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UK Research and Innovation

**Establishing materials
modelling marketplaces:
From interoperability to
cooperation**

**EMMC International
Workshop**

3rd March 2021



VIMMP

VIRTUAL MATERIALS
MARKETPLACE

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existentialcomics.com, 2nd March 2021

Establishing materials modelling marketplaces: From interoperability to cooperation

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Virtual Materials Marketplace (VIMMP)



<http://vimmp.eu/>

- Horizon 2020 project
 - Innovation action, grant agreement *no.* 760907
 - H2020 (NMBP-25-2017)
 - 4 years project – started on 1st January 2018

Objective: To support accelerating innovation in manufacturing industries by using electronic, atomistic, mesoscopic, and continuum materials modelling.

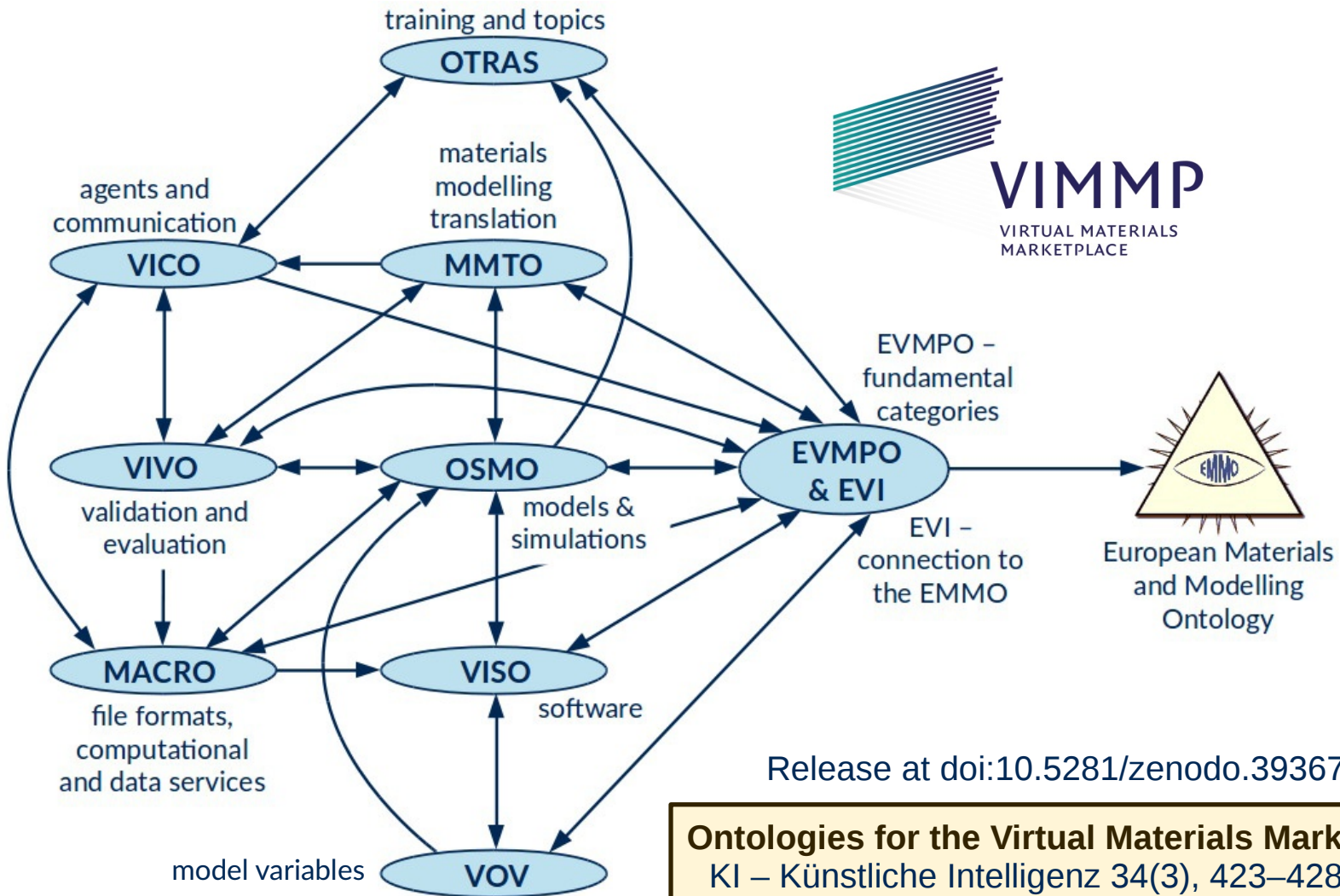
engineering challenges

modelling
& simulation

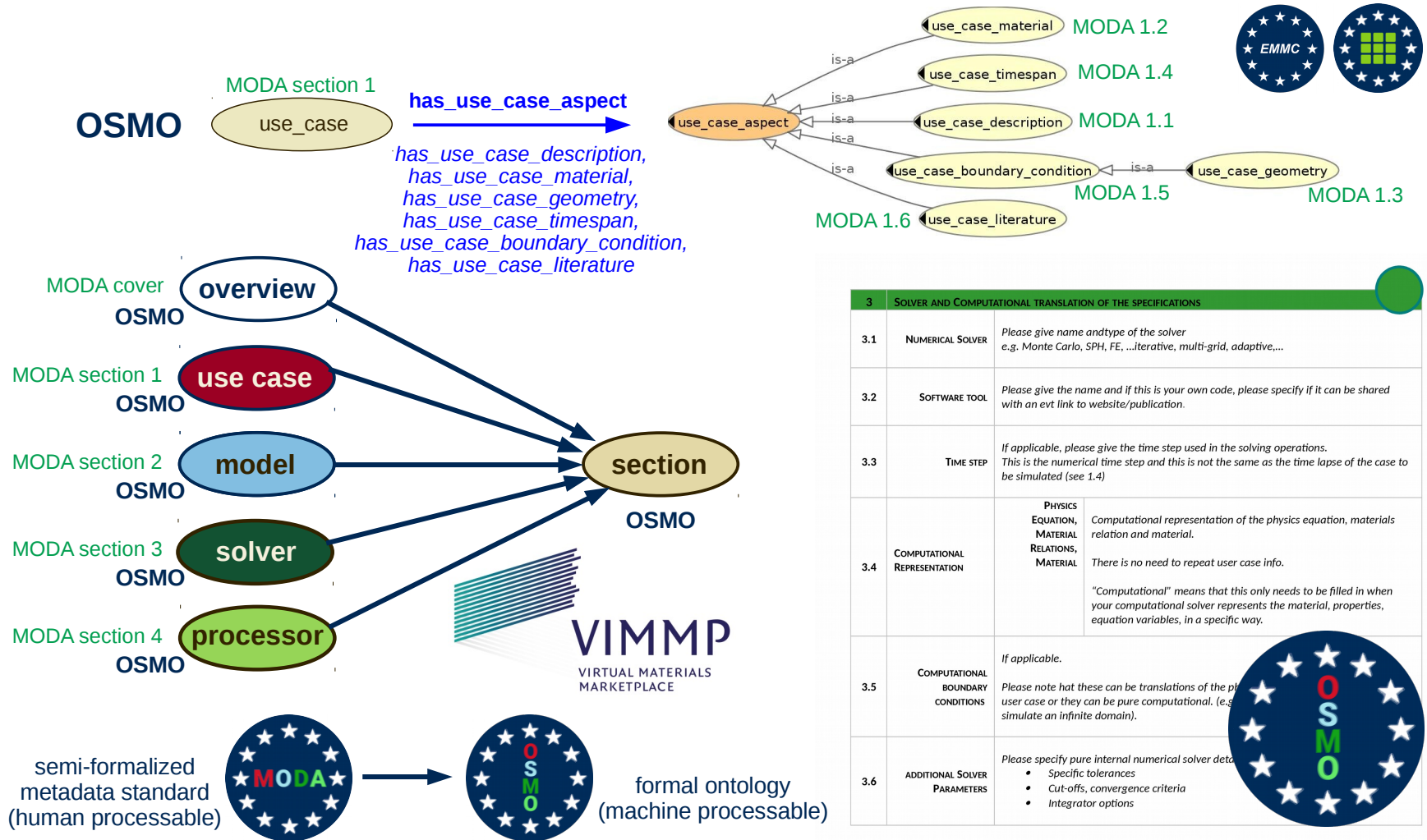
actionable decisions

materials modelling
“translation”

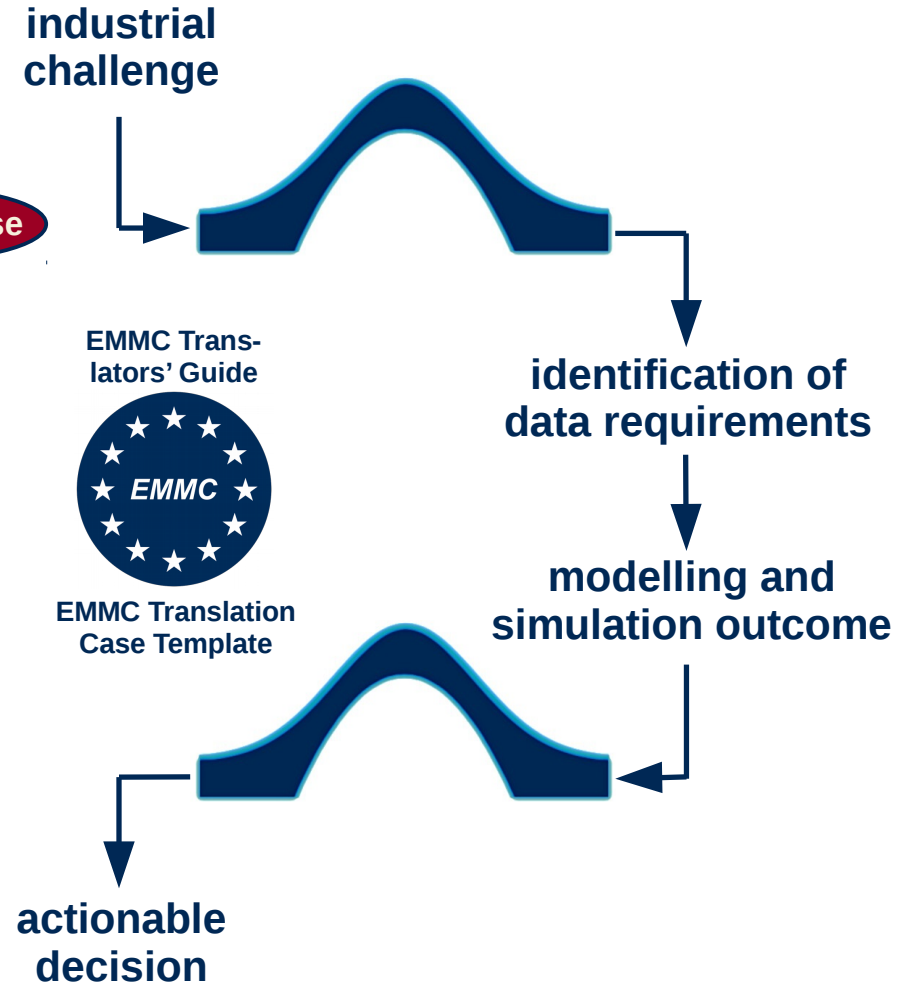
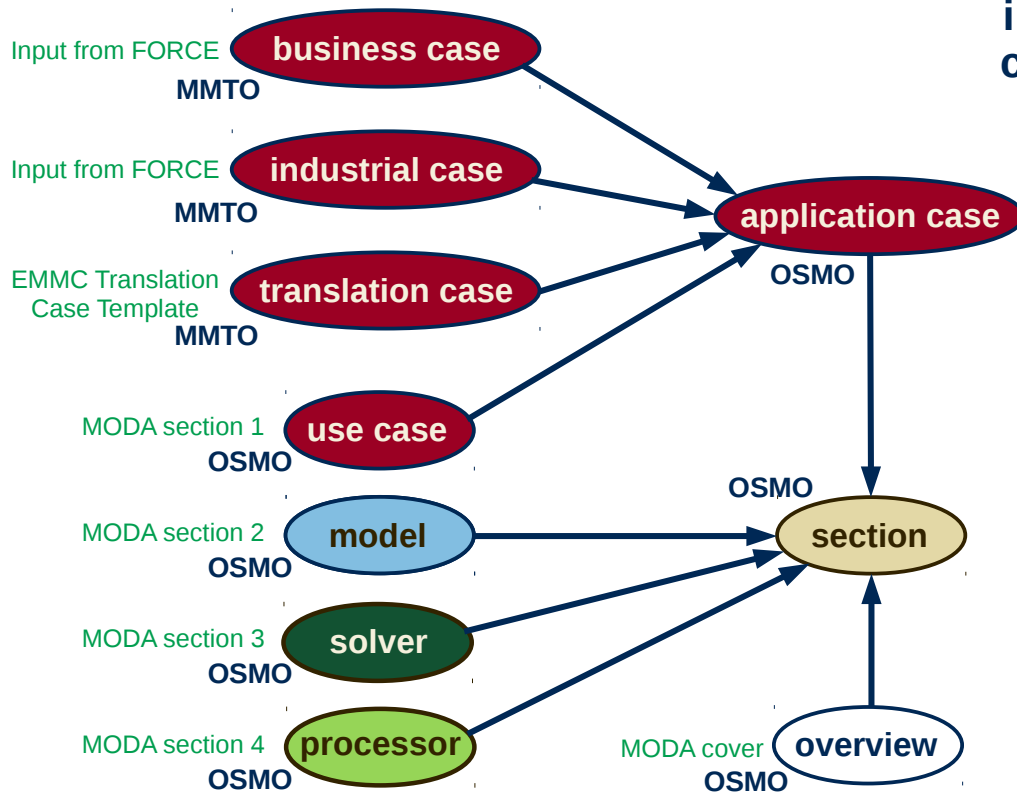
VIMMP system of marketplace-level domain ontologies



Provenance description of simulation results: OSMO



Materials Modelling Translation Ontology (MMTO)



M. T. Horsch, S. Chiacchiera, M. A. Seaton, I. T. Todorov, B. Schembera, P. Klein, N. A. Konchakova,
 "Pragmatic interoperability and translation [...],"
Proceedings of DAMDID/RCDL, 2020.

Alignment of domain ontologies with the EMMO

Relations covered by the European Materials and Modelling Ontology¹ (EMMO)

- 1) **Taxonomy**: Conceptual hierarchy (subclass relation)
- 2) **Semiotics**: Representation of physical entities by signs
- 3) **Mereotopology**: Spatiotemporal parthood and connectivity

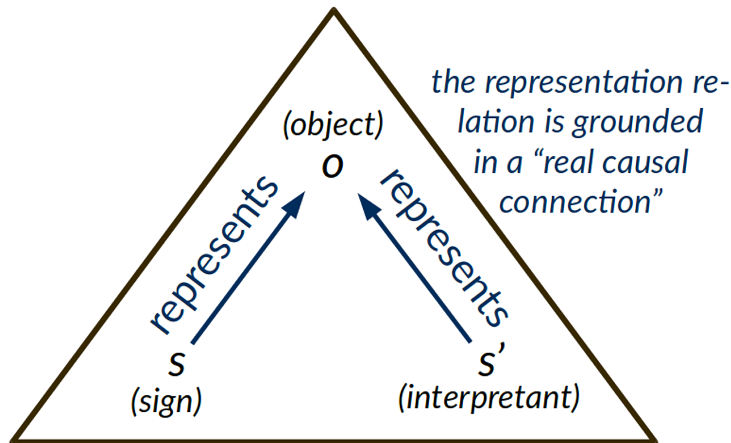
“represents” or “is sign for” will be abbreviated by **S**

semiosis



C. S. Peirce

Peircean semiotics

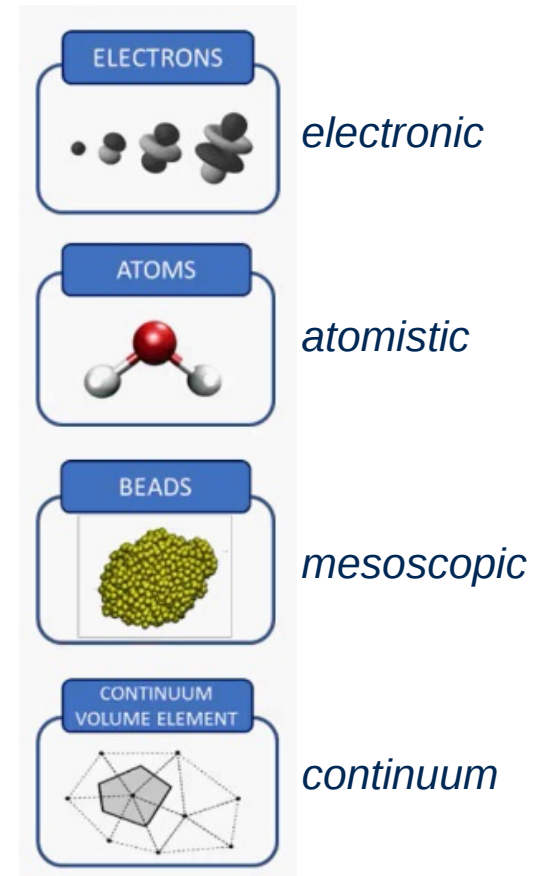
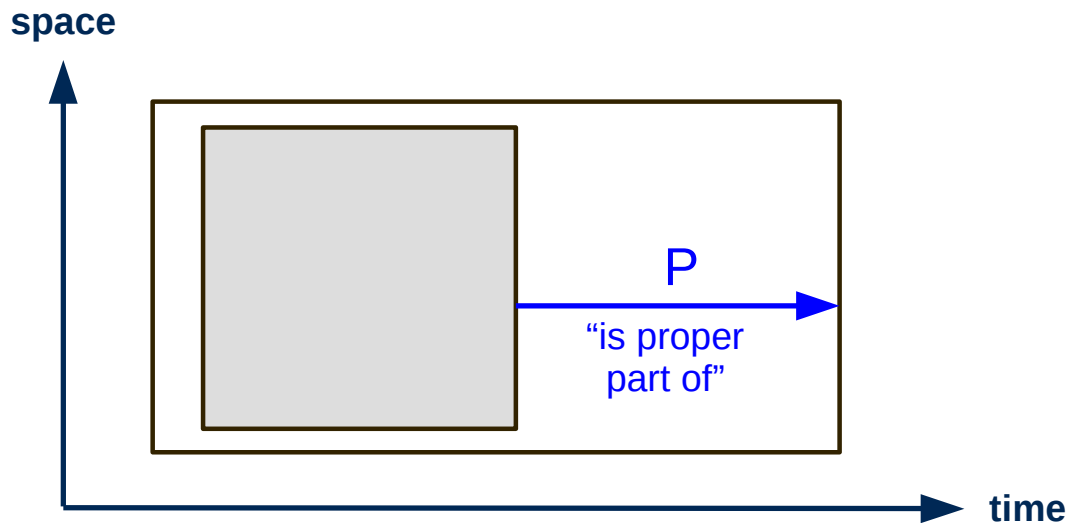


¹E. Ghedini, J. Friis, A. Hashibon, G. J. Schmitz, G. Goldbeck, *et al.*, 2020; <http://emmc.info/emmo-info/>.

Alignment of domain ontologies with the EMMO

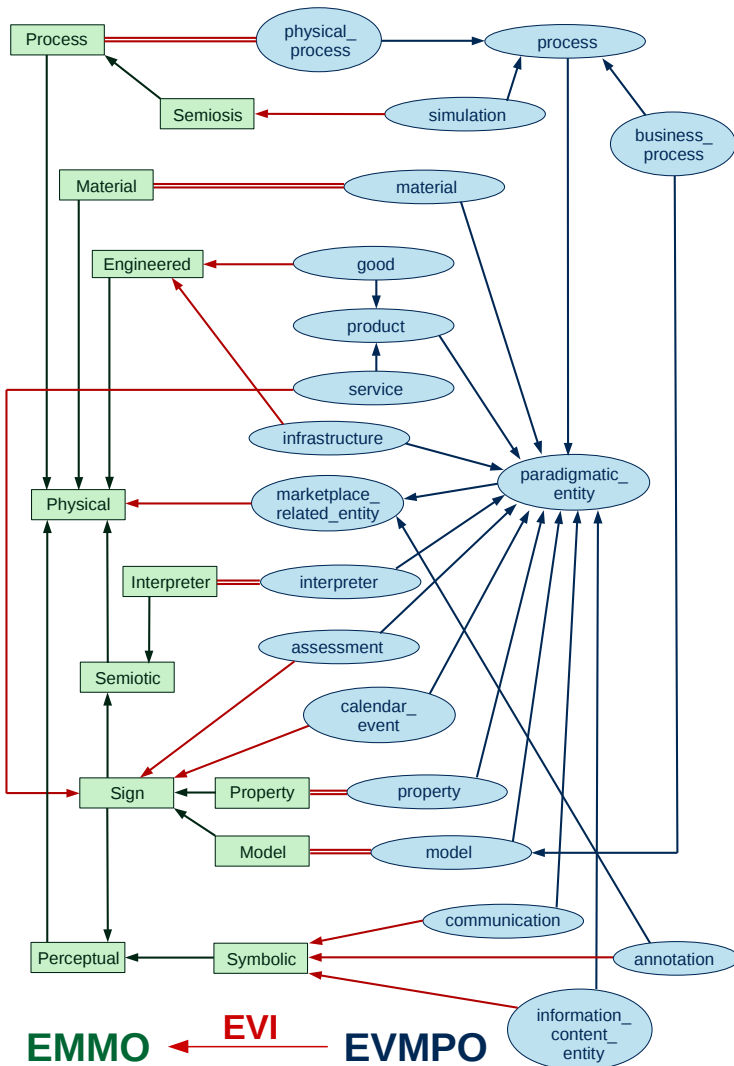
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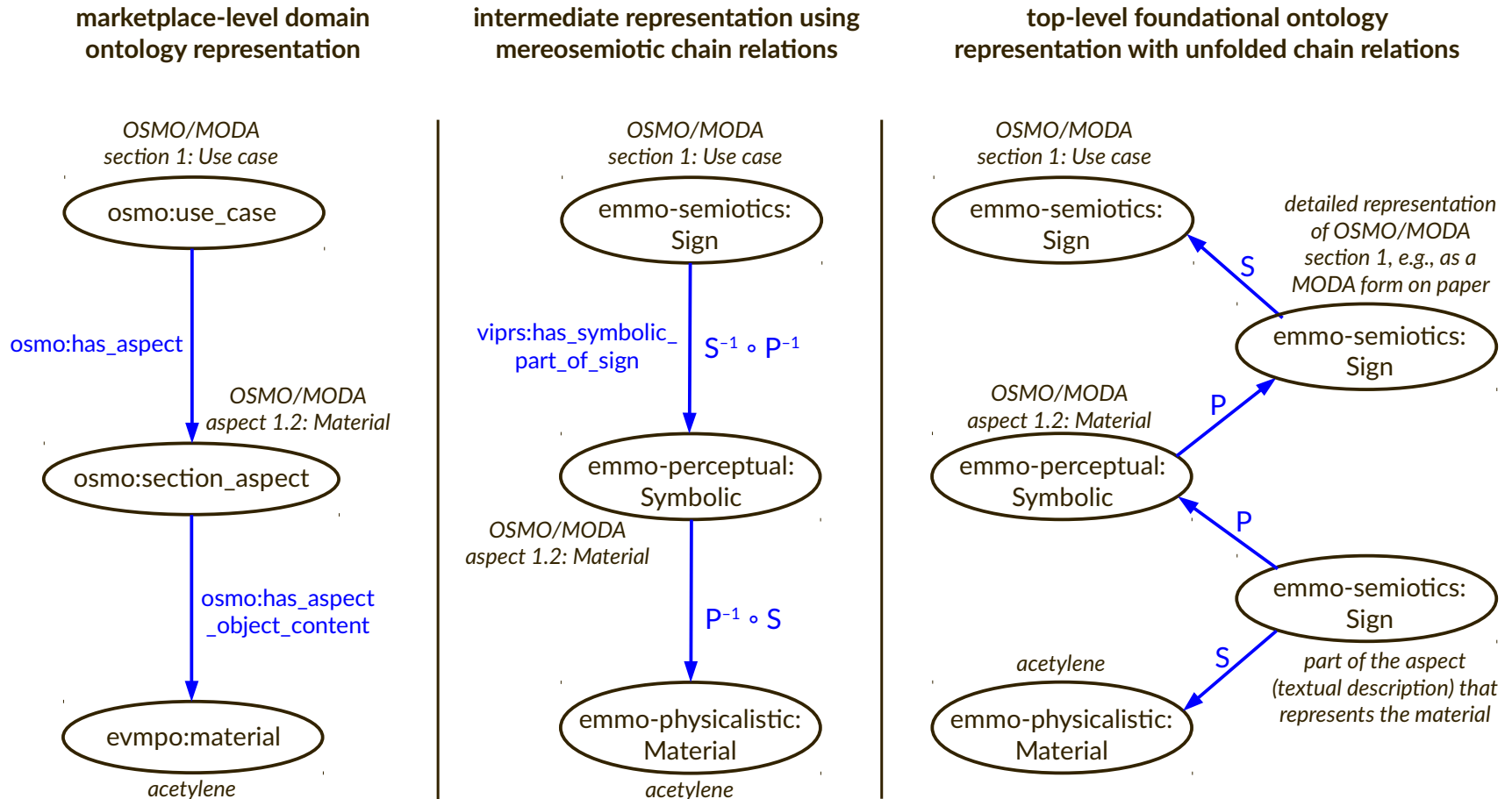
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Alignment of domain ontologies with the EMMO



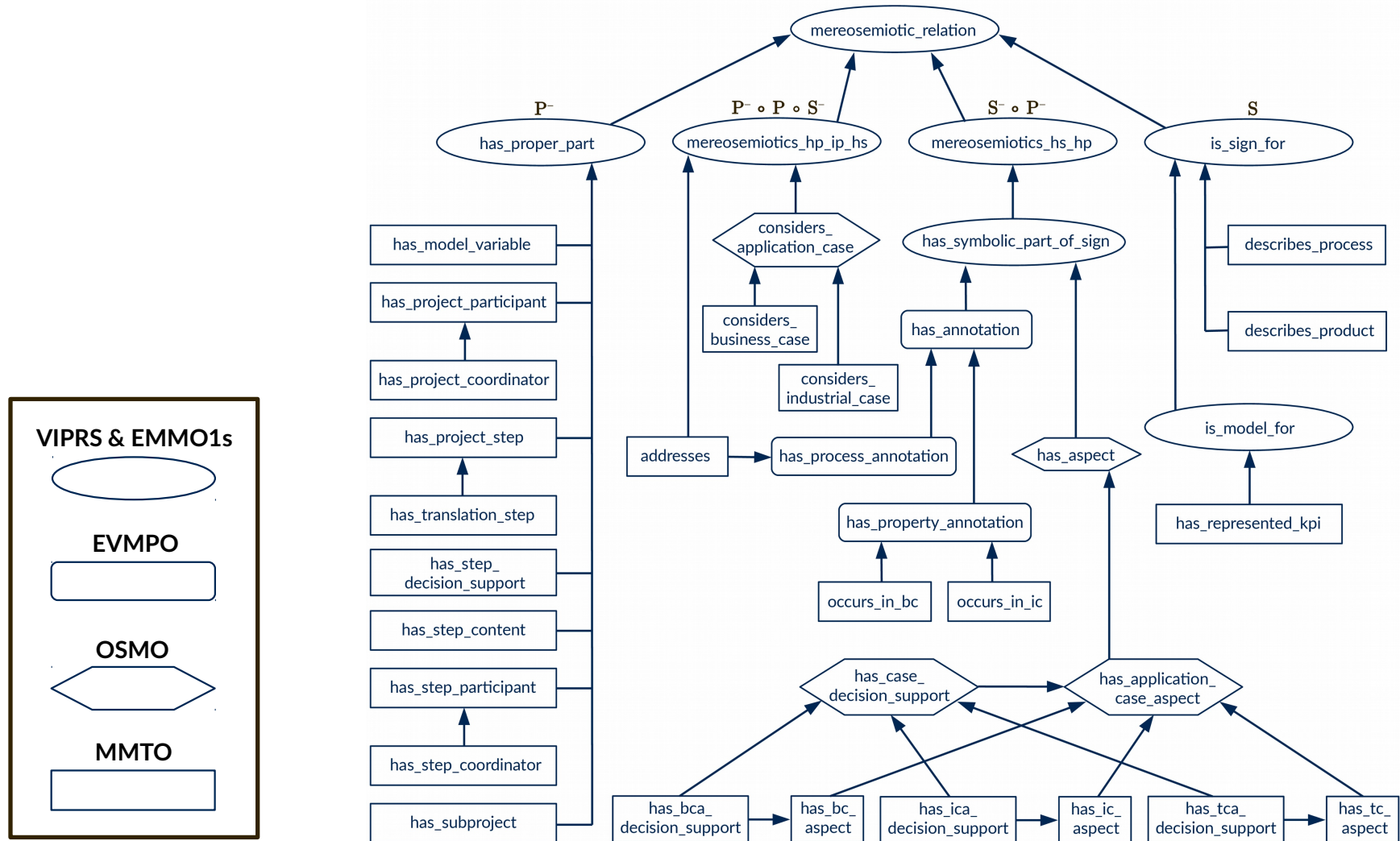
- (0) **annotation** (non-paradigmatic fundamental category), *i.e.*, anything in the knowledge graph that is not under (1) – (11)
- (1) **assessment**, *i.e.*, a proposition on accuracy or performance or an expression of trust
- (2) **calendar_event**, *i.e.*, a meeting or activity that is scheduled or can be scheduled; from W3C iCal ontology
- (3) **communication**, *i.e.*, a message or part of a message (*e.g.*, an attachment) that is communicated
- (4) **information_content_entity** from the Information Artifact Ontology; *e.g.*, a journal article, a data set, or a graph
- (5) **infrastructure**, *i.e.*, a digital platform infrastructure, *e.g.*, data access, hardware, or software
- (6) **interpreter**, *i.e.*, an item that can carry out a semiosis, as formalized by Peirce & the EMMO, creating an interpretant
- (7) **material**, *i.e.*, an amount of substance & part of an object
- (8) **model**, *i.e.*, a representamen that represents an object by direct similitude or within a mathematical framework
- (9) **process**, *i.e.*, temporal evolution of one or multiple entities
- (10) **product**, *i.e.*, a good or service that can be traded
- (11) **property**, *i.e.*, a representamen that is determined as an interpretant by observation, involving a specific observer

Alignment of domain ontologies with the EMMO¹

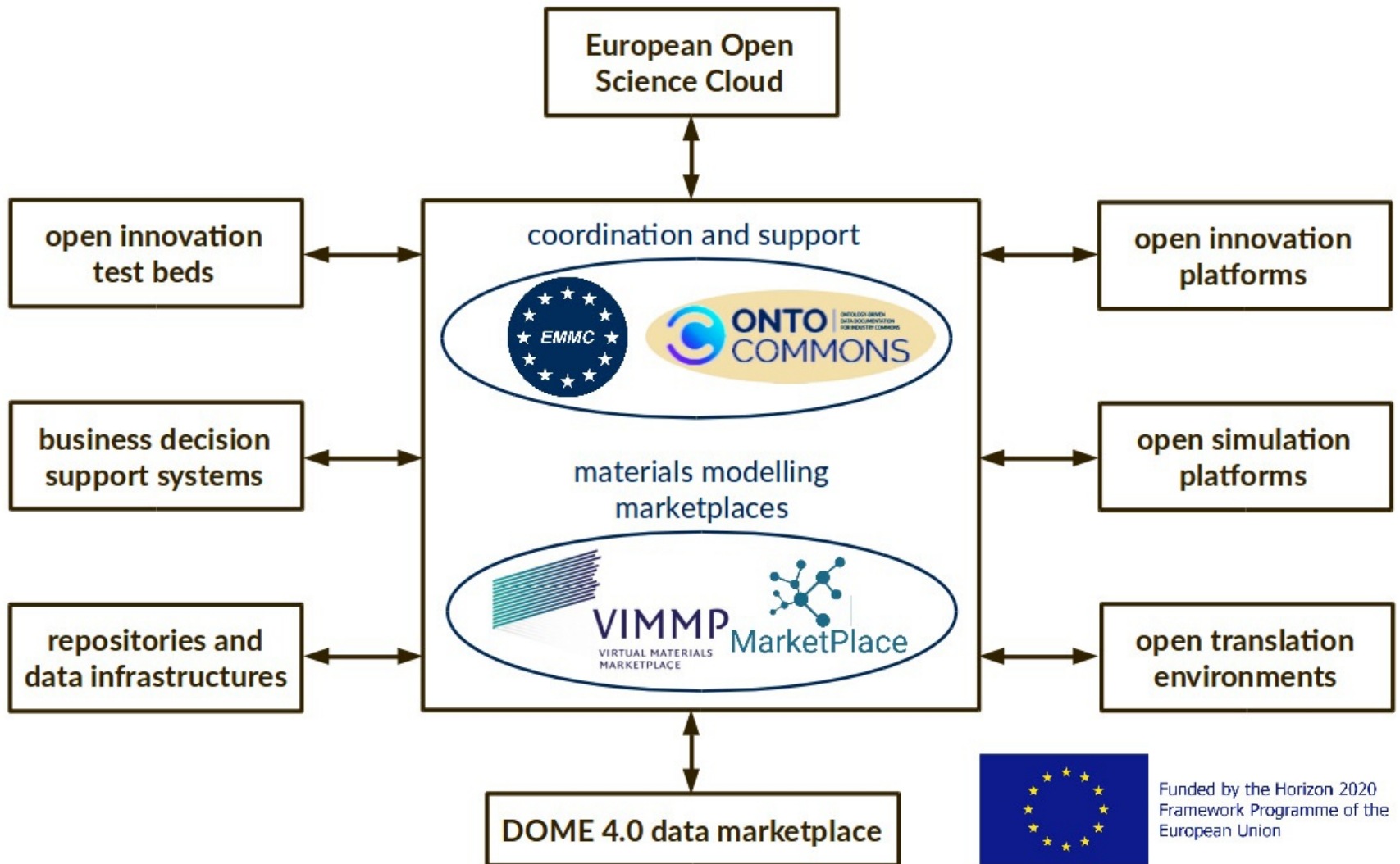


¹M. T. Horsch, S. Chiacchiera, W. L. Cavalcanti, B. Schembera, *Data Technology in Materials Modelling*.

Alignment of domain ontologies with the EMMO



From interoperability to cooperation



From interoperability to cooperation

1) What does it actually mean?

It could be a common interface, that allows users to do **simultaneous queries** of the databases (getting info) and/or **simultaneous posts** (putting info). It involves different levels:

- **Business level** - “How do users register/get access?”
- **Technical level** - “How can users do queries? And posts?”

Beside a GUI (for manual upload and search), the VIMMP database will be accessible via a REST API. The metadata are typically exchanged in JSON(-LD) format.

- **Content level** - “What can users look for?”

Depends on which type of data is stored, what properties are given in each marketplace/database.

2) What is the current status?

Hard to say, since many H2020 projects are working in this line (some just started), but platforms are not fully developed yet.

From interoperability to cooperation

3) Proposals? Focusing on the content level:

- Building on the EVMPO idea: **Agree** on a minimal set of concepts for which data will be stored and visible in the API. E.g., “translator” profiles, including “topic of expertise”.
- Otherwise (or for legacy work) provide a sort of **mediation schema**: A third model, with mappings to the two to be integrated.

4) Advantages?

The usual ones of interoperability, e.g., broader audience, better user/provider experience.

5) Difficulties and risks

Inter-project interactions are not straightforward, for legal reasons and due to timelines.

6) Discussion

How do we proceed? Can a task group be formed for this purpose?

Suggestion: Agree on a time for meeting in the lobby to discuss task group formation.

DORIC-MM 2021 workshop

Domain Ontologies for RDM in Industry Commons of Materials and Manufacturing

<https://ontocommons.eu/doric-mm-2021>

The banner is split into two main color sections: a dark blue left side and an orange right side. On the blue side, the 'ONTO COMMONS' logo is at the top left, with the tagline 'ONTOLOGY-DRIVEN DATA DOCUMENTATION FOR INDUSTRY COMMONS' to its right. Below this, a purple pill-shaped button contains the text 'ONLINE WORKSHOP', and a white pill-shaped button below it says '7 June 2021 - Full day'. The main title 'DORIC-MM 2021' is written in large, bold, white letters. At the bottom left, there are social media icons for Twitter and LinkedIn, with the text 'Follow us on' to their left. A white pill-shaped button at the bottom right of the blue section says 'SAVE THE DATE!'. On the orange side, there is a white rounded rectangle containing a blue icon with a laurel wreath, a factory, and a bar chart, with the text 'DORIC-MM 2021' below it. Underneath this is the 'ONTO COMMONS' logo and tagline, and at the bottom is the 'ESWC21' logo, which consists of a blue triangle with a white 'A' shape inside.

deadline extended – submit now (three to 16 pages)

Upcoming CECAM school supported by VIMMP



Simulation Workflows in Materials Modelling (SWiMM 2021)

15th – 26th March 2021
(digital event)

<https://www.cecama.org/workshop-details/27>

1. Industrial-accuracy data-driven model parameterization
2. Semantic interoperability and ontology-driven technology
3. Autotuning, load balancing, and task based parallelization
4. Salome and YACS: An integration platform for workflows
5. Simulation workflows with AiiDA and Materials Cloud
6. European Materials and Modelling Ontology
7. The Pyiron IDE for simulation workflows
8. preCICE multi-physics coupling library
9. Atomic Simulation Environment





Science and Technology Facilities Council

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