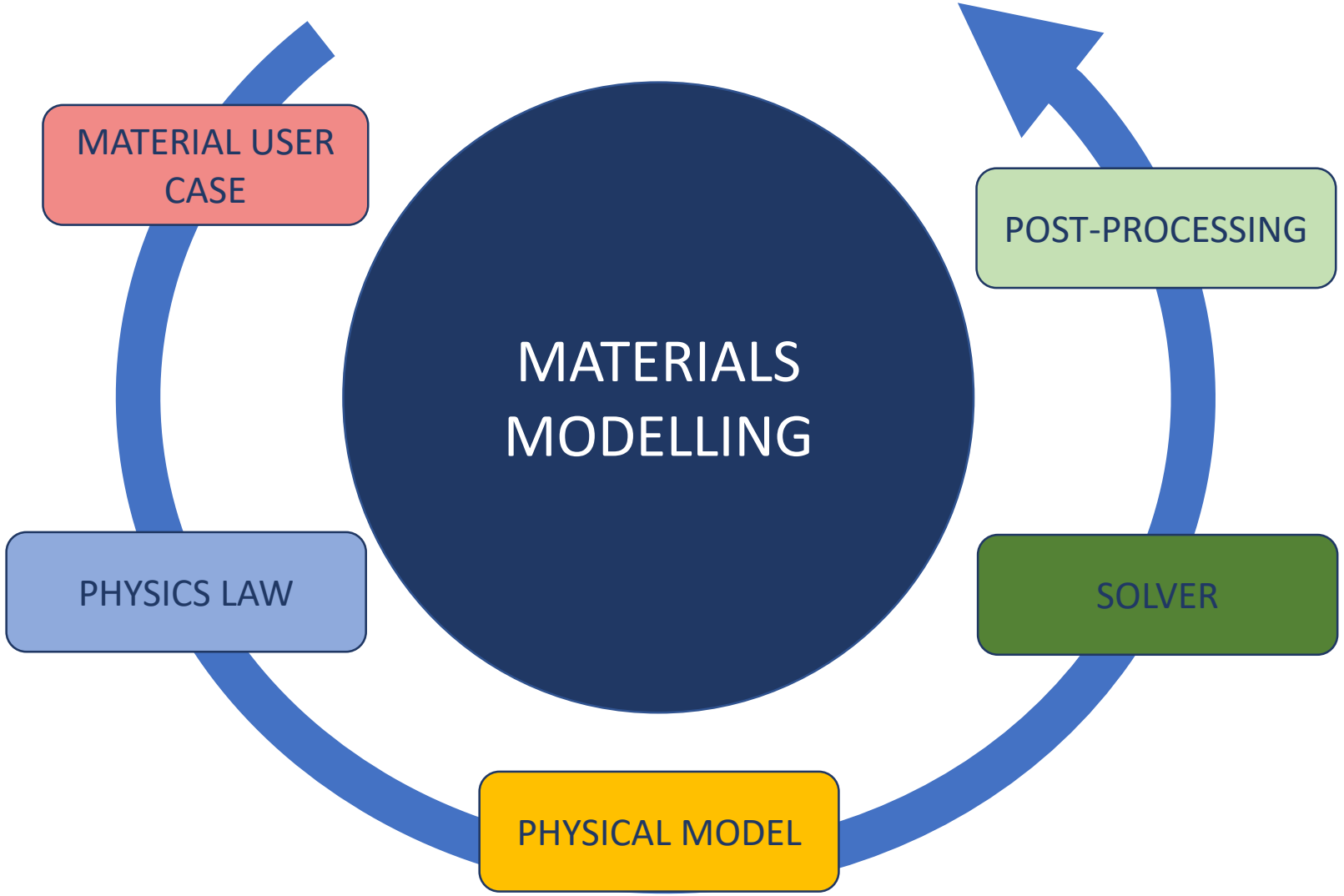
Fraunhofer

SINTEF

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



EMMO SCOPE AND OBJECTIVES

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 SCOPE AND OBJECTIVES

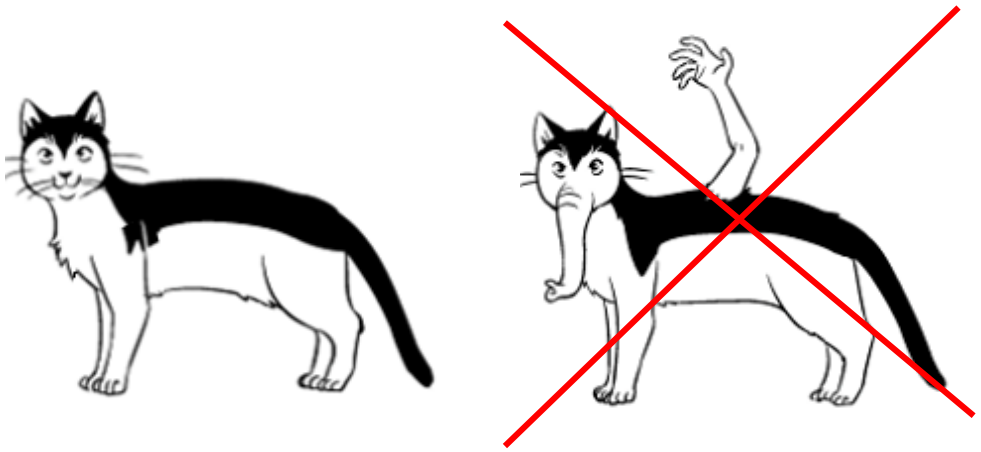
THE **EMMO** IS A MULTIDISCLIPLINARY EFFORTS WITHIN THE **EMMC** AIMED TO THE DEVELOPMENT OF A **STANDARD REPRESENTATIONAL FRAMEWORK** (THE ONTOLOGY) BASED ON CURRENT MATERIALS MODELLING KNOWLEDGE.

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.

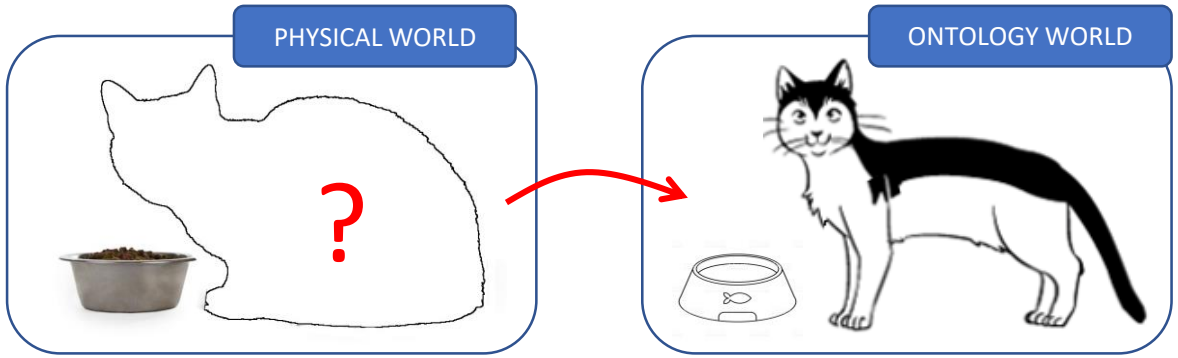
The EMMO does provide the consistency of the symbolic representation.

i.e. you cannot say everything in EMMO, but only what is realistic



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

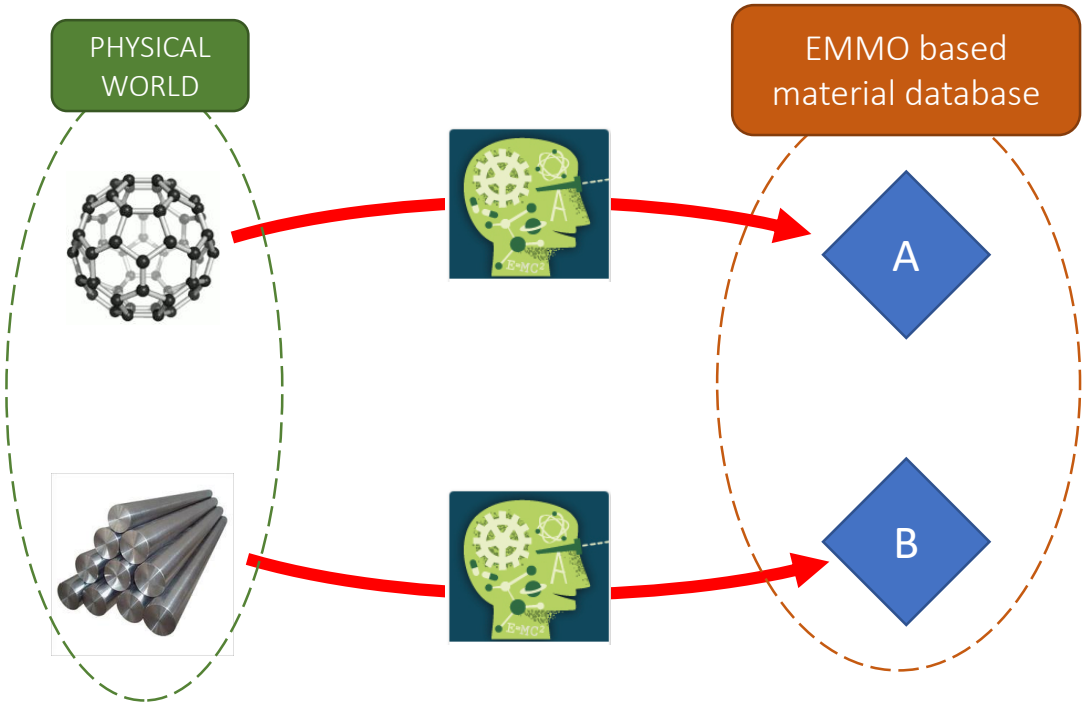
i.e. you can use symbolic representation to express something that is realistic in the EMMO but that does not exist (a realistic lie)



EMMO GENERAL USAGE EXAMPLES

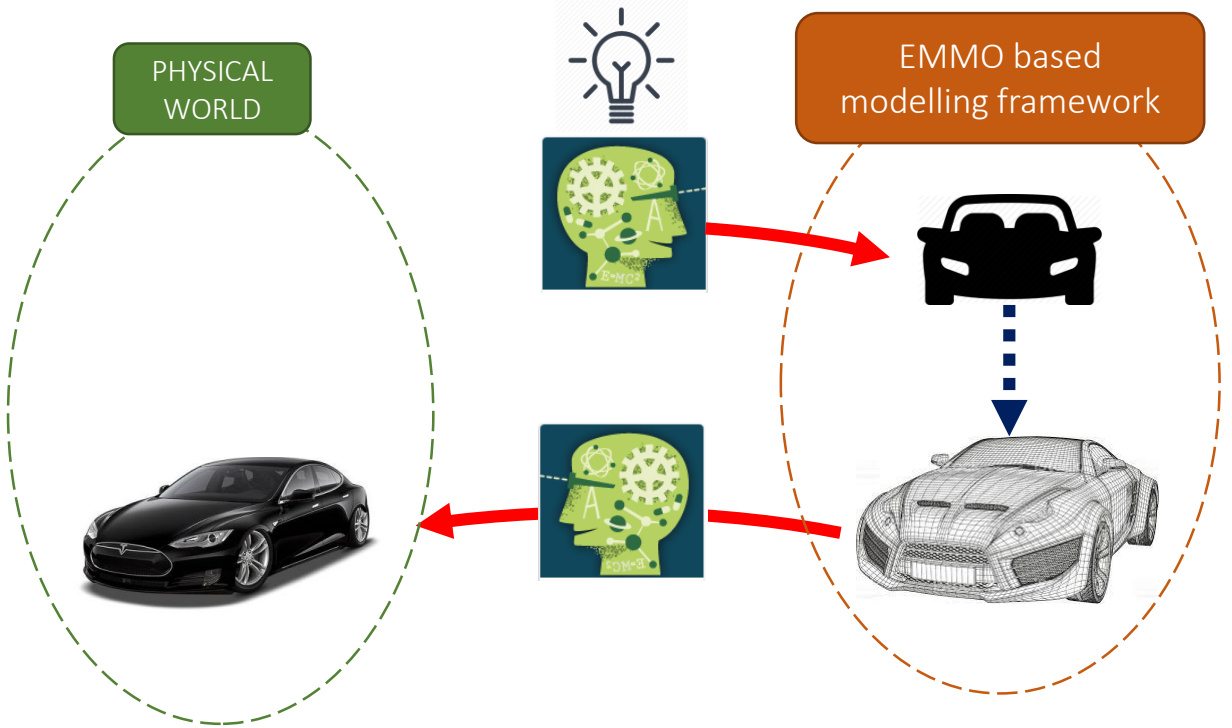
MATERIALS CHARACTERIZATION

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*

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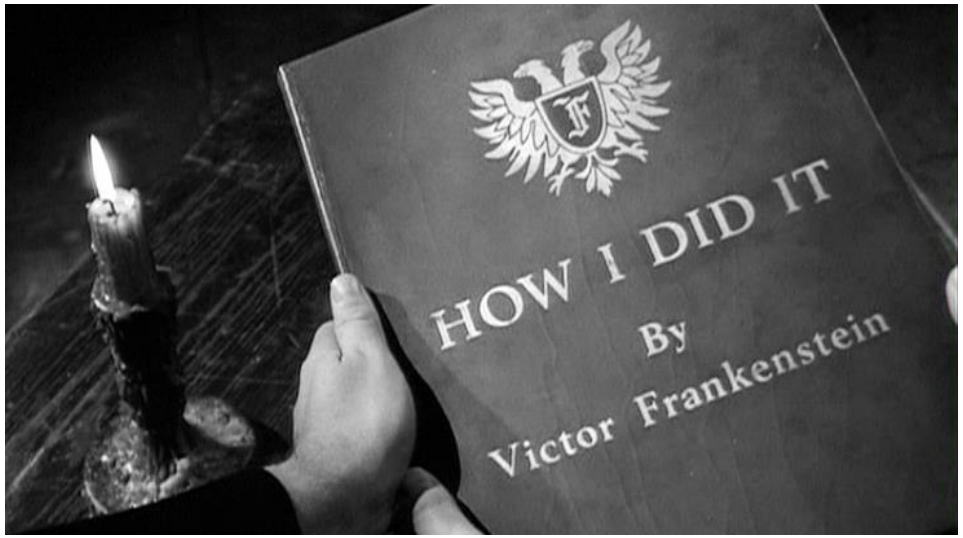
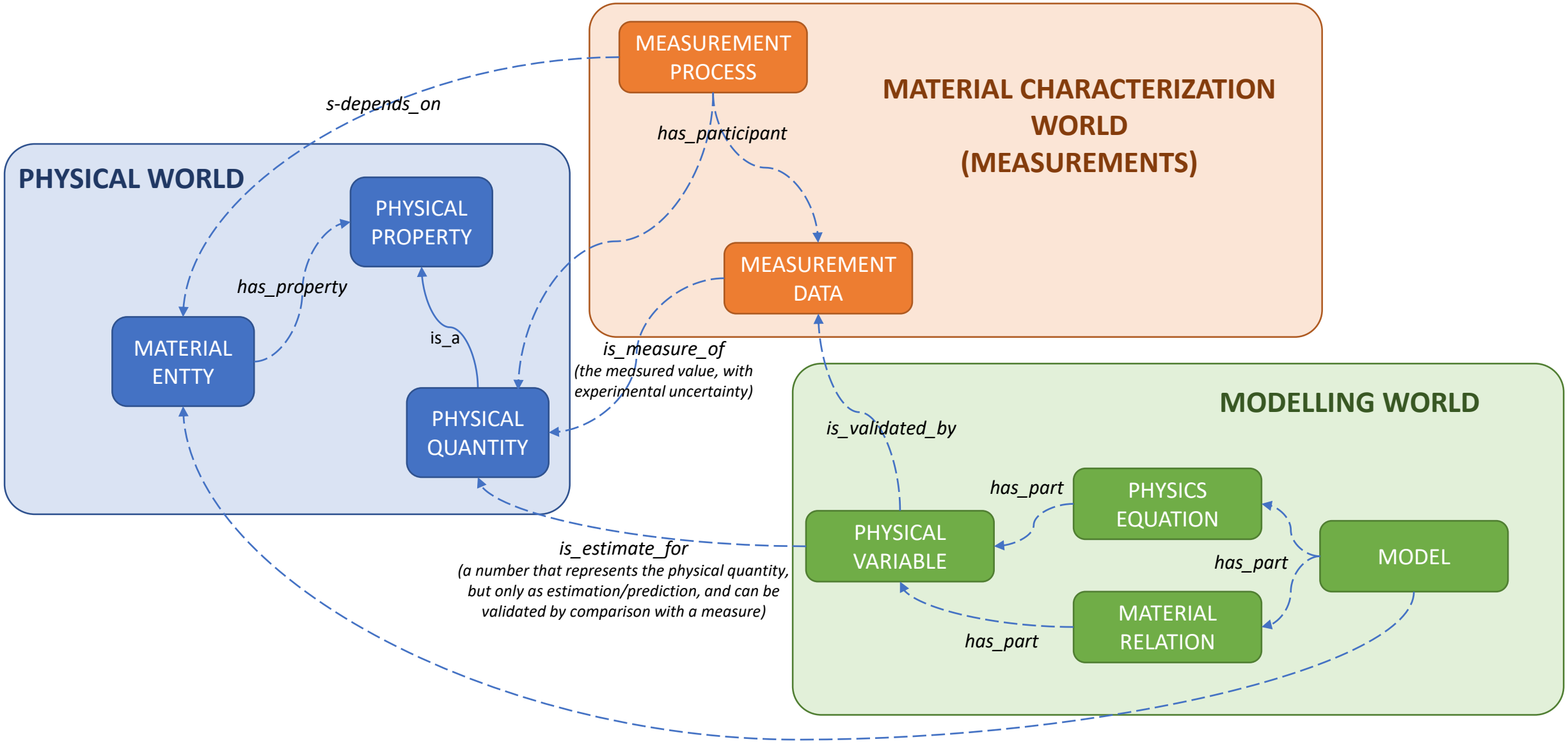
EMMO main objectives:

- provide a basic framework for the description of material science
- Provide efficient representation of physical entities granularity (polymer -> monomer -> atom -> nucleus -> …) to facilitate multiscale modelling
- include physical models and their relations with material entities
- categorize material properties to enable a material classification
- provide a framework for materials properties database



EMMO – THE THREE WORLDS



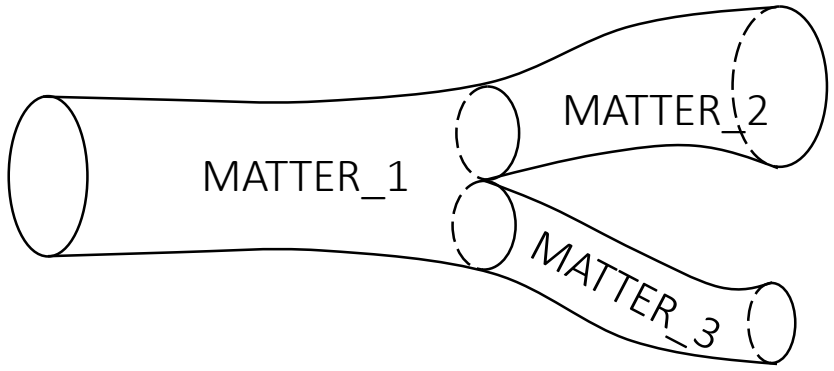
EMMO Physical World representation

Based on concept that a physical world entity is a **spacetime entity.**

Some mereological parts (regions) can be categorized in **matter** spacetimes or **field** spacetimes:

- **matter** is a subclass of **spacetime** that expresses some mass property.
- **field** is a subclass of **spacetime**, but expresses no mass property.

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

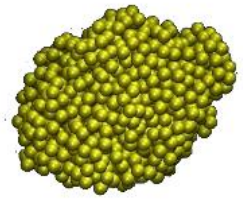


EMMO Mereology

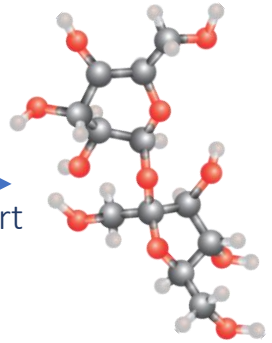
has_part

has_part

has_part

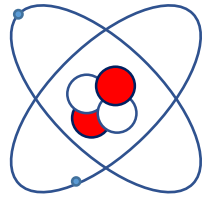


has_part

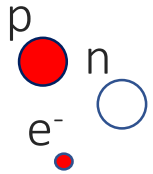


has_part

has_part



has_part



EMMO Material Entities are defined by a
Hierarchy of parthood relations,
Including the NEW concept of direct parthood

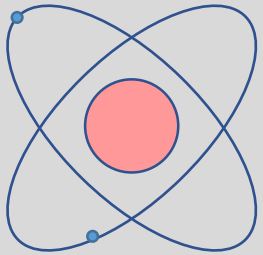
A representation of the granularity of materials entities that follows physics and materials science perspectives.

The basic idea is that the material can be represented at different levels of granularity, depending on **perspective**.

EMMO Mereology of Direct Parts Example

AXIOMS

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



n = 3

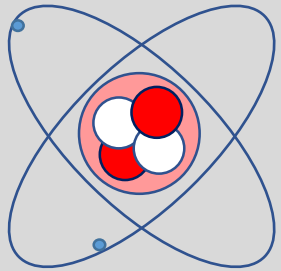
He nucleus **has_direct_parts**:
- neutron_1
- neutron_2
- proton_1
- proton_2

n = 4

THE **EMMO** DIRECT PARTHOOD RELATION CONCEPT 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).

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

EMMO Relations

- EMMO has very limited and strictly categorized relations:

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

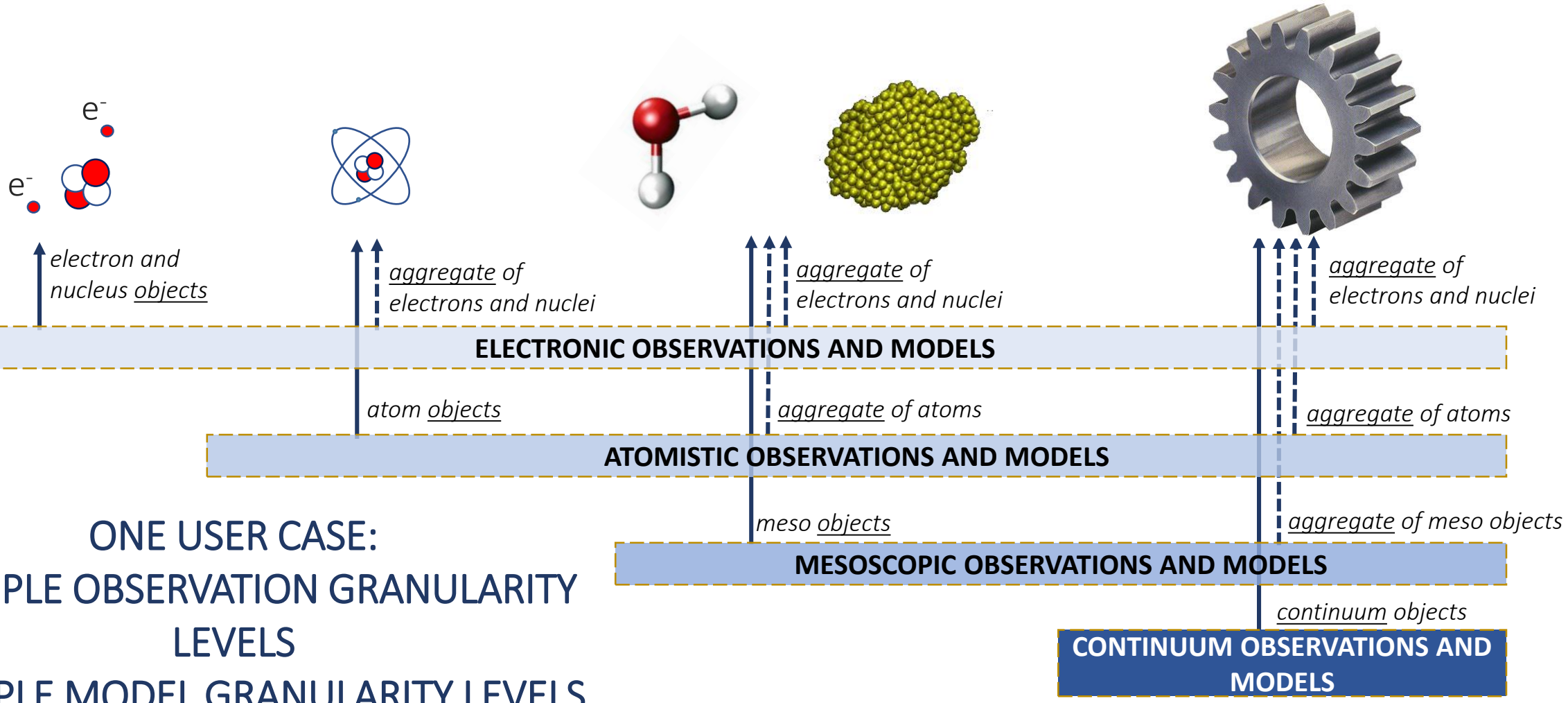
has_subdimensional_space (slicing) reduction of dimensionality of a physical or substrate

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)

EMMO MEREOLOGY FOR OBSERVATIONS AND MODELS

EACH material can be observed at different levels of granularity and can be modelled by different granularities.



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

ACKNOWLEDGEMENTS

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