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

VIMMP ontologies and metadata

VIMMP MVP Demo

17th October 2019

Fraunhofer IFAM

Bremen

VIMMP
VIRTUAL MATERIALS MARKETPLACE

Science & Technology Facilities Council

UK Research and Innovation

Ontologies (in a nutshell)

What are they?

In philosophy, Ontology is the “science of what is”.

In information science, an ontology is a formal (machine-readable) representation of knowledge within a certain domain. It identifies the categories (“classes”) that exist in the domain and the relations between them.

Why are they useful?

Ontologies allow 1) automatic reasoning, 2) easier exchange of information across heterogeneous sources.

What is the bigger picture?

The context is that of semantic technologies and semantic interoperability. Notably, the Semantic Web concept, an evolution of the World Wide Web that is based on semantics rather than ad-hoc links between resources (e.g., web-pages) was proposed in the 1990s.

Taxonomies

A taxonomy is a hierarchical classification.

Simpler than an ontology, has only sub-class relations (also called “is-a” relation). For example, think of taxonomies in botanics and zoology.

In most cases, its graph structure is an acyclic tree (Aristotelic approach). However, some authors allow multiple inheritance (i.e., a class can have multiple super-classes).

Metadata

Metadata are data that provide information about other data.

For example, given a text (data) one can annotate it with a title, author, language used etc (metadata). Given a software (data) one can annotate it with a version number, programming language etc (metadata).

In general, the concepts used as metadata can be just a list, or be organized in some structure. In our case, we use concepts belonging to ontologies and taxonomies.

The semantic web

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

Example

(1) Frank is_father_of Robert.

Human a Class.

Frank a Human.
Robert a Human.

Cardinality restriction:
Every human has exactly one father.

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.)

The semantic web

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

Example

(1) Frank is_father_of Robert.

Q: "Is Emanuele the father of Robert?"

Human a Class.

Frank a Human.
Robert a Human.

Cardinality restriction:
Every human has exactly one father.

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.)

Principle: No unique name assumption
Unless explicitly stated, individuals with different names can coincide.

The semantic web

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

Example

(1) Frank is_father_of Robert.

Human a Class.

Frank a Human.
Robert a Human.

Q: “Is Emanuele the father of Robert?”

A: “We don’t know.”

Cardinality restriction:
Every human has exactly one father.

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.)

Principle: No unique name assumption
Unless explicitly stated, individuals with different names can coincide.

The semantic web

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

Example

(1) Frank is_father_of Robert.

(2) Frank is_different_from Emanuele.

Q: “Is Emanuele the father of Robert?”

A: “No, he is not.”

Human a Class.

Frank a Human.
Robert a Human.

Cardinality restriction:
Every human has exactly one father.

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.)

Principle: No unique name assumption
Unless explicitly stated, individuals with different names can coincide.

The semantic web

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

Example

(1) Frank is_father_of Robert.

(2) Frank is_different_from Emanuele.

Q: “Is Emanuele the father of Robert?”

A: “No, he is not.”

(3) Frank is_father_of Anna.

Q: “How many children does Frank have?”

Human a Class.

Frank a Human.
Robert a Human.

Cardinality restriction:
Every human has exactly one father.

Anna is_different_from Robert.

“How many different entities X are there such that Frank is_father_of X?”

The semantic web

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

Example

(1) Frank is_father_of Robert.

(2) Frank is_different_from Emanuele.

Q: “Is Emanuele the father of Robert?”

A: “No, he is not.”

(3) Frank is_father_of Anna.

Q: “How many children does Frank have?”

A: “At least two.”

Human a Class.

Frank a Human.
Robert a Human.

Cardinality restriction:
Every human has exactly one father.

Anna is_different_from Robert.

“How many different entities X are there such that Frank is_father_of X?”

Open world assumption: More information could be available elsewhere.

Ontologies on the marketplace

How do we use them in a marketplace?

They cover all aspects of the marketplace. At the user interface, for the data ingest (i.e., to create entries about agents, products, services) and to guide search and browsing. Internally, they are the base of interoperability of the marketplace compontents.

How will this help/affect users and providers?

Ontologies define the “common language” used in the marketplace. Users will indirectly see them via the available keywords and search criteria and results (e.g., as when you search a movie on Netflix).

This vocabulary will not be frozen: there will be a policy to allow users/providers to request the addition of categories or to integrate sub-domain specific ontologies.

Providers can choose down to which level of detail to adhere to the proposed common language: the deeper the adherence, the deeper the interoperability with other services.

Ontology development on the basis of the EMMO

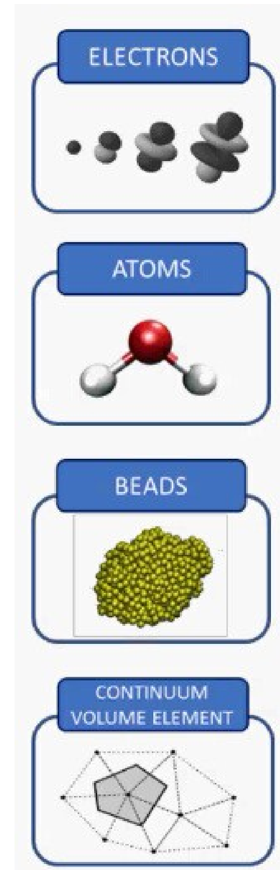
Types of relations covered by the European Materials & Modelling Ontology (EMMO)

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*)



electronic

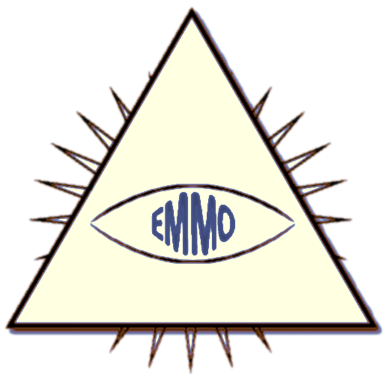
atomistic

mesoscopic

continuum

C. S. Peirce

object



sign

interpretant

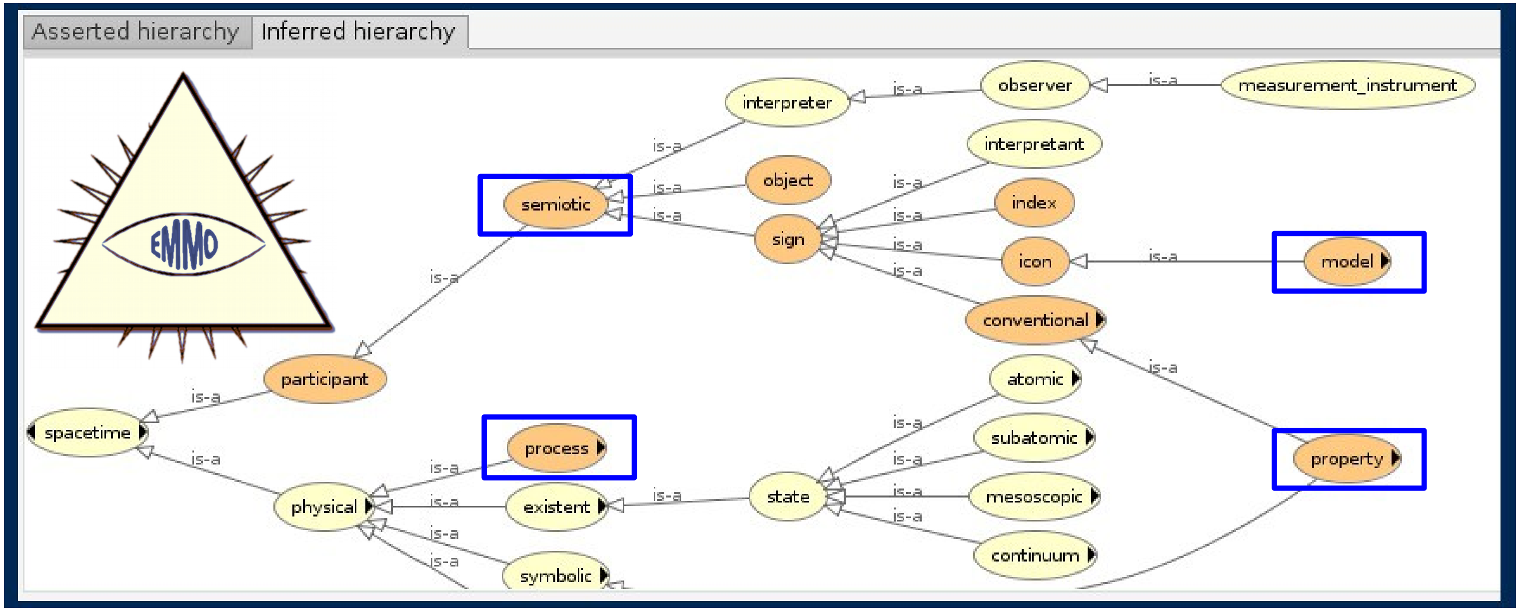
Ontology development on the basis of the EMMO

Types of relations

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"



Ontology development on the basis of the EMMO

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

MODA
CWA 17284
EMMO

VIMMP
VIRTUAL MATERIALS MARKETPLACE

European Virtual Marketplace Ontology (EVMPO)

Persons, institutions, stakeholders (CVIII)

Computational resources (MACRO)

Models and simulation workflows (OSMO)

Training services and competencies (OTRAS)

Communication and messages (VICO)

Validation, benchmarking, assessments (VIVO)

Translation, decision support (MMTO)

Software, quantities, variables (VISO + branches + VOV)

- **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)**

European Virtual Marketplace Ontology

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.

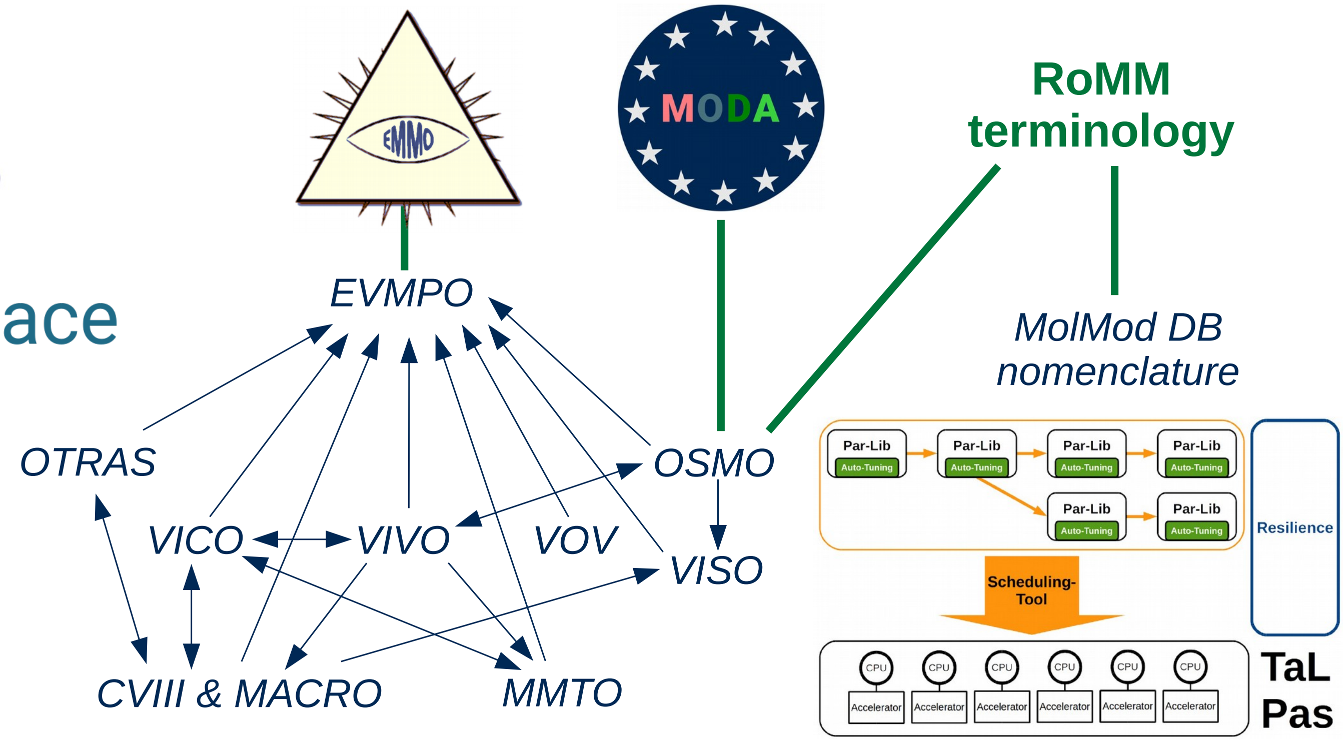
Recommendation: Any ontology at the marketplace level should follow the structure given by these categories as closely as possible.

VIMMP
VIRTUAL MATERIALS MARKETPLACE
MarketPlace

Fundamental paradigmatic categories:

(1) **assessment**, i.e., proposition on accuracy, performance of an entity, or of an entity's trust in another entity
(2) **calendar_event**, i.e., meeting or activity that is scheduled or can be scheduled, equivalent to Vevent from ICALTZD
(3) **communication**, i.e., statement or sequence of statements that can be communicated at a virtual marketplace
(4) **information_content_entity** as defined in the Information Artifact Ontology (IAO)
(5) **infrastructure**, i.e., virtual-marketplace infrastructure (e.g., data access, hardware, and software)
(6) **material** as defined in the European Materials Modelling Ontology (EMMO)
(7) **model**, i.e., entity that can be described by the 2nd section of MODA, equivalent to "model" from the EMMO
(8) **process**, i.e., temporal evolution of one or multiple entities note: **physical_process** is a subclass of EMMO "process"
(9) **product**, i.e., good or service that can be offered either at a virtual marketplace or off-site
(10) **property** as defined in the EMMO
(11) **role** as defined in the EMMO
(12) **simulation**, i.e., a simulation workflow (as in MODA)

Landscape of semantic assets developed by VIMMP



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 VIMMP

VISO – VImmp Software Ontology

VISO's main purpose is to describe software, addressing mostly its capabilities (both model and solver aspects), but also licensing, requirements (as libraries and operating systems) and compatibility[1] with other tools.

It will be used to structure the ingestion of information about software tools on the virtual marketplace. The same keywords will be then available to the users to browse the 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 language)

Categories at the upper level:

(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, as statistical mechanics, the RoMM models, fundamental physics equation, etc.

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

(9) **software_update** = Allows to describe the differences between two softwares. It has input/output the older/newer version of the software

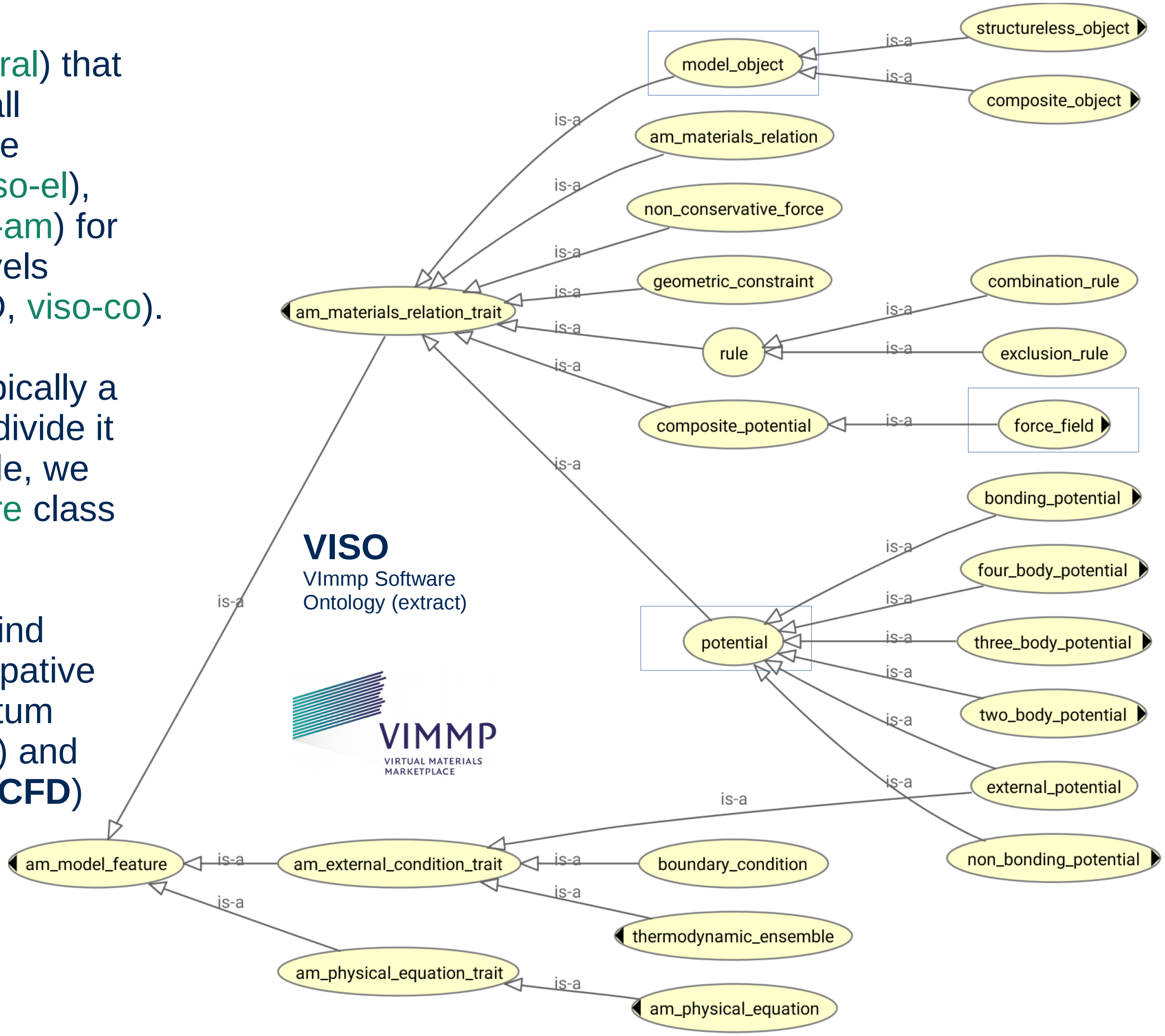
(10) **software_interface** = Interface between a software and a user or a client (i.e., a program or device)

VISO (2): The structure

Below an upper level (viso-general) that addresses aspects common to all software, we split VISO into three branches, i.e., electronic (EL, viso-el), atomistic-mesoscopic (AM, viso-am) for the two molecular granularity levels from RoMM, and continuum (CO, viso-co).

The model_feature class has typically a rich structure, so we further subdivide it into three classes. As an example, we show here the am_model_feature class and its subclasses.

VISO was designed having in mind Molecular Dynamics (**MD**), Dissipative Particle Dynamics (**DPD**), Quantum Density Functional Theory (**DFT**) and Computational Fluid Dynamics (**CFD**) models and tools.



VISO
VImmp Software Ontology (extract)

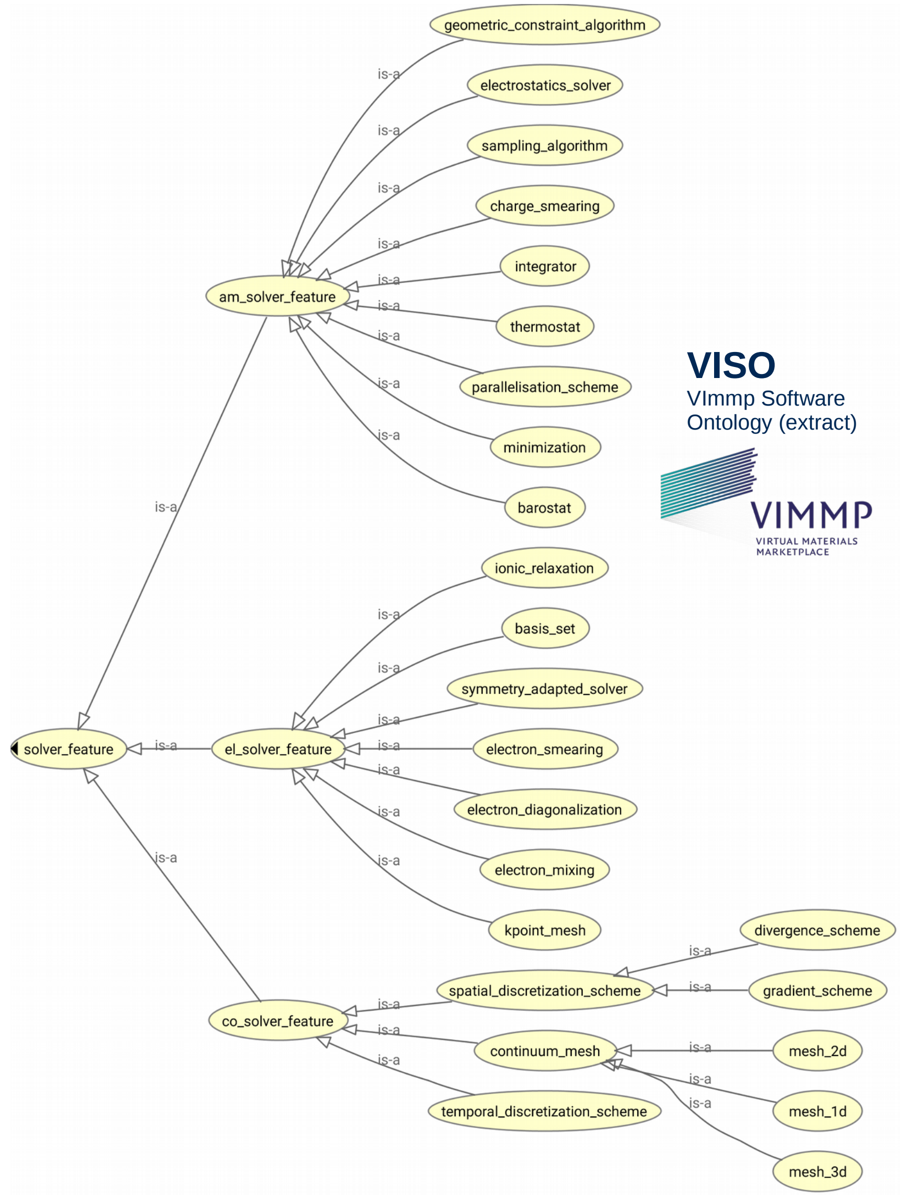
VISO (3): Solver features

Here, we show instead the solver_feature class and its subclasses, for the three branches.

This includes, for example, concepts as: geometric_constraint_algorithm, electrostatics_solver, integrator (in AM), ionic_relaxation, basis_set (in EL), spatial_discretization_scheme (in CO).

Main contributors of VISO:

Silvia Chiacchiera, Martin T. Horsch
Mara Chiricotto, Joshua D. Elliott (UoM)
Gianluca Boccardo (PoliTO)



VISO
VImmp Software Ontology (extract)

VISO (4): Relations and an example

The main relations between objects in VISO are:

has_feature = To describe the features of a software tool [Inverse: **is_feature_of**]

is_tool_for_model = Relates software tools and RoMM models

is_compatible_with = Asserts compatibility between software tools

is_distributed_by = Relates tools and agents [Inverse: **is_distributor_of**]

has_license = Relates software and license

requires = Relates a software tool to libraries and/or operating systems

can_run_on = Relates a software tool to operating systems

Some relations between objects and literals are:

is_free, **is_open_source**, **is_a_library**, **has_a_gui**

Example for a software tool (extract from a .TTL file):

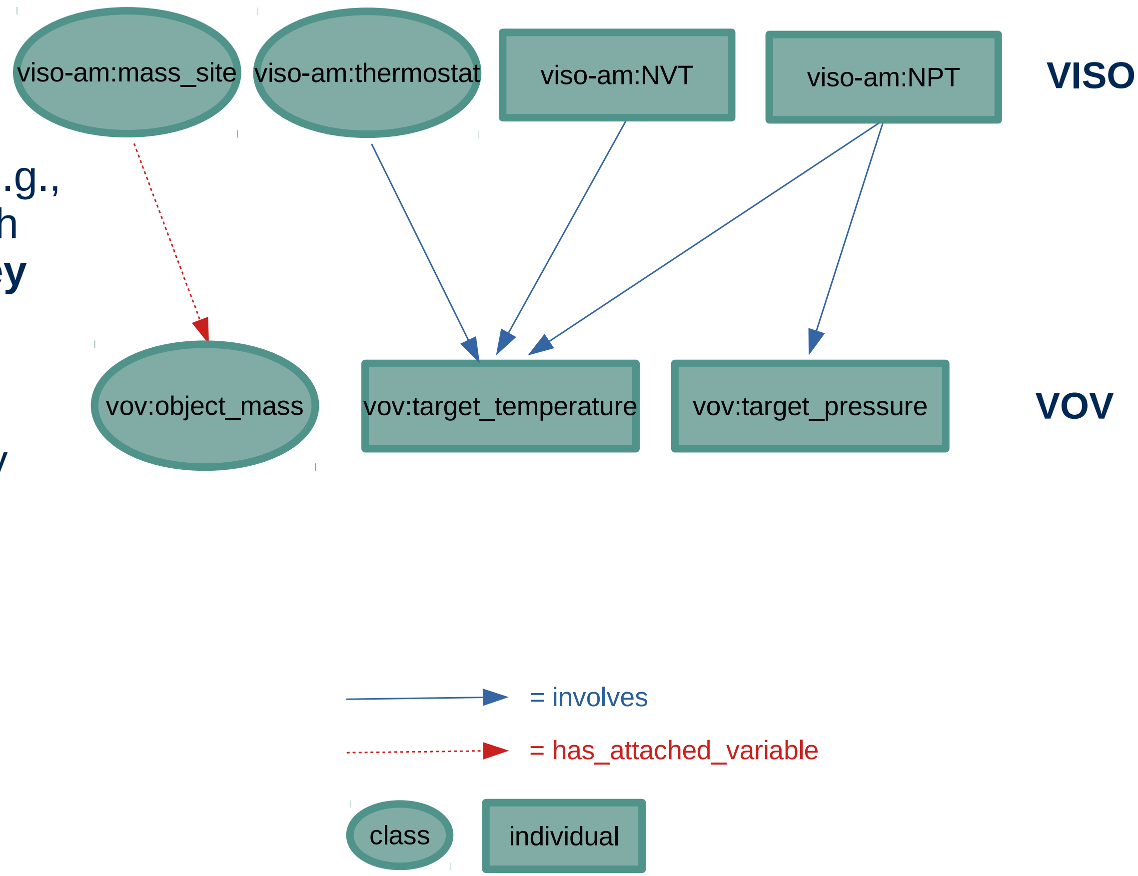
```
ex:DL_POLY a viso:software_tool;
  viso:is_free false;
  viso:is_free_to_academic true;
  viso:has_a_gui true;
  viso:is_open_source true;
  viso:is_a_library false;
  viso:is_distributed_by ex:STFC;
  rdfs:seeAlso
"https://www.scd.stfc.ac.uk/Pages/DL_POLY.aspx"^^xs:anyURI;
  viso:is_tool_for_model viso-am:MM;
  viso:is_tool_for_model viso-am:MD;
  viso:has_feature viso-am:DOMAIN_DECOMPOSITION;
  viso:has_feature viso-am:DIRECT_COULOMB_SUM;
  viso:has_feature viso-am:SPME;
  viso:uses_language viso:FORTRAN90;
  viso:has_feature viso-am:NVE;
  viso:has_feature viso-am:NVT;
  viso:has_feature viso-am:NPT;
  viso:has_feature viso-am:LENNARD_JONES_12_6;
  viso:has_feature viso-am:RIGID_BOND;
  viso:has_feature viso-am:VV;
  viso:has_feature viso-am:LFV;
  viso:is_compatible_with ex:PLUMED;
  viso:is_compatible_with ex:OPENKIM;
  a viso:simulation_engine.
```

VOV – Vimmp Ontology of Variables

The purpose of VOV is to **organize the variables** (in broad sense, including constants) that appear in modeling and simulations, **and to connect them to models and algorithms in which they are involved and to model objects** (e.g., entities entering a simulations, such as sites, rigid bodies) **to which they are attached**.

VOV is to be used in connection to VISO and OSMO, to further specify models, algorithms and workflows.

See the examples on the right.

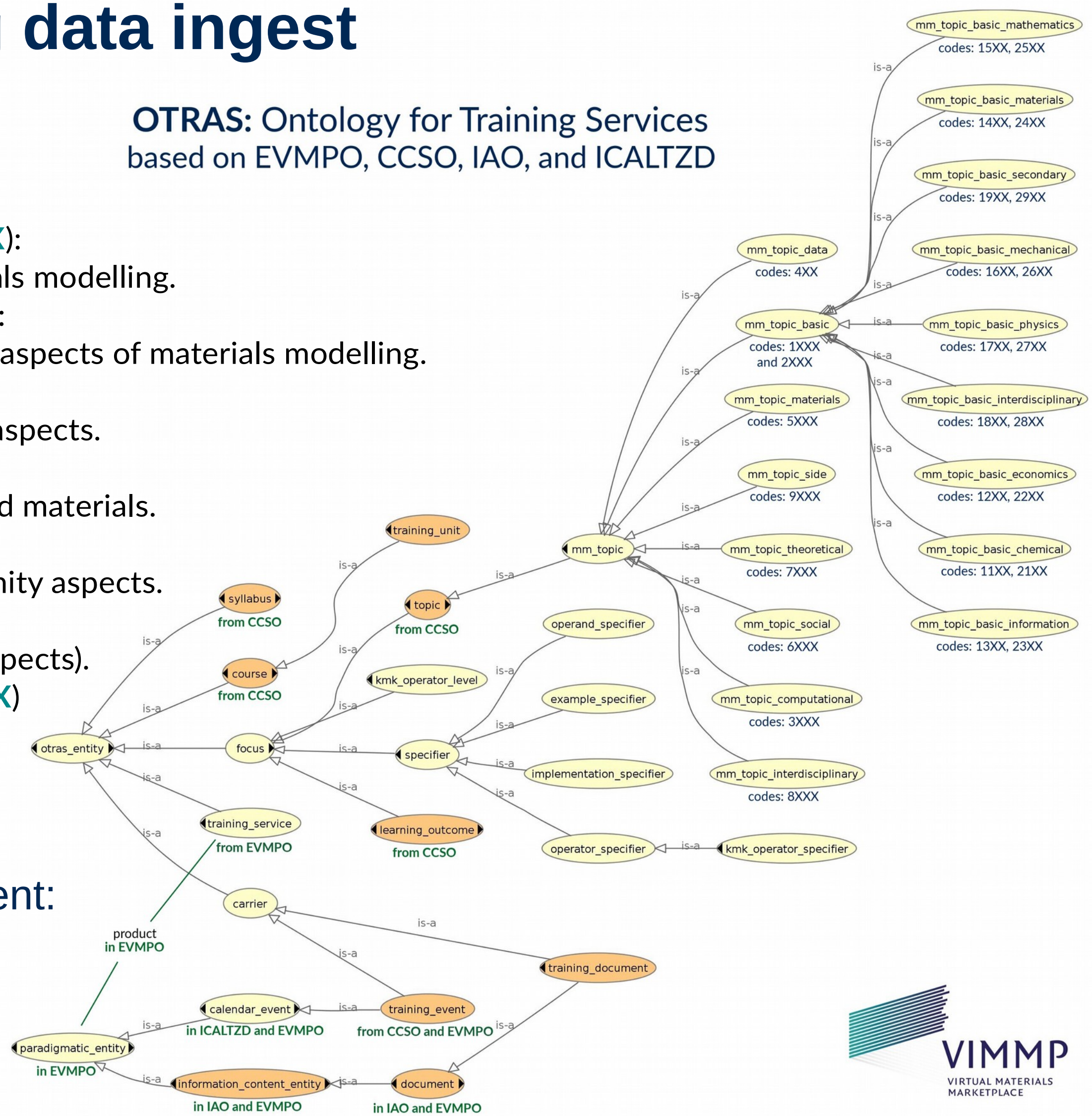


Ontology use during data ingest

The OTRAS ontology includes **topic** and **operator** catalogues.

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

OTRAS: Ontology for Training Services
based on EVMPO, CCSO, IAO, and ICALTZD



Pre-existing semantic assets considered for further development:

- **ACM Computing Classification System (CCS)**
- **APS Physics Subject Headings (PhysH)**

Ontology use during data ingest

Expert competency description: "The expert $\mathbf{X_1}$ can (accomplish) X_2 **with respect to topic $\mathbf{X_3}$** by doing $\mathbf{X_4}$; for example, $\mathbf{X_5}$." (Note: $\mathbf{X_4}$ and $\mathbf{X_5}$ are not required.)

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.
under 61XX: industrial
- 6120 chemical
- 6140 automotive, aerospace, etc.
- 6150 biotechnology
- 6155 food
- 6160 medicine
- 6165 paper
- 6170 electrical
- 6175 machinery
- 6180 metal (basic and fabricated)
- 6190 special topics

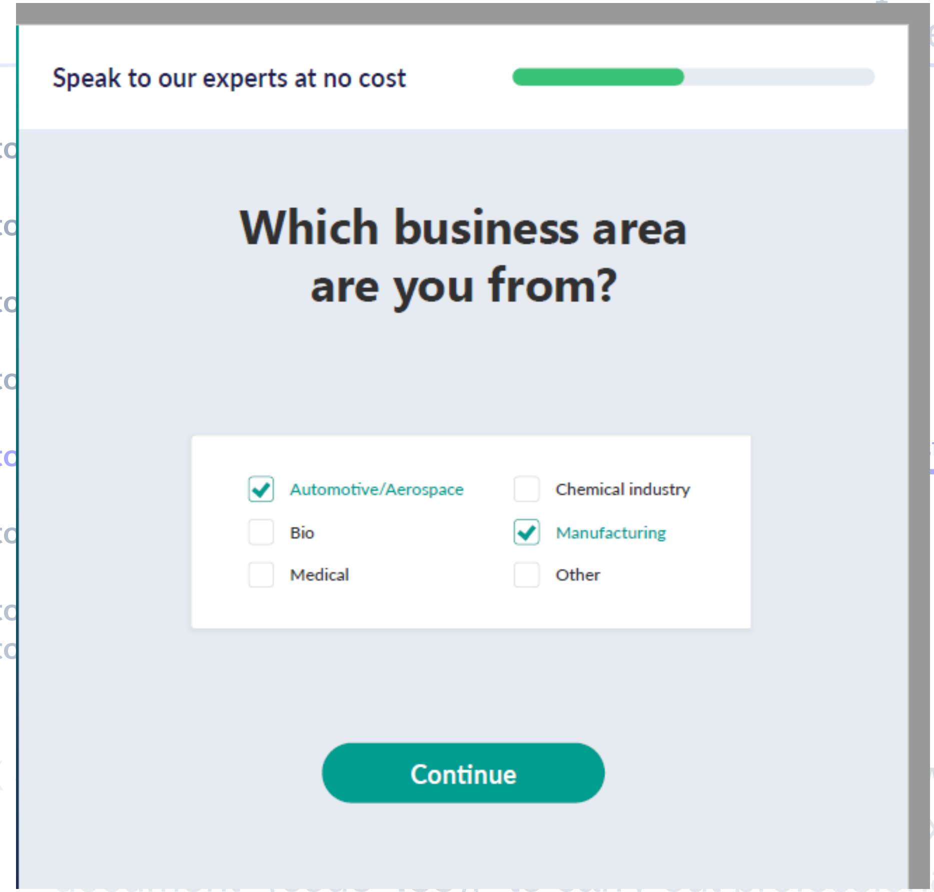
mm_topic_theoretical (codes 7XXX):
Theory (non-computational aspects).
mm_topic_interdisciplinary (codes 8XXX)
mm_topic_side (codes 9XXX):
Topics from other disciplines

4XX – Operators for **expert competencies:** "to review/evaluate critically" (code **420**), "to advise/manage" (code **425**), "to characterize experimentally" (code **430**), "to document" (code **435**), "to carry out professionally" (code **440**), "to correspond" (code **445**), "to teach" (code **450**), ..., "to innovate/develop" (code **480**).

Ontology use during data ingest

Expert competency description: “The expert X_1 can (accomplish) X_2 **with respect**
e: X_4 and X_5 are not required.)

mm_to
mm_to
mm_to
mm_to
mm_to
mm_to
mm_to
mm_to



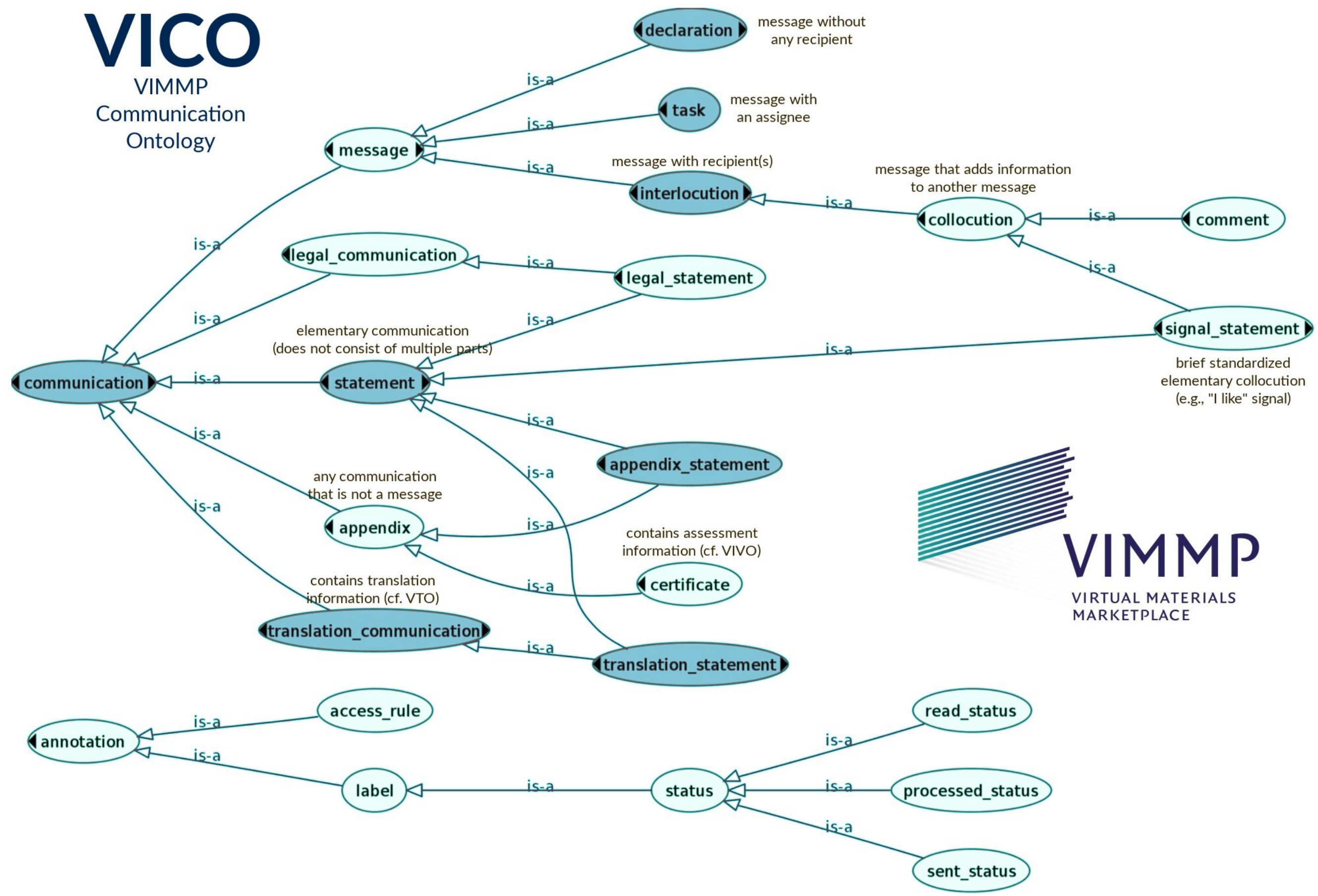
trial

- 6120 chemical
- 6140 automotive, aerospace, etc.
- 6150 biotechnology
- 6155 food
- 6160 medicine
- 6165 paper
- 6170 electrical
- 6175 machinery
- 6180 metal (basic and fabricated)
- 6190 special topics

4XX

/evaluate critically” (code **420**), “to
xperimentally” (code **430**), “to
ally” (code **440**), “to correspond”
(code **445**), “to teach” (code **450**), ..., “to innovate/develop” (code **480**).

Ontology use within the virtual marketplace framework

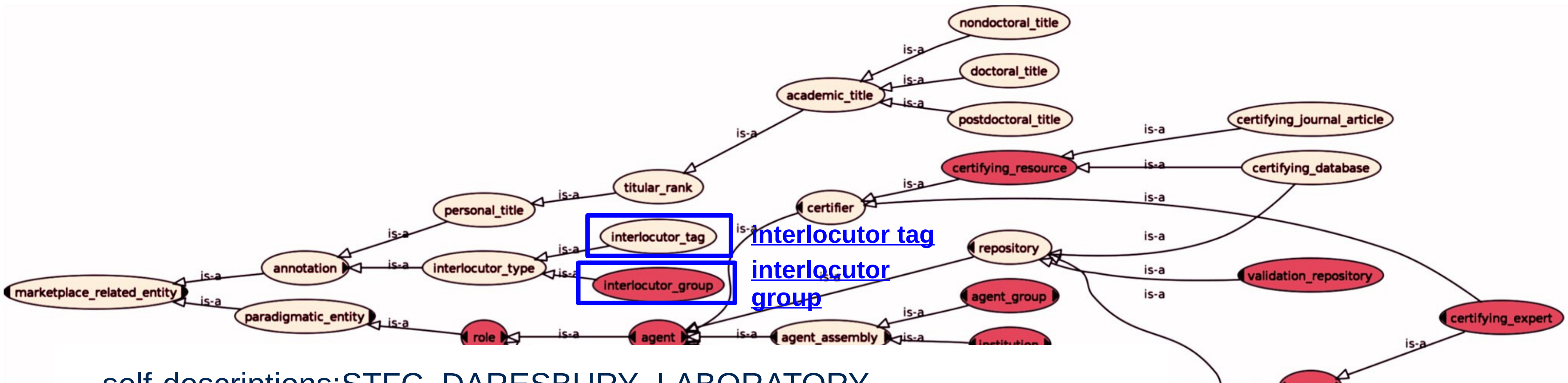


Virtual-marketplace stakeholder communication is formalized by VICO, taking into account specific requirements related to assessment and validation (VIVO) and translation.

VIMMP Validation Ontology (VIVO) Assessment Matrix

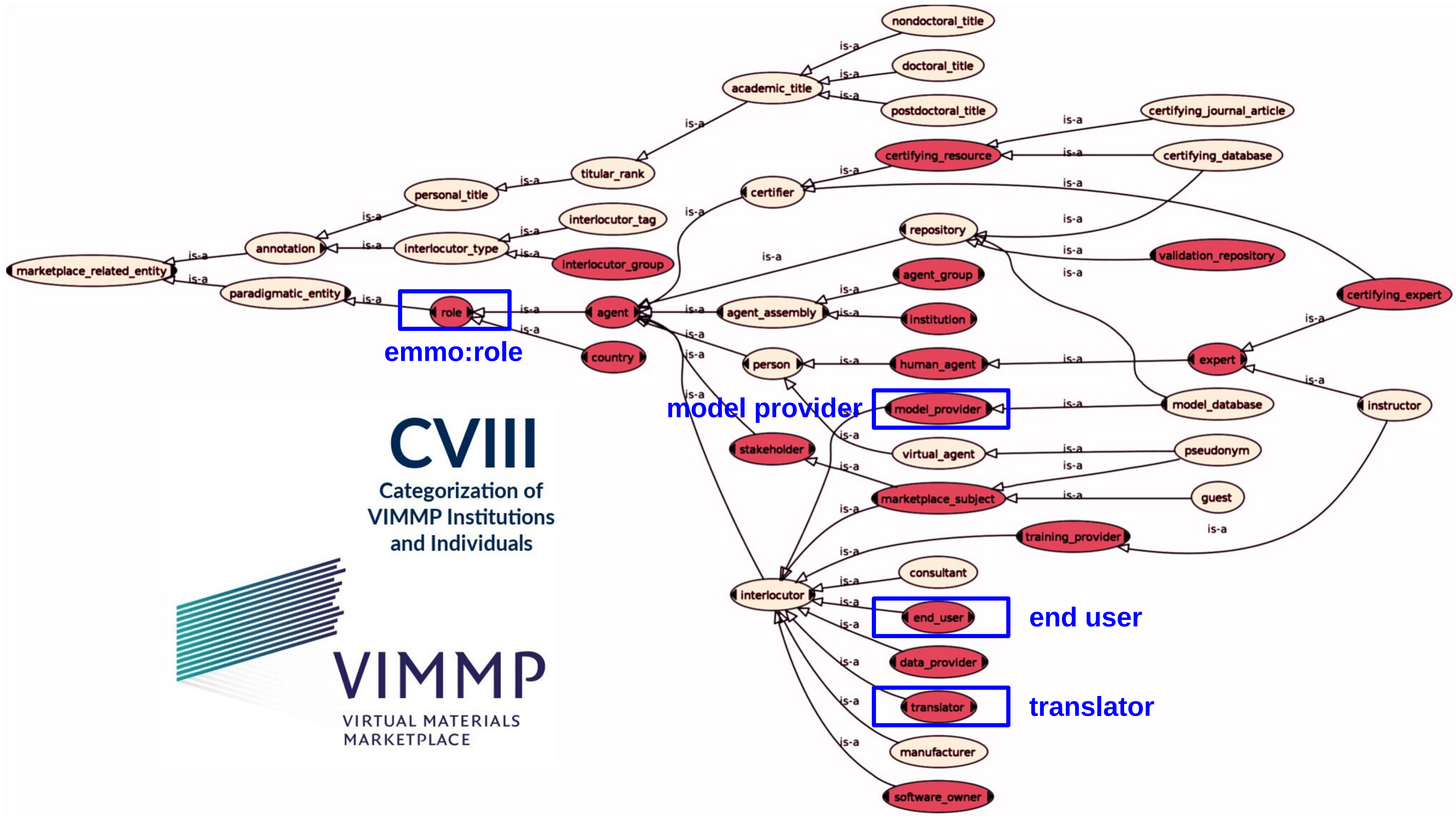
		accuracy			requirement			review		
		absolute	*relative*	*qualitative*	*(computing) time*	*space (memory)*	*other*	*endorsement*	*comment*	*revision*
	agent		-			-		+		
	data item		+			-			+	
	document			+		-			+	
	event		-				+	+		
data	**infrastructure**			+		+	+	+		
hardware	**infrastructure**						+	+		
software	**infrastructure**					+	+	+		
	meta-assessment		-			-			+	
	model		+				+		+	
	project		-				+	+		
data access	**service**		-			-		+		
hardware access	**service**									
software access	**service**									
training	**service**									
translation	**service**									
other	**service**									
	workflow		+			+			+	

Ontology use within the virtual marketplace framework

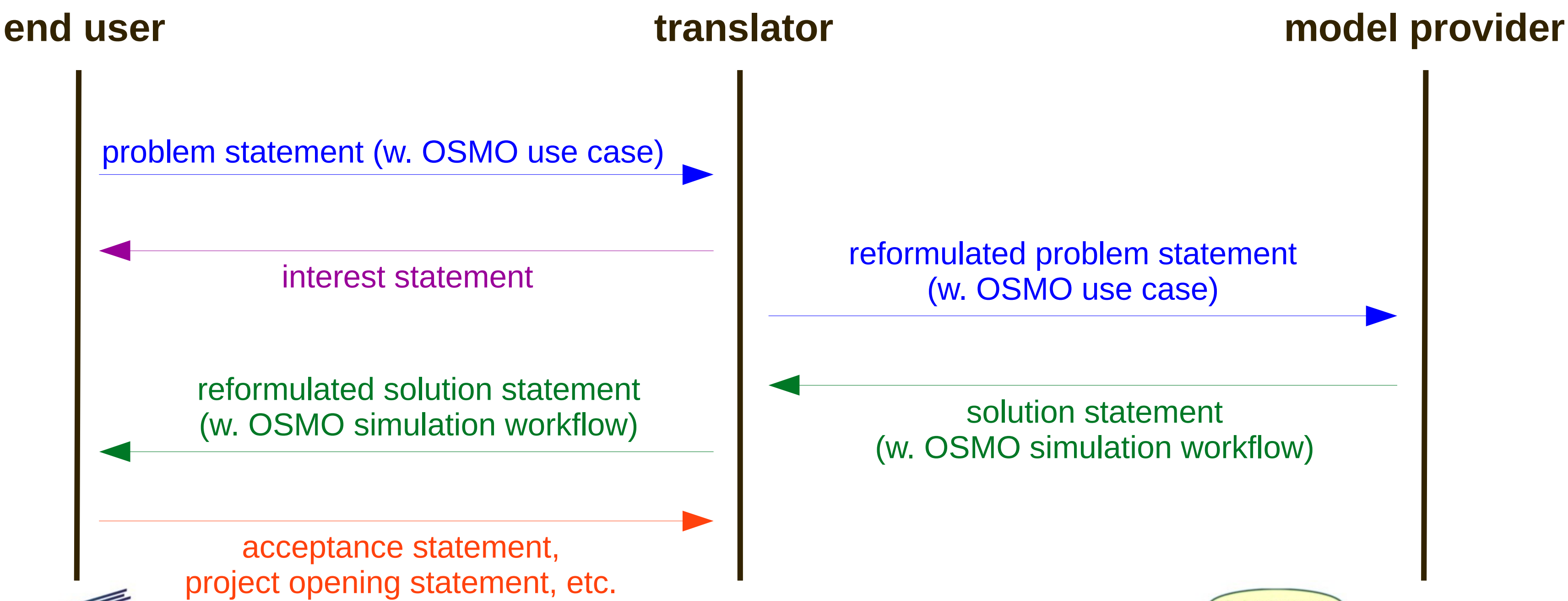


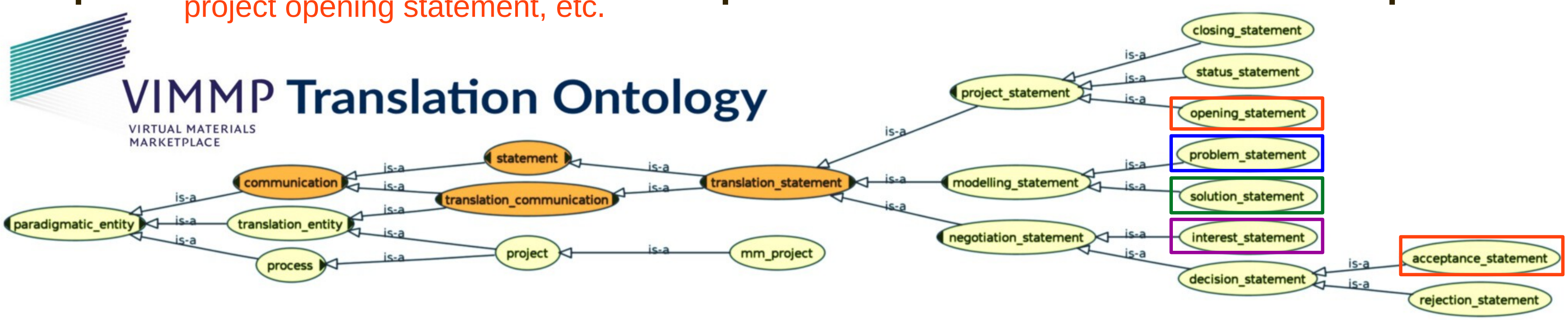
self-descriptions:STFC_DARESBURY_LABORATORY
  a cviii:institution, cviii:model_provider, cviii:software_owner, cviii:training_provider, cviii:translator;
  cviii:has_name "STFC Daresbury Laboratory"^^xs:string;
  cviii:has_interest
    otras:MM_TOPIC_3000, otras:MM_TOPIC_6120, otras:MM_TOPIC_7200, otras:MM_TOPIC_8350;
  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
  ].

Ontology use within the virtual marketplace framework

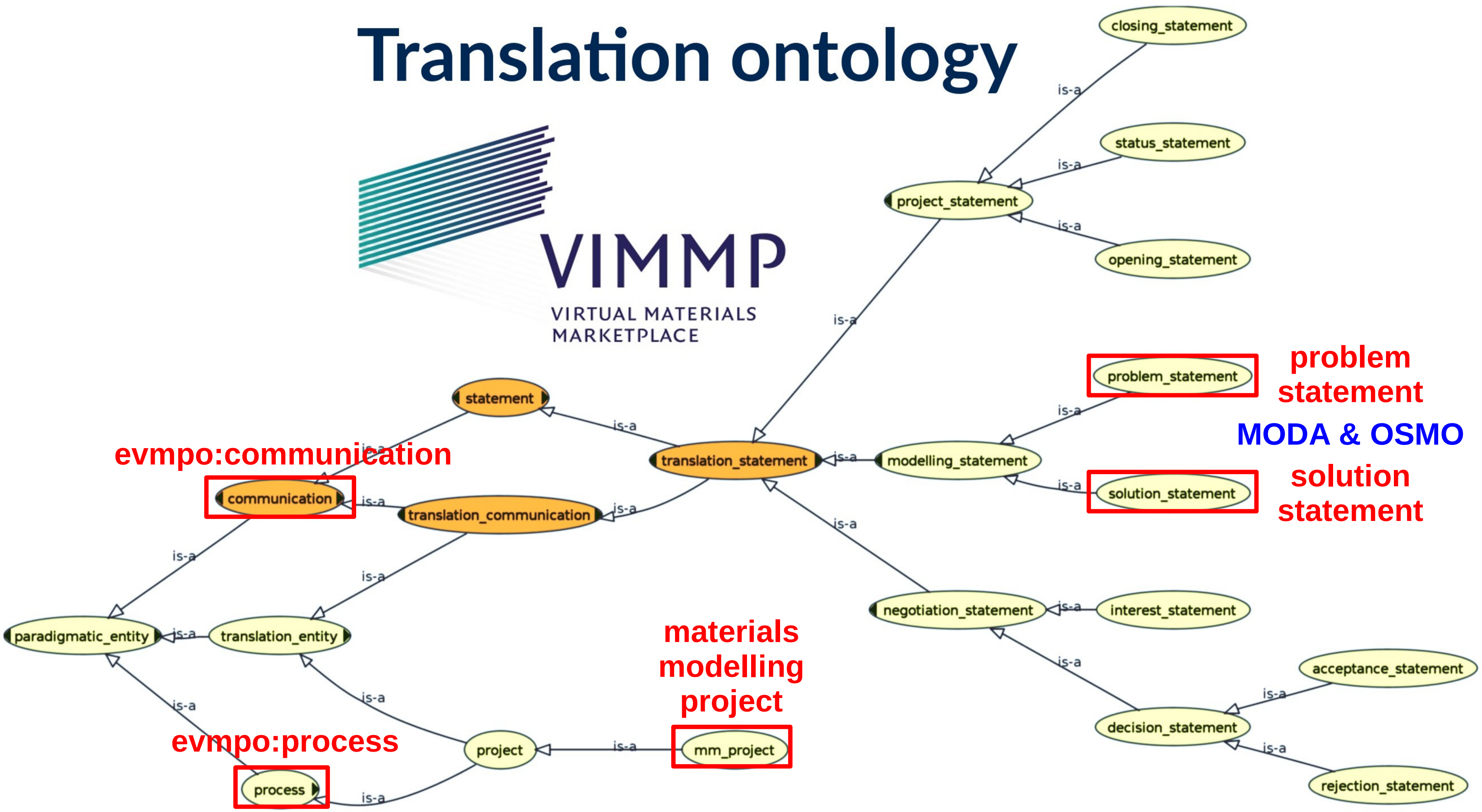


Semantic and pragmatic interoperability

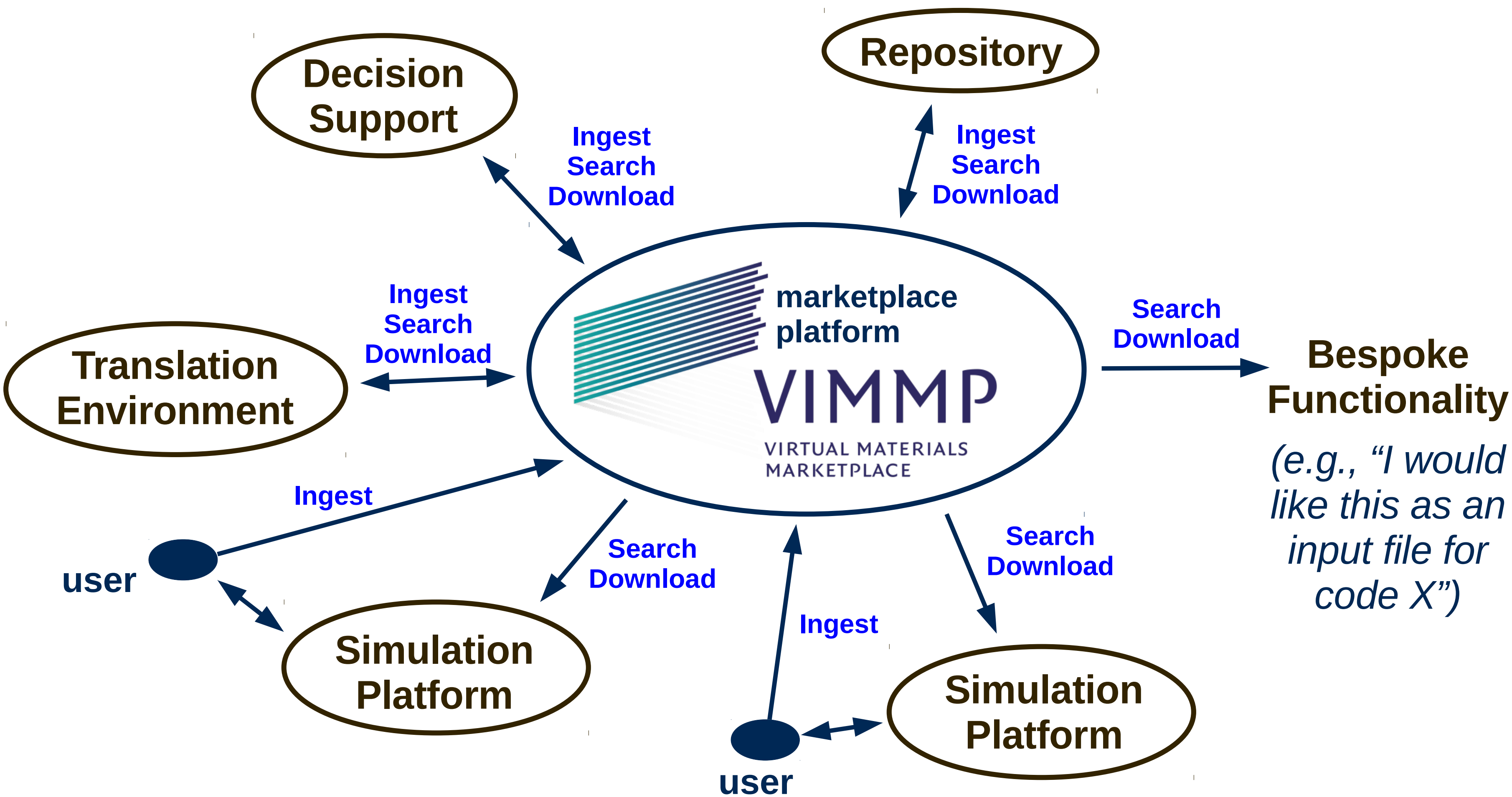




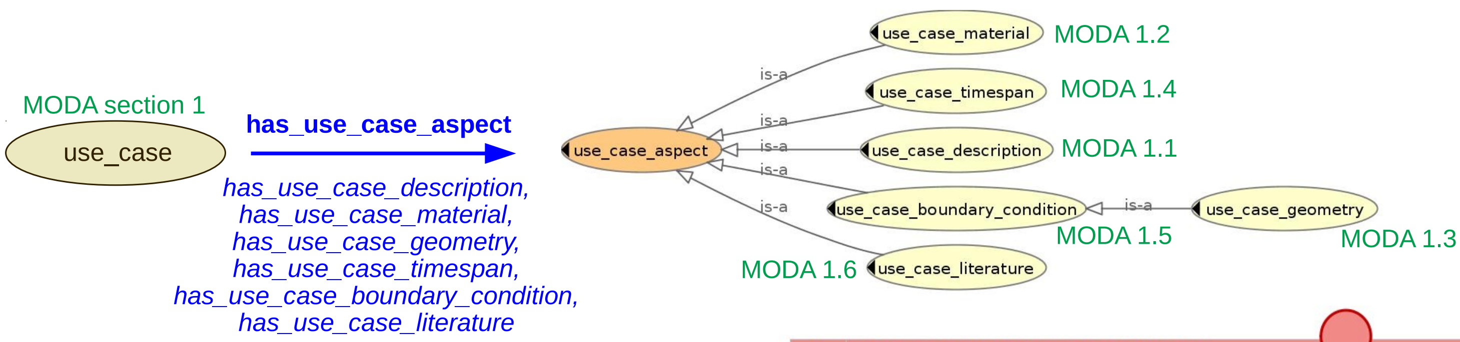
Semantic and pragmatic interoperability

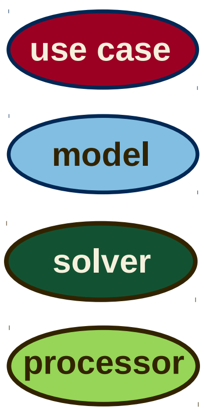


Interoperability and data provenance



Ontology use for data provenance characterization



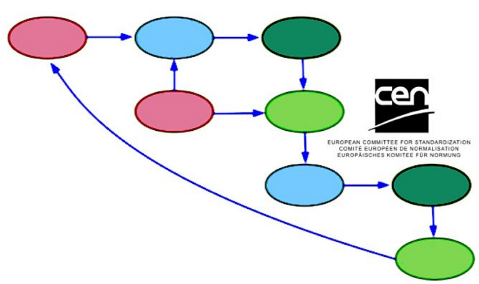


“sections”

“aspects”

OSMO

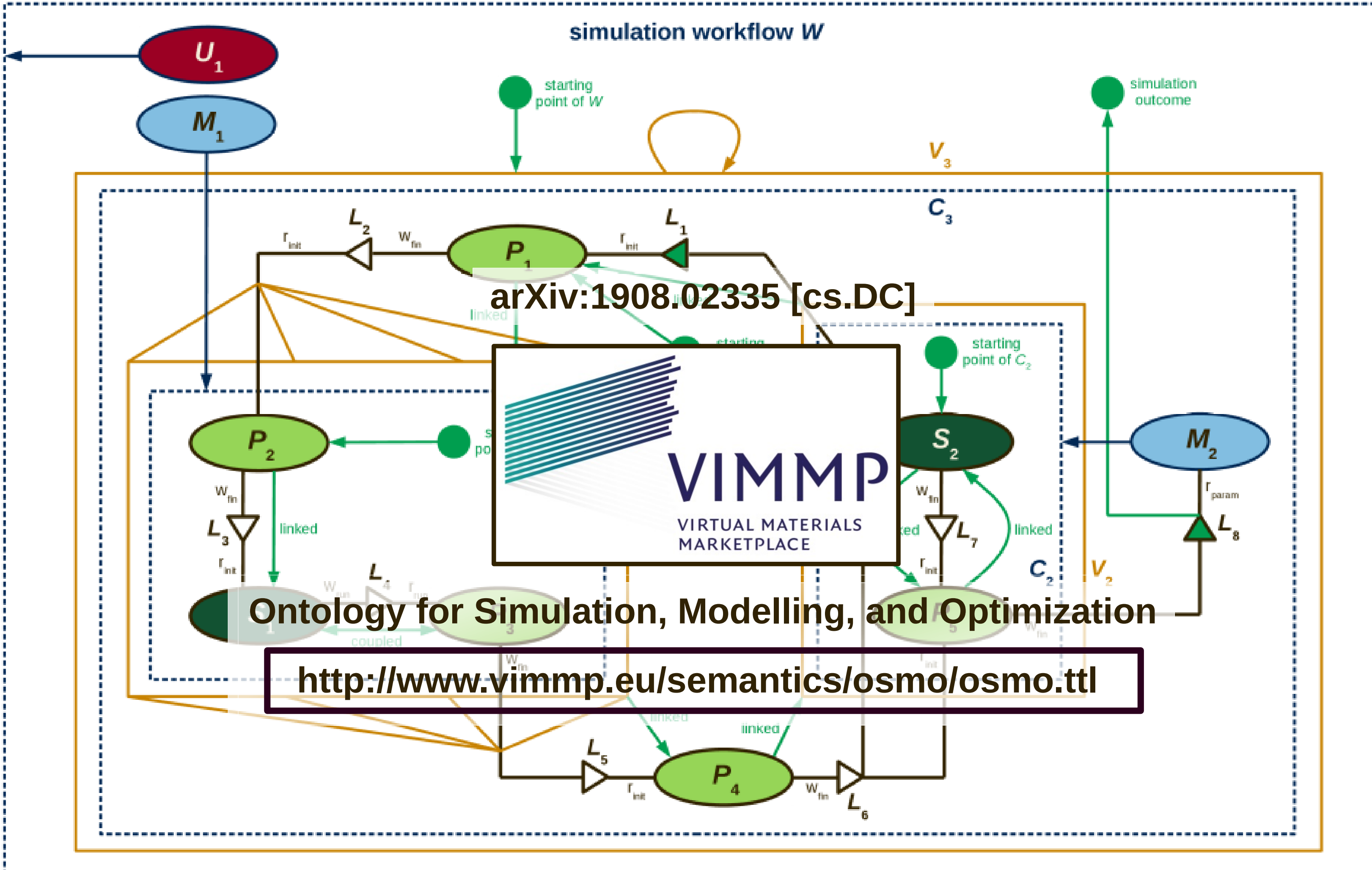
“graphs”



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).

VIMMP
VIRTUAL MATERIALS MARKETPLACE

Ontology use for data provenance characterization



arXiv:1908.02335 [cs.DC]

VIMMP
VIRTUAL MATERIALS MARKETPLACE

Ontology for Simulation, Modelling, and Optimization

http://www.vimmp.eu/semantics/osmo/osmo.ttl

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