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Performance Computing Center Stuttgart**,
P. Klein, **Fraunhofer ITWM**, N. A. Konchakova,
Helmholtz-Zentrum Geesthacht

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

13th October 2020

DAMDID 2020



VIMMP

VIRTUAL MATERIALS
MARKETPLACE

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 01.01.2018

To support accelerating innovation in manufacturing industries by using materials modelling solutions.

From Materials

Applying
Modelling

To Innovation

Virtual Materials Marketplace (VIMMP)



<http://vimmp.eu/>

- Horizon 2020 project
 - Innovation action, grant agreement no. 760907
 - H2020 (NMBP-25-2017)
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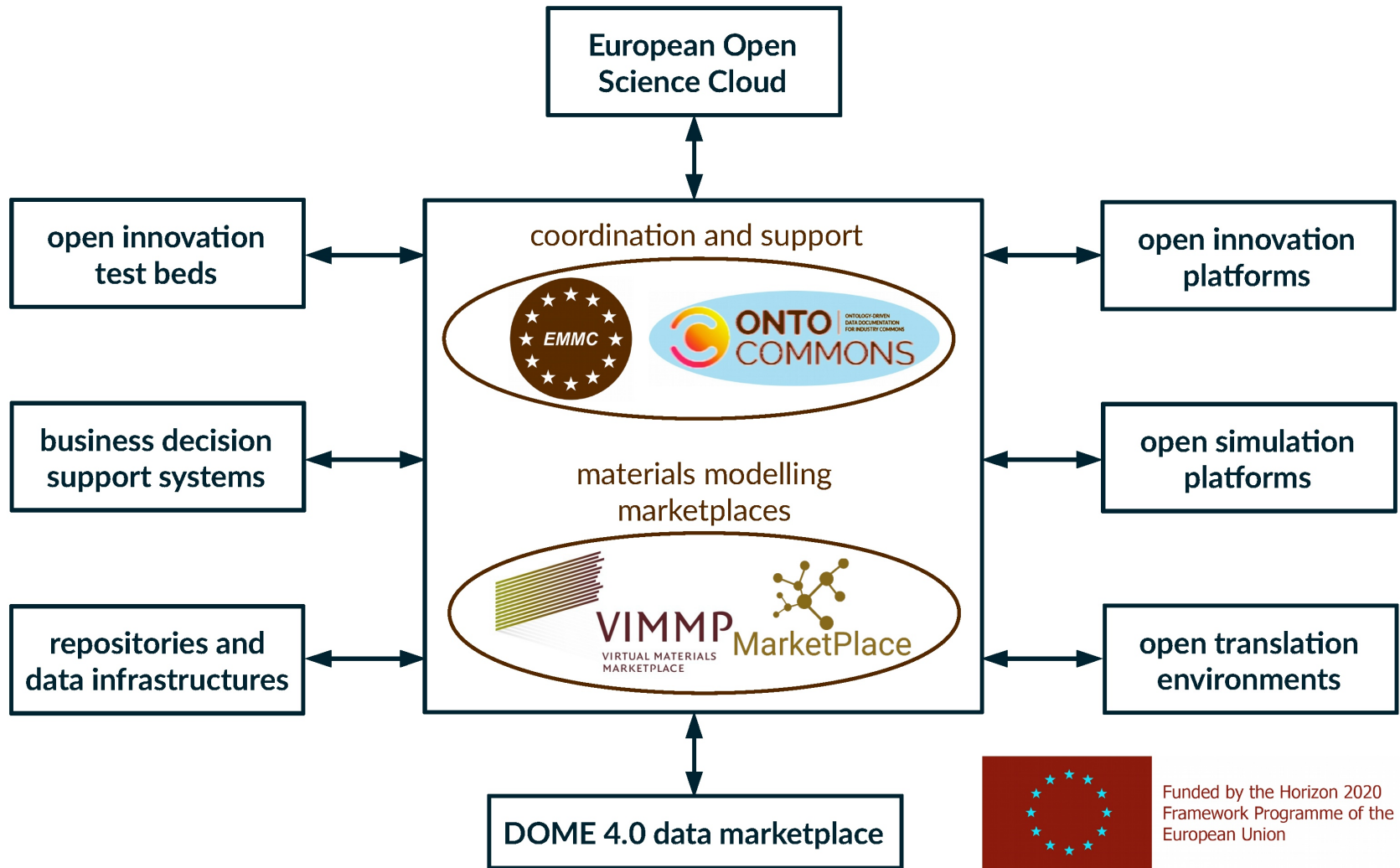
Marketplaces Can Transform Entire Industries

amazon
Retail Marketplace

airbnb
Housing Marketplace

UBER
Transportation Marketplace

European digital platforms in materials modelling



Funded by the Horizon 2020 Framework Programme of the European Union

European Materials Modelling Council



<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

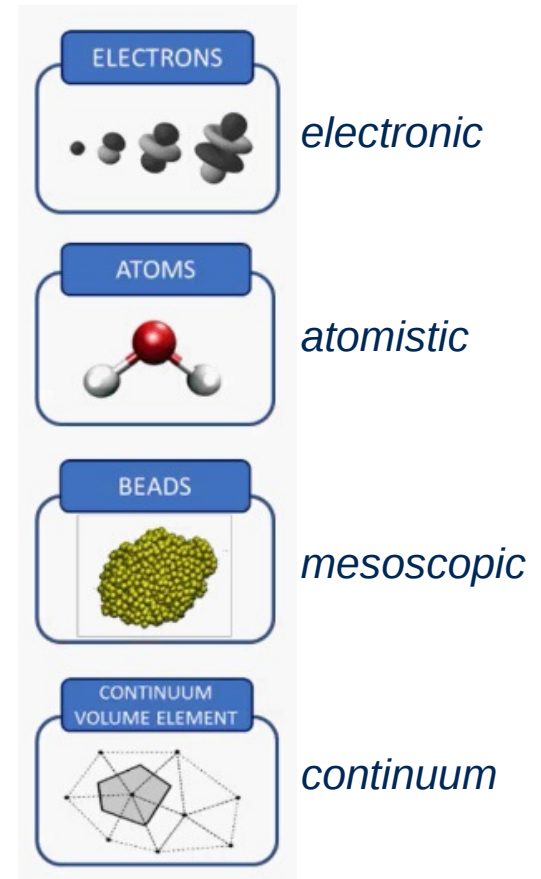
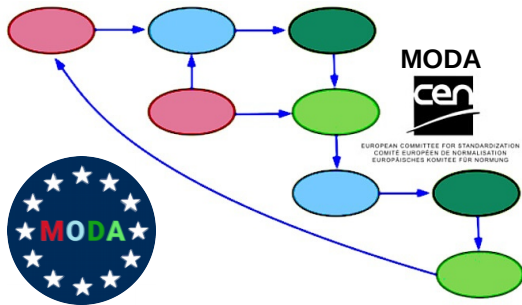
MODA

CWA 17284

Review of Materials Modelling (compendium)

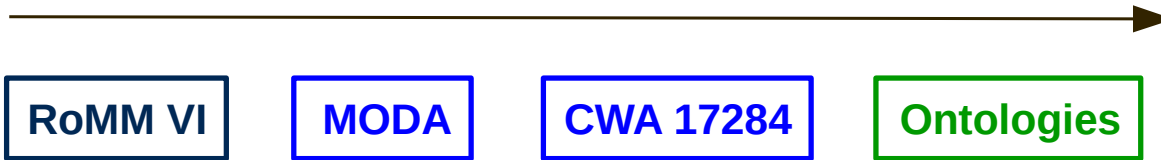
MODA (“Model Data”)

CEN workshop agreement



Knowledge representation in materials modelling

Community-governed development of metadata standards

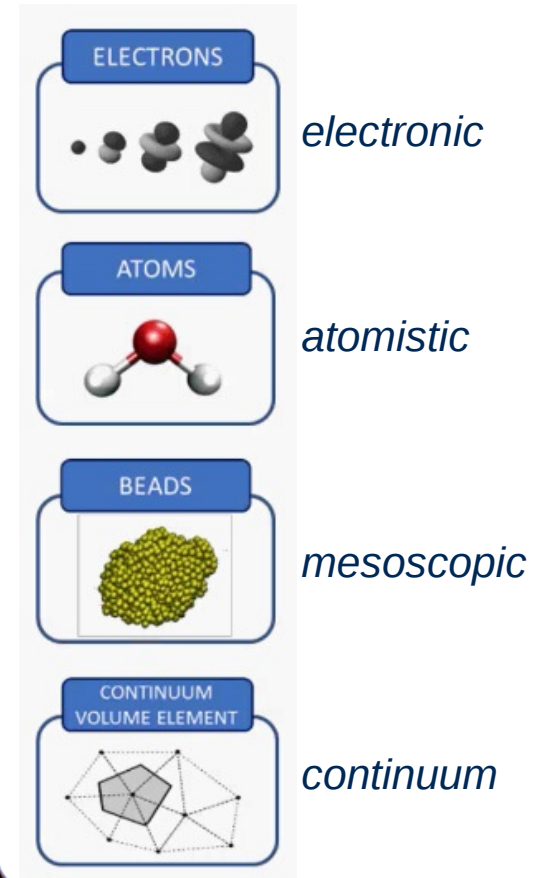
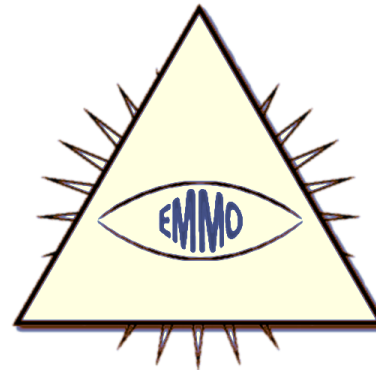
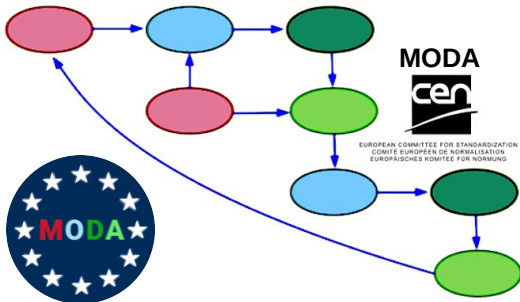


Review of Materials Modelling (compendium)

MODA (“Model Data”)

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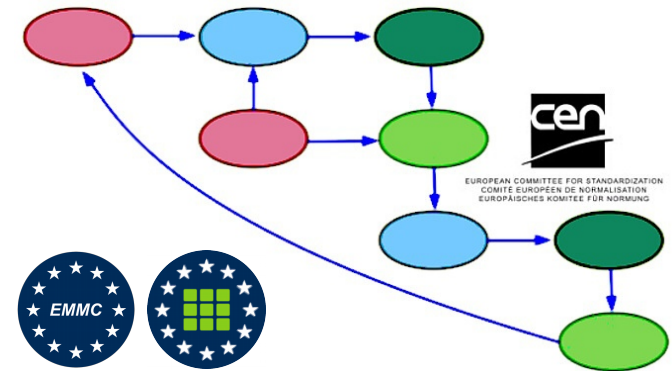
Domain ontologies
EMMO top-level ontology



Provenance description of simulation results: MODA

1 ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	<p>ASPECT OF THE USER CASE TO BE SIMULATED</p> <p><i>Describe the aspects of the user case textually.</i></p> <p><i>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)</i></p> <p><i>Also the result of pre-processing necessary to translate the user case specifications to values for the physics variables of the entities can be documented here.</i></p>
1.2	<p>MATERIAL</p> <p><i>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.</i></p>
1.3	<p>GEOMETRY</p> <p><i>Size, form, picture of the system (if applicable)</i></p> <p><i>Note that computational choices like simulation boxes are to be documented in chapter 3.</i></p>
1.4	<p>TIME LAPSE</p> <p><i>Duration of the case to be simulated.</i></p> <p><i>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.</i></p>
1.5	<p>MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS</p> <p><i>If relevant, please list the conditions to be simulated (if applicable). These can be boundary, initial and global conditions.</i></p> <p><i>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.</i></p> <p><i>Note: These conditions will be expressed in physics relations in Ch 2.4</i></p> <p><i>Please specify the values used for parameters and from which database these are taken. If pre-processing was needed please specify the methodology.</i></p>
1.6	<p>PUBLICATION ON THIS DATA</p> <p><i>Publication documenting the simulation with this single model (if available and if not already included in the overall publication).</i></p>

MODA workflow description



MODA section 1

use case

MODA section 2

model

MODA section 3

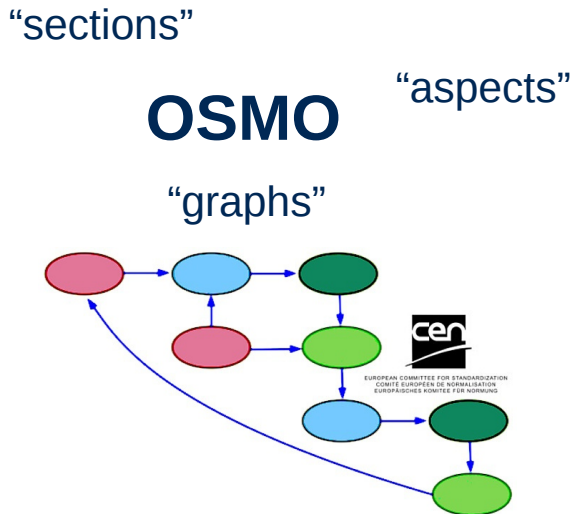
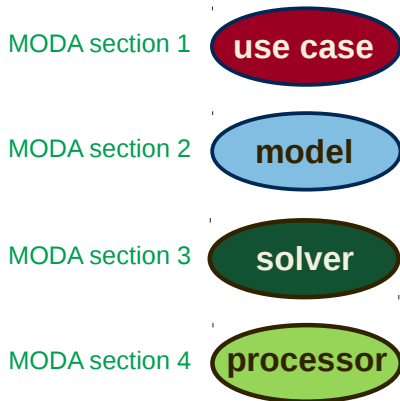
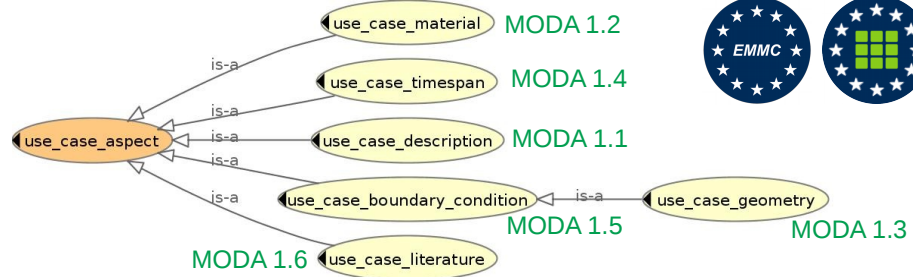
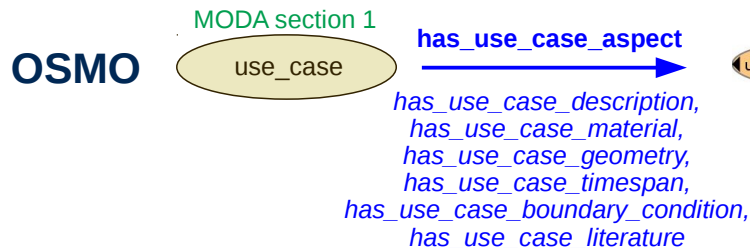
solver

MODA section 4

processor



Provenance description of simulation results: OSMO

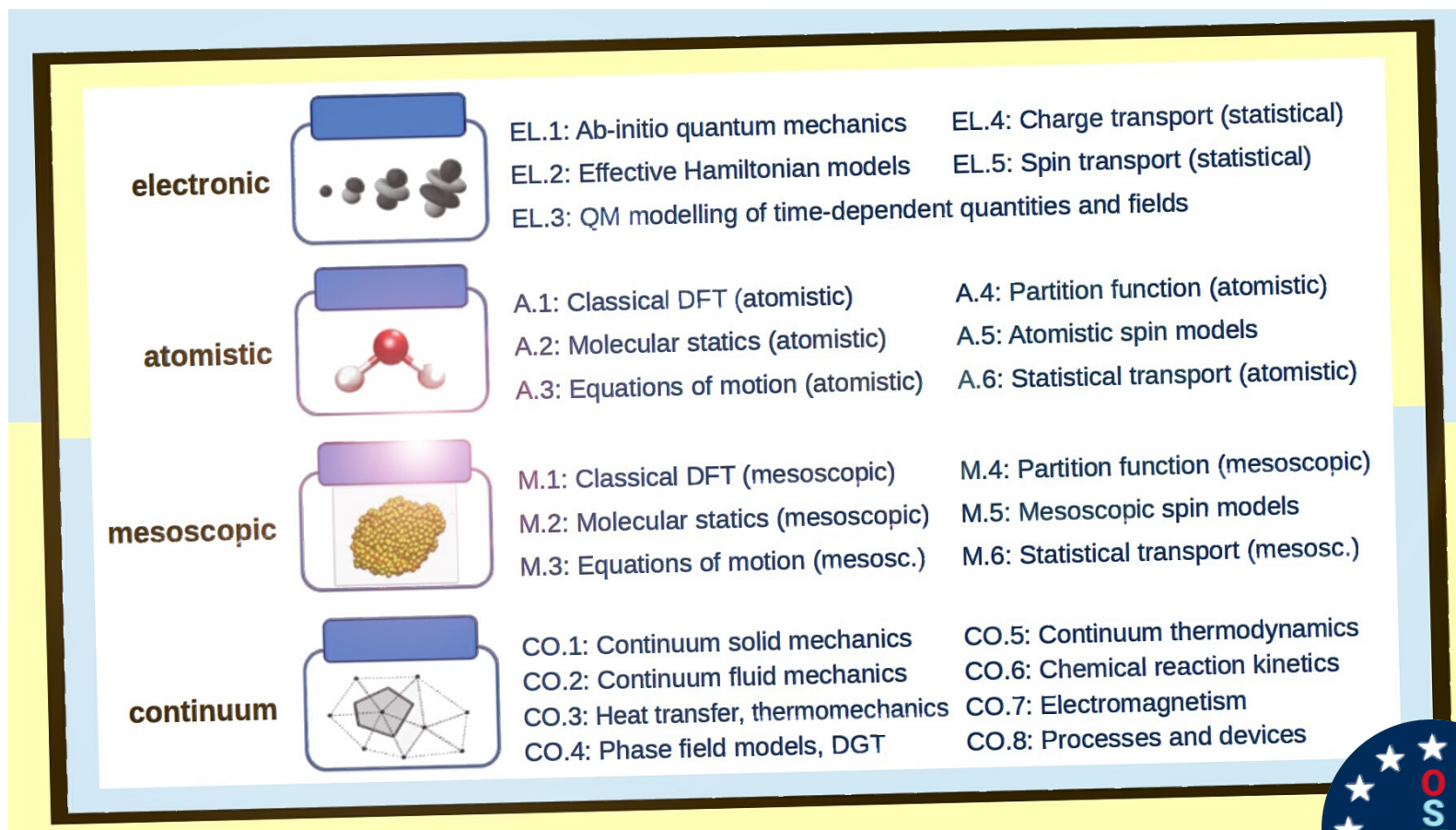


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1.2	MATERIAL	Describe the chemical composition. ...and the values used for properties and from which database these are taken. If pre-processing was needed please specify the methodology.
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1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	<p>If relevant, please list the conditions to be simulated. These can be boundary, initial and global conditions.</p> <p>E.g. heated walls, external pressures and be Please note that these might appear as term conditions, and this will be documented in Ch 2.4</p> <p>Note: These conditions will be expressed in Ch 2.4</p> <p>Please specify the values used for parameters are taken. If pre-processing was needed please</p>
1.6	PUBLICATION ON THIS DATA	Publication documenting the simulation with this and if not already included in the overall publication).

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



Provenance description of simulation results: OSMO

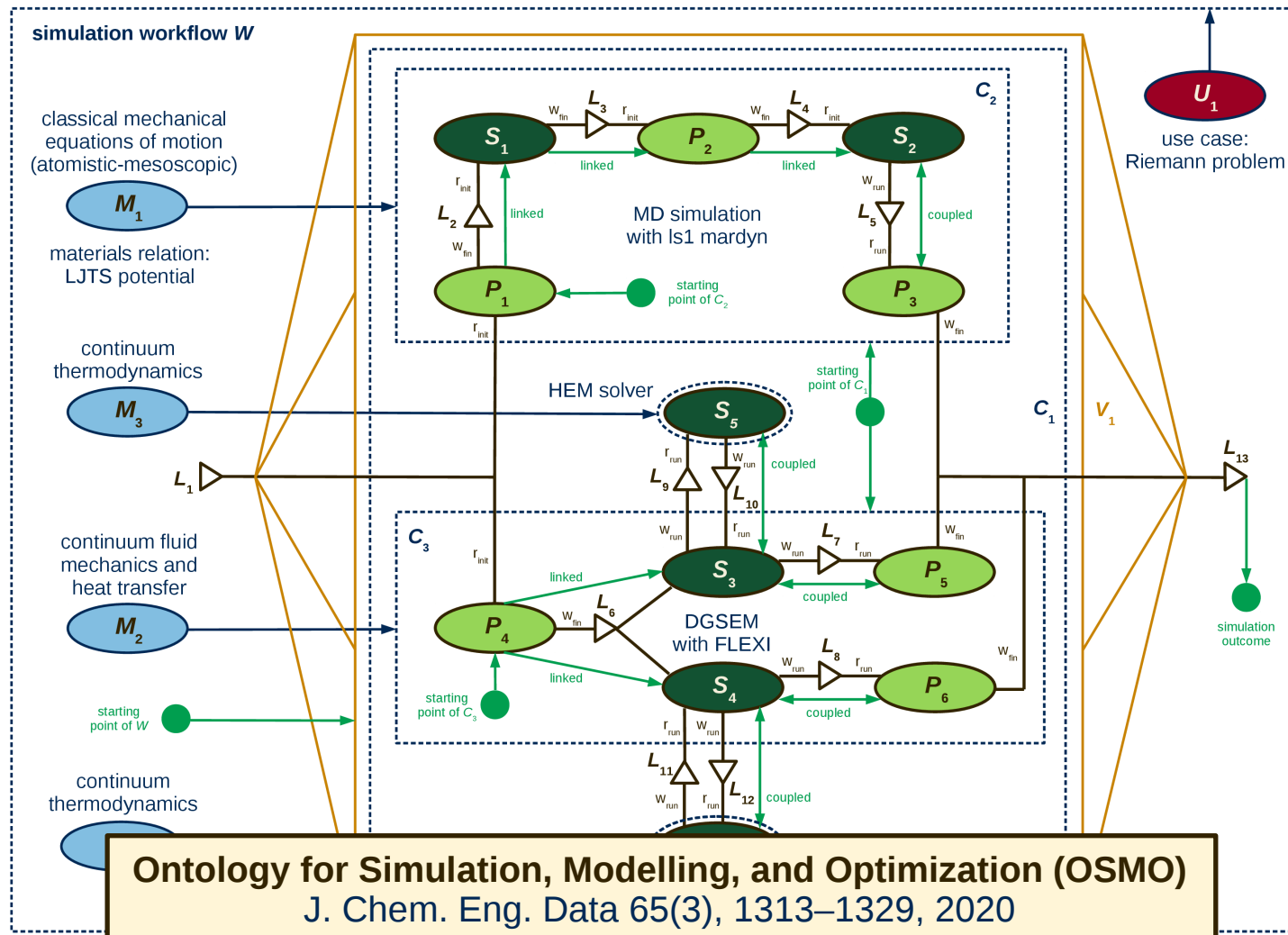


Ontology for Simulation, Modelling, and Optimization

J. Chem. Eng. Data 65(3), 1313–1329, 2020



Provenance description of simulation results: OSMO



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

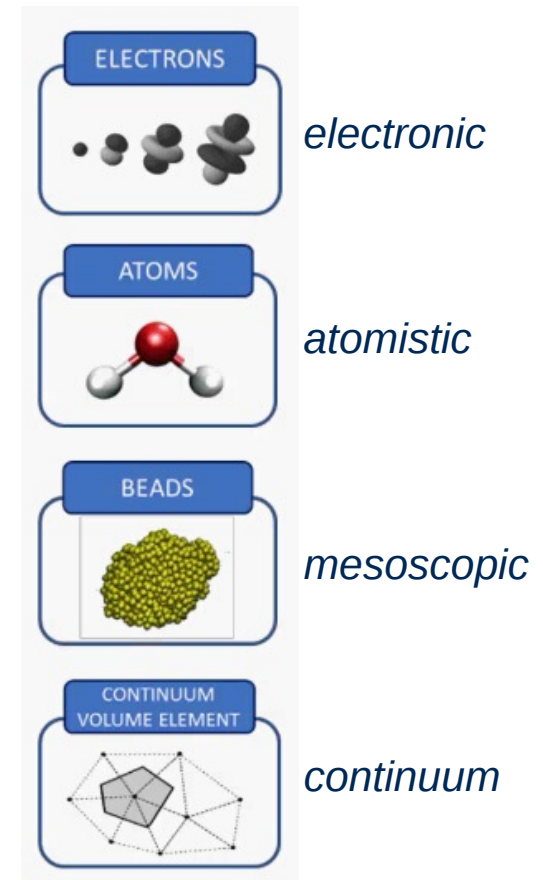
For all elements of the graph notation, there are corresponding concepts and relations from the ontology OSMO.



Community-governed top-level interoperability layer

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

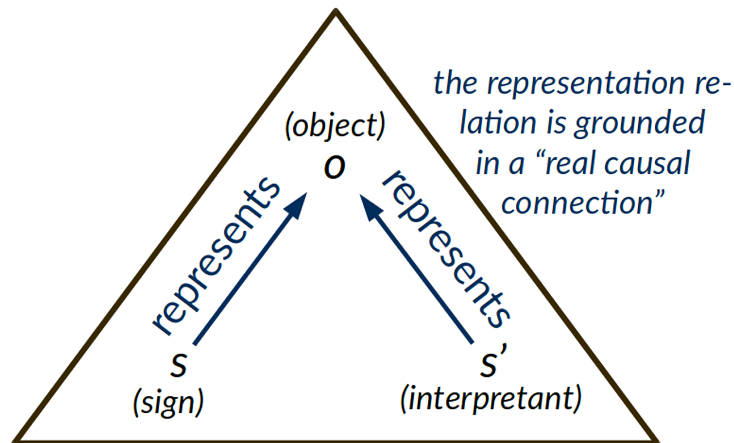


Peircean semiotics

semiosis



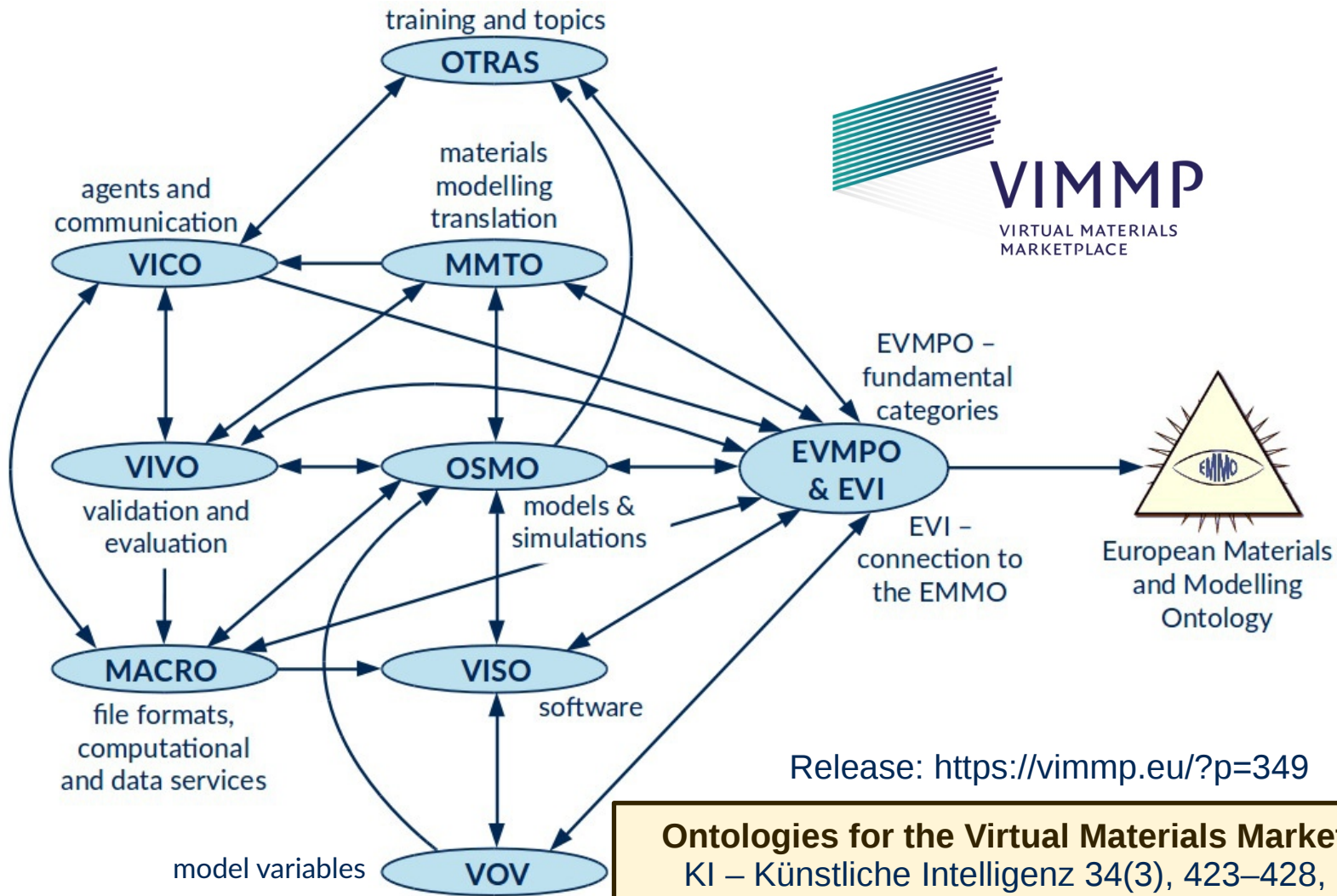
C. S. Peirce



the semiosis, a process by which a new representamen, the interpretant, is created

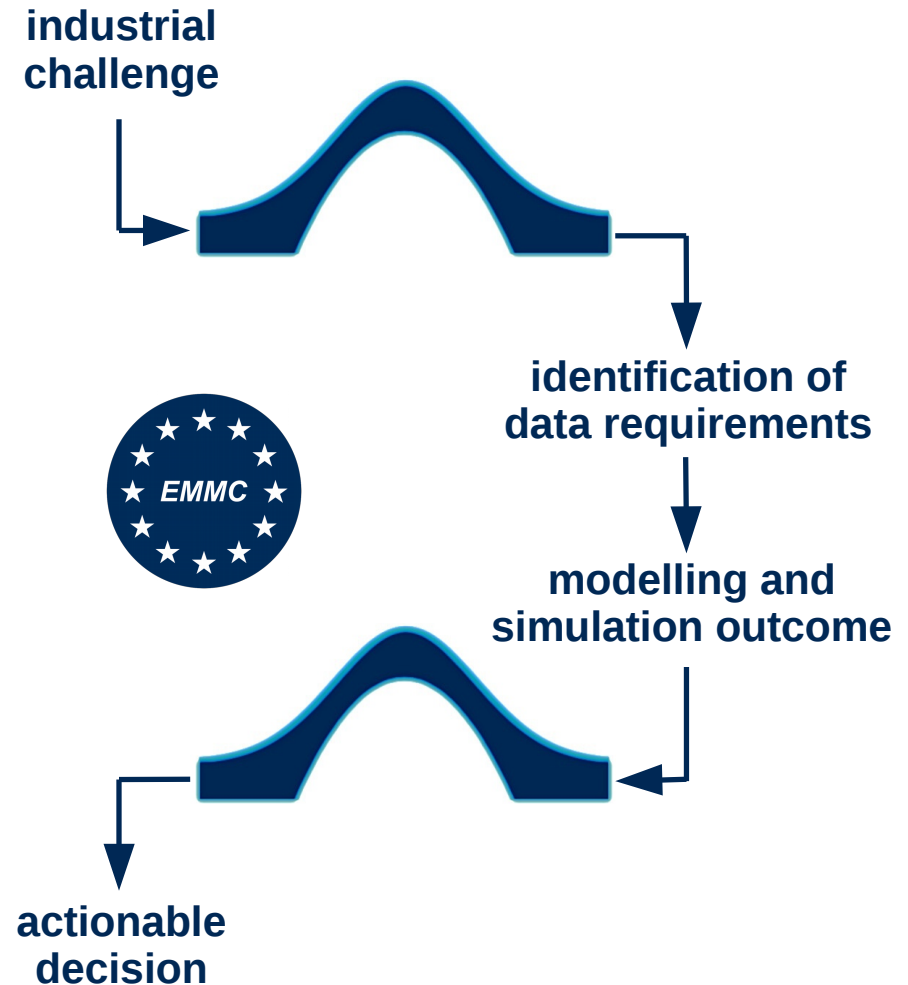
¹E. Ghedini, J. Friis, A. Hashibon, G. J. Schmitz, G. Goldbeck, et al., 2020; <http://emmc.info/emmo-info/>.

System of marketplace-level domain ontologies

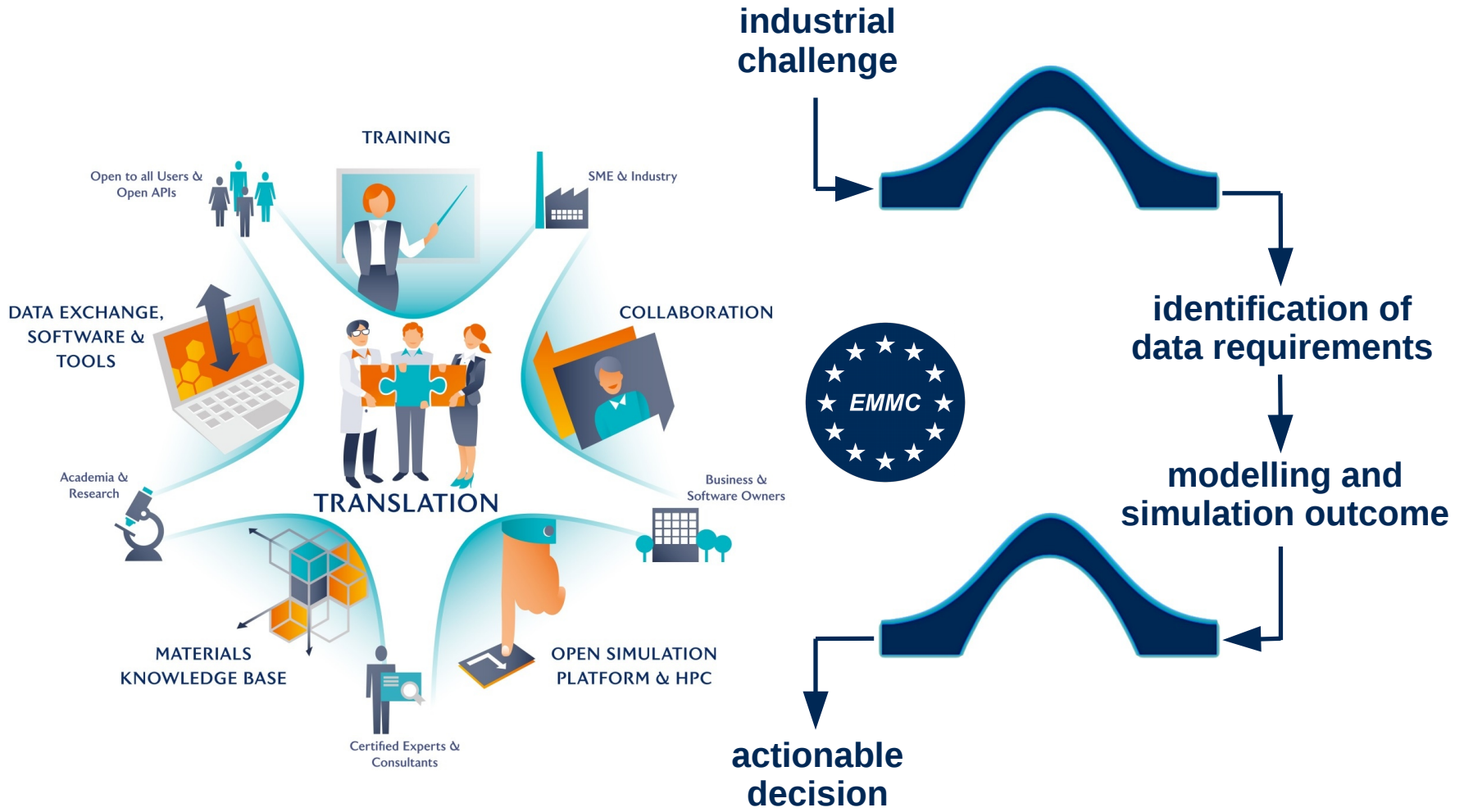


Translation in materials modelling

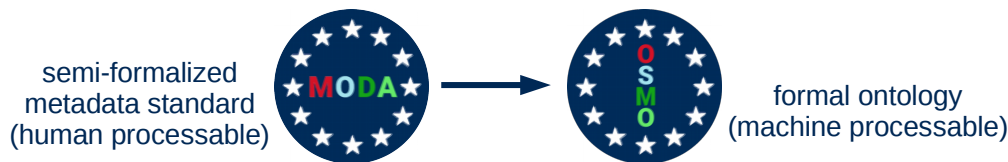
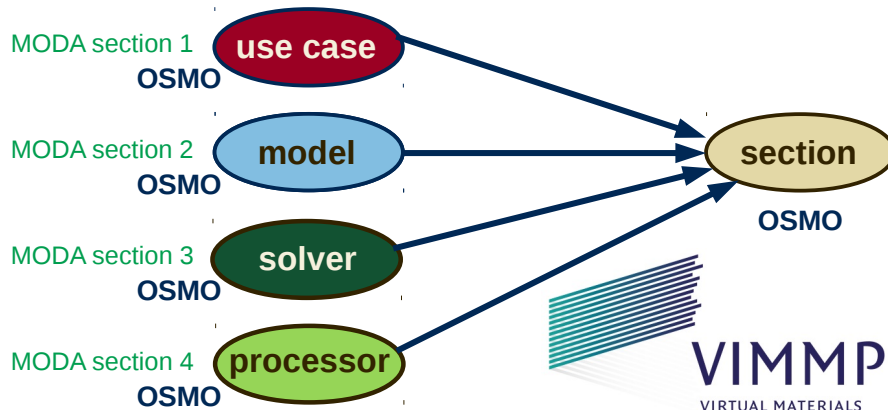
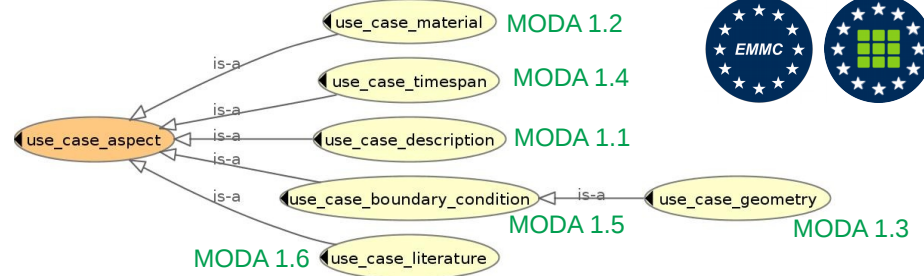
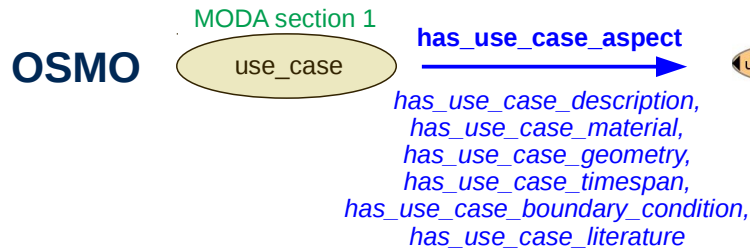
Task: Facilitate the translation of industrial R&D challenges into solutions using scalable and quantitatively reliable materials modelling and simulation.



Translation in materials modelling

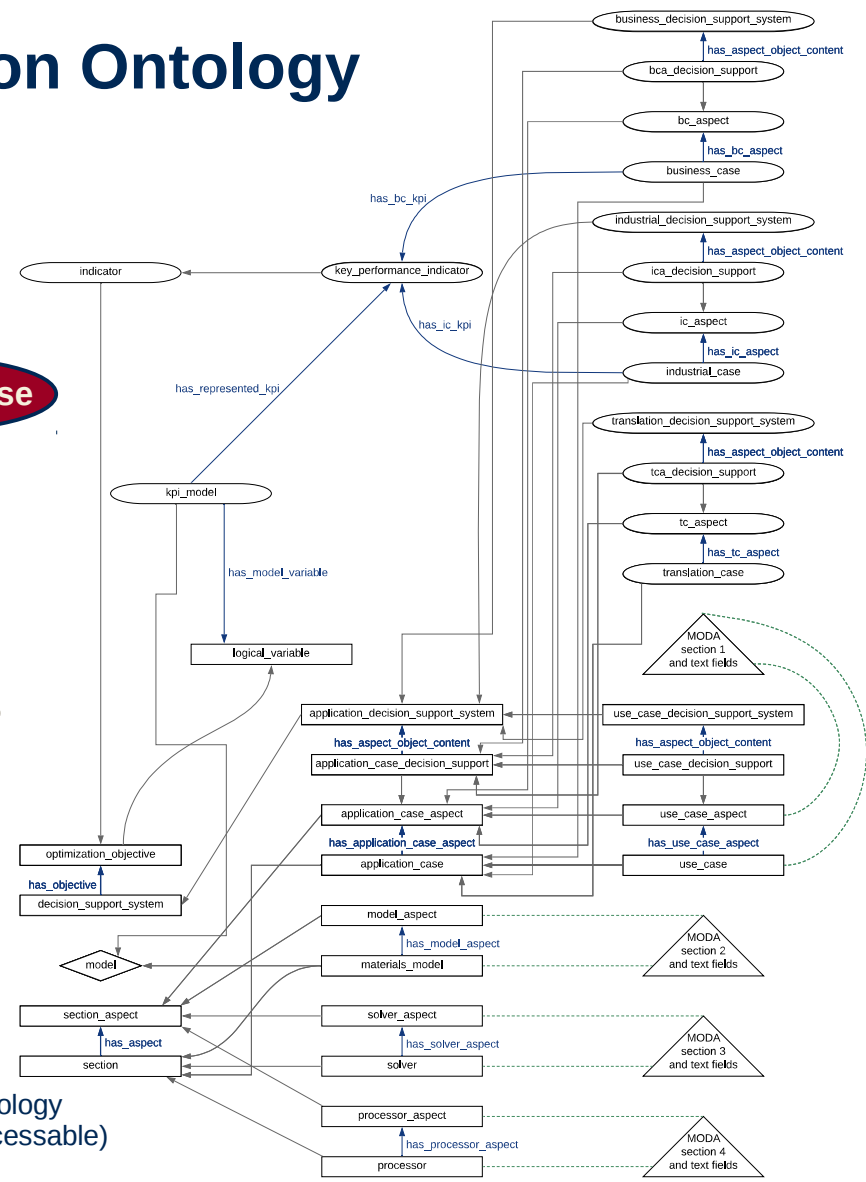
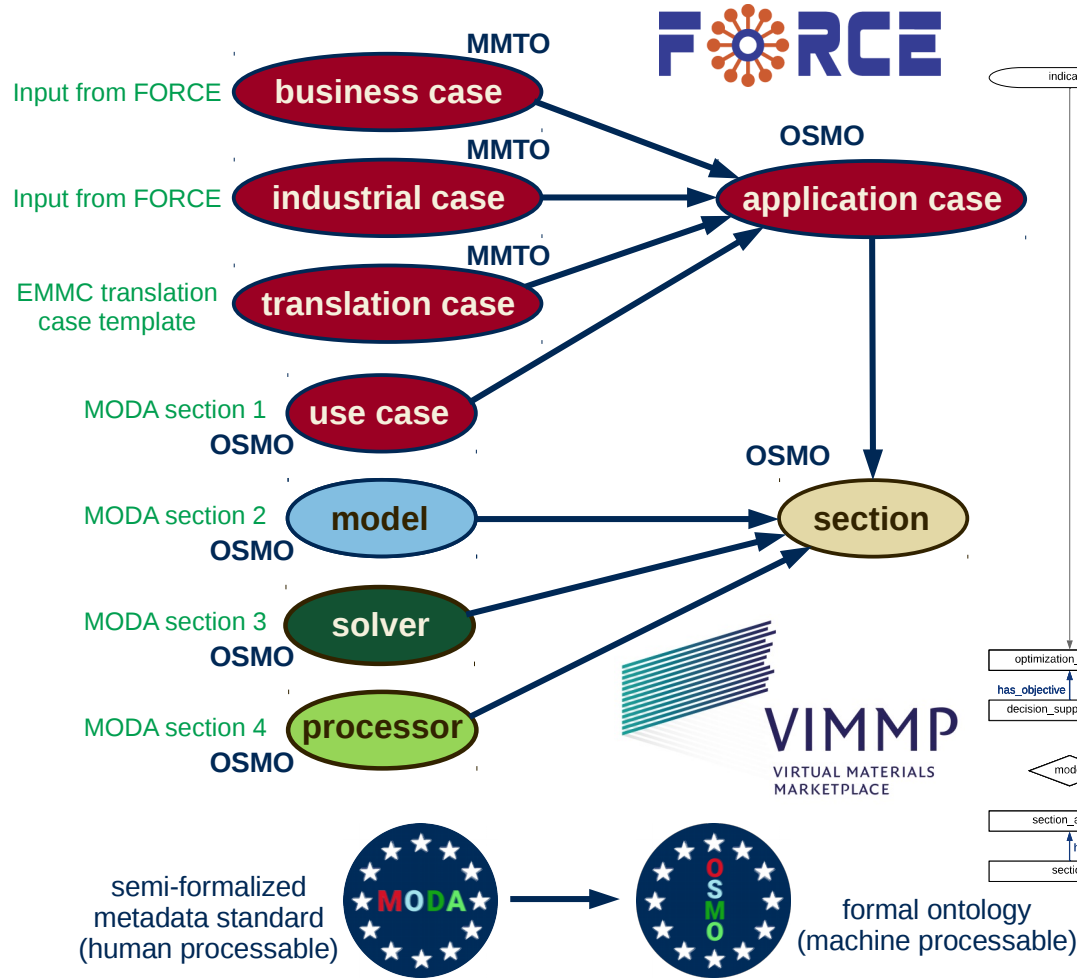


Ontologization of EMMC metadata standards

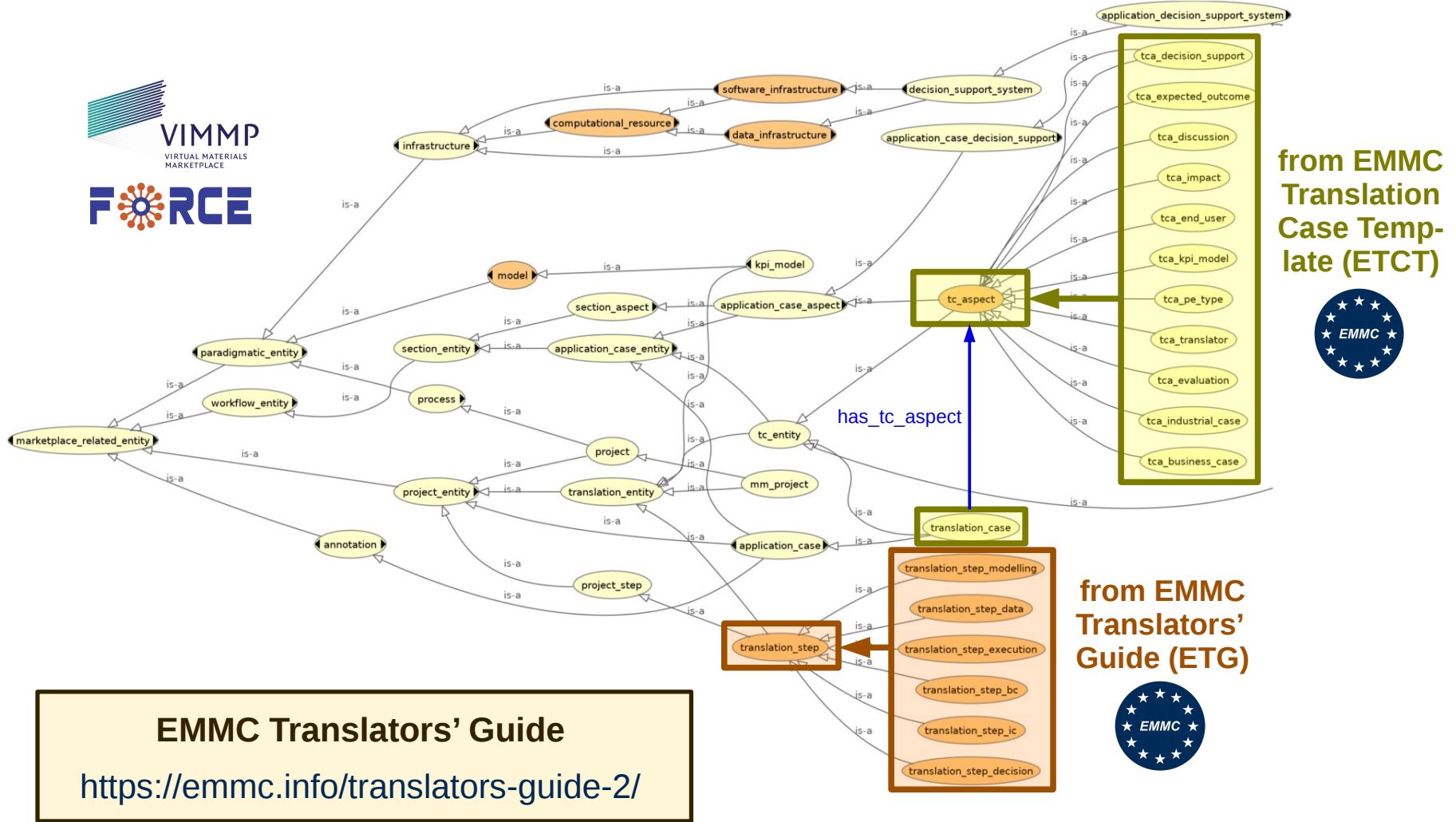


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Materials Modelling Translation Ontology



Materials Modelling Translation Ontology



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.
- 3300, 7300 continuum
 - 3320, 7320 physical equation CO.1
 - 3330, 7330 physical equation CO.2
 - etc.


Speak to our experts at no cost




Which class of model?






Electronic


Atomistic


Mesoscopic


Continuum

I don't know

electronic		EL.1: Ab-initio quantum mechanics EL.2: Effective Hamiltonian models EL.3: QM modelling of time-dependent quantities and fields	EL.4: Charge transport (statistical) EL.5: Spin transport (statistical)
atomistic		A.1: Classical DFT (atomistic) A.2: Molecular statics (atomistic) A.3: Equations of motion (atomistic)	A.4: Partition function (atomistic) A.5: Atomistic spin models A.6: Statistical transport (atomistic)
mesoscopic		M.1: Classical DFT (mesoscopic) M.2: Molecular statics (mesoscopic) M.3: Equations of motion (mesosc.)	M.4: Partition function (mesoscopic) M.5: Mesoscopic spin models M.6: Statistical transport (mesosc.)
continuum		CO.1: Continuum solid mechanics CO.2: Continuum fluid mechanics CO.3: Heat transfer, thermomechanics CO.4: Phase field models, DGT	CO.5: Continuum thermodynamics CO.6: Chemical reaction kinetics CO.7: Electromagnetism CO.8: Processes and devices

VIMMP ontology-based translation router

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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

Speak to our experts at no cost

Which class of model?

Electronic

Atomistic

Mesosopic

Continuum

I don't know

Speak to our experts at no cost

Which business area are you from?

Automotive/Aerospace

Bio

Medical

Chemical industry

Manufacturing

Other

Continue

VIMMP ontology-based translation router

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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

Speak to our experts at no cost

Which class of model?

<input checked="" type="checkbox"/> Electronic	<input type="checkbox"/> Atomistic
<input type="checkbox"/> Mesoscopic	<input type="checkbox"/> Continuum

I don't know

Speak to our experts at no cost

Which business area are you from?

<input checked="" type="checkbox"/> Automotive/Aerospace	<input type="checkbox"/> Chemical industry
<input type="checkbox"/> Bio	<input checked="" type="checkbox"/> Manufacturing
<input type="checkbox"/> Medical	<input type="checkbox"/> Other

Continue

Speak to our experts at no cost

Which material class are you interested in?

<input type="checkbox"/> Metal	<input type="checkbox"/> Composites
<input type="checkbox"/> Polymer	<input type="checkbox"/> Other
<input type="checkbox"/> Ceramic	

Continue

Data management on the VIMMP back end

The screenshot shows the VIMMP back end interface. At the top, there are filters for 'Lifecycle Status' and 'Expertise in the Materials'. A search bar contains the word 'fluid'. A dropdown menu is open, showing a search bar and a list of expertise categories: 5200 fluid (checked), 5450 electrolyte (checked), 5300 bio, 5350 ceramic, 5400 composite, and 5500 metal. Below the dropdown, a table displays search results. The table has columns for 'Created On', 'Information Package Profile', and 'Expertise in the Materials'. The results are as follows:

Created On	Information Package Profile	Expertise in the Materials
2020/May/04 11:22:43 (+01:00)	Translator	5700 polymer, 5400 composite,...
2020/May/04 11:25:27 (+01:00)	Translator	5200 fluid, 5450 electrolyte, 56...
2020/May/04 11:43:13 (+01:00)	Translator	5700 polymer, 5200 fluid, 5450...
2020/May/04 11:33:29 (+01:00)	Translator	5200 fluid, 5500 metal, 5650 o...
2020/May/04 11:38:11 (+01:00)	Translator	5700 polymer, 5200 fluid, 5450...

The screenshot shows a table of properties and a detailed view of the '@hasDocumentTopic' property. The table has columns for 'Property Name', 'Preferred Label', 'Definition', 'Property Type', 'Default Group', and 'Deactivated'. The properties are as follows:

Property Name	Preferred Label	Definition	Property Type	Default Group	Deactivated
@hasCitedB...	ISBN		Text	VIMMP Pro...	no
@hasCitedB...	Number of ...		Integer	VIMMP Pro...	no
@hasCitedci...	Video durati...		Integer	VIMMP Pro...	no
@hasCitedPr...	Number of s...		Integer	VIMMP Pro...	no
@hasCodeList	CodeList	CodeList pro...	Code List	Custom Pro...	no
@hasDocu...	Topic (codes)		Code List	VIMMP Pro...	no
@hasExtern...	External URL		Link	VIMMP Pro...	no
@hasFeature	Feature		Code List	VIMMP Soft...	no

The detailed view of '@hasDocumentTopic' shows the following properties:

- Property Name: @hasDocumentTopic
- Property Type: Code List
- Preferred Label: Topic (codes)
- Definition: http://purl.vimmp.eu/ontologies/otras/otras.ttl#has_document_topic
- Default Group: VIMMP Properties
- Information Package Property: yes



The present work is a collaboration of UKRI STFC Daresbury Laboratory with:



Geesthacht	–	Natalia A. Konchakova
Kaiserslautern	–	Peter Klein
Stuttgart	–	Björn Schembera

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

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The statements made herein do not necessarily have the consent or agreement of the VIMMP Consortium. They represent the opinion and findings of the authors.

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Kaiserslautern – Peter Klein
Stuttgart – Björn Schembera

**Formulations and
Computational
Engineering (FORCE)**

H2020 GA no. 721027



<http://www.the-force-project.eu/>

**EMMC Coordination
and Support Action**

H2020 GA no. 723867



<http://emmc.info/>

**Virtual Materials
Marketplace (VIMMP)**

H2020 GA no. 760907



<http://vimmp.eu/>

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