M. Horsch, S. Chiacchiera, **UK Research and Innovation**,
G. Mogni, D. Toti, G. Goldbeck, **Goldbeck Consulting**,
P. Schiffels, and W. Cavalcanti, **Fraunhofer IFAM**

Semantic interoperability based on the European Materials and Modelling Ontology

13th January 2021

ECCOMAS 2020/21

VIMMP
VIRTUAL MATERIALS MARKETPLACE

Science and Technology Facilities Council

VIMMP
VIRTUAL MATERIALS MARKETPLACE

Virtual Materials Marketplace (VIMMP)

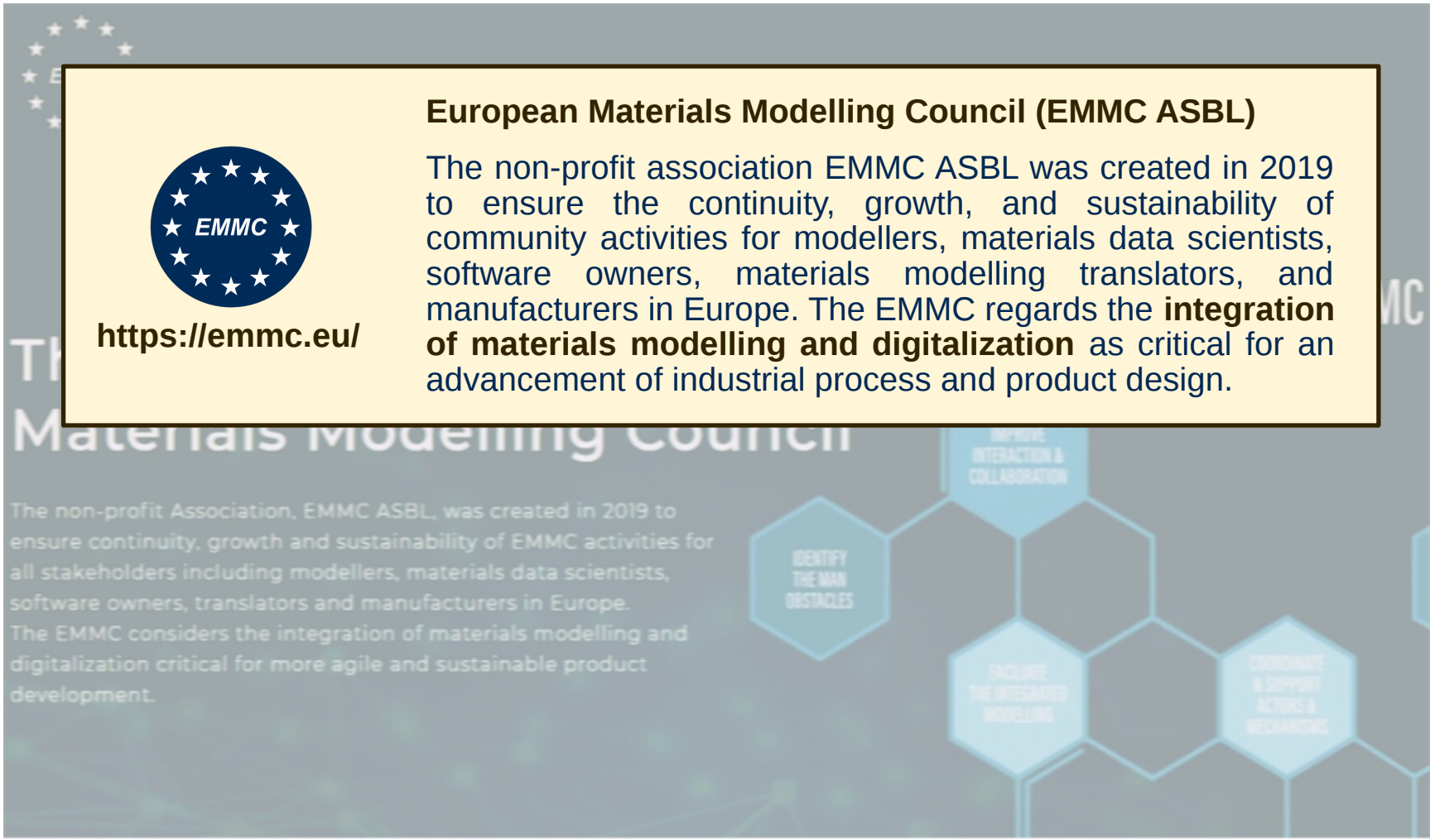
VIMMP
VIRTUAL MATERIALS MARKETPLACE

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.

Community governed metadata standards



Community governed metadata standards

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.

Knowledge representation in materials modelling

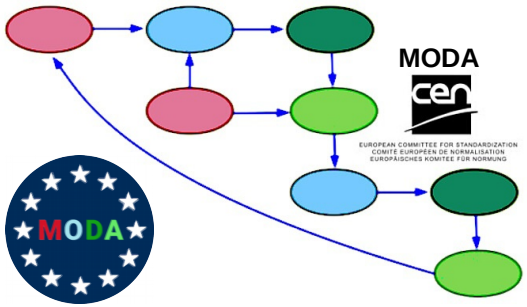
Community-governed development of metadata standards

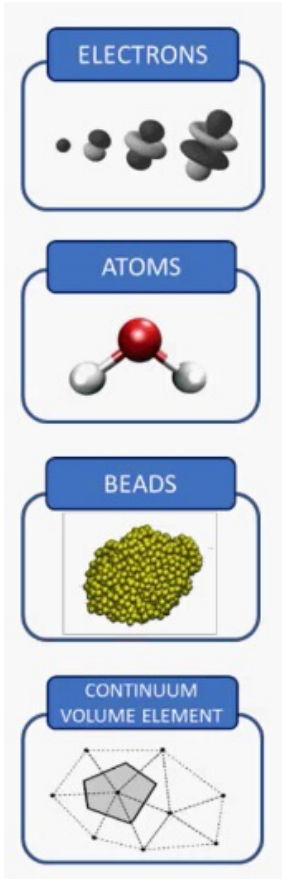
RoMM VI **MODA** **CWA 17284**

Review of Materials Modelling (compendium)

MODA (“Model Data”)

CEN workshop agreement





electronic

atomistic

mesoscopic

continuum

Knowledge representation in materials modelling

Community-governed development of metadata standards

RoMM VI **MODA** **CWA 17284** **Ontologies**

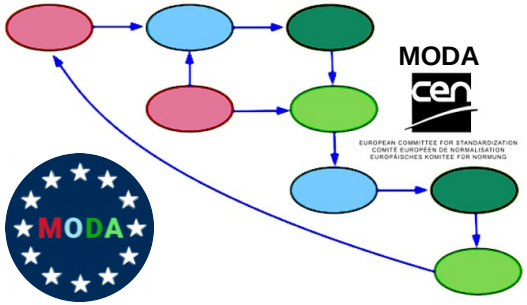
Review of Materials Modelling (compendium)

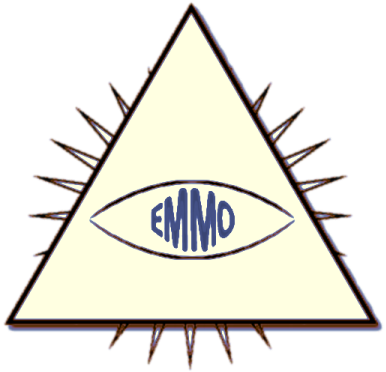
MODA (“Model Data”)

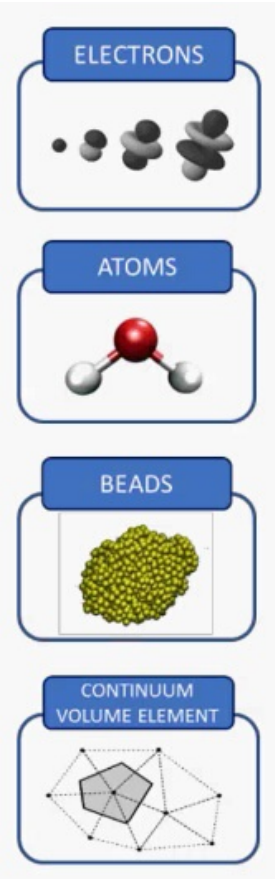
CEN workshop agreement

Domain ontologies

EMMO top-level ontology







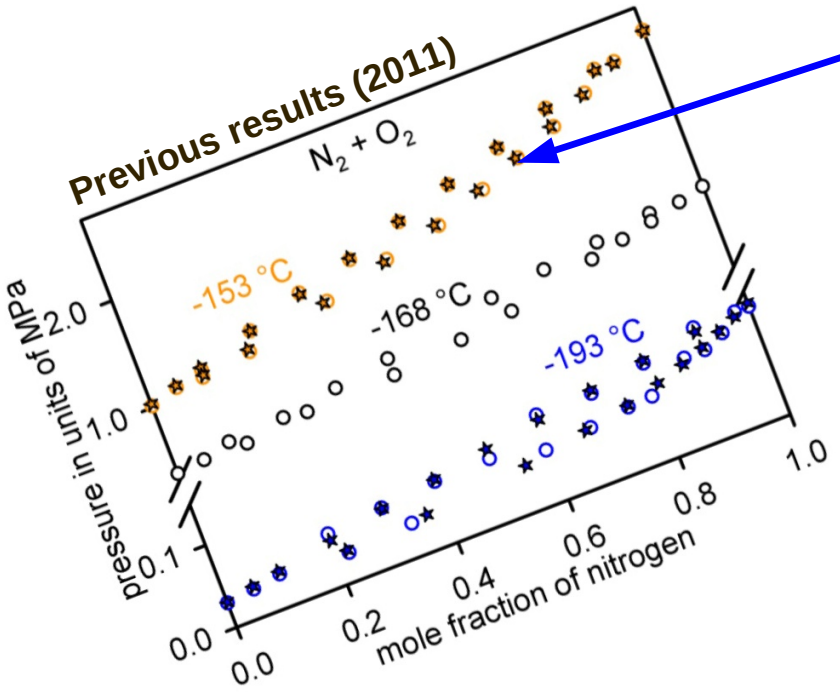
electronic

atomistic

mesoscopic

continuum

Provenance description of simulation results

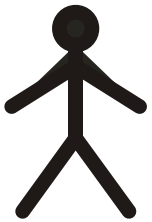


What values did *x* and *p* have?

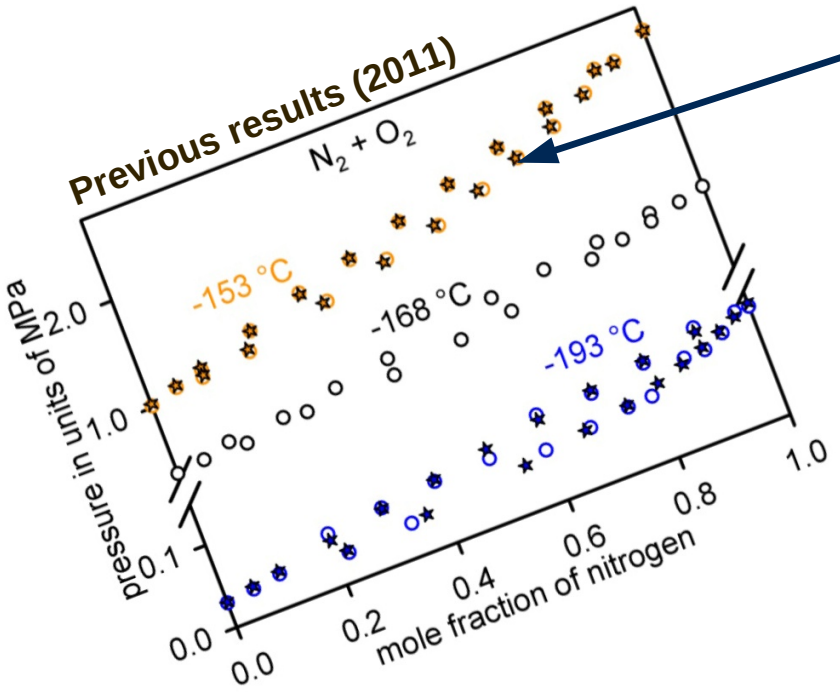
How was the data point obtained?

What is the margin of error, how was the error defined, and what software (or experimental setup) was used?

ask the person who carried out the work back in 2011



Provenance description of simulation results



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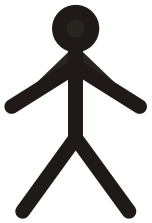
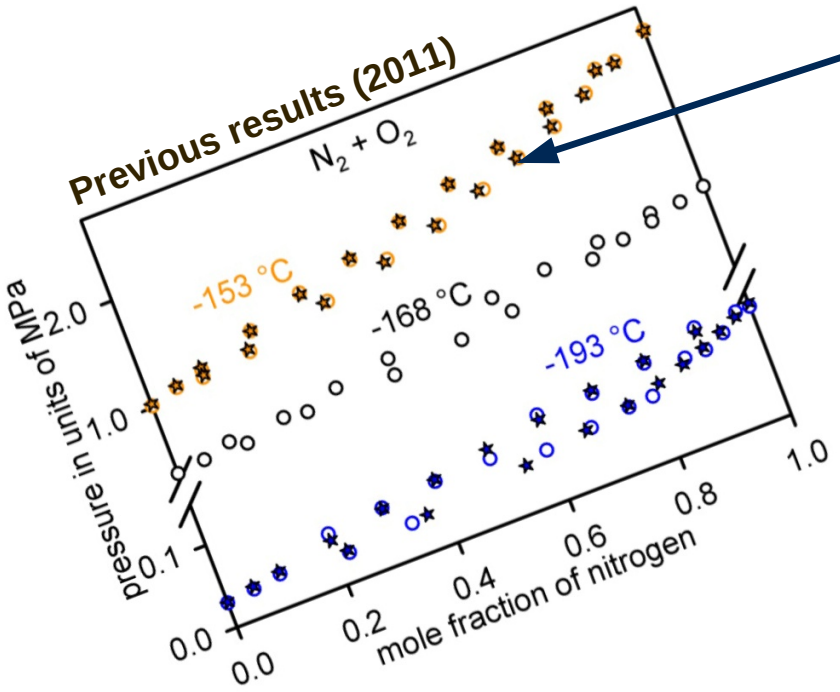


"I remember."

Provenance description of simulation results



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How was the data point obtained?

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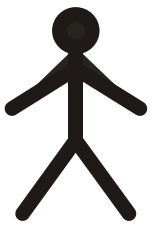


"I remember.
Haha, joke. Of course I don't."

Good practice in managing research data:

Make all data findable, accessible, interoperable, and reusable (FAIR).

Provenance description of simulation results: MODA

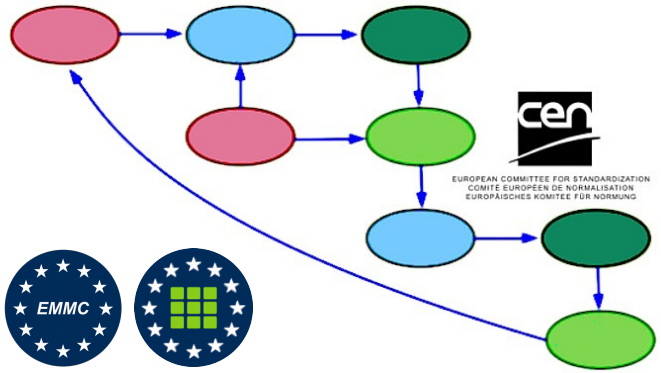
MODA
MOdelling DAta providing a description
for <*user-case name*>
simulated in project <*acronym*>

Data Owner [*name*, *organisation*, *e-mail*]

	OVERVIEW of the SIMULATION		
1	**USER CASE**	*General description of the User Case. One sentence is enough.* *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 IV 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 MINING METHODOLOGY	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 (including 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.* *This should include the reason why a particular aspect of the user case is to be simulated with a particular model.*	

Workflow picture

<Please insert your workflow picture >

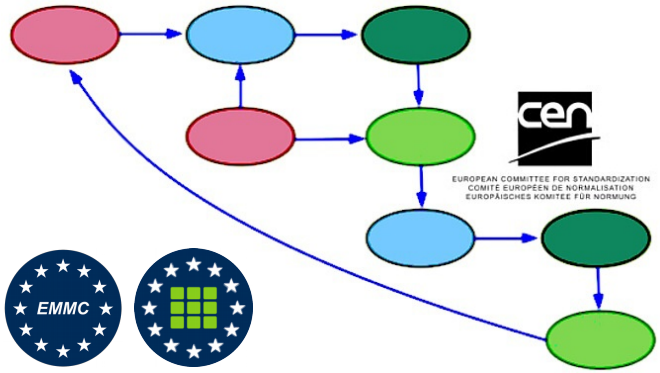


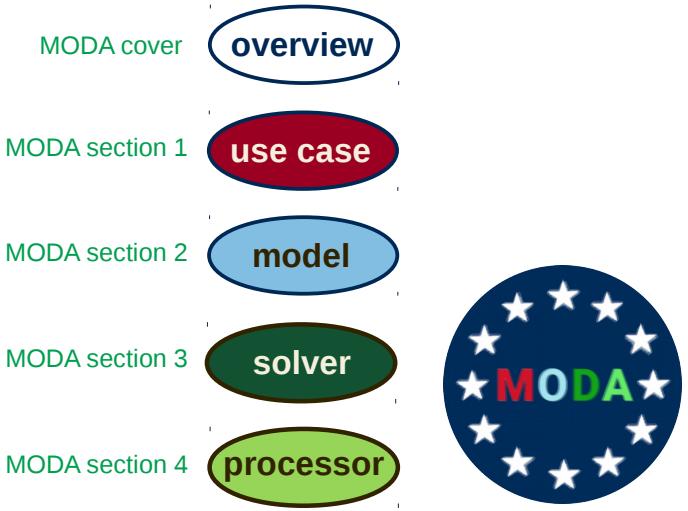
MODA cover **overview**

MODA

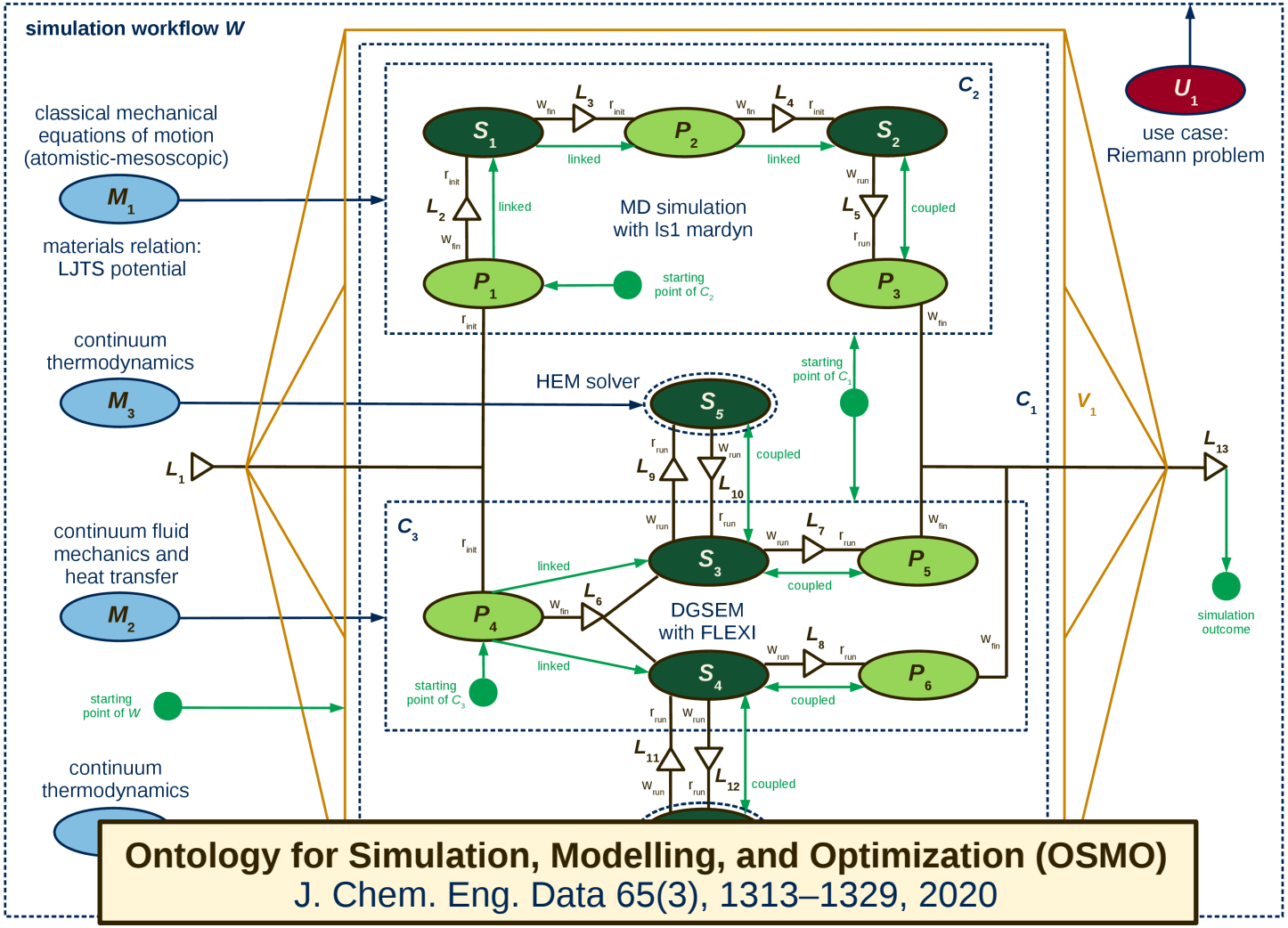
Provenance description of simulation results: MODA

3	Solver and Computational translation of the specifications		
3.1	Numerical Solver	*Please give name andtype of the solver* *e.g. Monte Carlo, SPH, FE, ...iterative, multi-grid, adaptive,...*	
3.2	Software tool	*Please give the name and if this is your own code, please specify if it can be shared with an evt link to website/publication.*	
3.3	Time step	*If applicable, please give the time step used in the solving operations.* *This is the numerical time step and this is not the same as the time lapse of the case to be simulated (see 1.4)*	
3.4	Computational Representation	Physics Equation, Material Relations, Material	*Computational representation of the physics equation, materials relation and material.* *There is no need to repeat user case info.* *"Computational" means that this only needs to be filled in when your computational solver represents the material, properties, equation variables, in a specific way.*
3.5	Computational boundary conditions	*If applicable.* *Please note hat these can be translations of the physical boundary conditions set in the user case or they can be pure computational. (e.g. a unit cell with mirror b.c. to simulate an infinite domain).*	
3.6	Additional Solver Parameters	*Please specify pure internal numerical solver details (if applicable), like* • *Specific tolerances* • *Cut-offs, convergence criteria* • *Integrator options*	





Provenance description of simulation results: OSMO

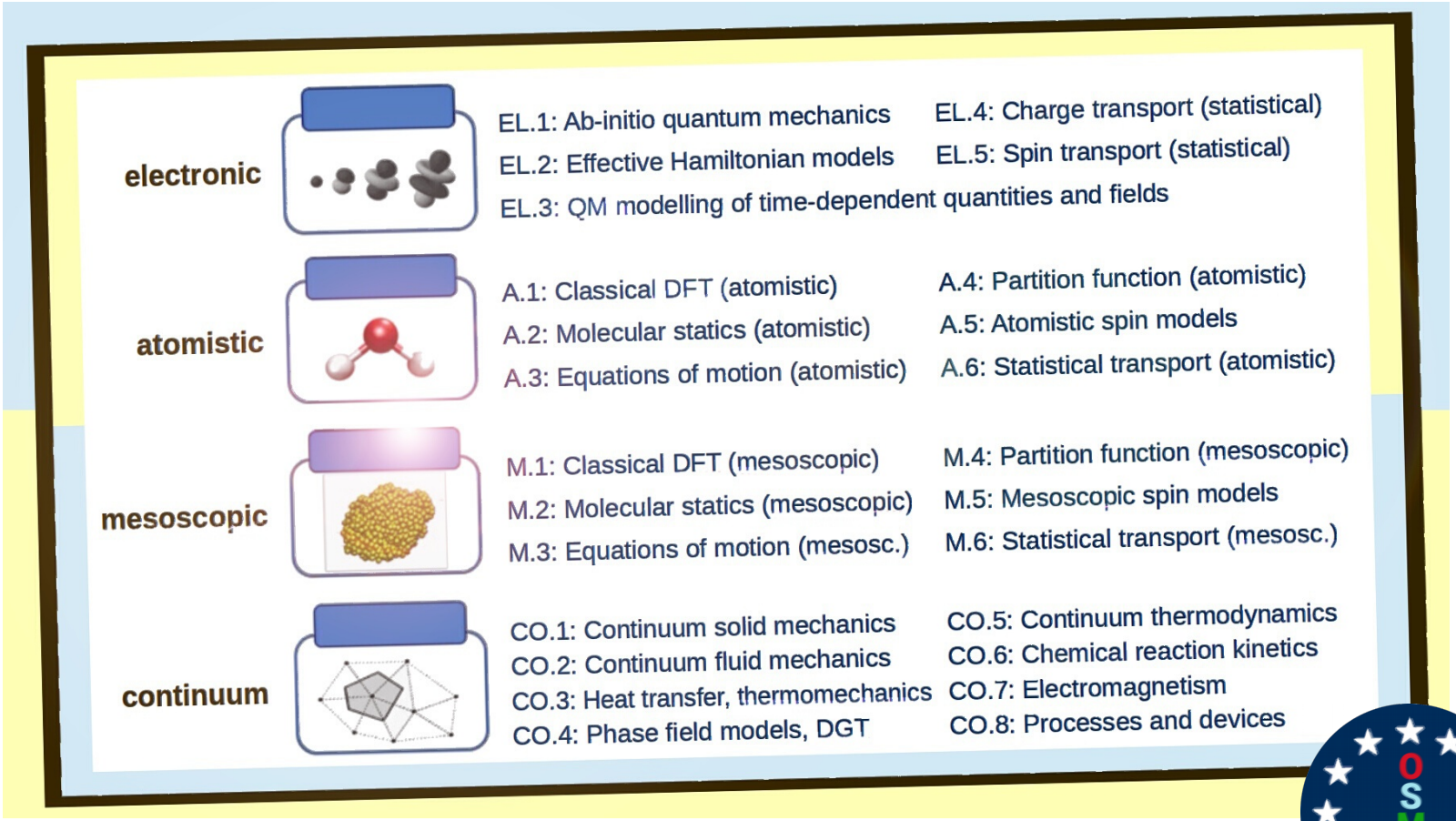


Ontology for Simulation, Modelling, and Optimization (OSMO)
J. Chem. Eng. Data 65(3), 1313–1329, 2020

OSMO-based **provenance description** as an extension of the MODA workflow meta-data standard:

For all elements of the graph notation, there are corresponding concepts and relations from the ontology OSMO.

Provenance description of simulation results: OSMO



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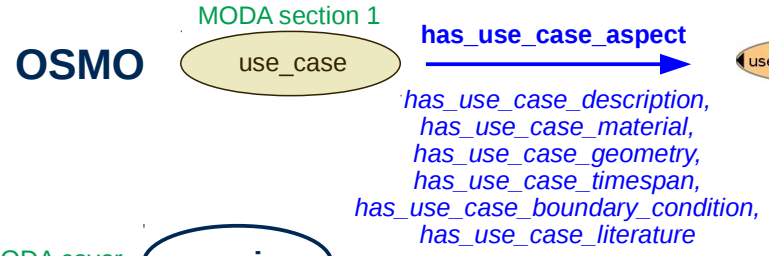

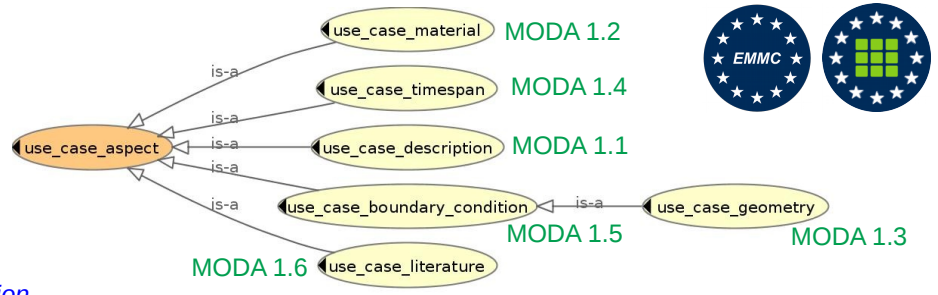

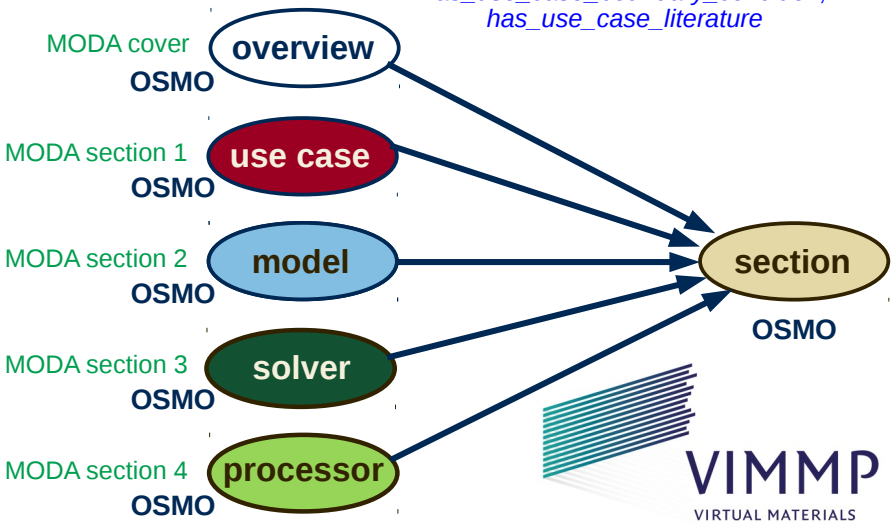

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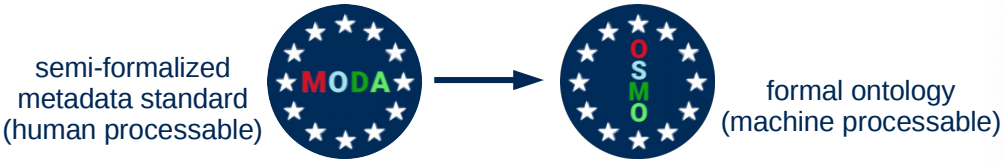
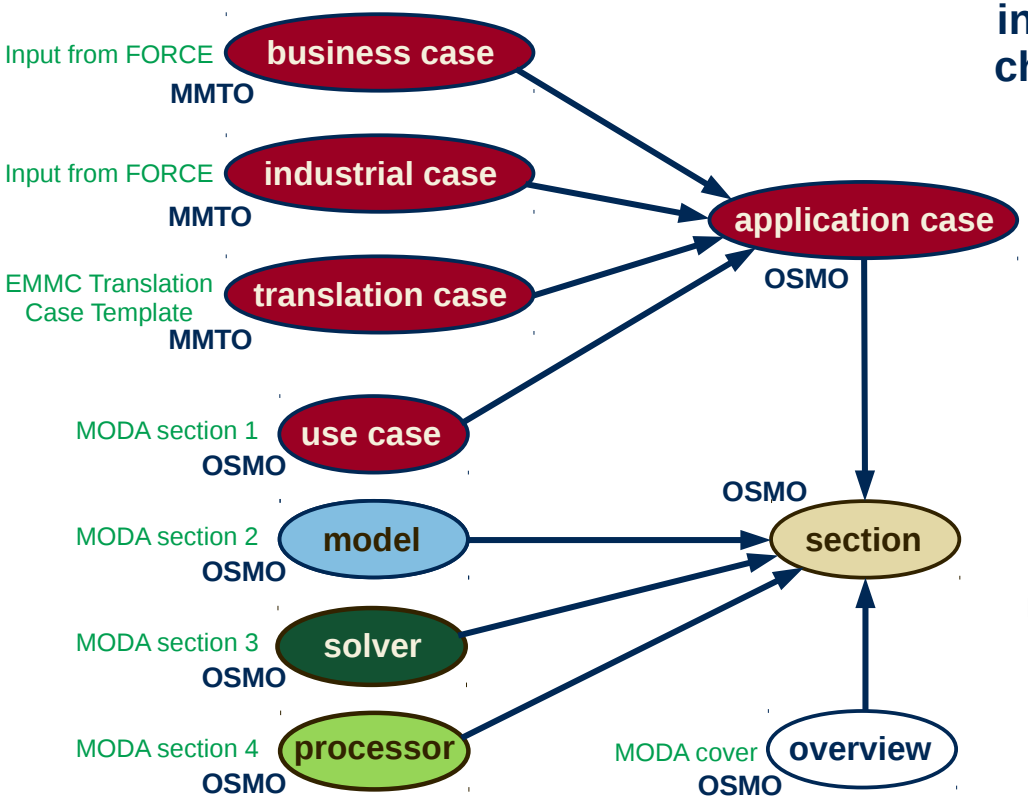
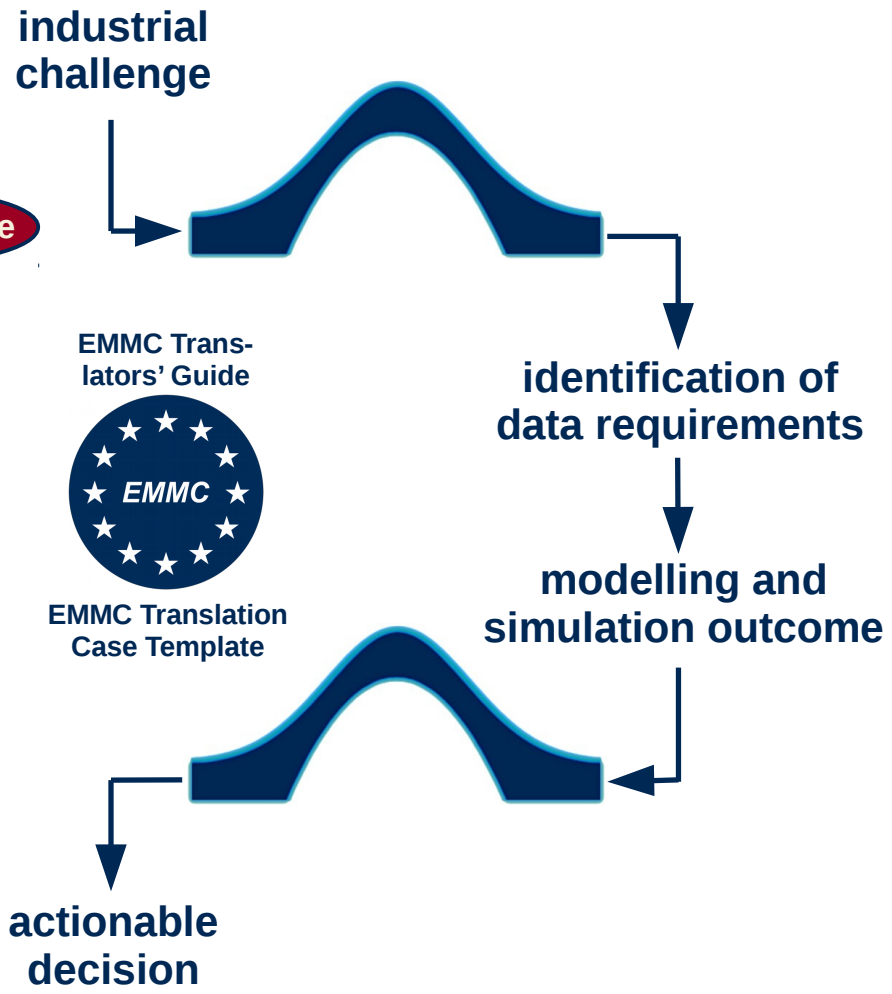


Materials Modelling Translation Ontology (MMTO)





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**.

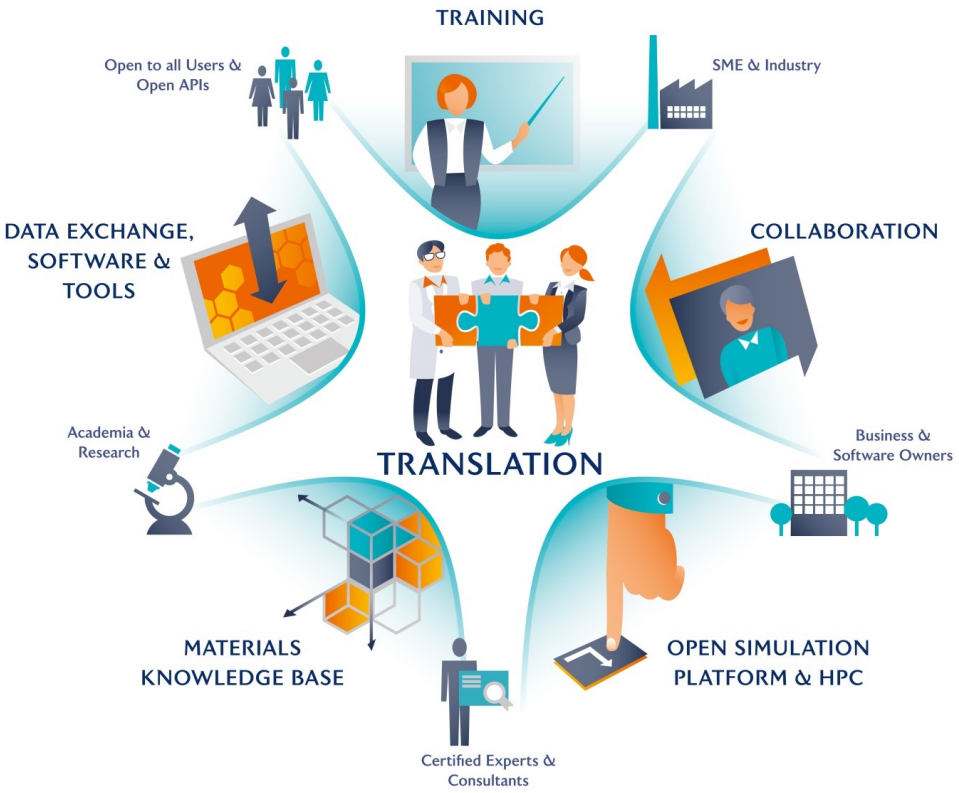
Science and Technology Facilities Council

EMMC

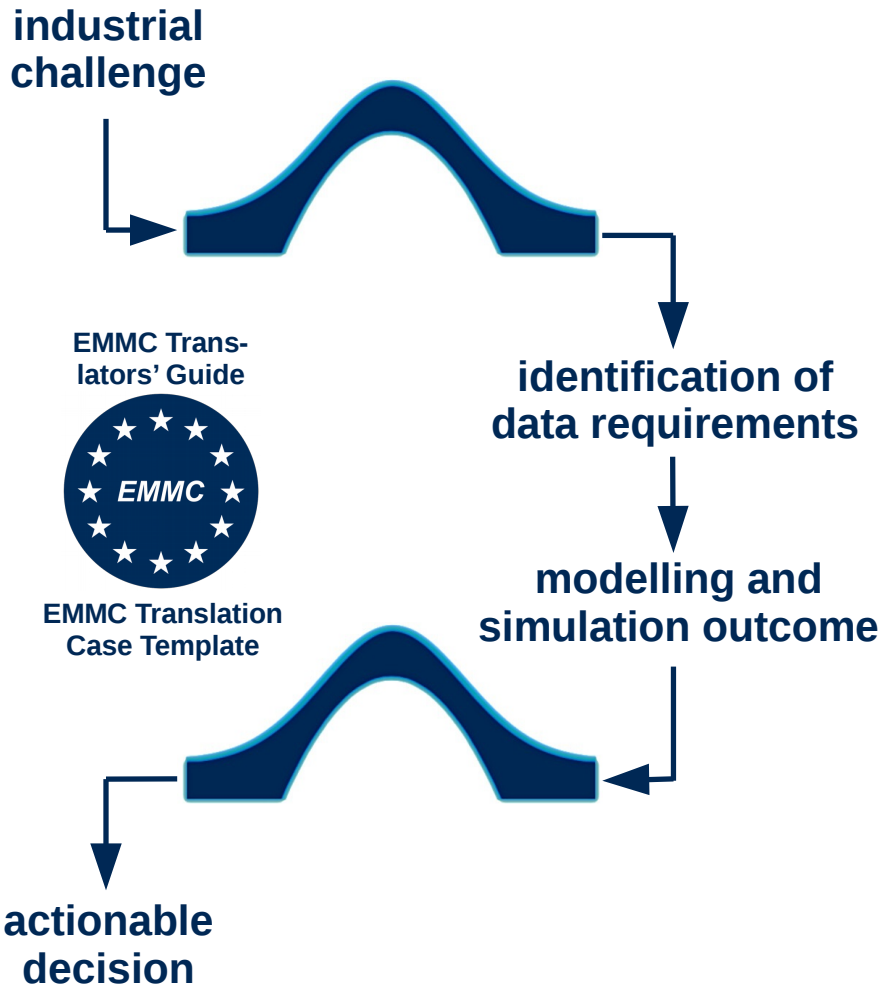
FORCE

VIMMP VIRTUAL MATERIALS MARKETPLACE

“Translation” and the Virtual Materials Marketplace



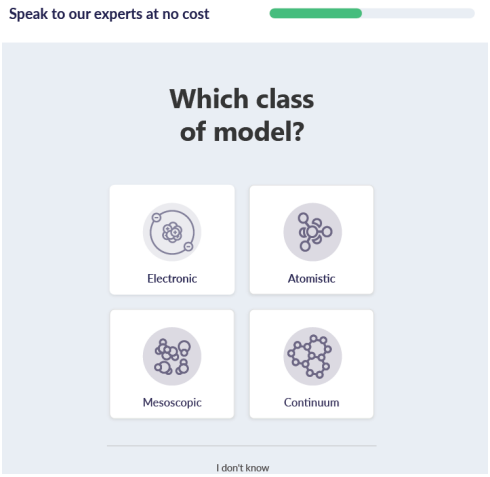
M. T. Horsch, S. Chiacchiera, M. A. Seaton, I. T. Todorov, B. Schembera, P. Klein, N. A. Konchakova, “Pragmatic interoperability and translation [...],” *Proceedings of DAMDID/RCDL*, **2020**.

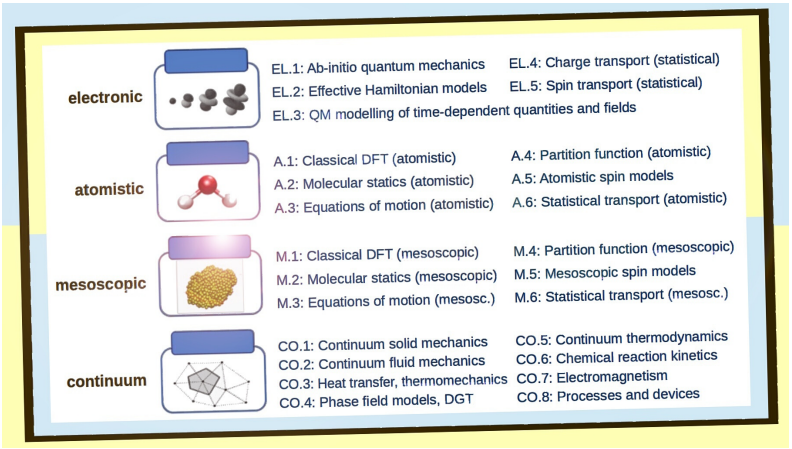


Matchmaking: VIMMP translation router

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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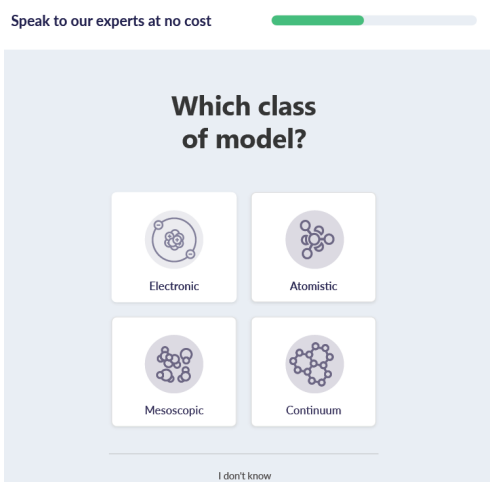
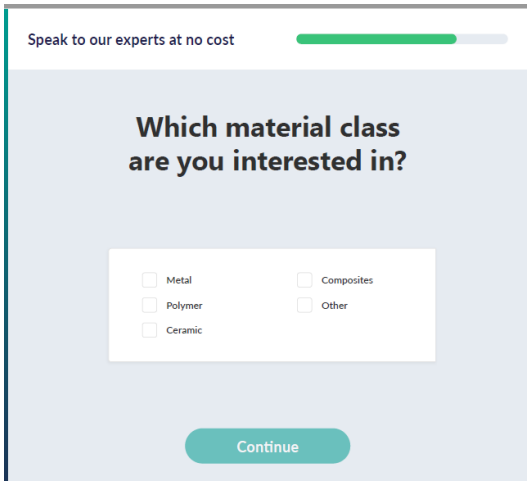
Topics from other disciplines.

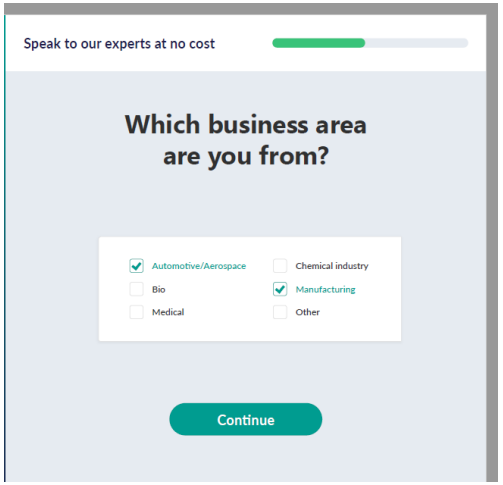
under 61XX: industrial

6120 chemical
6130 petrochemical
6140 transport
- 6142 aerospace
- 6144 automotive
- 6148 railway

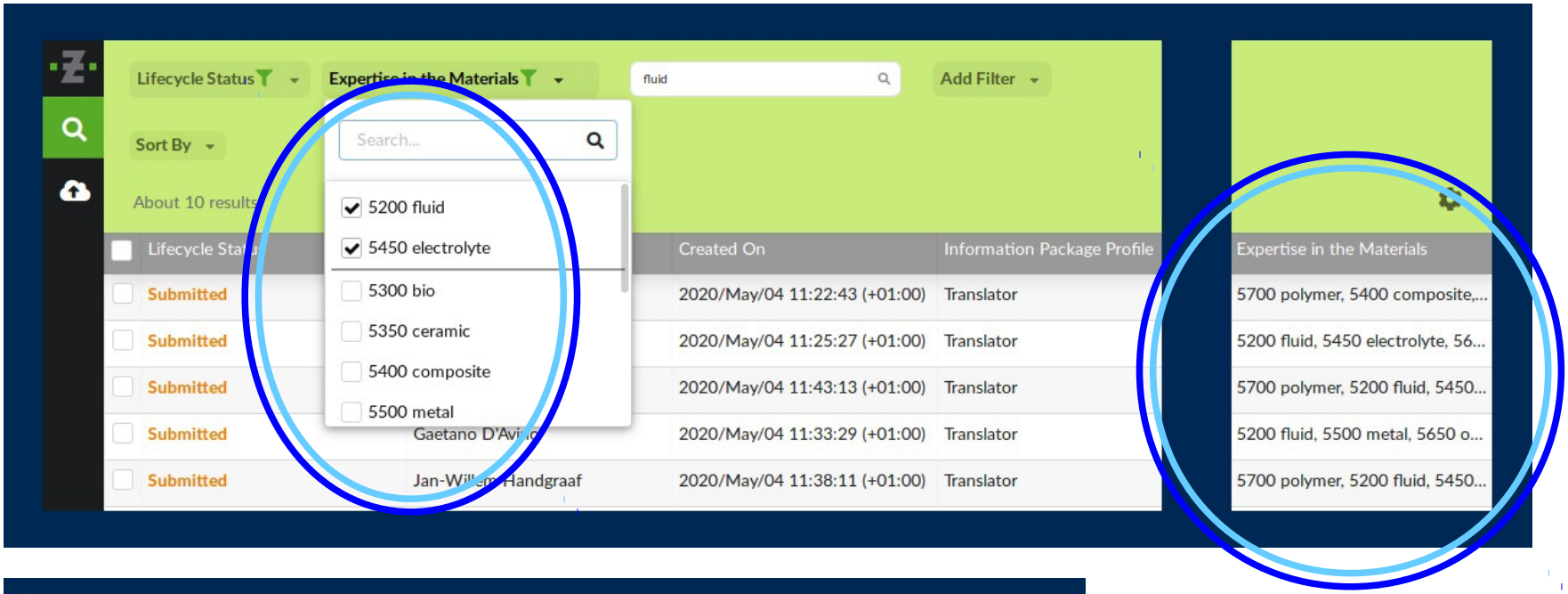
6150 biotechnology
6155 food
6160 medicine
6165 paper
6170 electrical
6175 machinery
6180 metal (basic and fabricated)
6190 special topics

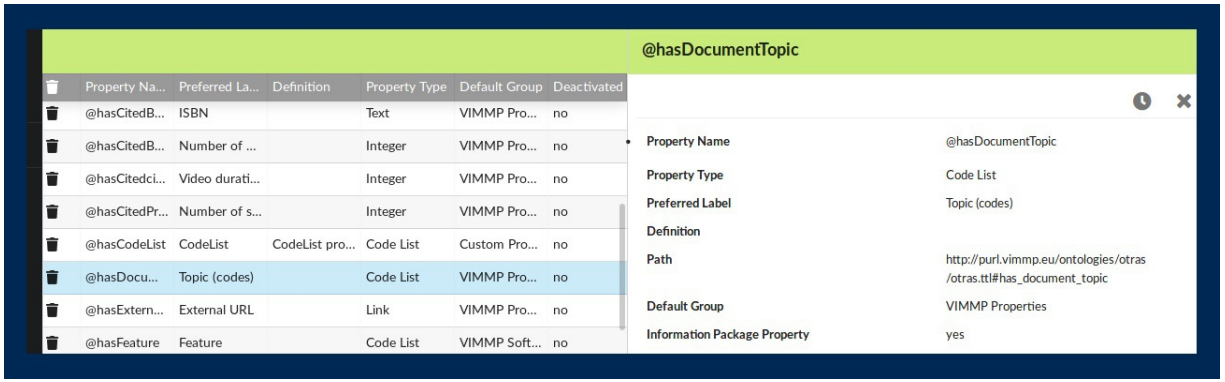






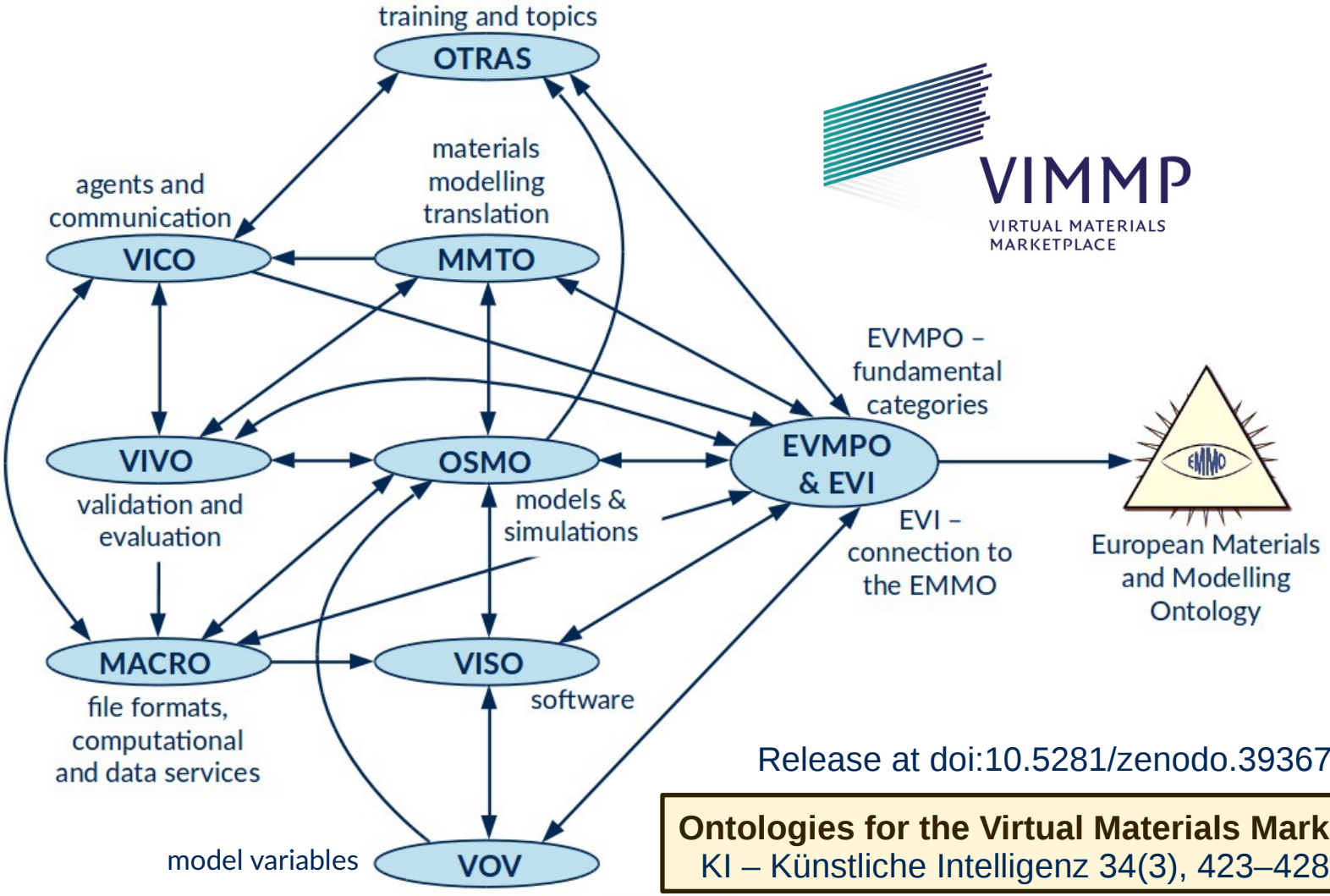
Data management on the VIMMP backend





OSTHUS

VIMMP system of marketplace-level domain ontologies

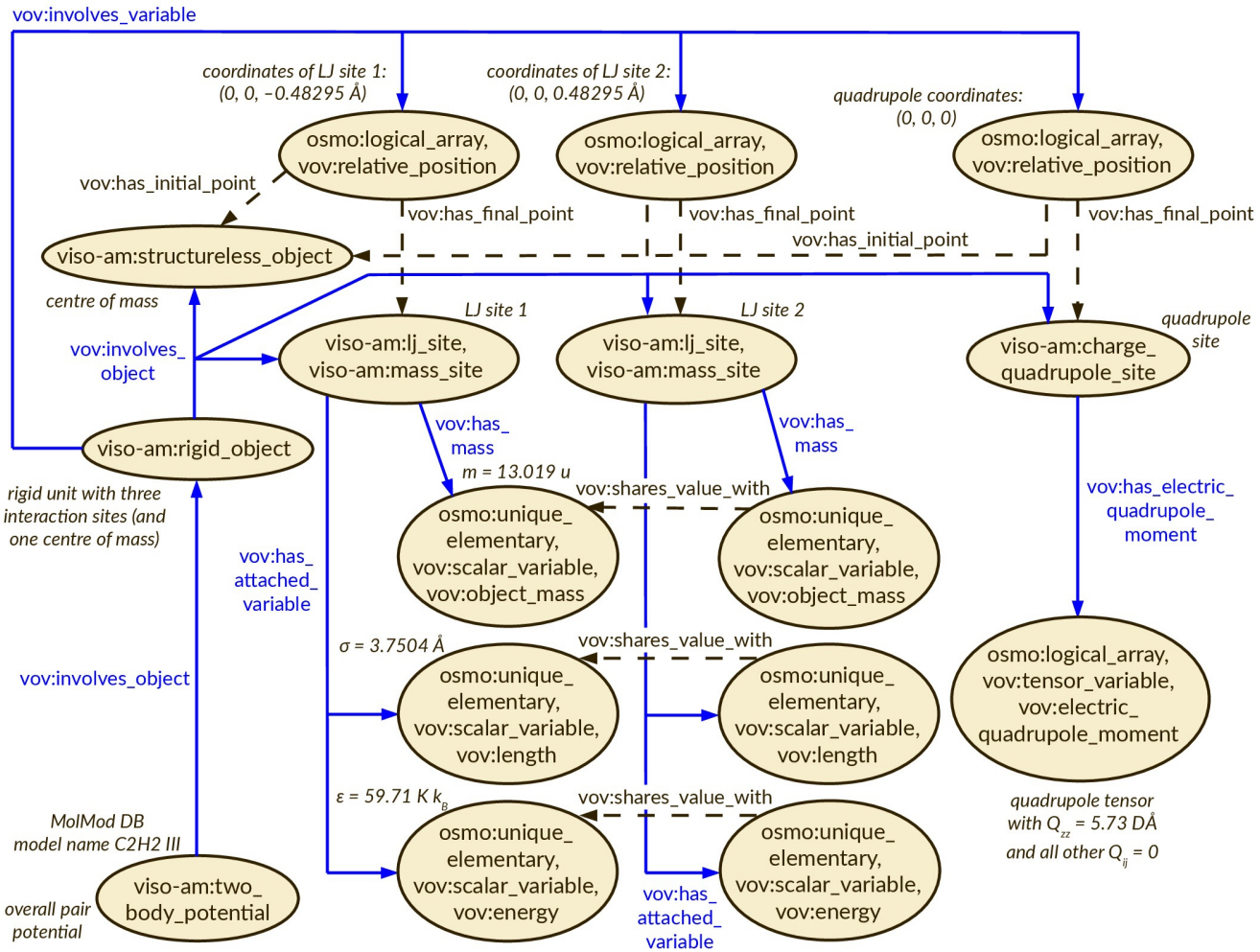


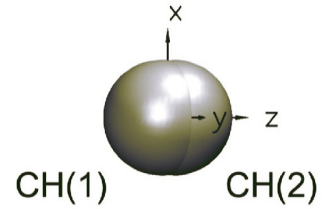
VIMMP
VIRTUAL MATERIALS MARKETPLACE

Release at doi:10.5281/zenodo.3936795

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

Example: Knowledge graph for a molecular model



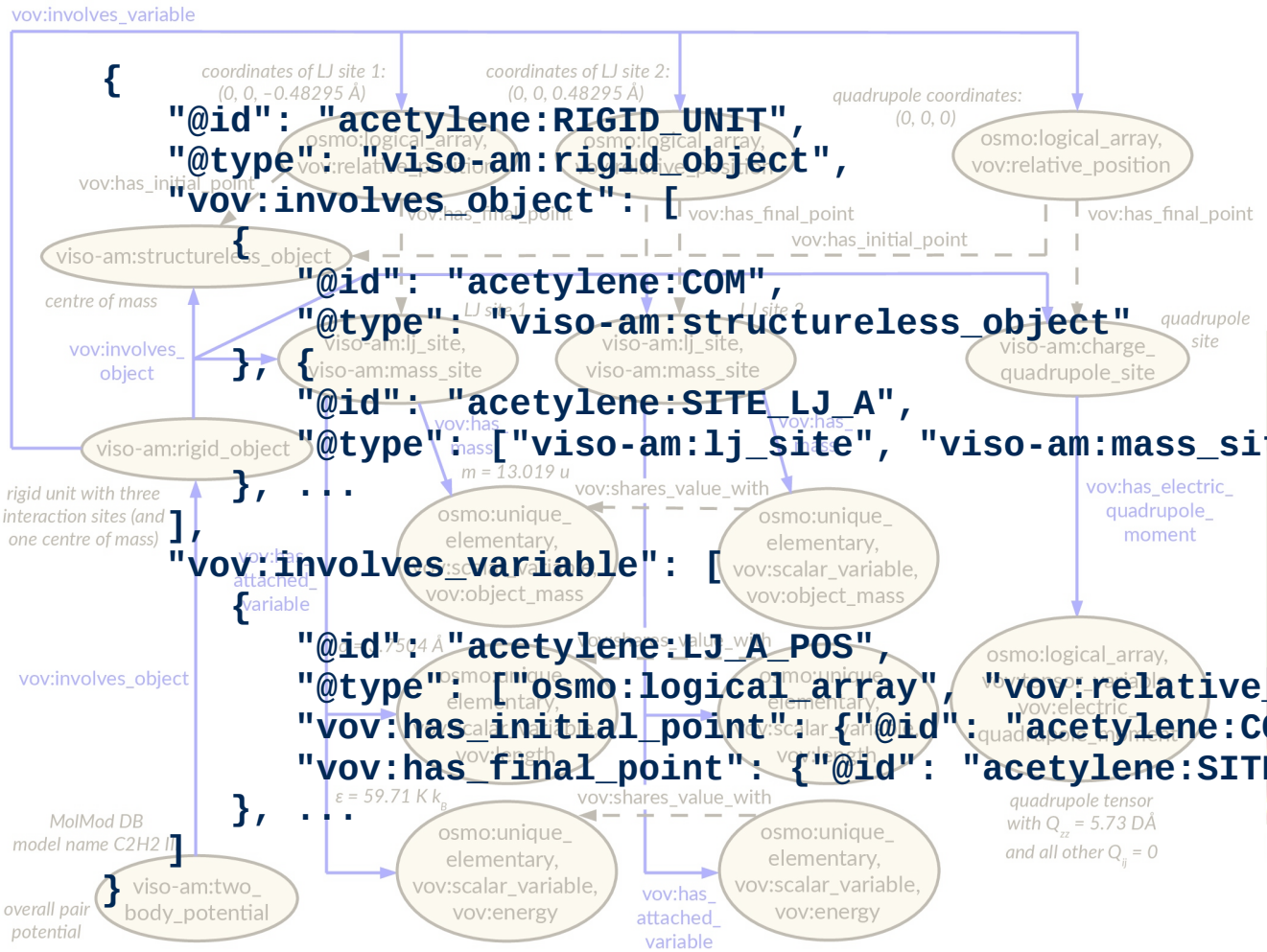


MolMod DB (Molecular Model Database)

http://molmod.boltzmann-zuse.de/

pair potentials for over 150 molecular fluids

Example: Knowledge graph for a molecular model

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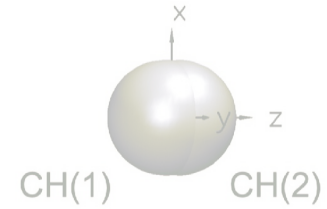
}
```



MolMod DB
(Molecular Model Database)

http://molmod.boltzmann-zuse.de/

pair potentials for
over 150 molecular fluids

Alignment of domain ontologies with the EMMO[1]

European Materials and Modelling Ontology[1] (EMMO)

1) **Taxonomy**: Conceptual hierarchy (subclass relation)

2) **Semiotics**: Representation of physical entities by signs

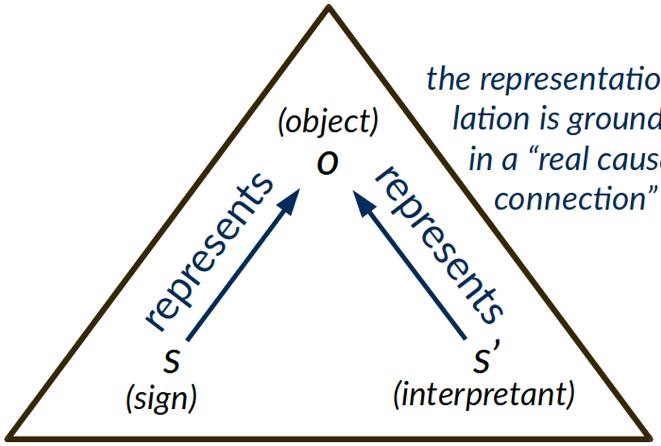
3) **Mereotopology**: Spatiotemporal parthood and connectivity

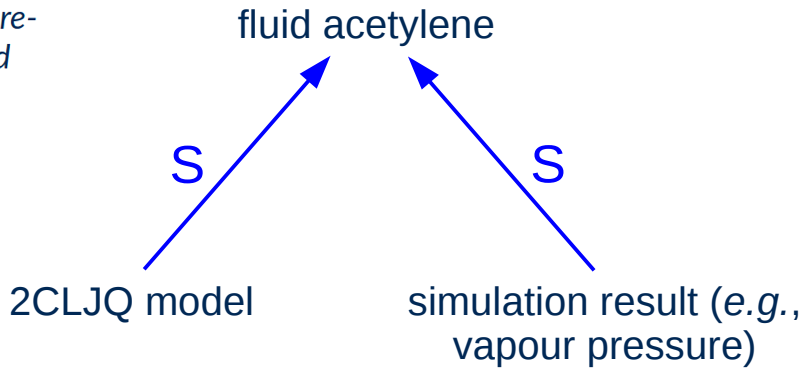
"represents" or **"is sign for"** will be abbreviated by **S**

Peircean semiotics

semiosis

C. S. Peirce





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

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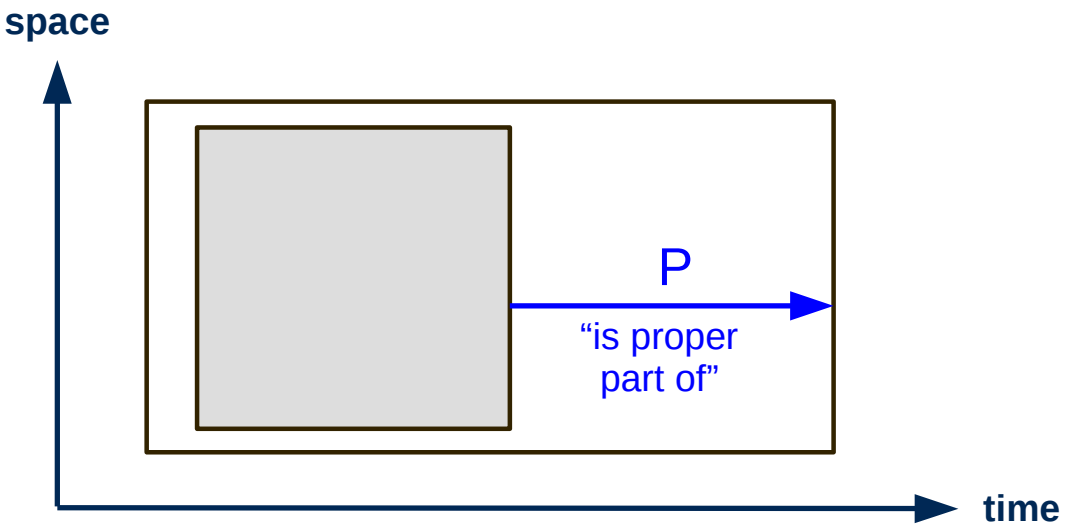

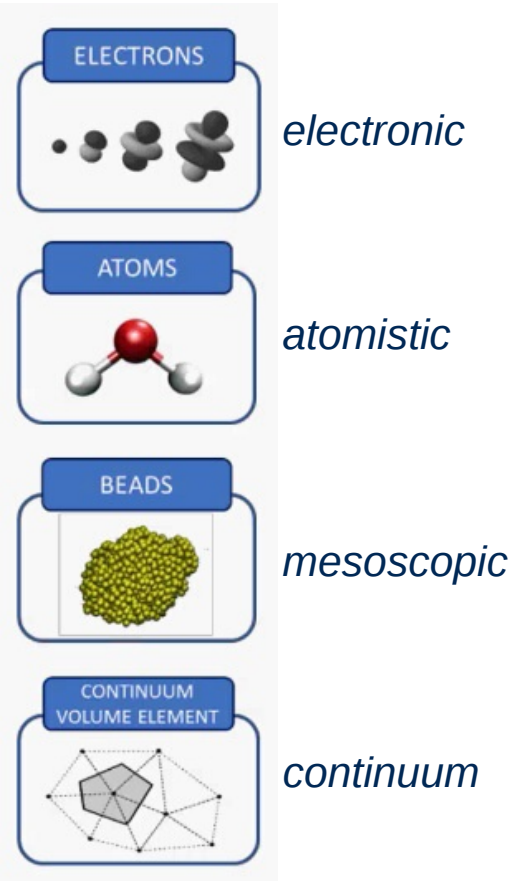

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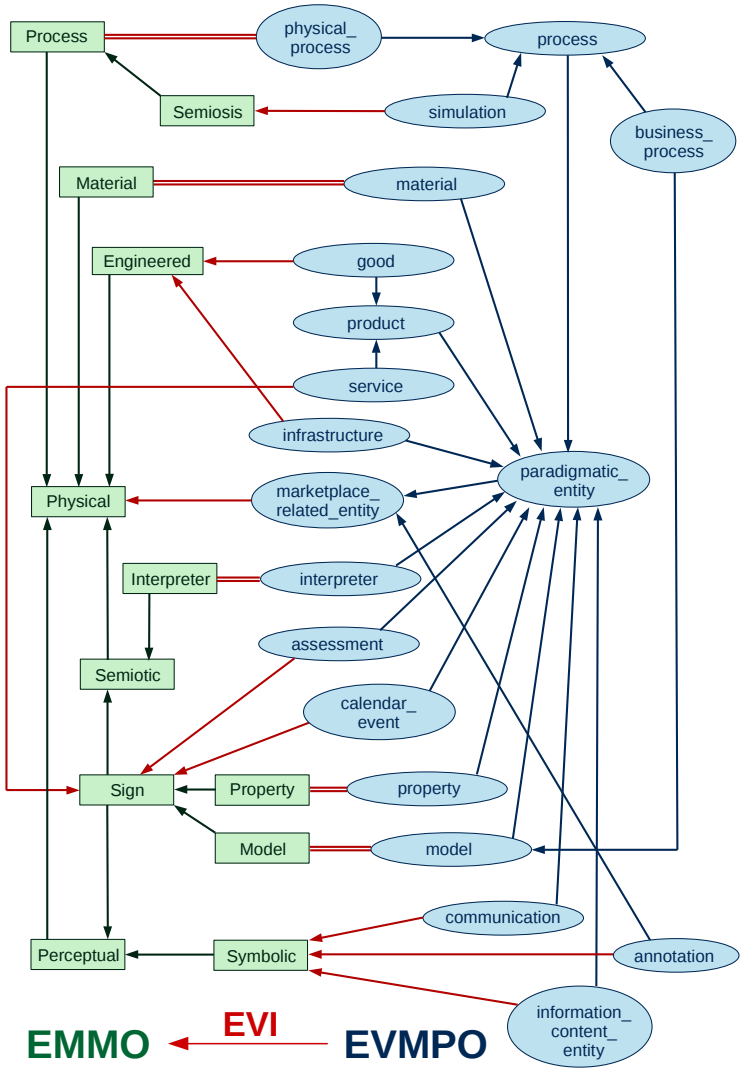
Alignment of domain ontologies with the EMMO



(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

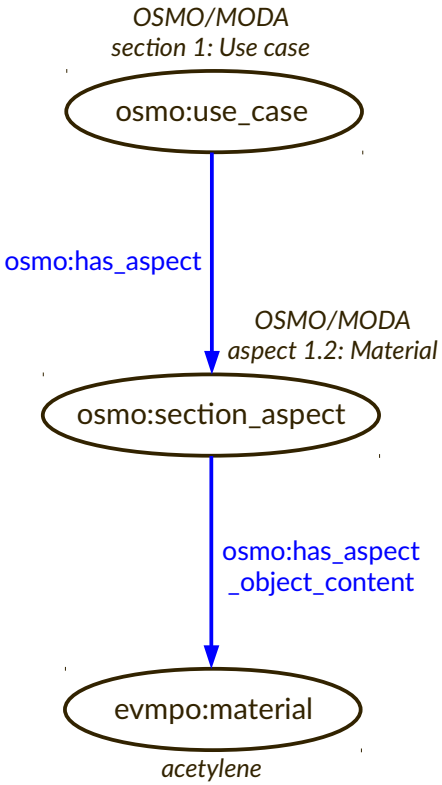
(9) **process**, *i.e.*, temporal evolution of one or multiple entities

(10) **product**, *i.e.*, a good or service that can be traded

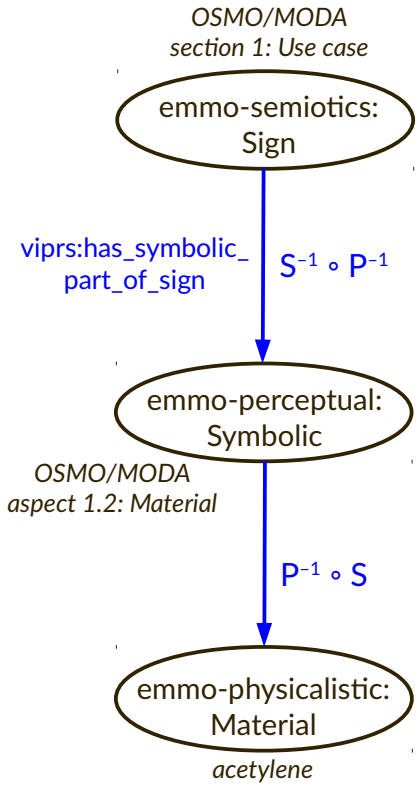
(11) **property**, *i.e.*, a representamen that is determined as an interpretant by observation, involving a specific observer

Alignment of domain ontologies with the EMMO[1]

marketplace-level domain ontology representation

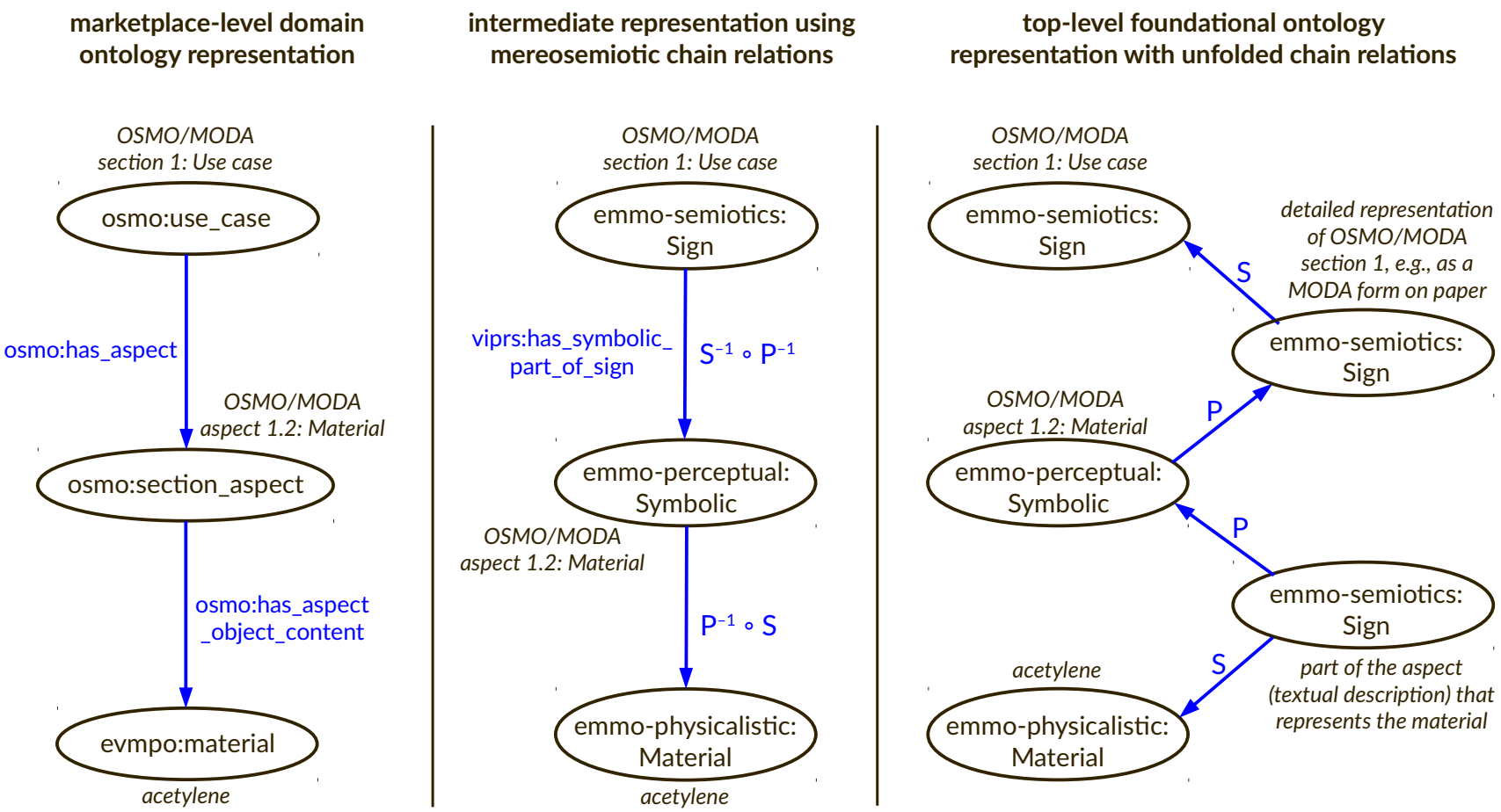


intermediate representation using mereosemiotic chain relations



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

Alignment of domain ontologies with the EMMO[1]



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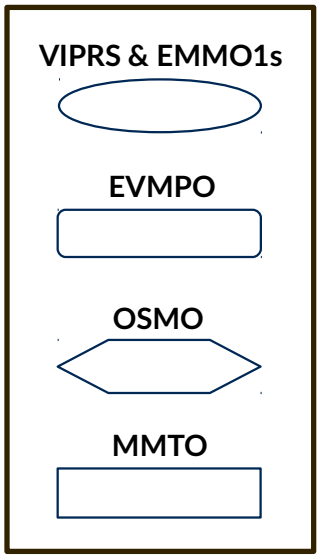
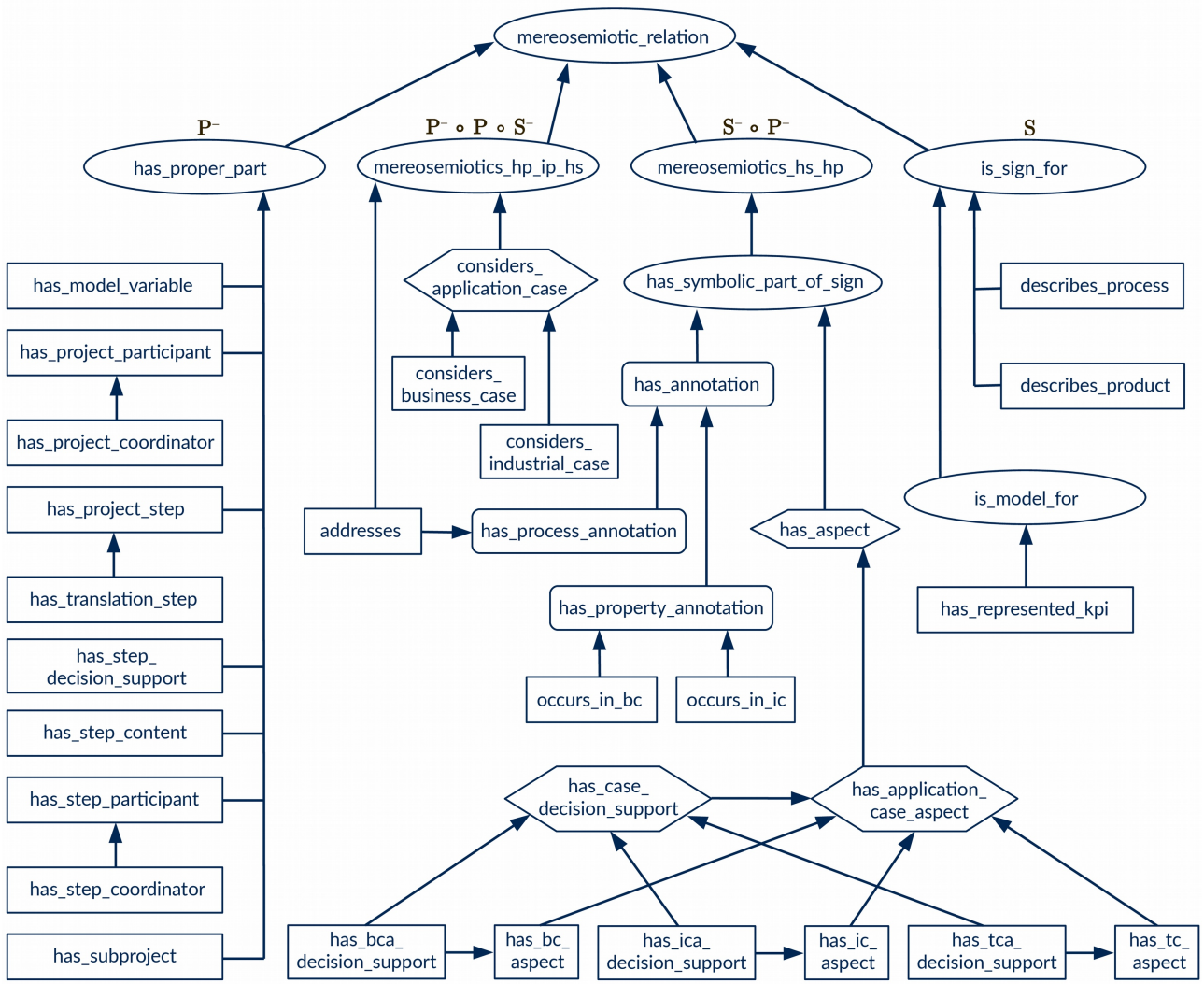
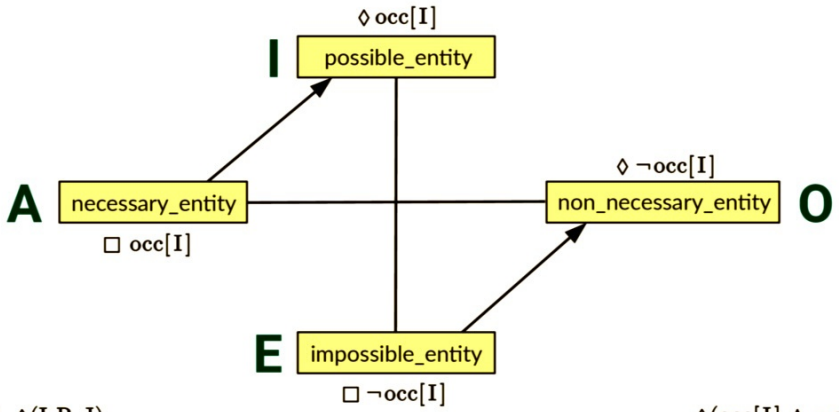




VIMMP Primitives (VIPRS) and modal relations[1]

design pattern

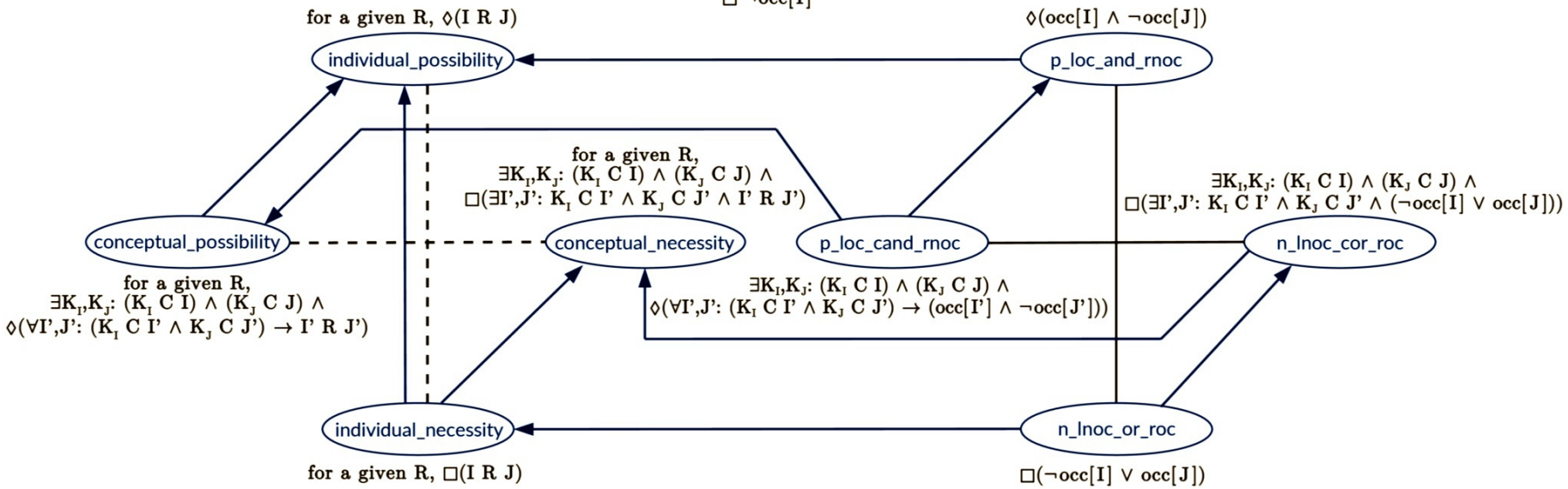
modal squares of opposition



□φ ≡ φ is necessary

◊φ ≡ φ is possible

occ[X] ≡ X occurs



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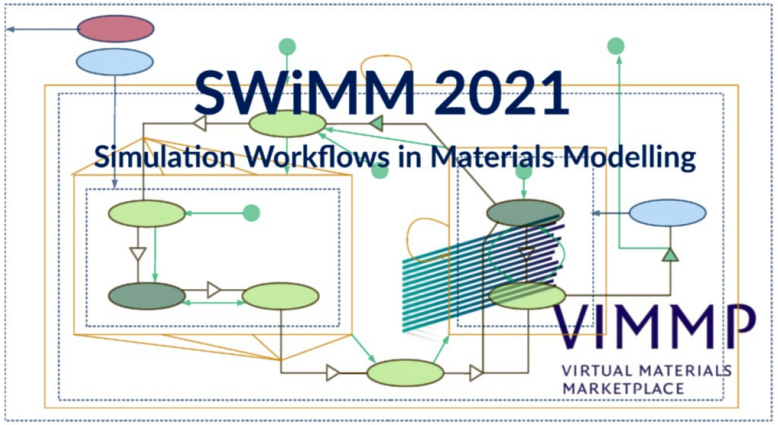
CECAM school “SWiMM 2021” supported by VIMMP



Simulation Workflows in Materials Modelling

15th – 26th 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. European Materials and Modelling Ontology
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

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