European Materials & Modelling Ontology

Emanuele Ghedini (University of Bologna)

Gerhard Goldbeck (Goldbeck Consulting Ltd)

Adham Hashibon (Fraunhofer IWM)

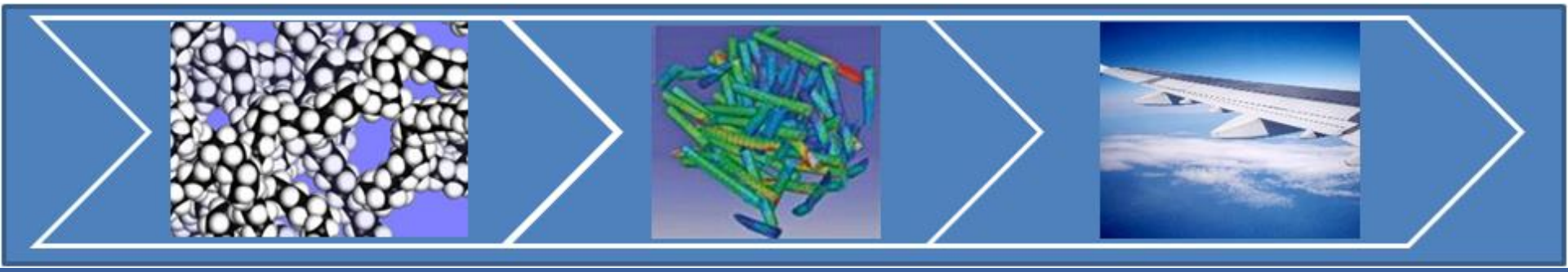
Georg J. Schmitz (ACCESS)

Jesper Friis (SINTEF)

https://github.com/emmo-repo/EMMO

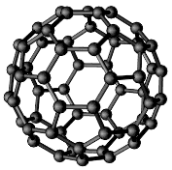
Application Domain

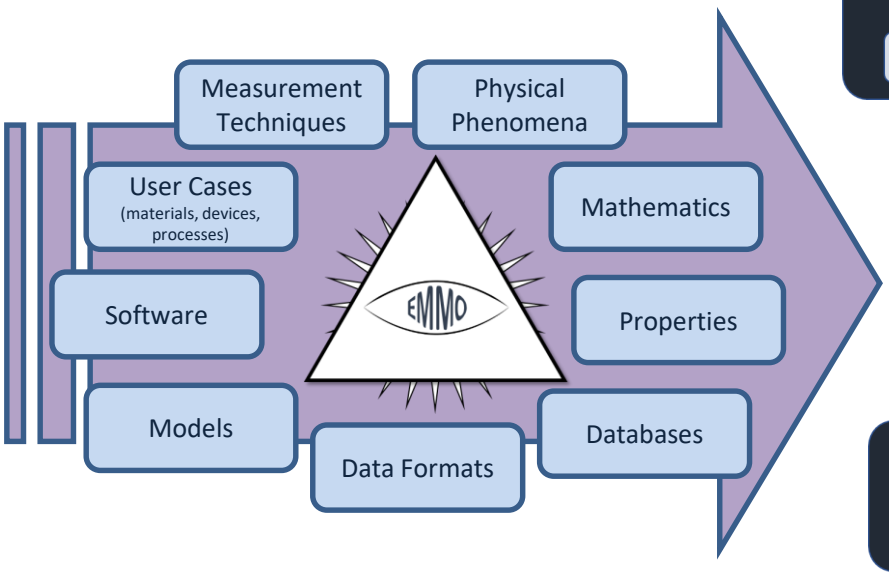
- Applied Sciences, including applications in
  - Materials science: modelling, characterisation etc
  - Chemistry: modelling, analytical, formulations etc
  - Physics: e.g. representations of a system in terms of different interpretations of quantum mechanics
  - Engineering: components and systems, processes etc

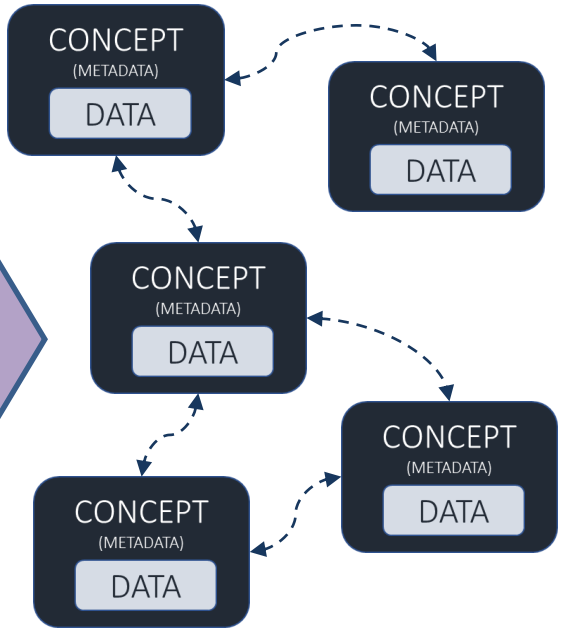


Intended Purpose

- EMMO is a **tool connecting** Materials User Cases to Models, Characterisation etc, incl. Inference, organising concepts according to scientific and mereotopological principles
- EMMO supports Interoperability, Data organisation, Databases integration, Translation etc.







USER CASE
From real world entities at different scales…

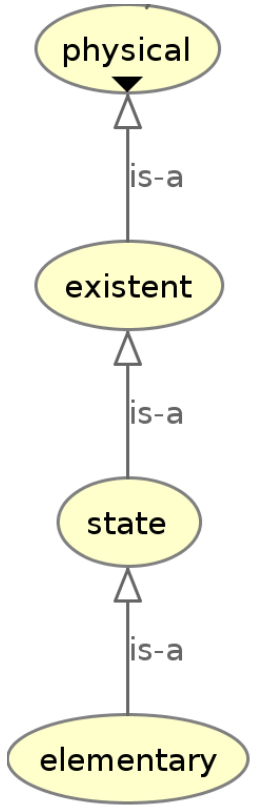
ONTOLOGY
…through a formal knowledge-based representational system…

INFORMATION
…to a digital representation and knowledge management.

Representation "of the world"

continuum, discrete, quantum mechanics?

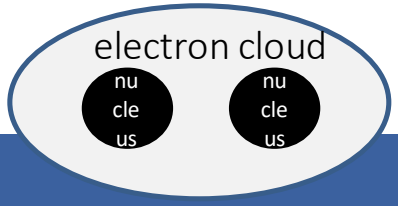
- **4D**: Real world entities exists only in full **spacetime:**
  - a physical object **is** a topological subspace of the 4D universe
- **Elementary**: 'fundamental/indivisible' physical object: hence space is discrete.
- **Causality***:* Interactions between physical objects require them to be topologically connected.
- **Existent**: made of sub parts, as defined by interpreter:
  - Enables different quantum mechanical representations to be expressed, e.g.



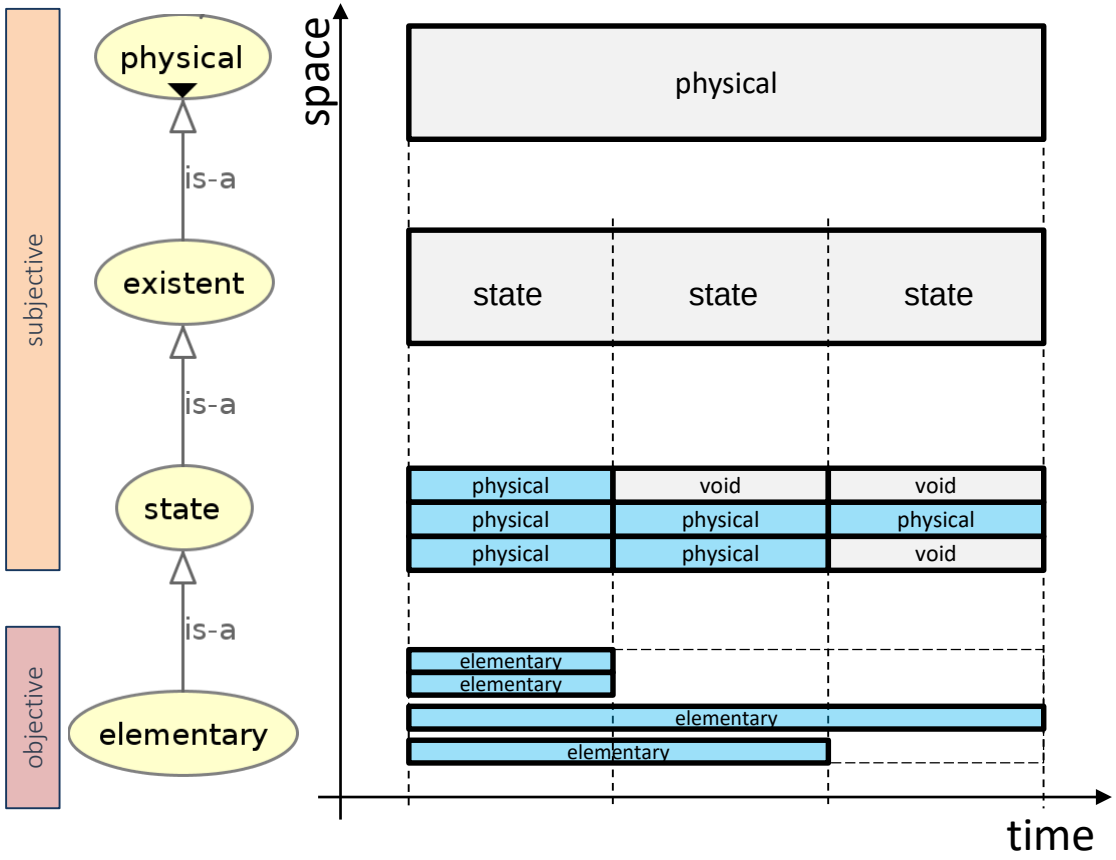
fully entangled system

Atom or molecule

electron and nucleus un-entangled (Born-Oppenheimer approximation)



Representation of the world



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

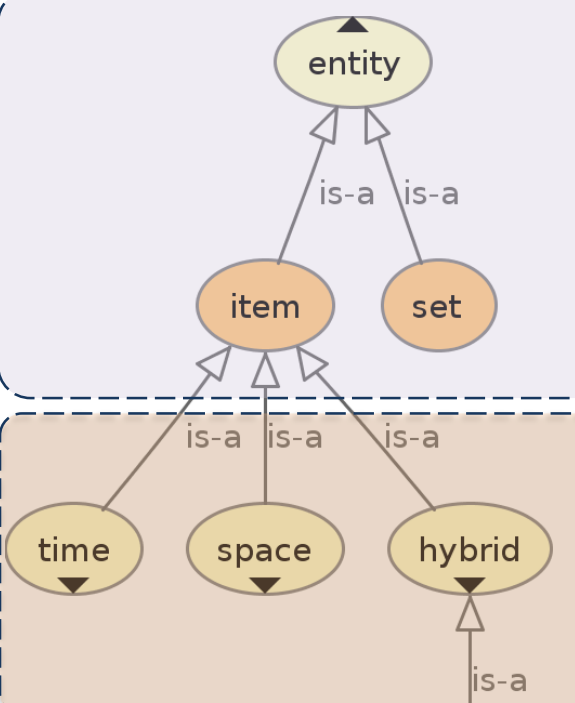
- **elementary** as the fundamental, non-divisible, constituent of entities (i.e. atomistic mereology)
- **state** as a **physical** whose parts have a constant cardinality during its life time (similar to endurants)
- **existent** as a succession of **state**s (similar to perdurants)

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

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, a furniture component in a IKEA ontology)

Upper level concepts



ABSTRACT CONCEPTUAL LEVEL

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

Abstract concepts are represented as the **set**s that concretize them (e.g. friendship is the collection of all friendship acts)

GEOMETRIC/TOPOLOGICAL LEVEL

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

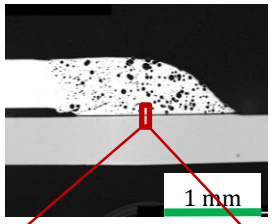
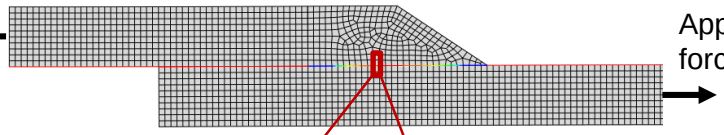
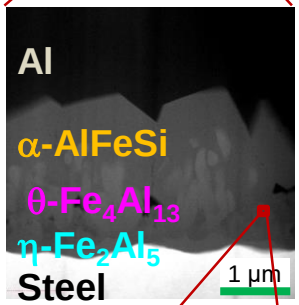
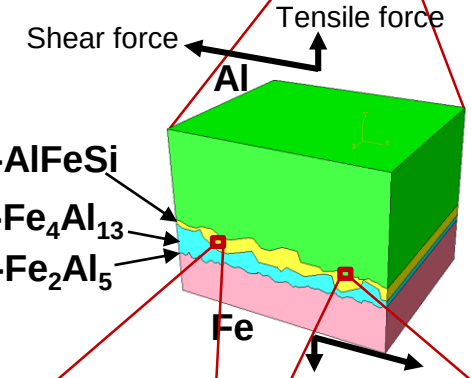
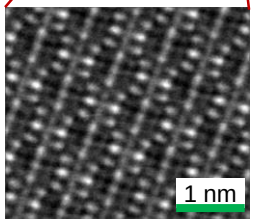
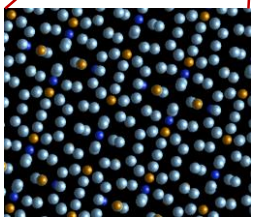
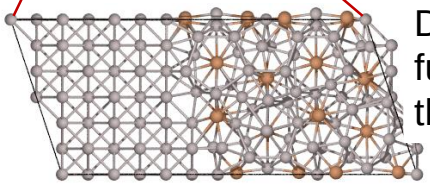
PHYSICAL LEVEL

Real world entities exists only in full 4D **spacetime** (3D space and 1D time).

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

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

Interoperability user case

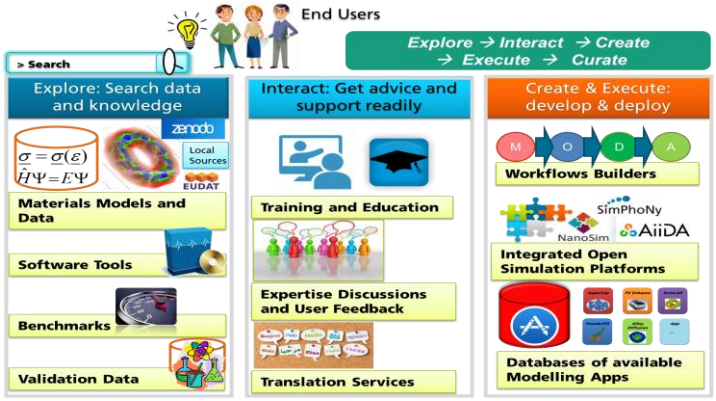
Scale	Real world	Model	Transferred properties
Component Welded structure		Finite element 	• Mechanical response • Cohesive behaviour (cohesive elements)
Microstructure Intermetallic phases and interfaces		 Finite element	*Interface* • Work of separation • Work of sharing *Bulk* • Elastic constants
Atomistic/ electronic Atomistic crystal and interface structures		  Density functional theory	• Atomistic structures

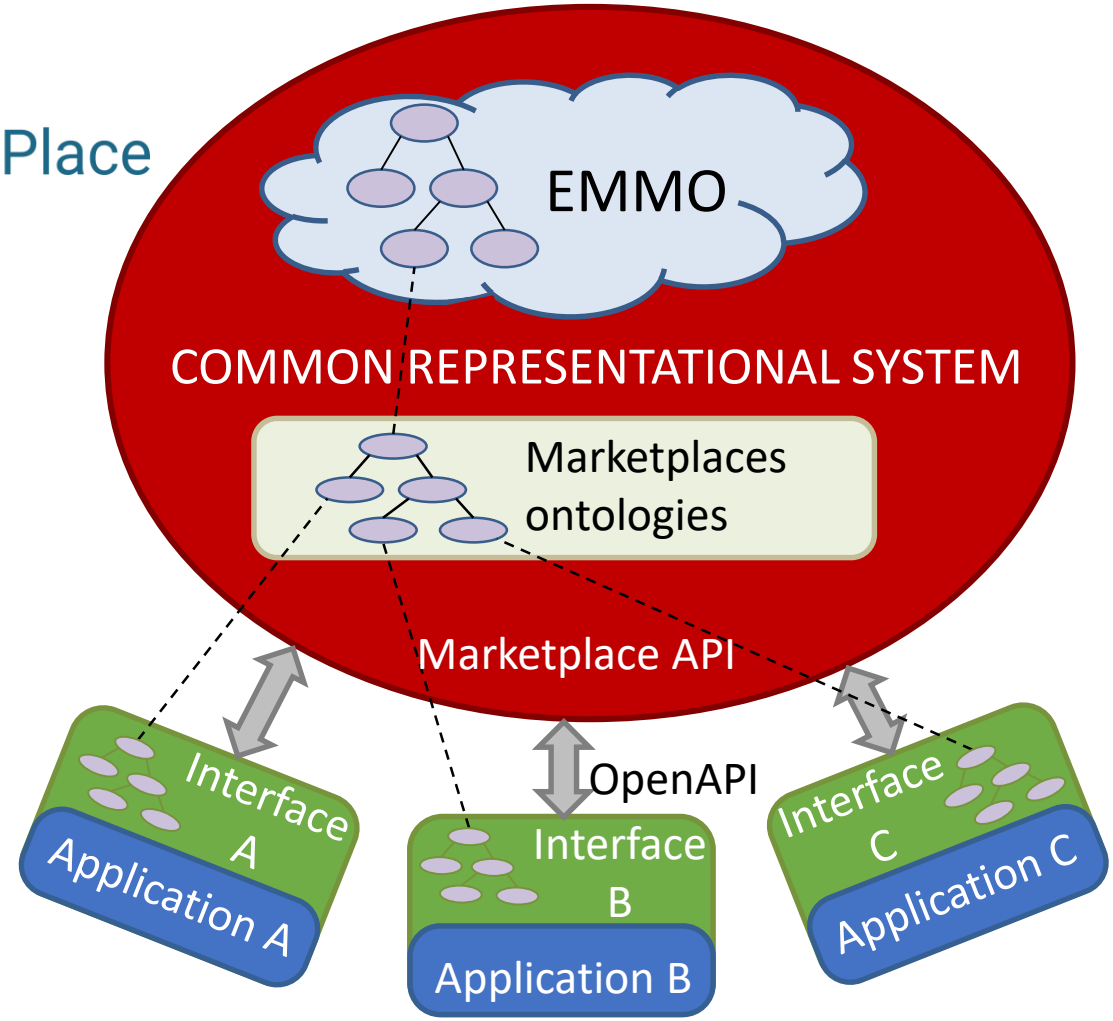
Marketplaces Use Case

Mapping between ontologies

VIMMP VIRTUAL MATERIALS MARKETPLACE

MarketPlace





EMMO implementations in current EU projects

VIMMP
VIRTUAL MATERIALS MARKETPLACE

MarketPlace

FORCE

Formulations and Computational Engineering

SimDOME

Digital Ontology-based Modelling Environment for Simulation of materials

EOSC-Pillar

APACHE

Active & intelligent PAckaging materials and display cases as a tool for preventive conservation of Cultural Heritage

OYSTER

Open characterisation and modelling environment to drive innovation in advanced nano-architectured and bio-inspired hard/soft interfaces

INTERSECT

*Interoperable Material-**to-Device** simulation box for disruptive electronics*

ReaxPRO

SOFTWARE PLATFORM FOR MULTISCALE MODELLING OF REACTIVE MATERIALS AND PROCESSES

Intended Purpose
(Summary from all mentioned projects)

- **Computational representation**
  - of top-down and bottom-up workflows including the user case and all computational details and GUI elements
- **Wrapper development**
- **Dataspaces**
- **Marketplace services**
- **Integrated materials modelling workflows**
- **Coupling and Linking**
- **Characterisation**
- **Pre and post processing**
- **Manufacturing processes (as far as needed for the demonstration cases)**

Overlaps with other taxonomies and/or ontologies

- EMMO is a tool.
- There is no application of EMMO (yet) which would overlap with existing semantic assets.
- EMMO allows for semantic connection to existing domain ontologies.

Main relations

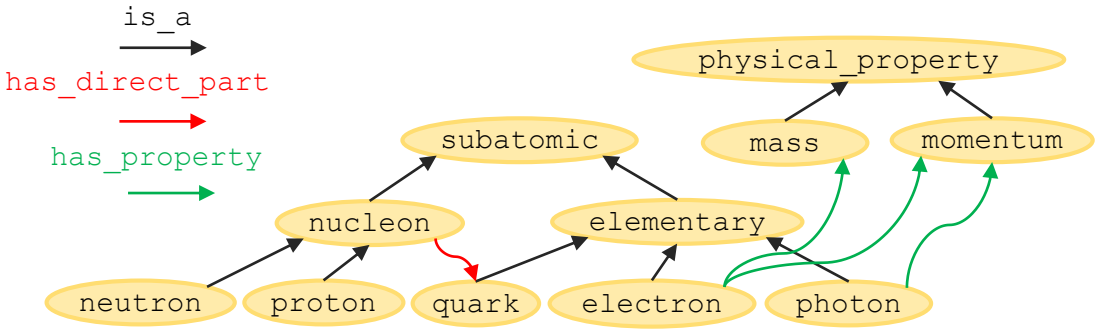
Only 4 primitive families

TAXONOMY
Classification
Ex: `is_a`

MEREOTOPOLOGY
Parthood and *Slicing*
Ex: `has_part`

SEMIOTIC
Representation
Ex: `has_property`

SET THEORY
Membership
Ex: `has_member`

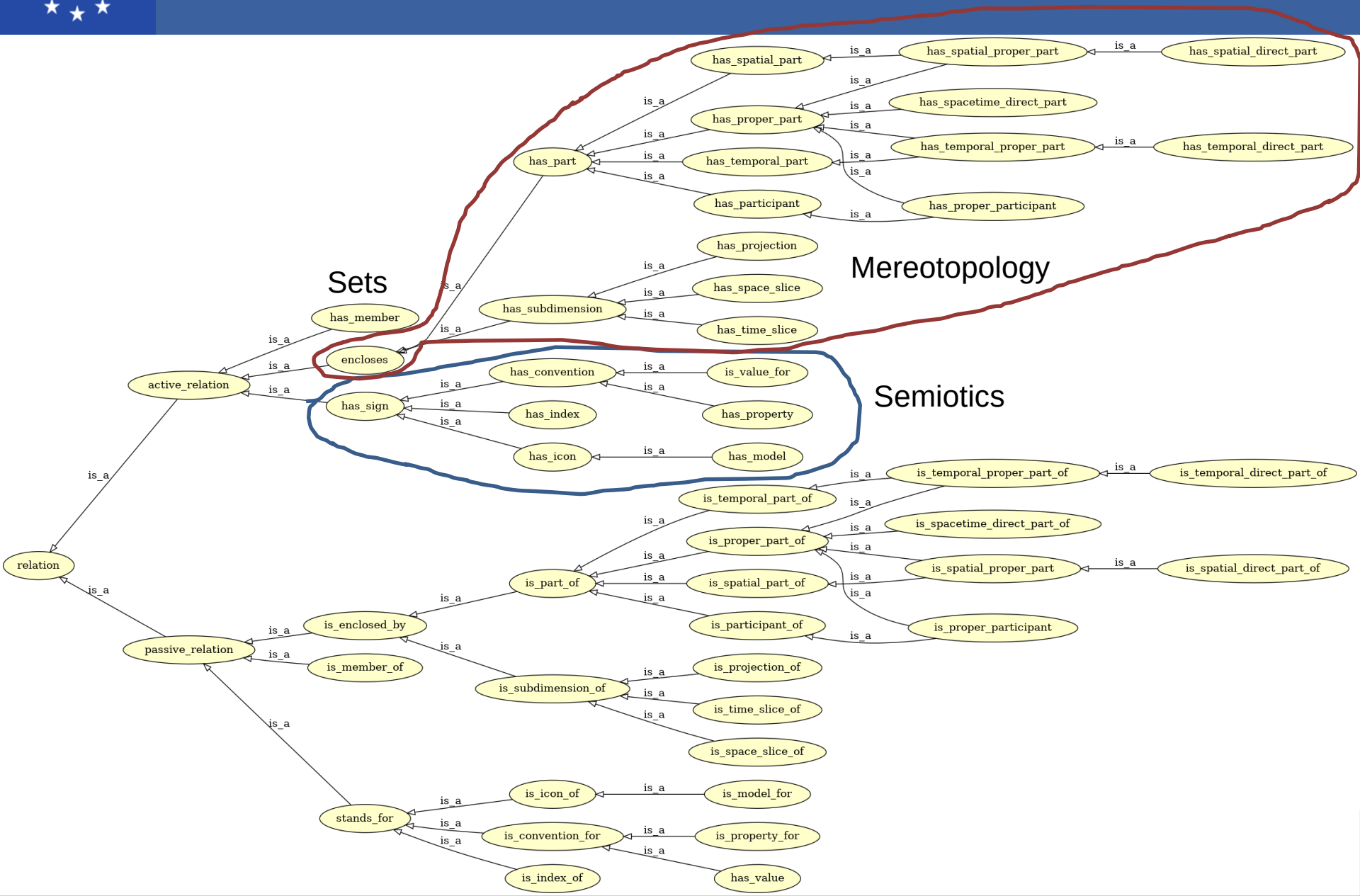


Items that unfolds in space and time
Granularity (multi-scale modelling)

Signs that stands for something else
Represents real-world objects

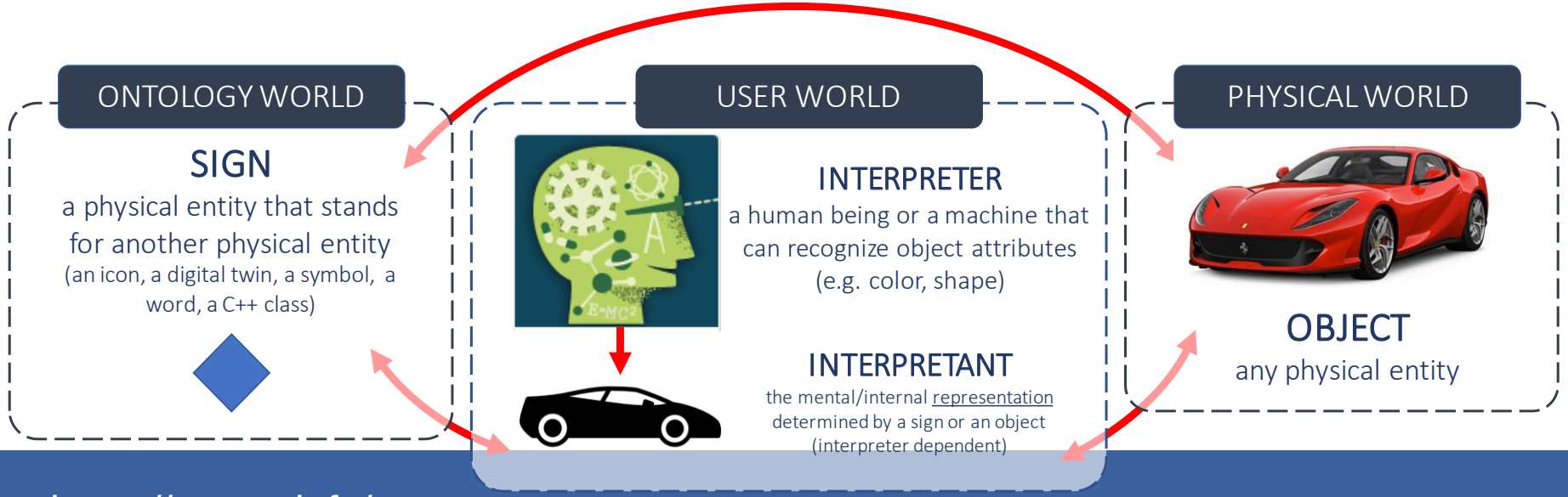
Abstract collections of items

EMMO relations



Knowledge represented

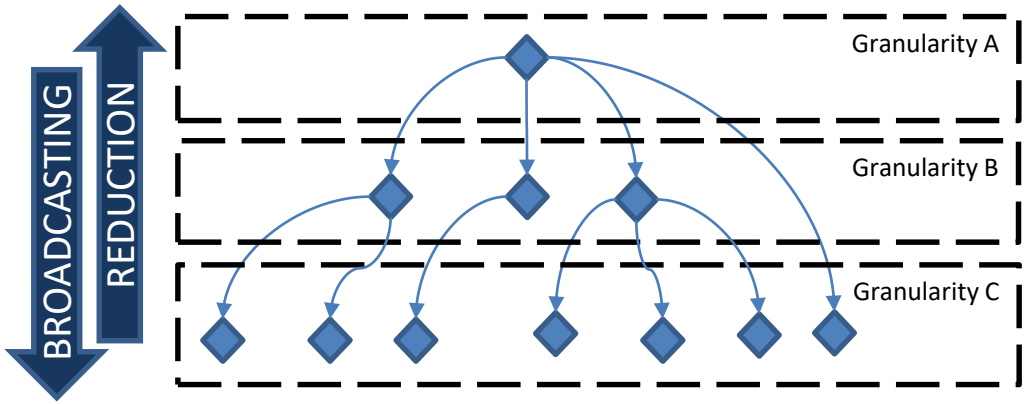
- Semiotics, Nominalism, Mereotopology, Set Theory
- EMMO is rooted in a strict form of nominalism
  - Real-world objects are represented by signs, where the relation between signs and object only exists via the interpreter: non-existence of universals!
  - everything (i.e. signs, interpreters and objects) exists in space and time. There are no abstract objects outside space and time.



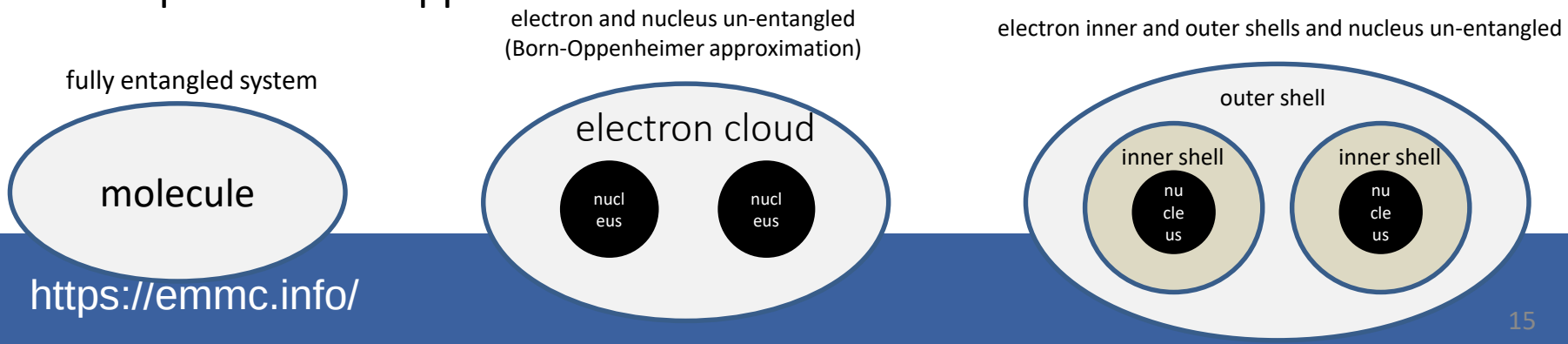
Representing granularity

- EMMO covers continuum and discrete representations

By defining the mereological relation of **direct parthood**, **EMMO** is able to describe entities as made of parts at different level of **granularity**. The individuals form a directed rooted tree



- EMMO covers quantum systems: declaring parts based on the relevant QM interpretation or approximation

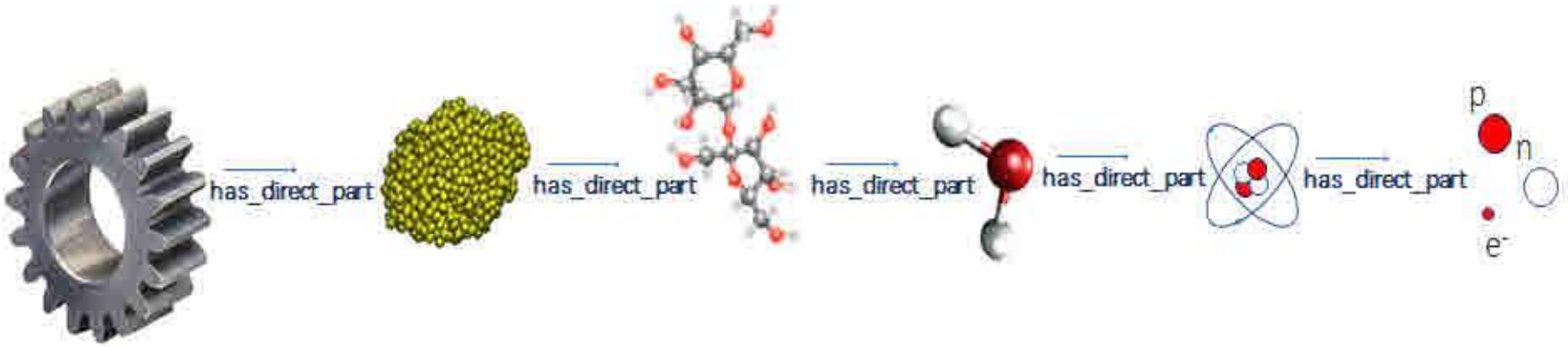


Capturing of materials

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

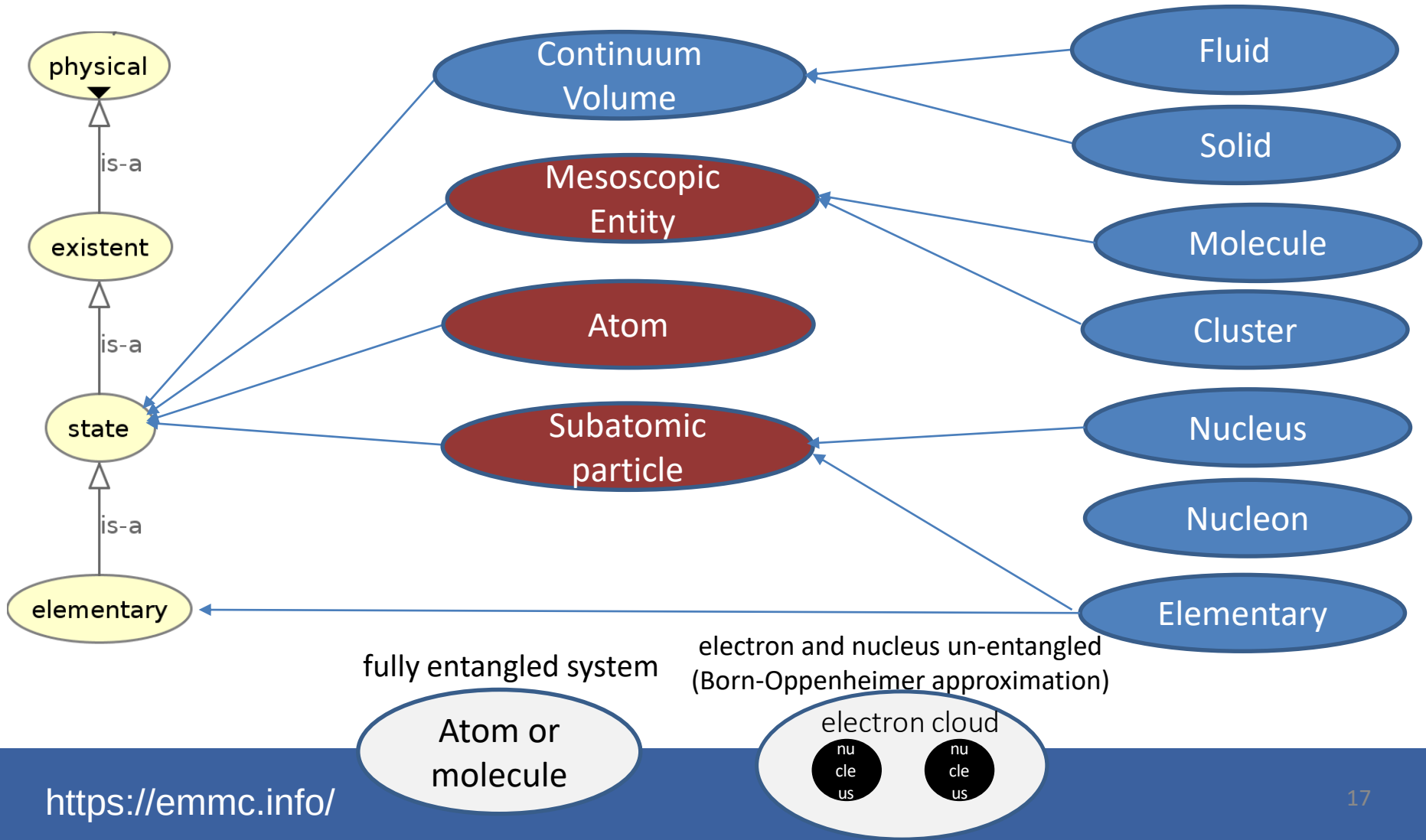
Material can be represented at different levels of granularity.

Hierarchy of structure can be univocally defined.



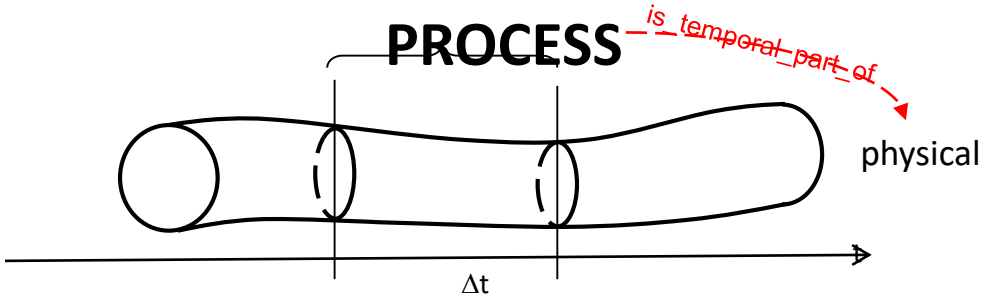
- **Elementary:** the fundamental, non-divisible, constituent of entities

Capturing of materials



Representation of processes

- EMMO is about describing the 'real world', i.e. things that we perceive (we can interact with). The real world is within a 4D spacetime.
- Real world objects can be processes: objects evolving in time.
- Classes of processes can be defined as required/relevant, e.g.
  - 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.
  - MANUFACTURE: A process aiming at altering properties of objects towards a desired property

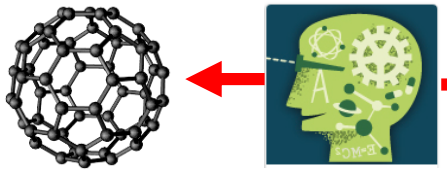


Capturing manufacturing

- EMMO Physicals can represent any real world object and process, including manufacturing.
- See also previous slide on Processes.

Connection between physical properties, materials models and measurement

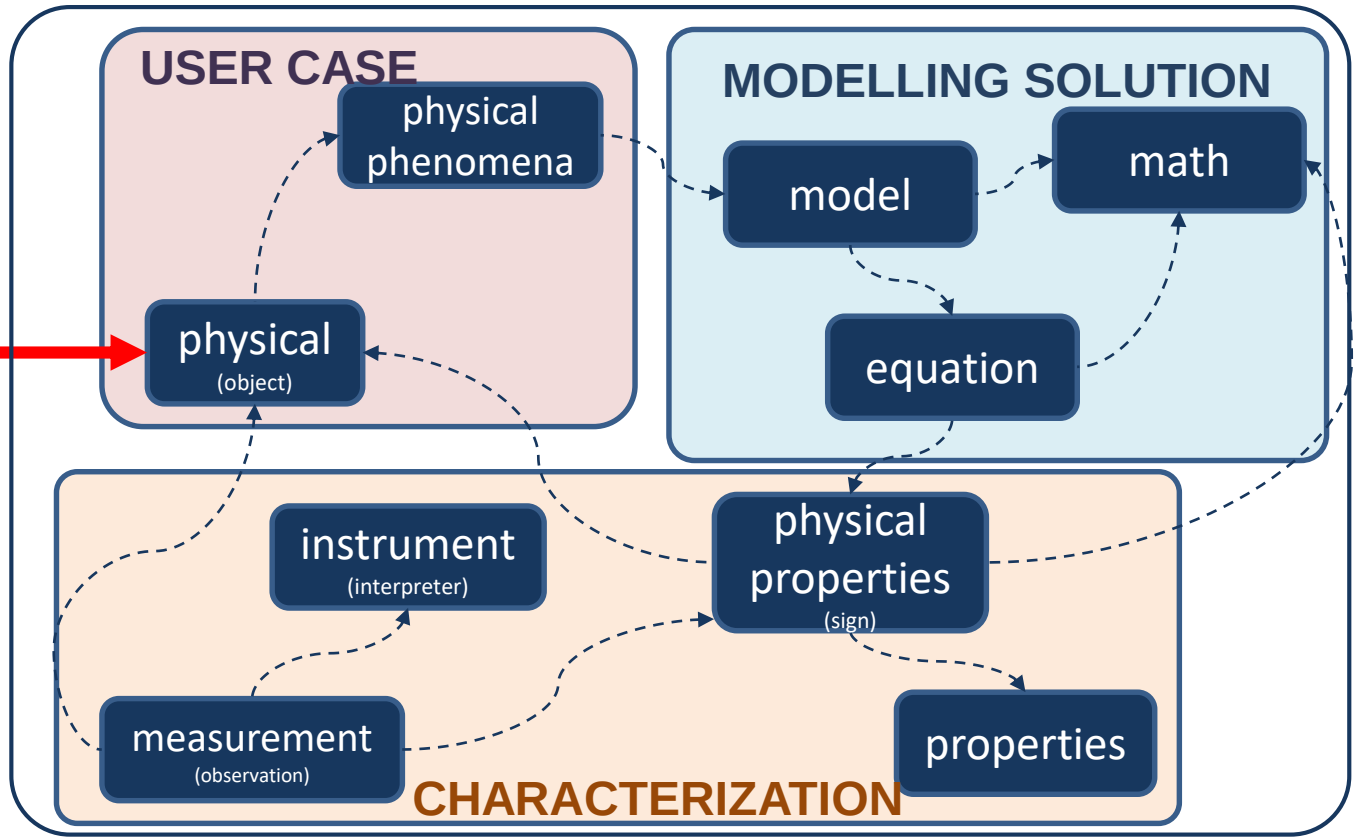
Horizontal interoperability: one user case, multiple modelling solutions.



real world entity

interpreter

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



Representation language and Implementation

- EMMO is implemented in OWL-DL (Description Logic)
- It draws on Mereotopology (MT) which is a First Order Logic (FOL) theory,
- FOL MT can be used as a tool at the EMMO 'Interpreter' level, to enable understanding what EMMO OWL entities stand for in the real world.
- Future work may develop a FOL version of EMMO.

- EMMO and EMMO python tools are available on: https://github.com/emmo-repo/EMMO
- More info: https://emmc.info/emmo-info/

European Materials Modelling Council

This project has received funding from the EU H2020 project:

EMMC-CSA H2020-NMPB-2016-2017 GA n. 723867