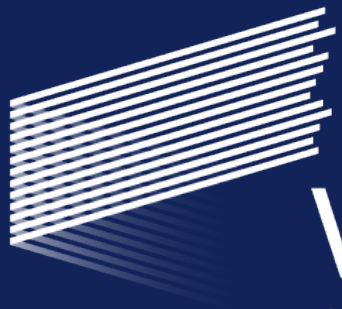
Martin T. Horsch, Silvia Chiacchiera,
Michael A. Seaton, Ilian Todorov
STFC Daresbury Laboratory
UK Research and Innovation

Ontology-based pragmatic interoperability between open platforms in materials modelling



VIMMP
VIRTUAL MATERIALS MARKETPLACE

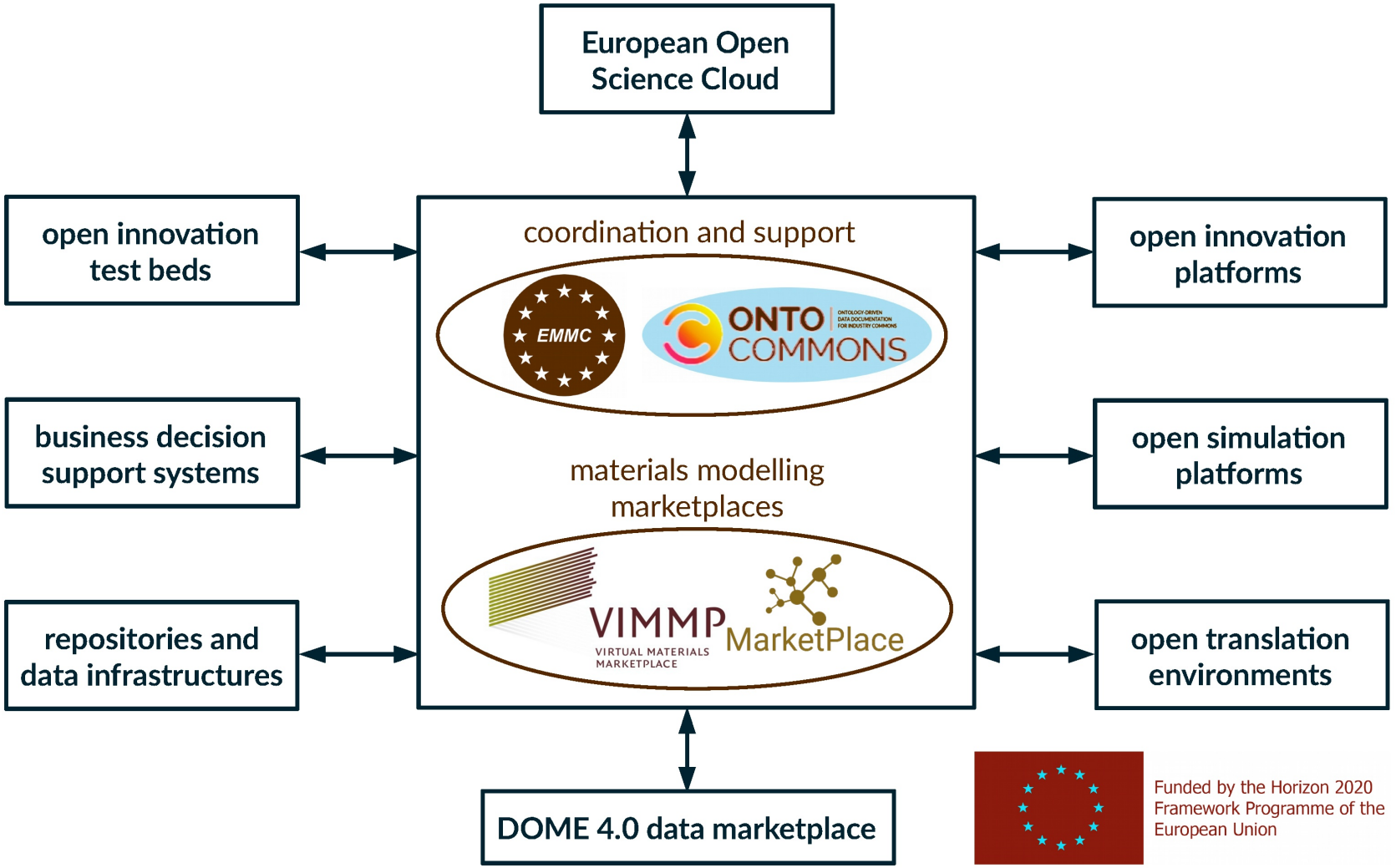
22nd September 2020

MSE Congress

Science and Technology Facilities Council

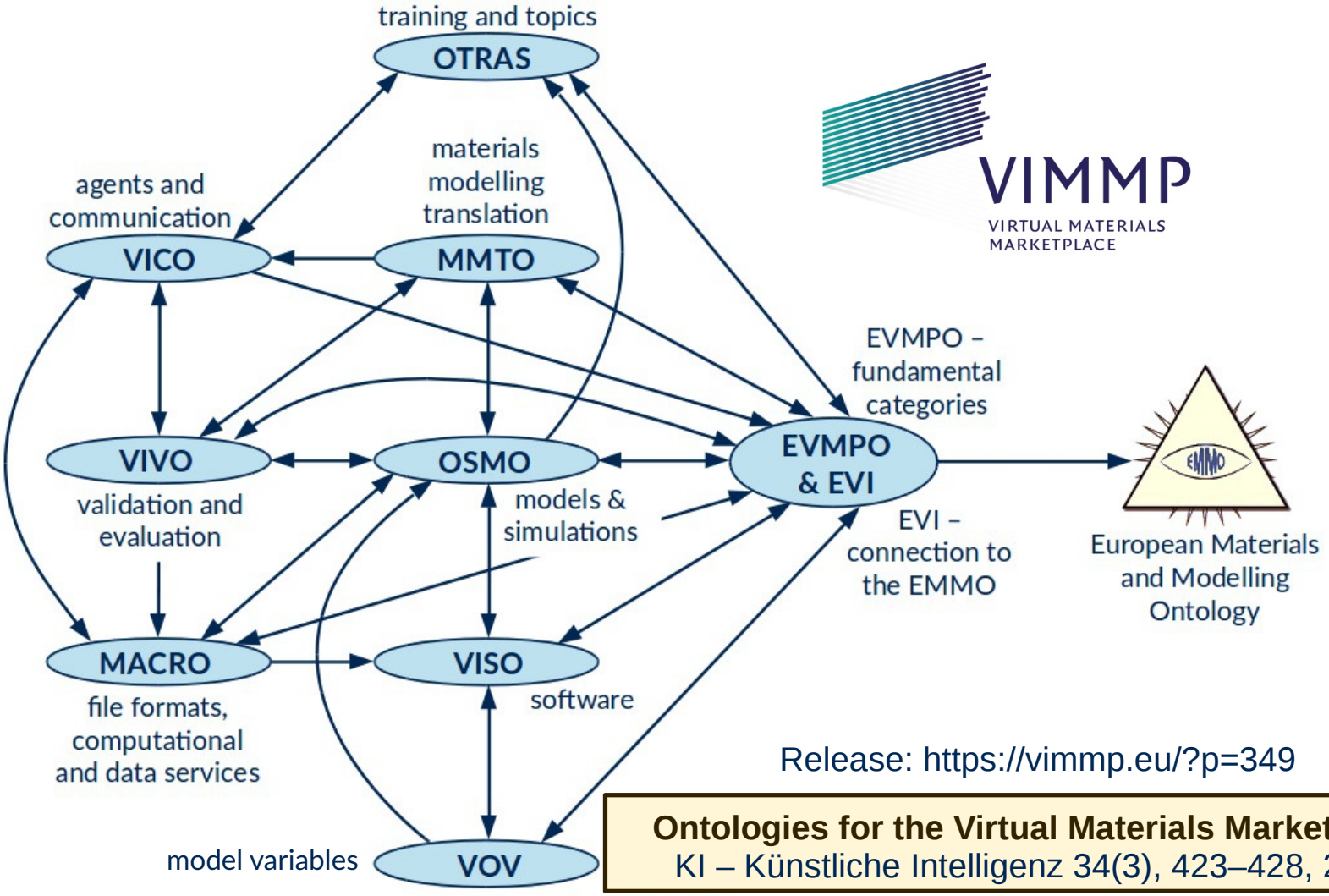
VIMMP
VIRTUAL MATERIALS MARKETPLACE

European digital platforms in materials modelling



Funded by the Horizon 2020 Framework Programme of the European Union

European digital platforms in materials modelling



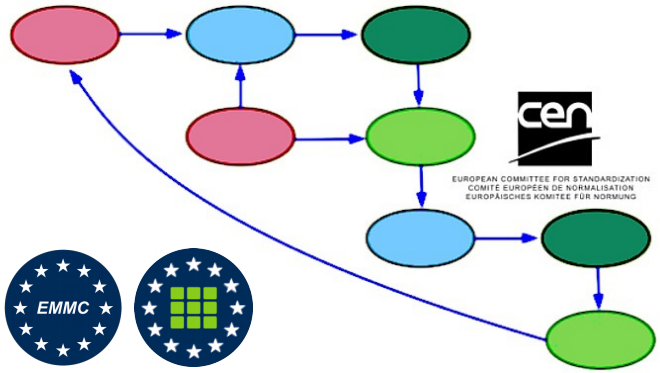
Release: https://vimmp.eu/?p=349

Ontologies for the Virtual Materials Marketplace
KI – Künstliche Intelligenz 34(3), 423–428, 2020

Provenance description of simulation results

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 would have been calculated by another model should not be included (but 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 van be documented here.*
1.2	Material	*Describe the chemical composition, ...and the values used for properties and from which database these are taken. If pre-processing was needed please specify the methodology.*
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 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).* *These can be boundary, initial and global conditions.* *E.g. heated walls, external pressures and bending forces.* *Please note that these might appear as terms in the PE or as boundary conditions, and this will be documented in the relevant chapters.* *Note: These conditions will be expressed in physics relations in Ch 2.4* *Please specify the values used for parameters and from which database these are taken. If pre-processing was needed please specify the methodology.*
1.6	Publication on this data	*Publication documenting the simulation with this single model (if available and if not already included in the overall publication).*

MODA workflow description



MODA section 1 — use case

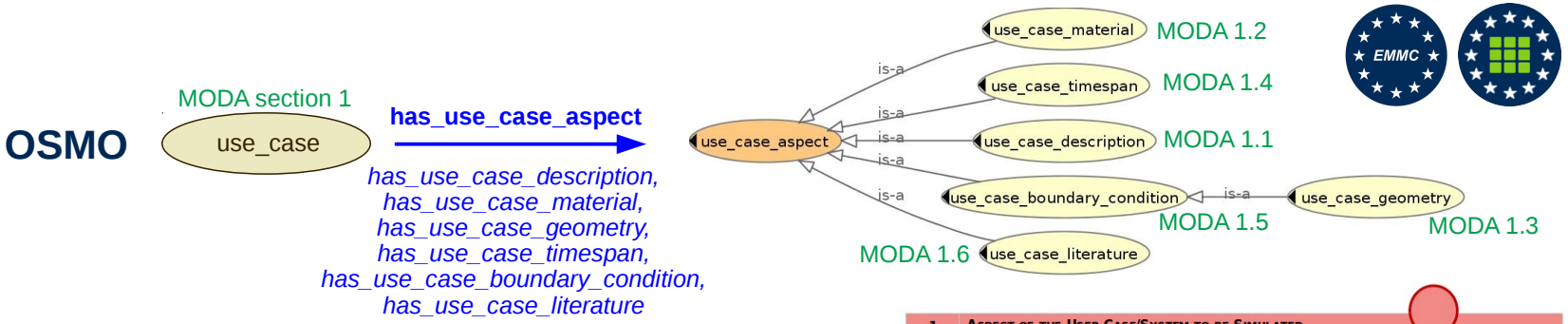
MODA section 2 — model

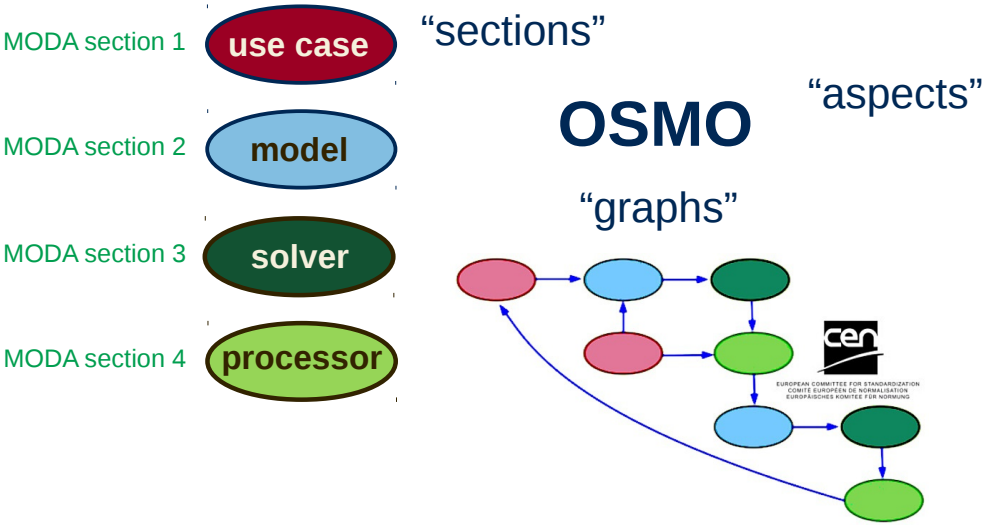
MODA section 3 — solver

MODA section 4 — processor

MODA

Provenance description of simulation results





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Ontology for Simulation, Modelling, and Optimization
J. Chem. Eng. Data 65(3), 1313–1329, 2020

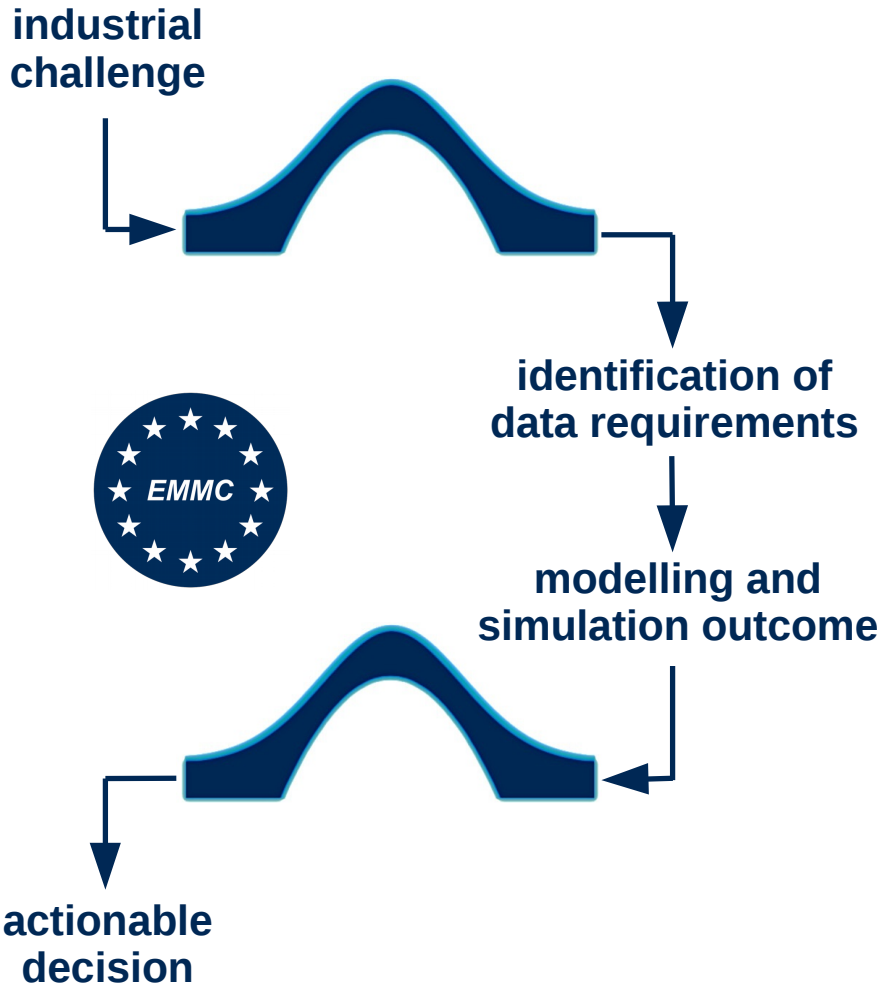
Translation in materials modelling

INPRODAT

Task: Facilitate the translation of industrial R&D challenges into solutions using scalable and quantitatively reliable materials modelling and simulation.

Pragmatic interoperability and translation of industrial engineering problems into modelling and simulation solutions

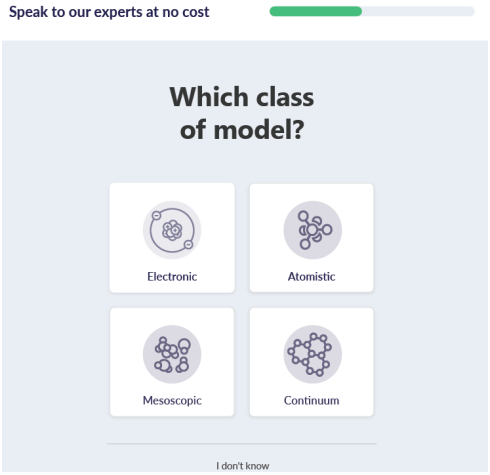
DAMDID 2020, doi:10.5281/zenodo.3949803

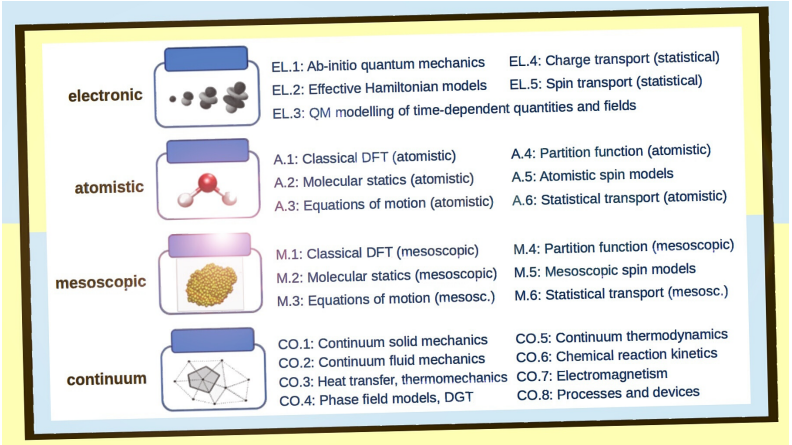


VIMMP ontology-based translation router

mm_topic_basic (codes **1XXX** and **2XXX**):
Basic prerequisites for materials modelling.
mm_topic_computational (codes **3XXX**):
Computational and numerical aspects of materials modelling.
mm_topic_data (codes **4XXX**):
Data science and technology aspects.
mm_topic_materials (codes **5XXX**):
Topics related to fluid and solid materials.
mm_topic_social (codes **6XXX**):
Social, economic, and community aspects.
mm_topic_theoretical (codes **7XXX**):
Theory (non-computational aspects).
mm_topic_interdisciplinary (codes **8XXX**)
mm_topic_side (codes **9XXX**):
Topics from other disciplines.

- 3100, 7100 electronic
  - 3120, 7120 physical equation EL.1
  - 3130, 7130 physical equation EL.2
  - *etc.*
- 3200, 7200 atomistic and mesoscopic
  - 3220, 7220 equations A.1 and M.1
    - 3222, 7222 physical equation A.1
    - 3225, 7225 physical equation M.1
  - 3230, 7230 equations A.2 and M.2
    - *etc.*
  - *etc.*
- 3300, 7300 continuum
  - 3320, 7320 physical equation CO.1
  - 3330, 7330 physical equation CO.2
  - *etc.*





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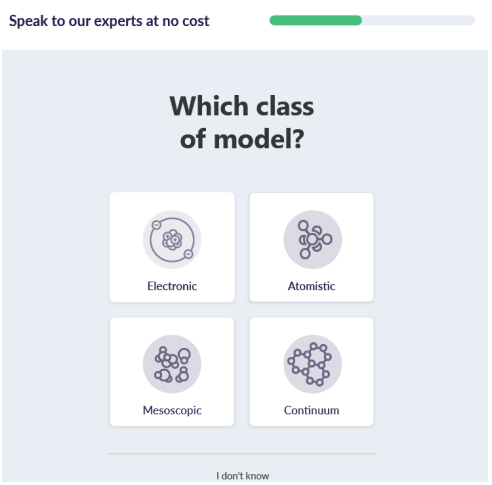
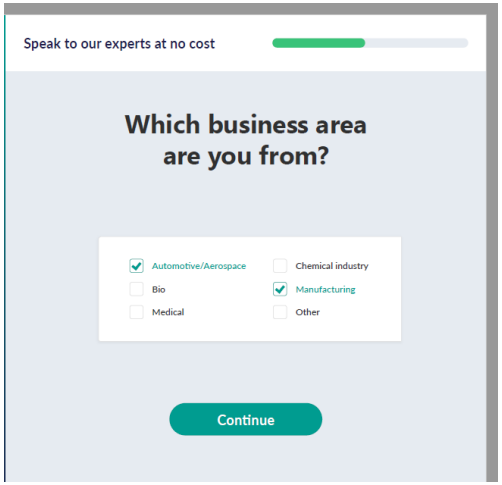
mm_topic_side (codes **9XXX**):
Topics from other disciplines.

under 61XX: industrial

- 6120 chemical
- 6130 petrochemical
- 6140 transport
  - 6142 aerospace
  - 6144 automotive
  - 6148 railway
- 6150 biotechnology
- 6155 food
- 6160 medicine
- 6165 paper
- 6170 electrical
- 6175 machinery
- 6180 metal (basic and fabricated)
- 6190 special topics





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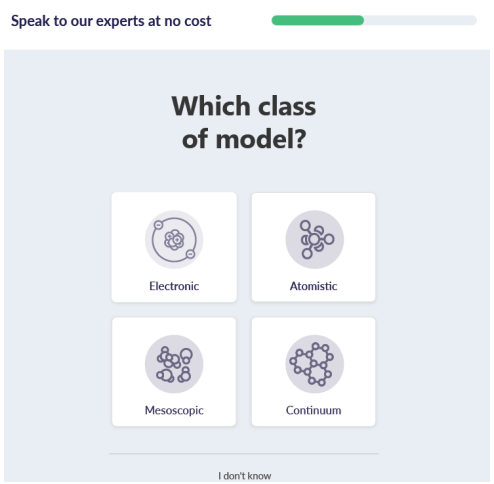
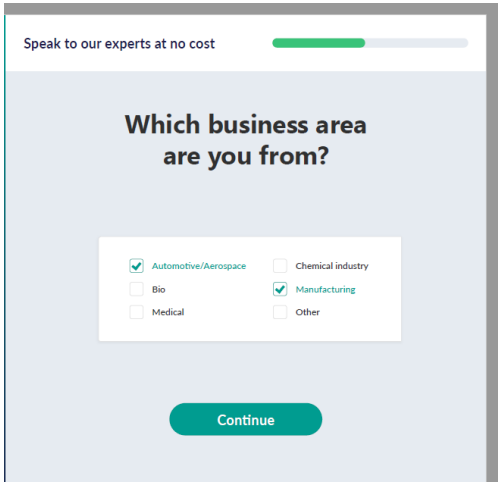
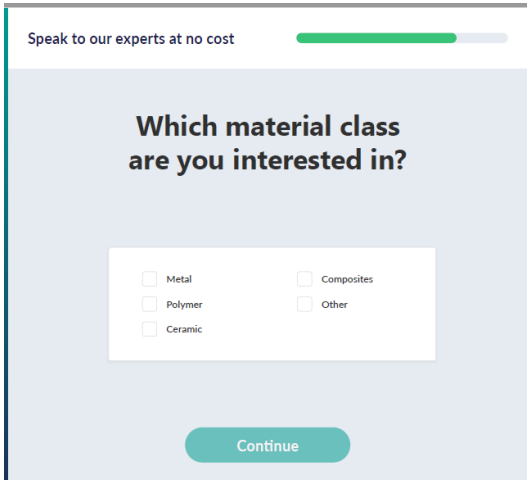
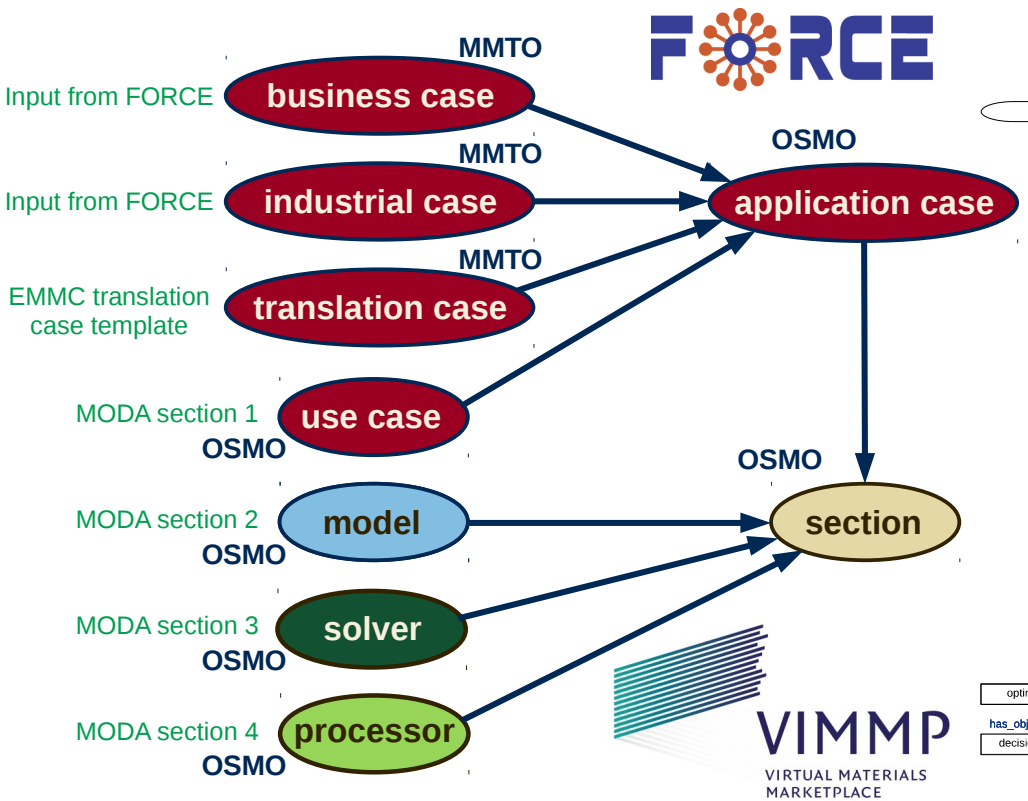
5100 general
5200 fluid
5300 bio
5350 ceramic
5400 composite
5450 electrolyte
5500 metal
5550 mineral
5600 nano
5650 organic
5700 polymer
5750 semiconductor
5800 ultracold
5850 unstable
5900 special topics

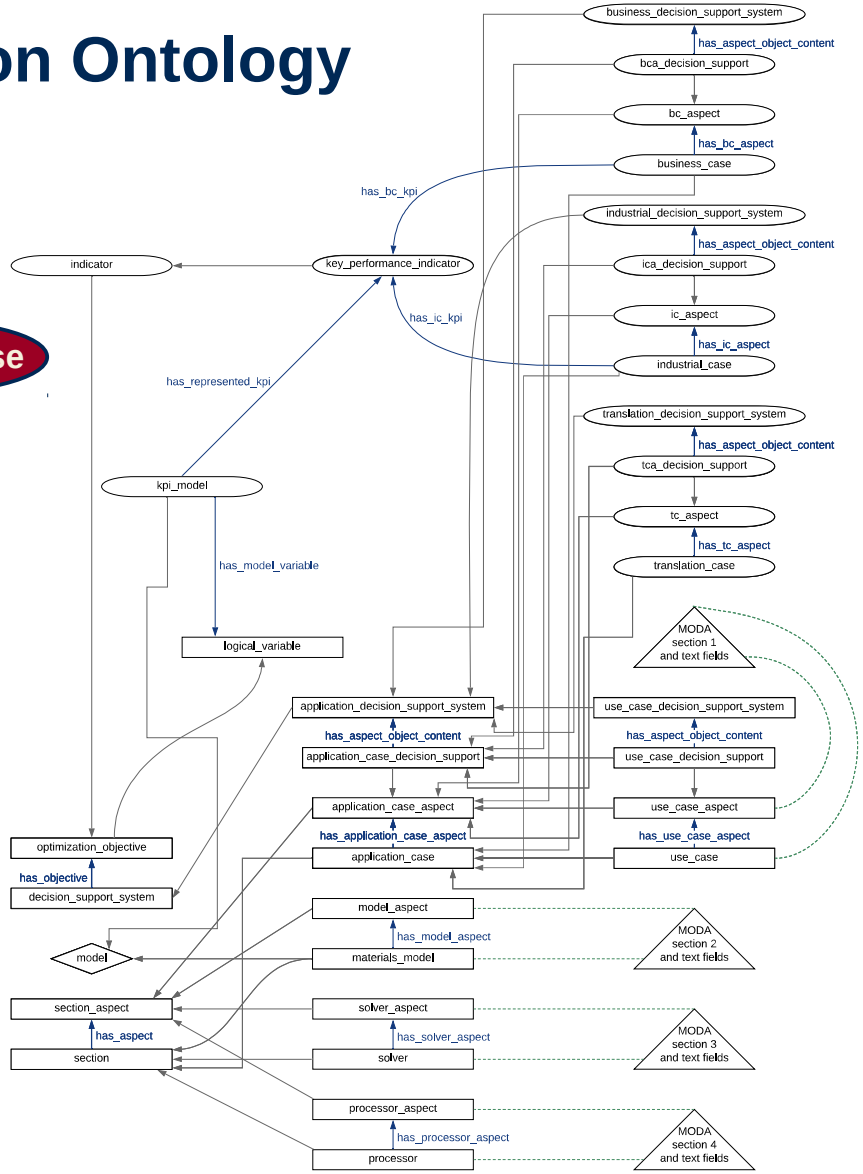






Materials Modelling Translation Ontology

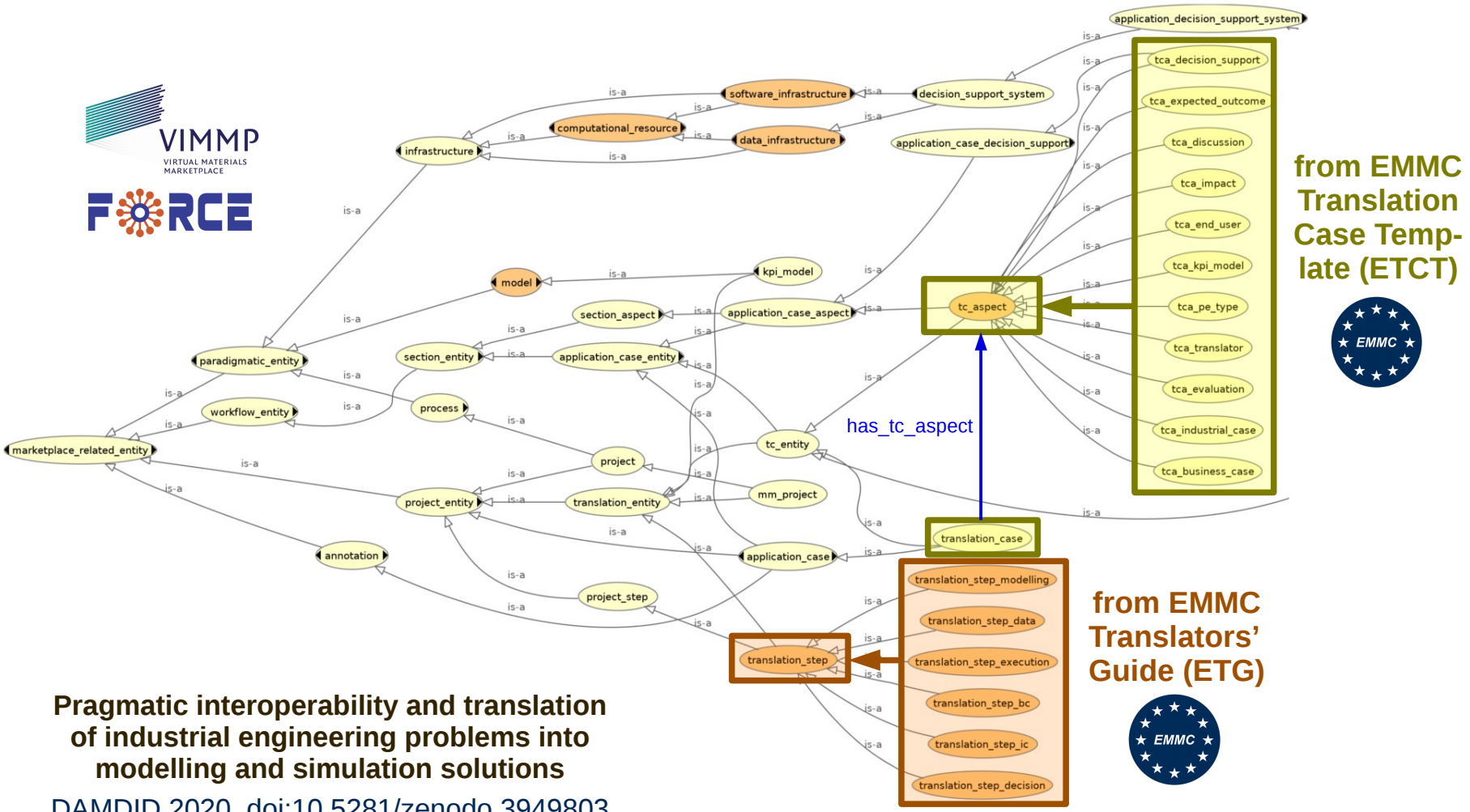




Pragmatic interoperability and translation of industrial engineering problems into modelling and simulation solutions

DAMDID 2020, doi:10.5281/zenodo.3949803

Materials Modelling Translation Ontology



Pragmatic interoperability and translation of industrial engineering problems into modelling and simulation solutions

DAMDID 2020, doi:10.5281/zenodo.3949803

EVMPO: Agreed and jointly used by MarketPlace+VIMMP

Fundamental paradigmatic categories:

(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

The EVMPO provides a structure for the marketplace-level ontologies by formulating **fundamental paradigmatic categories** that correspond to irreducible terms which are seen as constitutive to the virtual-marketplace paradigm.

Relations defined in the EVMPO: **has_annotation** & subproperties (has_assessment_annotation etc.) with **annotation** as the fundamental non-paradigmatic category.

Conceptual EMMO alignment

(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

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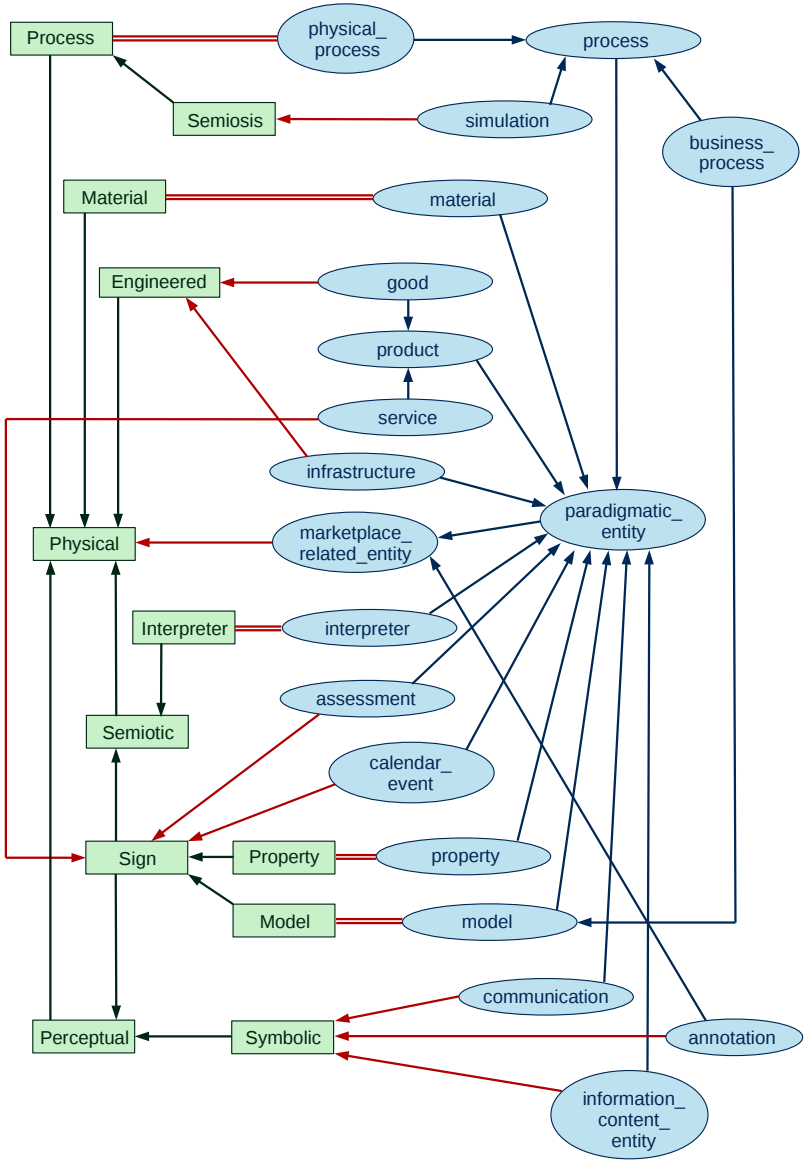
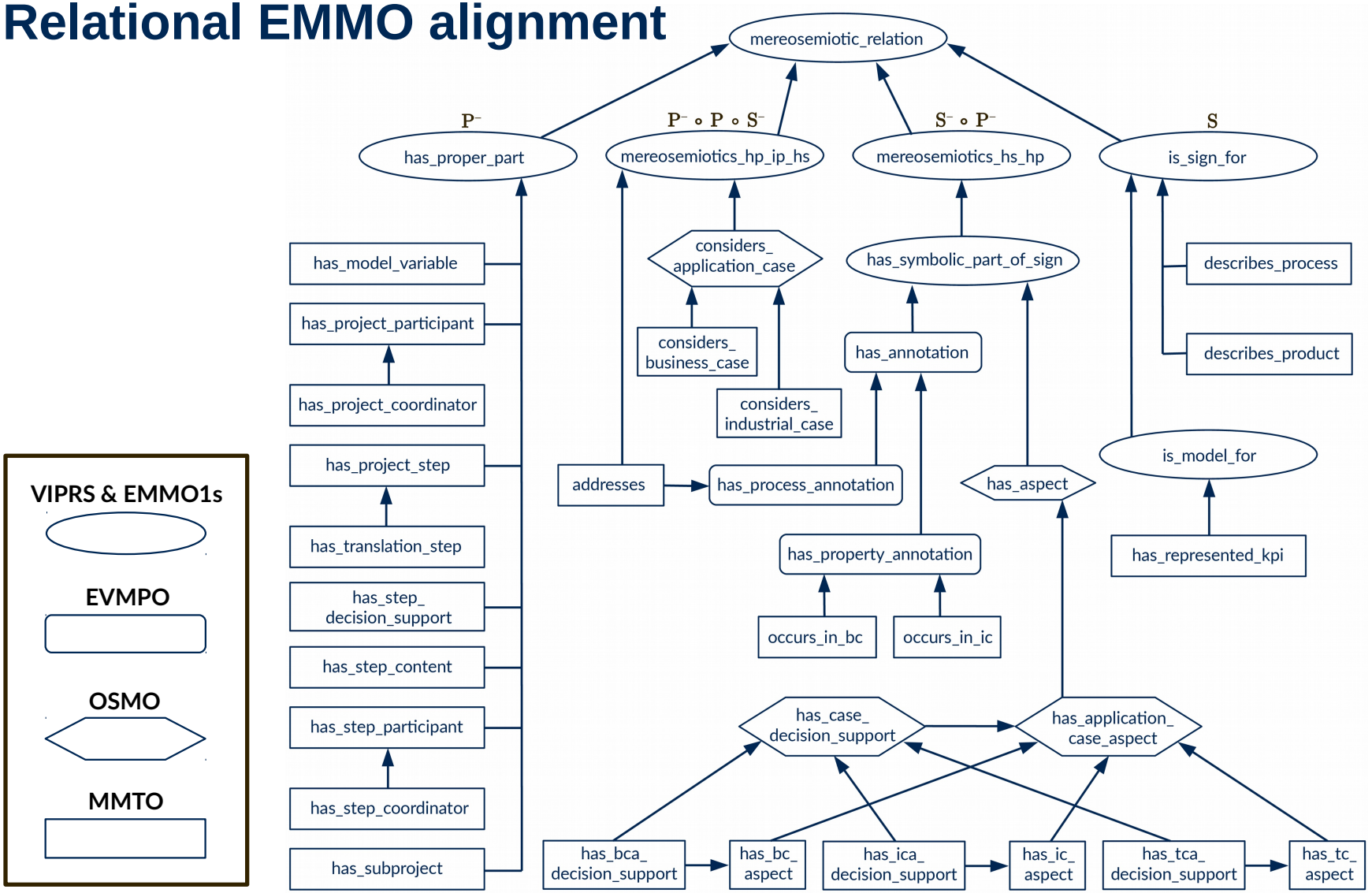
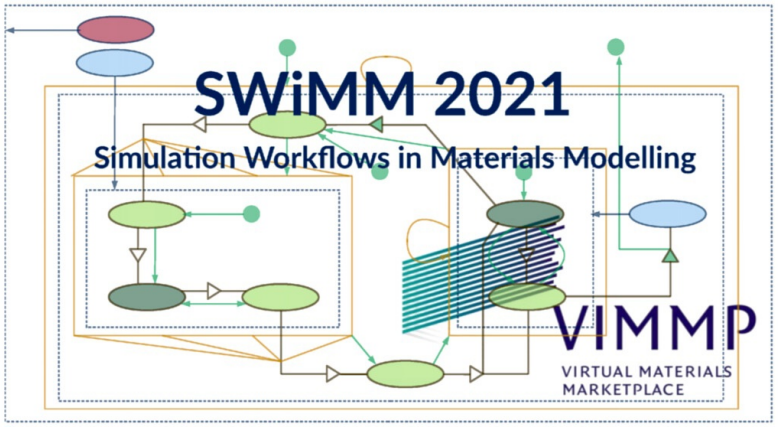


Relational EMMO alignment



Announcement: CECAM school on simulation workflows



Simulation Workflows in Materials Modelling

15th – 19th March 2021

CECAM HQ
École Polytechnique Fédérale de Lausanne

https://www.cecam.org/workshop-details/27

cecam
Centre Européen de Calcul Atomique et Moléculaire

1. Salome and YACS: An integration platform for workflows
2. Industral-accuracy data-driven model parameterization
3. Autotuning, load balancing, and task based parallelization
4. Semantic interoperability and ontology-driven technology
5. Harnessing EMMO towards applications
6. The Pyiron IDE for simulation workflows
7. The atomic simulation environment Python library
8. Complex workflows with AiiDA and Materials Cloud

Science and Technology Facilities Council

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement no. 760907.

VIMMP
VIRTUAL MATERIALS MARKETPLACE

Join and support the EMMC work on digitalization!

https://emmc.eu/

European Materials Modelling Council (EMMC ASBL)

The non-profit association EMMC ASBL was created in 2019 to ensure the continuity, growth, and sustainability of community activities for modellers, materials data scientists, software owners, materials modelling translators, and manufacturers in Europe. The EMMC regards the **integration of materials modelling and digitalization** as critical for an advancement of industrial process and product design.

EMMC Focus Area on Digitalization

In computational engineering, digitalization encompasses aspects of representing, managing, accessing, and utilizing digital information about products, components, materials, their behaviour, and their processing.