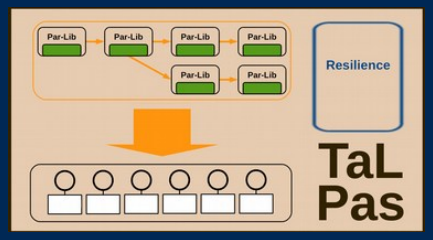


Martin Thomas Horsch, Silvia Chiacchiera,
Michael A. Seaton, and Ilian T. Todorov
STFC Daresbury Laboratory
UK Research and Innovation

Ontology development for virtual marketplaces in materials modelling

22nd October 2019

CAPE-OPEN Annual Meeting

Amsterdam

VIMMP
VIRTUAL MATERIALS MARKETPLACE

Science & Technology Facilities Council | UK Research and Innovation

VIMMP VIRTUAL MATERIALS MARKETPLACE

Ontologies in computational engineering

Semantic technology can facilitate the integration of diverse data and software components into a coherent framework, permitting multiple platforms to become interoperable. **Ontologies** are semantic assets that **characterize individuals (objects), the classes to which they belong, and their properties**, i.e., the possible relations between them.

Triples: Individual Relation Individual. (Subject Predicate Object.)

Example: Frank is_father_of Robert.

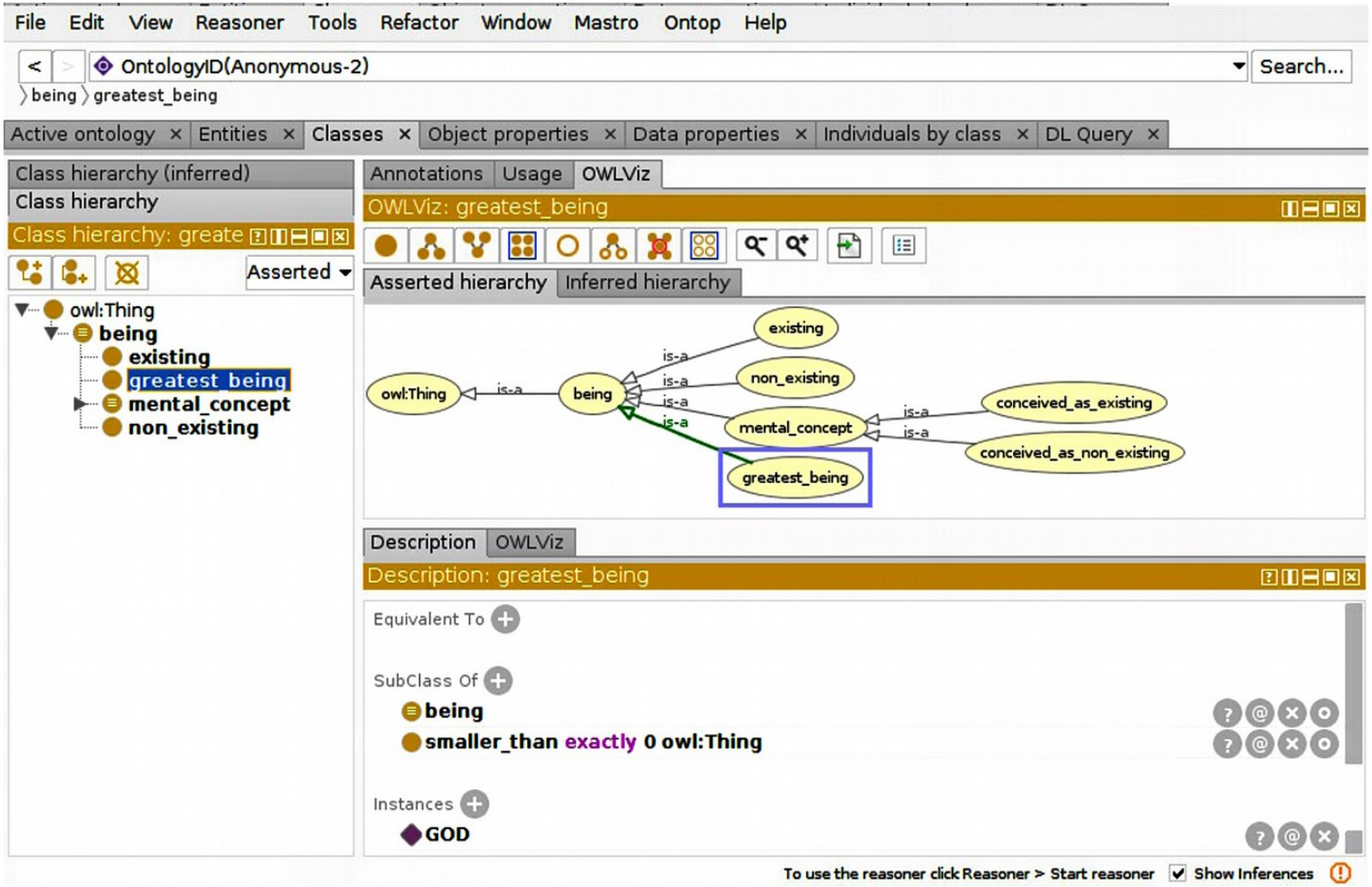
- Resource description framework (RDF): Basic semantic-web approach to specify triples.
- Web ontology language (OWL) and OWL Description Language (OWL DL): Approach for specifying ontologies, i.e., including rules that can be processed by automated reasoning.
- Terse triple language (TTL): Common syntax for denoting triples from RDF and OWL DL.

Semantic web principle: Open world assumption

Since relevant information may distributed over the entire semantic web, rather than the presently considered source only, the **available knowledge is assumed to be incomplete**.

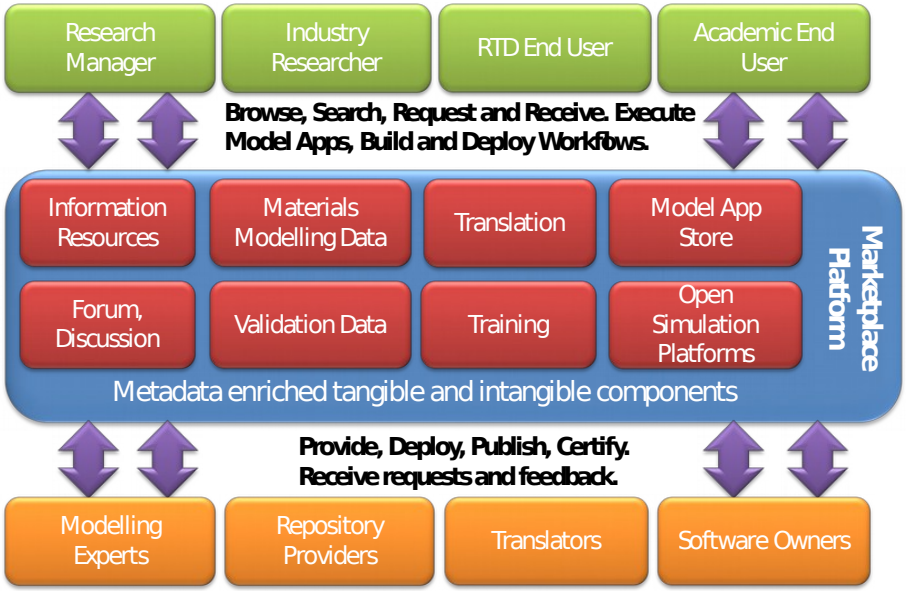
(Contrast with a closed, monolothic database architechture.)

Ontologies in computational engineering: *Protege* tool



VIMMP: The Virtual Materials Marketplace

VIMMP Marketplace concept: To serve its participants and facilitate exchange, e.g., between materials **model providers**, industrial & academic client **end users**, and **translators**.

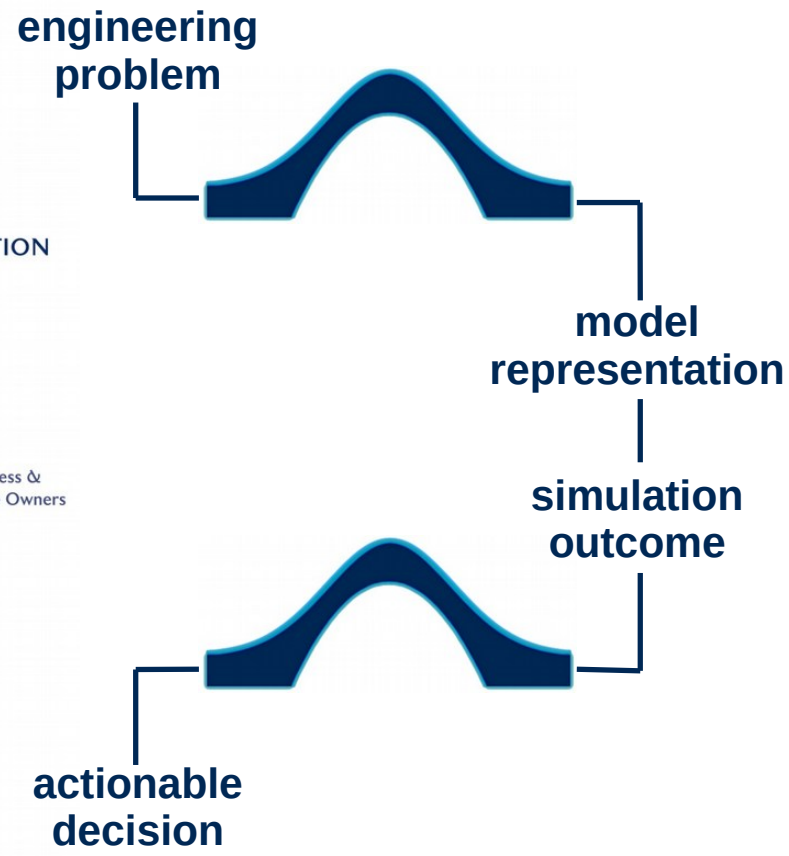


Coordination:

Fraunhofer IFAM

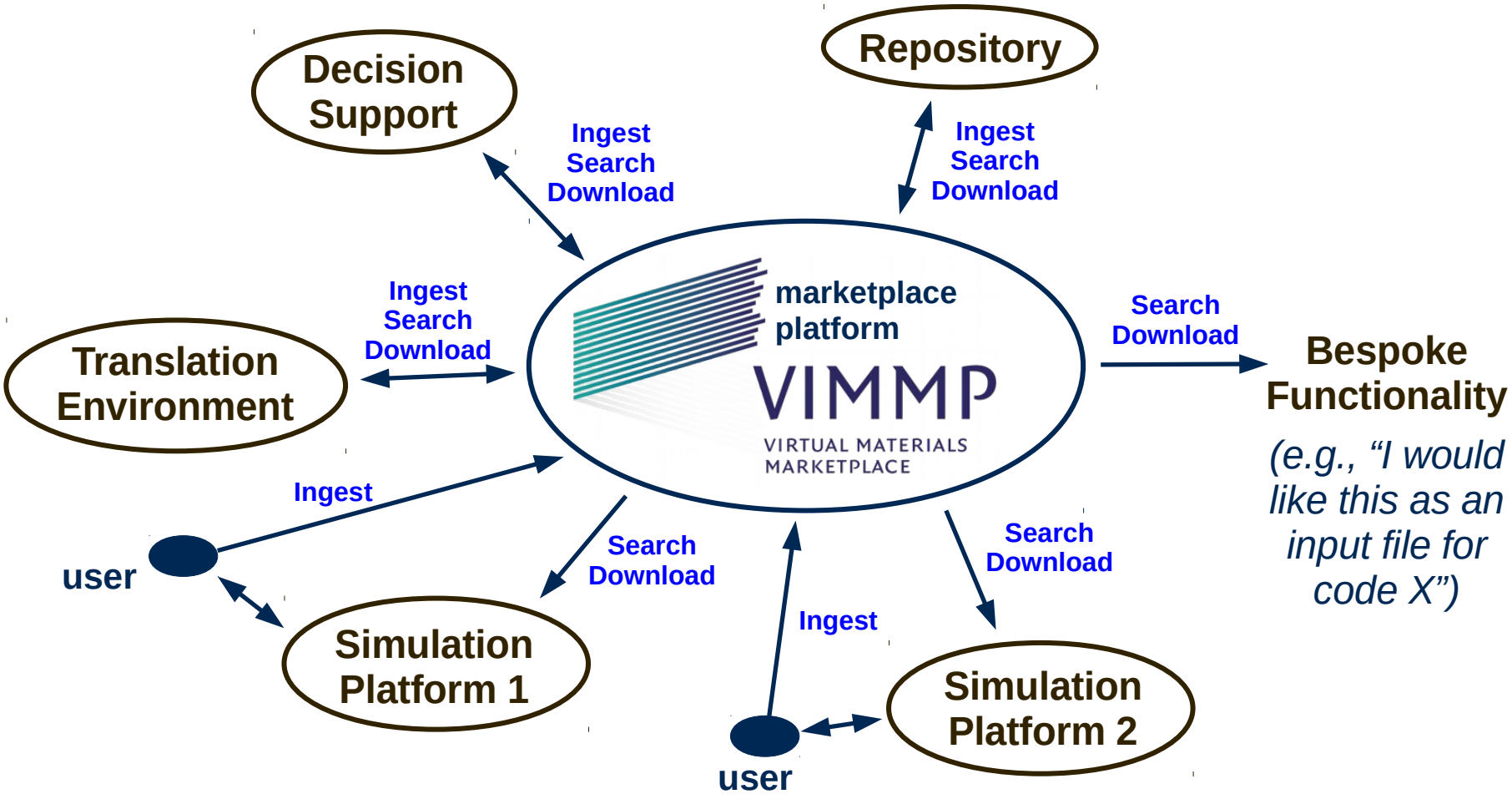
Funded by the Horizon 2020 Framework Programme of the European Union

The **VIMMP Marketplace** will provide end-user interfaces to information resources, discussion forums, databases and repositories, translation and training services, validated models and modelling software, and the ability to utilise open simulation platforms to build and deploy workflows via cloud-based computing resources.



VIMMP will facilitate the **translation of industrial R&D challenges into materials modelling solutions**, and connect potential users and providers of modelling and simulation related services to each other, as an **open two-sided virtual marketplace**.

Interoperability in materials modelling



Interoperability in materials modelling

Semantic asset development guided by the European Materials Modelling Council

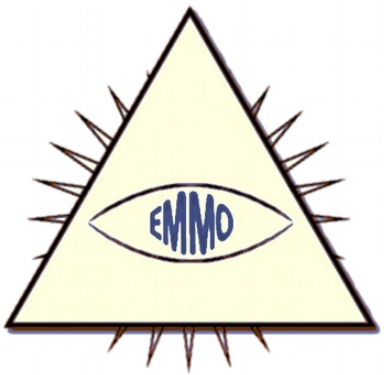
RoMM VI → **MODA** → **CWA 17284** → **Ontologies**

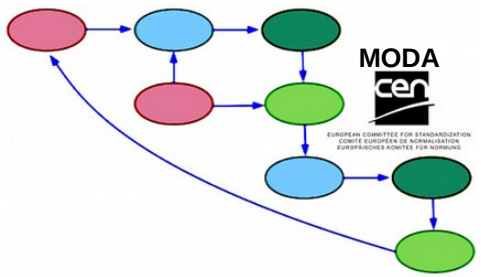
Semi-formalized terminology or vocabulary

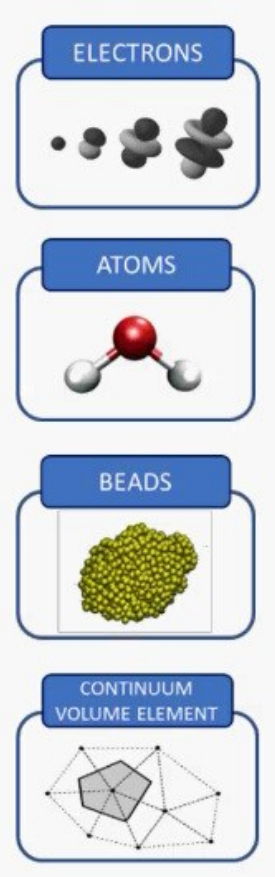
MODA workflow graph language

CEN European standard

European Materials and Modelling Ontology (EMMO)







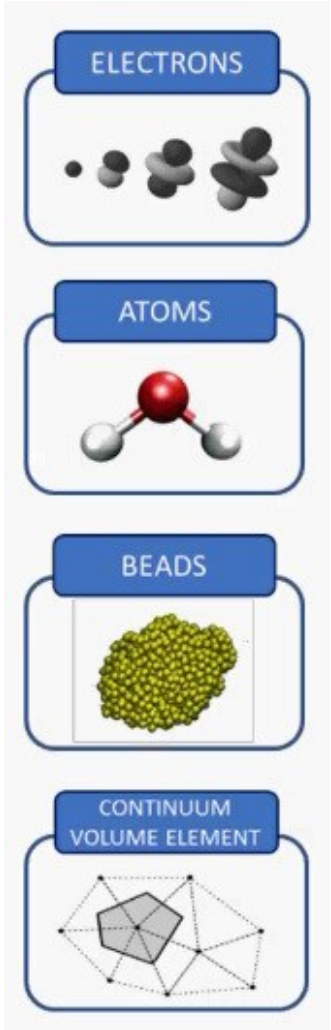
electronic

atomistic

mesoscopic

continuum

Physical equation taxonomy from RoMM and OSMO



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)

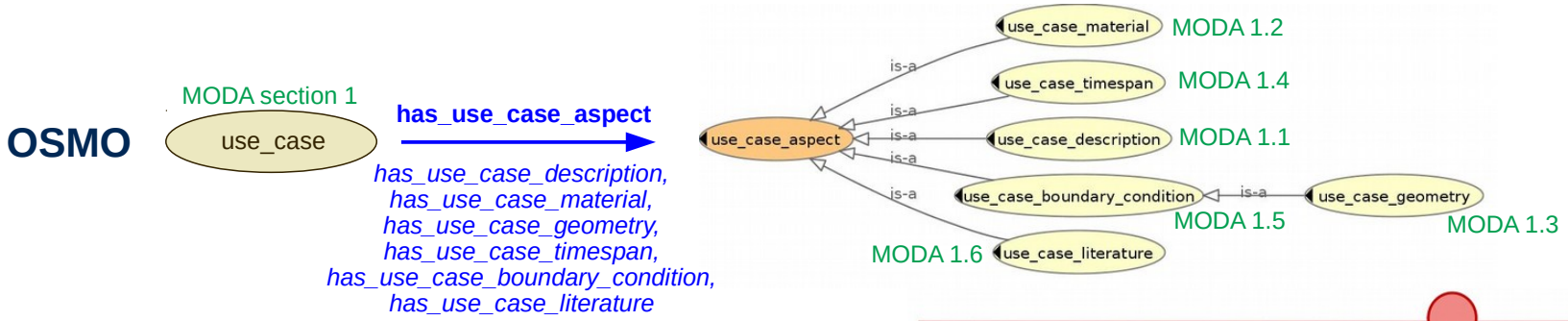
mesoscopic

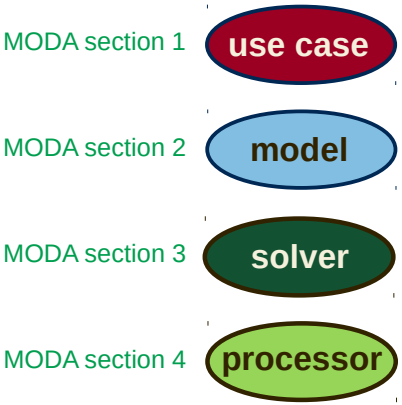
M.1: Classical DFT (mesoscopic)
M.2: Molecular statics (mesoscopic)
M.3: Equations of motion (mesosc.)
M.4: Partition function (mesoscopic)
M.5: Mesoscopic spin models
M.6: Statistical transport (mesosc.)

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

Simulation workflows following MODA and OSMO



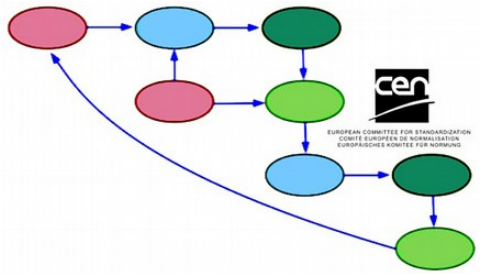


"sections"

"aspects"

OSMO

"graphs"

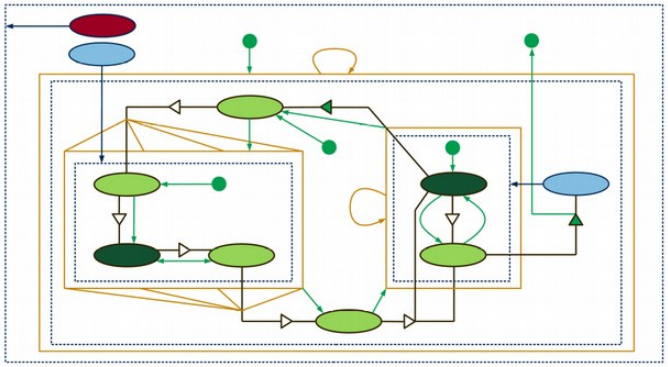


1	Aspect of the User Case/System to be Simulated	
1.1	Aspect of the User Case to be Simulated	*Describe the aspects of the user case textually.* *No modelling information should appear in this box. This case could also be simulated by other models in a benchmarking operation!* *The information in this 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).*

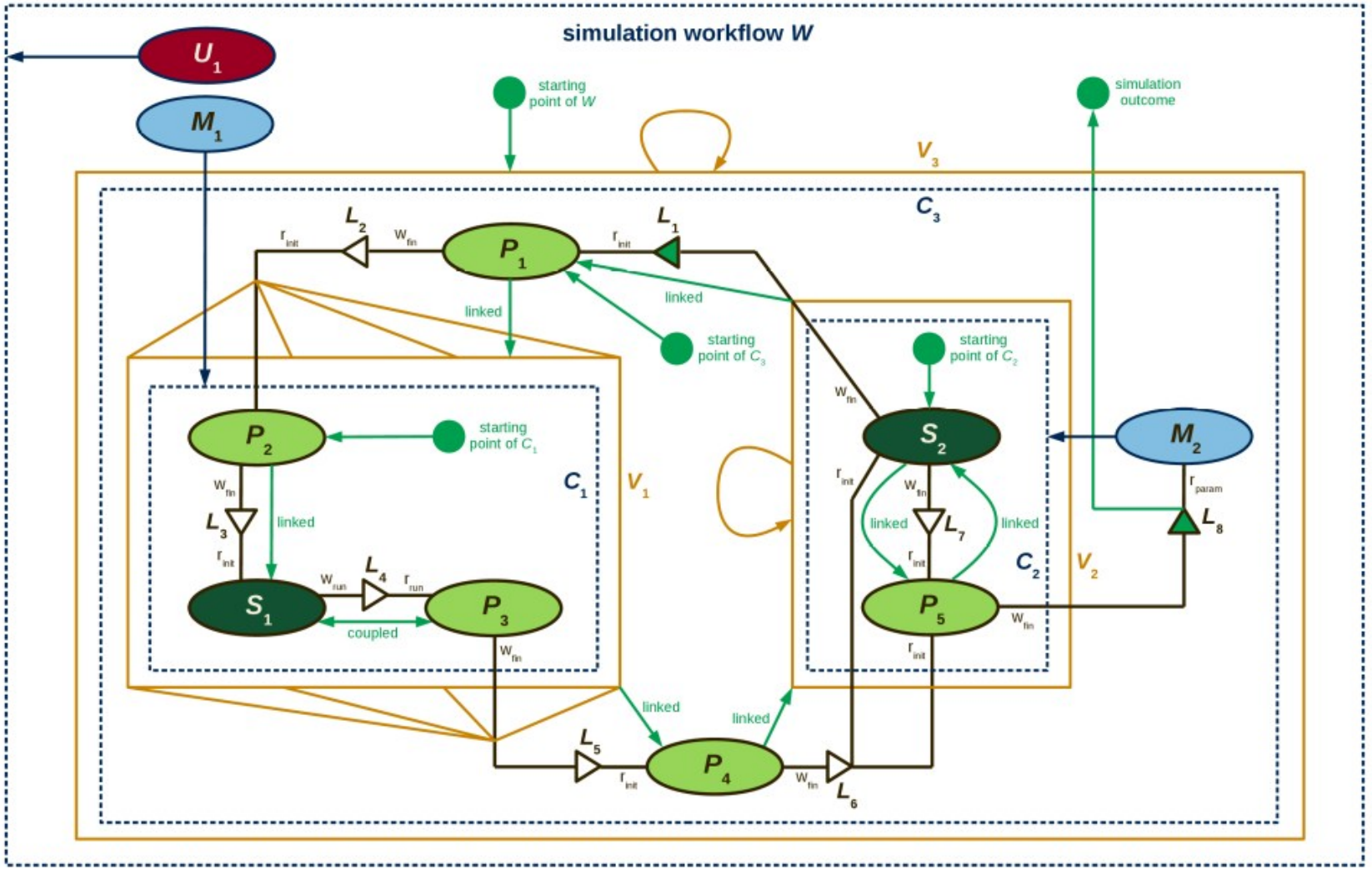
Simulation workflows following MODA and OSMO

Logical (i.e., non-technical) workflow description following the approach from RoMM and MODA

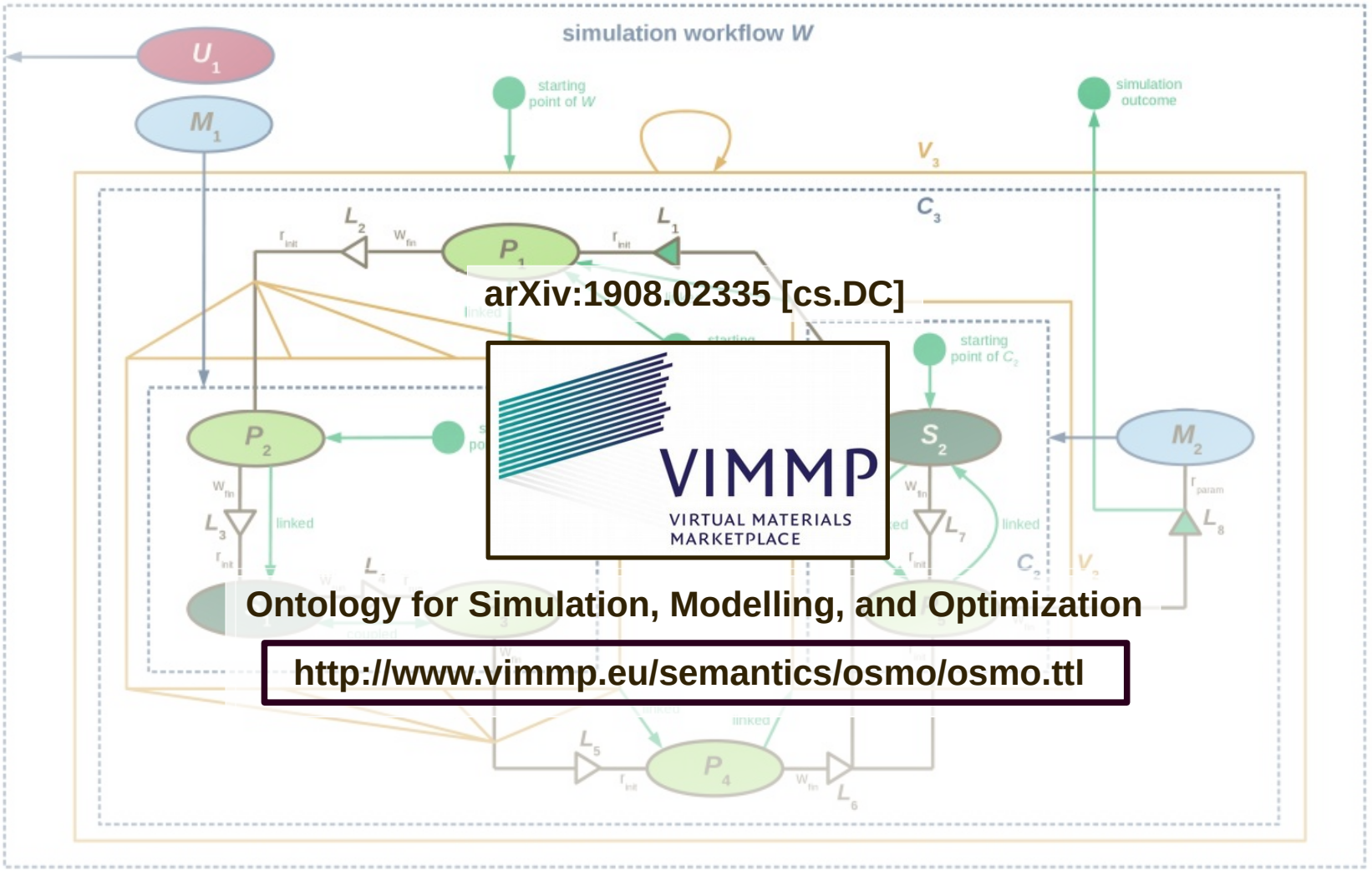
Ontology-level formalization by OSMO



Simulation workflows following MODA and OSMO



Simulation workflows following MODA and OSMO



European Materials and Modelling Ontology[1]

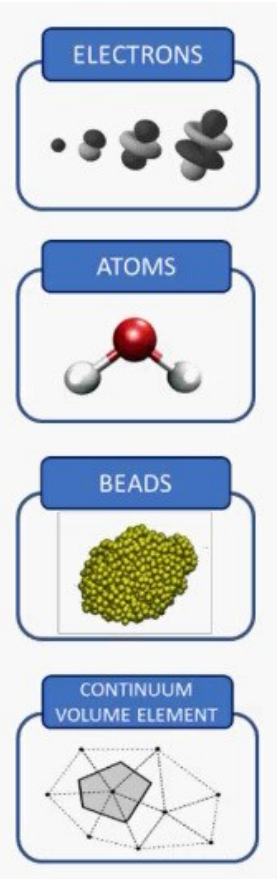
Types of relations covered by the European Materials & Modelling Ontology (EMMO)

1) **Taxonomy**: Subclass relation (between classes)

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

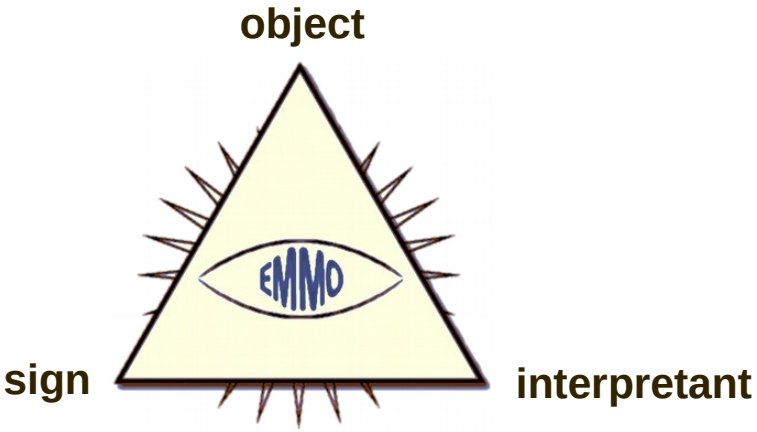
3) **Mereotopology**: Parthood (of a part in a *fusion*) and slicing

4) **Set theory**: Membership (of an element in a *set*)



"semiosis"

C. S. Peirce



[1]E. Ghedini, J. Friis, G. Schmitz, G. Goldbeck, **2019**; see http://emmc.info/emmo-info/.

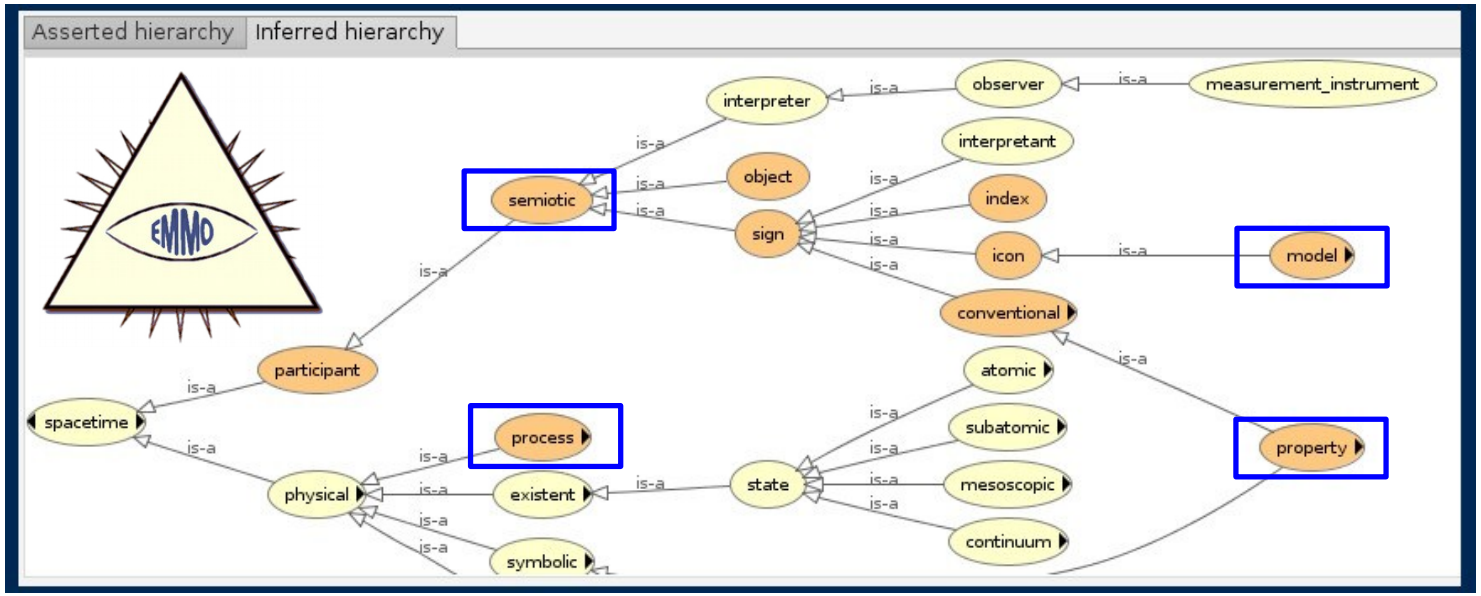
European Materials and Modelling Ontology[1]

Types of relations from EMMO

1) **Taxonomy**: Subclass relation
2) **Semiosis**: Representation by *signs*
3) **Mereotopology**: Parthood and slicing
4) **Set theory**: Membership

Branches and important classes from EMMO

1) "material"
2) "process"
3) "quantitative property"
4) "model"
5) "qualitative property"
6) "semiotic"



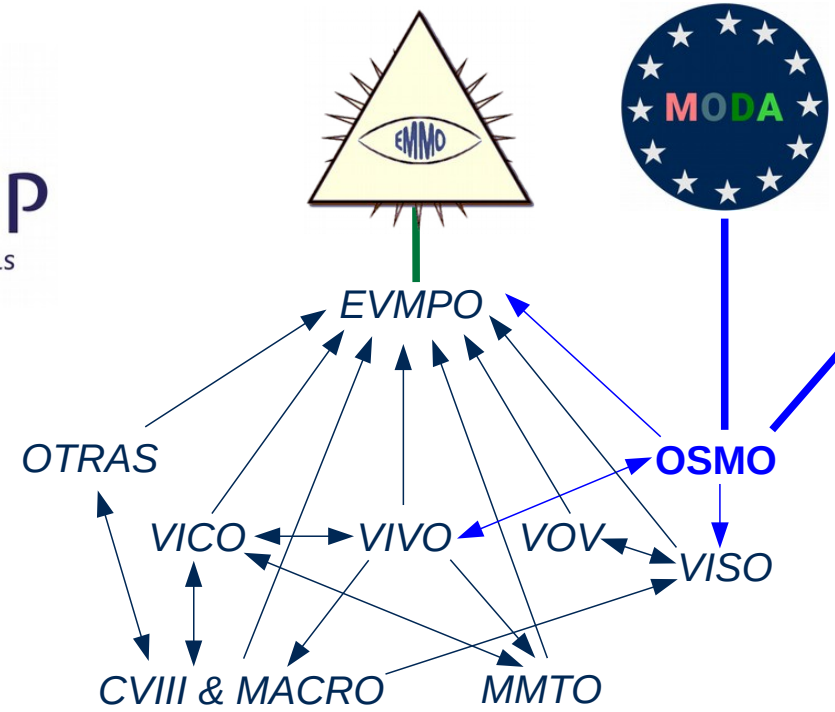
[1]E. Ghedini, J. Friis, G. Schmitz, G. Goldbeck, **2019**; see http://emmc.info/emmo-info/.

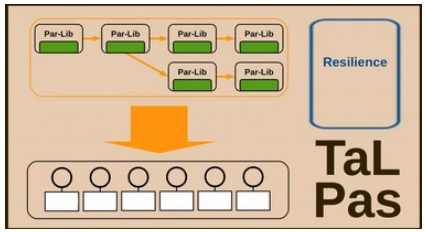
VIMMP ontologies based on EMMO and EVMPO

MODA Graph Language, CEN Workshop Agreement 17284, and EMMO (Ghedini *et al.*)

- **Upper level: EMMO extended by European Virtual Marketplace Ontology (EVMPO)**
- **Marketplace-level ontologies: VIMMP in coordination with the MarketPlace project**
- **Subdomains: VOV, VISO branches (electronic, atomistic-mesoscopic, continuum)**

VIMMP ontologies based on EMMO and EVMPO



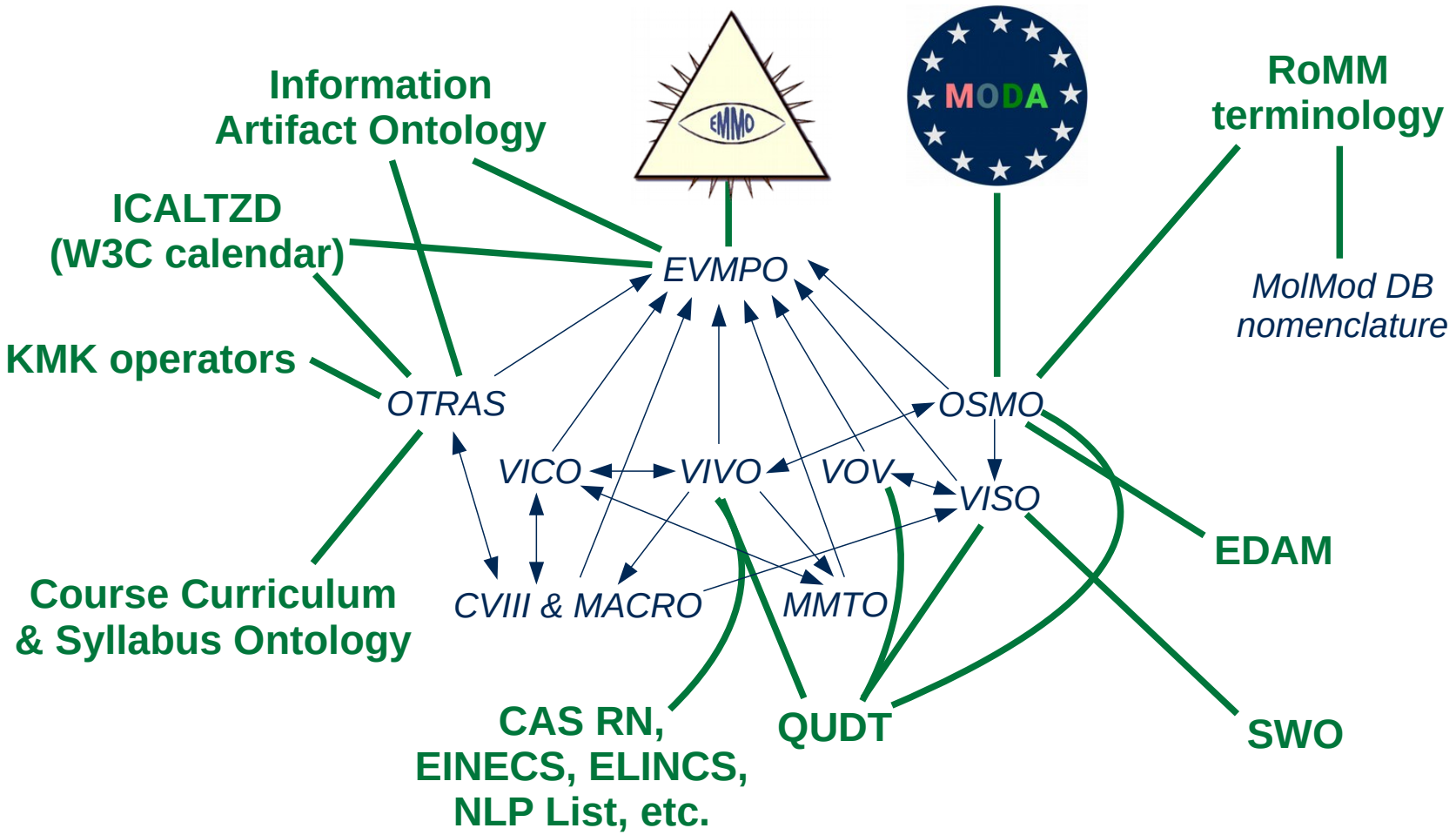


EMMC line of semantic asset development:

1) **Review of Materials Modelling (RoMM)**
2) **CWA 17284 – Model Data (MODA)**
3) **European Materials & Modelling Ontology (EMMO)**

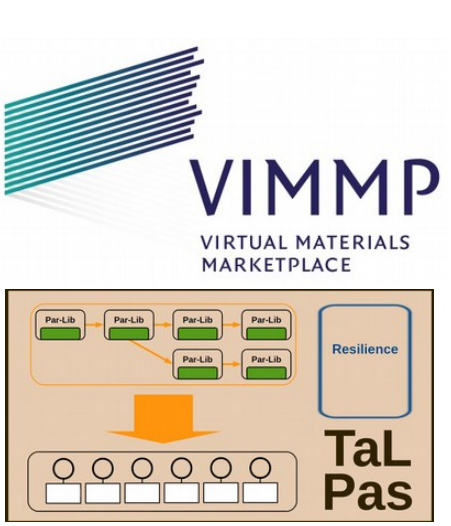
Blue: Semantic assets co-developed by the Virtual Materials Marketplace (VIMMP) project
OSMO: Ontology for Simulation, Modelling, and Optimization

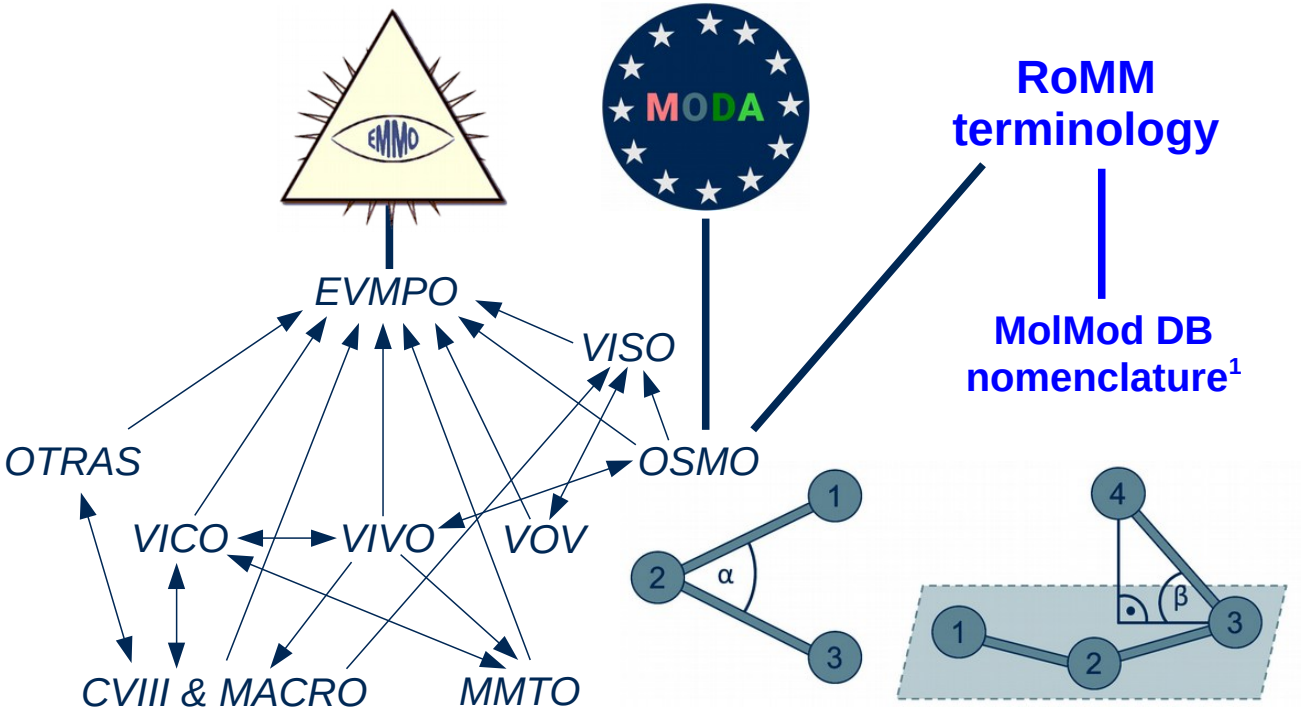
VIMMP ontologies based on EMMO and EVMPO



Blue: Semantic assets co-developed by the Virtual Materials Marketplace (VIMMP) project
Green: Connected external semantic assets

Molecular model nomenclature and database





1	$name_1$	-	-	-	-	-	-
2	$name_2$	1	$distance_2$	-	-	-	-
3	$name_3$	2	$distance_3$	1	$angle_3$	-	-
4	$name_4$	3	$distance_4$	2	$angle_4$	1	$dihedral_4$
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
n	$name_n$	n-1	$distance_n$	n-2	$angle_n$	n-3	$dihedral_n$

Z-matrix formalism for the site coordinates of multi-site models[1, 2]

[1]S. Stephan, M. Horsch, J. Vrabec, H. Hasse, *Mol. Sim.* 45(10), 806 – 814, **2019**.
[2]J. Parsons, J. B. Holmes, J. M. Rojas, J. Tsai, C. E. M. Strauss, *J. Comput. Chem.* 26(10), 1063 – 1068, **2005**.

Molecular model nomenclature and database

Geometry

Types and positions
of interaction sites

Dispersion and repulsion

Lennard-Jones or Mie potential:
Size and energy parameters

Electrostatics

Point charge or multipole
(point dipole or quadrupole):
Magnitude and orientation

Computational Molecular Engineering

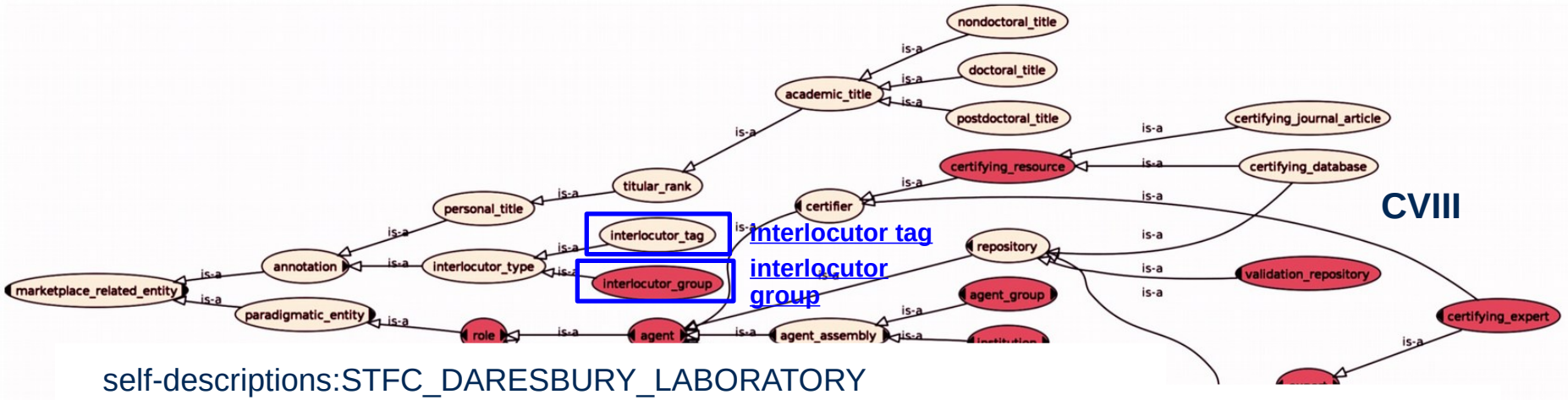
Molecular Model Database (MolMod DB)

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

pair potentials for over 150 molecular fluids

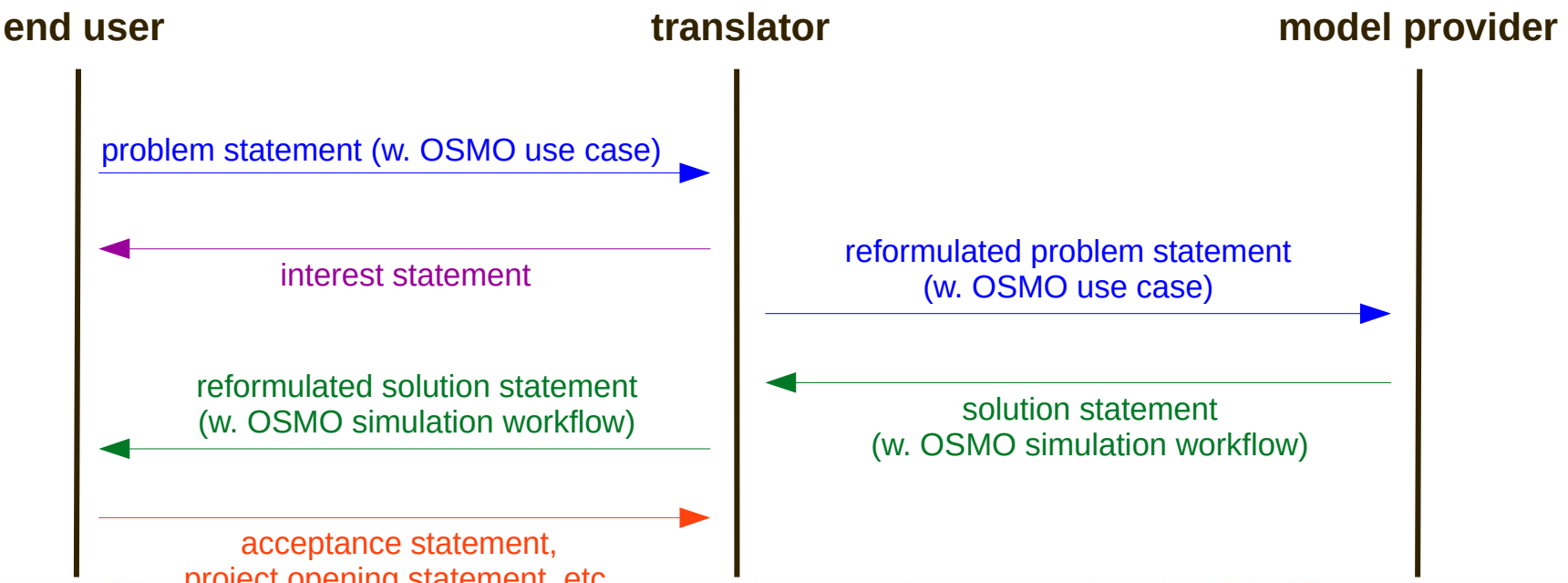
[1]S. Stephan, M. Horsch, J. Vrabec, H. Hasse, *Mol. Sim.* 45(10), 806 – 814, **2019**.

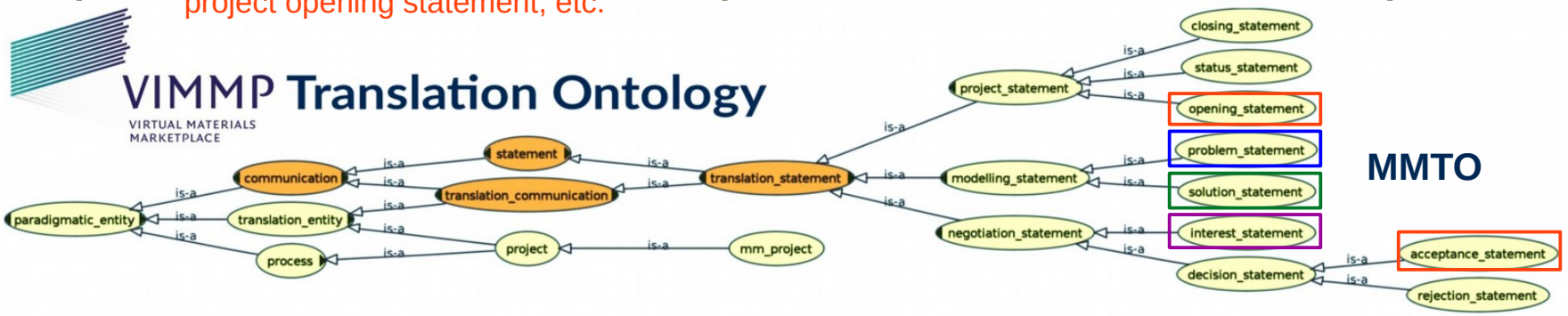
VIMMP ontologies related to marketplace interactions




```
self-descriptions:STFC_DARESBURY_LABORATORY
   a cviii:institution, cviii:model_provider, cviii:software_owner, cviii:training_provider, cviii:translator;
   cviii:has_name "STFC Daresbury Laboratory"^^xs:string;
   cviii:has_interest
      otras:MM_TOPIC_3000, otras:MM_TOPIC_6120, otras:MM_TOPIC_7200, otras:MM_TOPIC_8350;
   cviii:has_interlocutor_tag [
      cviii:is_academic true;
      cviii:is_based_in lcc-codes:UnitedKingdomOfGreatBritainAndNorthernIreland;
      cviii:is_in_group
         cviii:IG_MODEL_PROVIDER, cviii:IG_SOFTWARE_OWNER,
         cviii:IG_TRAINING_PROVIDER, cviii:IG_TRANSLATOR;
      cviii:is_for_profit false;
      cviii:is_nuclear true;
      cviii:is_sme false
   ].
```

VIMMP ontologies related to marketplace interactions





VIMMP Software Ontology (VISO)

The purpose is of VISO to describe software, addressing its capabilities (both model and solver aspects) as well as licensing, requirements (e.g., libraries and operating systems), and compatibility[1] with other tools.

It is employed to structure the data ingest for software tools at the virtual marketplace. The same keywords are available to the users to browse tools and compare them.

[1] Following E. Ghedini (EMMC), we distinguish between compatibility and interoperability, namely:

Compatibility = ability to exchange information directly, no need to interface
Interoperability = ability to exchange information through a common intermediate standard

Top categories within VISO (below EMMO and EVMPO):

(1) **agent** = an entity (individual, group, institution) that can potentially act on a virtual marketplace

(2) **software** = a computer program; can be a software tool, a compiler, or an operating system

(3) **license** = regulation of the right to use, modify and distribute something, in this case software.

(4) **programming_language** = a language that can be used to write software.

(5) **solver_feature** = capability of a software tool, intended as a numerical algorithm which is implemented.

(6) **model_feature** = capability of a software tool, intended as a model aspect that can be addressed.

(7) **modelling_related_entity** = high level concept related to modelling, such as statistical mechanics, the RoMM models, physical equation, etc.

(8) **property** = a feature that can be measured or computed

(9) **software_update** = allows to describe the differences between two softwares; connects an older to a newer version of the software

(10) **software_interface** = interface between a software and a user or a client (i.e., a program or device)

VIMMP Software Ontology: Versioning and tool updates

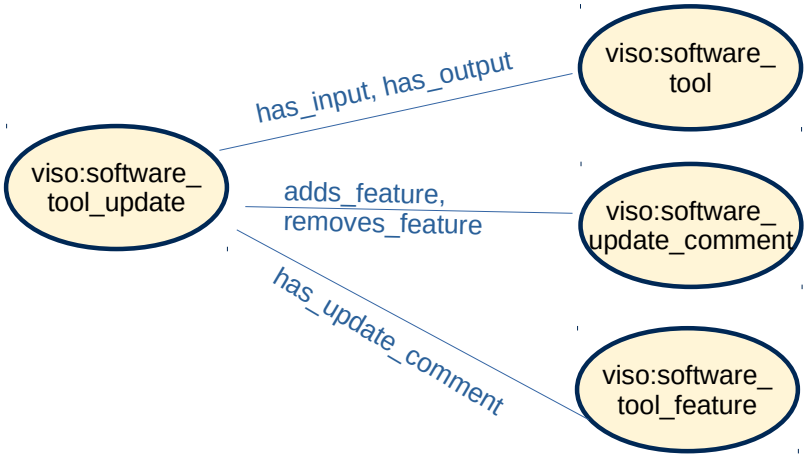
Example: the update of CODEX from version 1.0 to 2.0 removes the feature DIRECT_COULOMB_SUM and adds SPME. Also, trajectory format changes.

Description in TTL syntax:

```
ex:CODEX_1.0
  viso:has_main_name "CODEX"^^xs:string;
  viso:has_version_identifier "1.0"^^xs:string;
  viso:has_feature viso-am:LANGEVIN_BAROSTAT.

ex:CODEX_2.0
  viso:has_main_name "CODEX"^^xs:string;
  viso:has_version_identifier "2.0"^^xs:string.

ex:UPDATE_CODEX_1TO2 a viso:software_tool_update;
  viso:has_input ex:CODEX_1.0;
  viso:has_output ex:CODEX_2.0;
  viso:adds_feature viso-am:SPME;
  viso:removes_feature viso am:DIRECT_COULOMB_SUM;
  viso:has_update_comment "Trajectory formats have
  changed, postprocessors need to be adapted."^^xs:string.
```



A reasoner may deduce that:

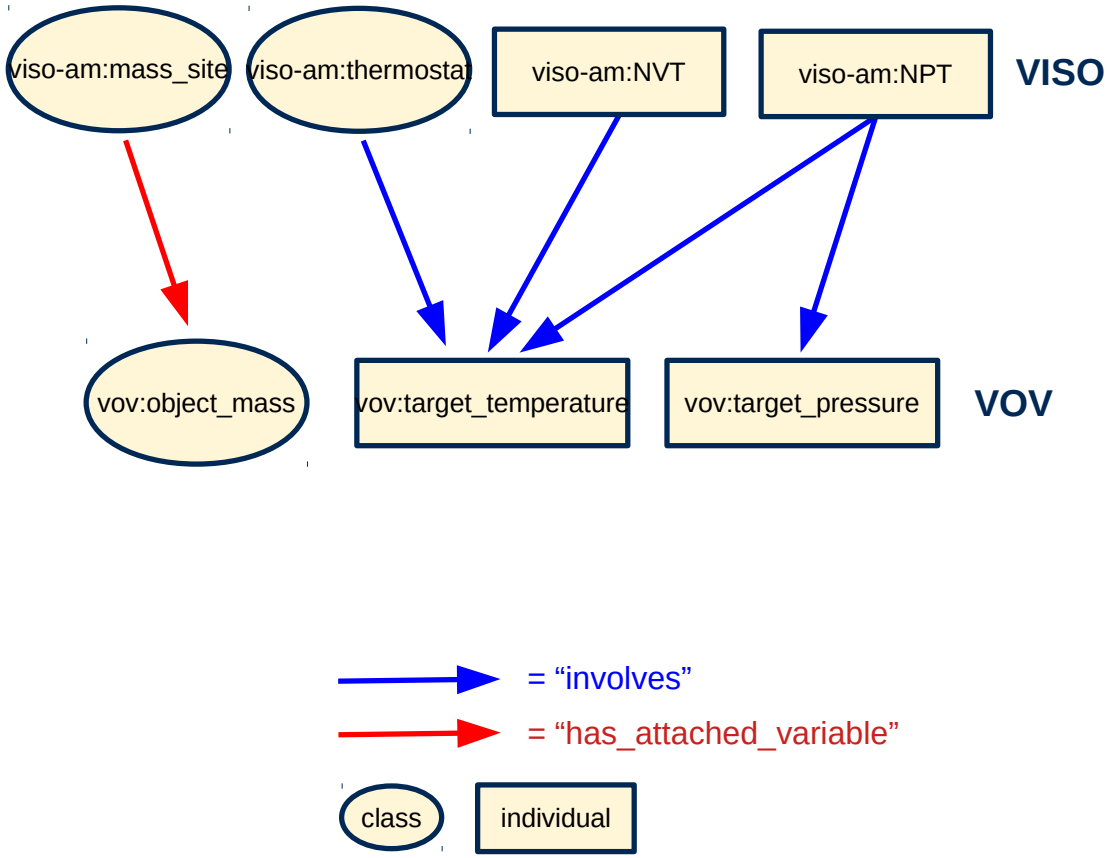
```
ex:CODEX_1.0 viso:has_newer_version ex:CODEX_2.0;
  viso:has_not_feature viso-am:SPME;
  viso:has_feature viso-am:DIRECT_COULOMB_SUM.

ex:CODEX_2.0 viso:has_older_version ex:CODEX_1.0;
  viso:has_feature viso-am:SPME;
  viso:has_not_feature viso-am:DIRECT_COULOMB_SUM.
```

VIMMP Ontology of Variables (VOV)

The purpose of VOV is to **organize variables** (in a broad sense, including constants) that appear in materials modelling and to connect them to **models in which they are involved** as well as to **model objects to which they are attached** (i.e., to entities entering a simulation, such as sites, rigid bodies, volume elements, etc.).

The perspective of the present development is to use VOV in combination with OSMO and VISO to describe what quantities are exchanged in workflows and specified for models and solvers.



European Materials Modelling Council

Association with seat in Belgium, open to individual and corporate membership.

https://emmc.info/the-emmc-mission/

The mission of the EMMC is to bring materials modelling closer to the demands of industry!

The existing **foundations** in terms of discrete and continuum models, open simulation platforms, interoperability based on metadata schema **are further strengthened**, and roadmaps are established for future actions.

A new **collaborative and integrative approach** will bring materials modelling benefits to manufacturers: The **EMMC Marketplace**, a digital European hub to ease the access of industry to materials modelling and **data repositories,** development of the **translators** role and function, **training** and **validation of software.**

The EMMC promotes integration of materials modelling into state of the art **Business Decision Support Systems (BDSS)**. Materials modelling must be associated with clear economic impacts and become an integral **part of product life cycle management** in European industry.

The EMMC enhances **the interaction and collaboration** between all stakeholders engaged in different types of materials modelling, including discrete and continuum modellers, software owners, translators and manufacturers.

The EMMC networks with all existing activities taking place in the field of materials modelling, and builds on existing activities in Europe.

The EMMC elaborates methodologies and supports the development and implementation of open, widely endorsed metadata schema for interoperability and standards based on the **European Materials Modelling Ontology (EMMO)** framework.

EMMC INTERNATIONAL WORKSHOP 2019

EVENTS

"Digitalization of Knowledge and Industrial Technologies - Towards Horizon Europe" - University of Bologna, Thursday 7th November 2019
Thursday, November 7, 2019

all events

OPEN JOBS

postdoc position on soft matter tribology, EU applicants only
Lecce ▸ Italian Institute of Technology ▸ Full Time

Innovation Manager
Sci-tech Daresbury, Warrington, UK ▸ STFC Hartree Centre ▸ Full Time

use the portal at http://emmc.info/ and join the association at http://emmc.eu/

Conclusion

The **European Materials Modelling Council** is an organization dedicated to supporting platforms and infrastructures, such as the Virtual Materials Marketplace (VIMMP), which interoperate on the basis of **semantic assets including RoMM, MODA/OSMO, and EMMO** extended by EVMPO. This is early work in progress with a perspective for substantial additional funding from Horizon LEIT-NMBP projects in the near future.

The EMMC and CoLaN are organizations with a similar purpose. It would be adviseable to work on a **convergence** between the EMMC-guided and the CoLaN-guided interoperability solutions as far as this is feasible without abandoning the basic approach. Possible benefit:

- CAPE-OPEN PMCs and PMEs could be included as building blocks of workflows and simulation solutions available, e.g., at **virtual marketplaces** and **open innovation platforms**. They could import data and simulation results from such infrastructures.
- The EMMC and VIMMP approach is focused on **“translation” services** provided by professional “translators”. The **CoLaN community** can provide such bespoke services.
- Joint participation in projects can be explored (e.g., B2B cases for **data marketplaces**, a CAPE-OPEN **ontology**, integration of **molecular modelling** into CAPE-OPEN, etc.).

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VIMMP
VIRTUAL MATERIALS MARKETPLACE