Ontologies on marketplaces: VIMMP

19\textsuperscript{th} August 2019

Marketplaces EMMC Expert Group Meeting

Bremen
European Virtual Marketplace Framework

http://the-marketplace-project.eu/

http://emmc.info/

http://vimmp.eu/
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.

**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
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)
Ontology development for materials marketplaces

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

- MODA
- CWA 17284
- EMMO

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 services and BDSS (discussed tomorrow)
- Materials modelling software (VISO + branches of VISO)

- Upper level: EMMO extended by European Virtual Marketplace Ontology (EVMPO)
- Marketplace-level ontologies: VIMMP in coordination with the MarketPlace project
- Subdomain-specific VISO branches (electronic, atomistic-mesoscopic, continuum)
Competencies and topics in materials modelling

The training ontology will include **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

Pre-existing semantic assets to be considered for further development:

- ACM Computing Classification System (CCS)
- APS Physics Subject Headings (PhysH)
Representation of simulation workflows

(1) Use Case
(2) Model
(3) Solver
(4) Processor

“sections”

OSMO

“aspects”

“graphs”

1. Aspect of the User Case/System to be Simulated

1.1 ASPECT OF THE USER CASE TO BE SIMULATED

OSMO:

- has_use_case_aspect
- has_use_case_description
- has_use_case_material
- has_use_case_geometry
- has_use_case_timespan
- has_use_case_boundary_condition
- has_use_case_literature

1.2 MATERIAL

- has_use_case_material

1.3 GEOMETRY

- has_use_case_geometry

1.4 TIME LAPSE

- has_use_case_timespan

1.5 MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS

- has_use_case_boundary_condition

1.6 PUBLICATION ON THIS DATA

- has_use_case_literature

MODA sections:

- MODA 1.1
- MODA 1.2
- MODA 1.3
- MODA 1.4
- MODA 1.5
- MODA 1.6
Ontology for Simulation, Modelling, and Optimization

To facilitate the integration of MODA into virtual marketplace infrastructures, simulation workflow semantics need to be provided at a machine-readable level of formalization.

Following the approach of the EMMC community, OSMO was developed: The ontology version of MODA.

By OSMO, simulation workflow semantics from MODA can be integrated into the ongoing ontology development work in materials modelling. OSMO is one of the marketplace-level ontologies shared in the EVMPO development group.
Simulation workflows in OSMO

Ontology for Simulation, Modelling, and Optimization

http://www.vimmp.eu/semantics/osmo/osmo.ttl
Virtual-marketplace stakeholder communication is formalized by VICO, taking into account specific requirements related to assessment and validation (VIVO) and translation (VTO).
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VIMMP ontologies and their relation to existing assets

Blue: Own semantic assets
Green: Related external semantic assets with a connection
Black: Not connected

ICALTZD (W3C calendar)
KMK operators
CCS (ACM), PhysH (APS)
Course Curriculum & Syllabus Ontology

Information Artifact Ontology

OTRAS
EVMPO
OSMO

VICO
VIVO
VISO

CVIII & MACRO

Cas RN, EINECS, ELINCS, NLP List, etc.

QUDT

EMMC Translators’ Guide

EngMeta Metadata Schema
Citation File Format
SWO
OntoSoft

RoMM Terminology
CAPE-OPEN, OntoCAPE

Friend of a Friend Ontology

Blue: Own semantic assets
Green: Related external semantic assets with a connection
Black: Not connected
VISO – VImmp Software Ontology

VISO’s main purpose is to describe the 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.

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

\[1\] 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)
VIS0 (2): The structure

Below an upper level (viso-general) that addresses aspects common to all software, we split VIS0 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 subdivide it into three classes: physical_equation_trait, materials_relation_trait, and external_condition_trait.

As an example, we show here the am_model_feature class and its subclasses.
VISO (3): 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.
```
**VISo (4): Related assets**

- **High level of description** (for code browsing, comparing)

Ontologies that describe the software for a scientist end user have been developed in other areas: for example, the Software Ontology (SWO)\(^1\) for life sciences and OntoSoft\(^2\) for geosciences. The latter has been used for a portal (http://www.ontosoft.org/portal/#list).

We are evaluating these works to see whether the domain-independent parts can be re-used within viso-general. **Our peculiarity and main focus are therefore the domain and sub-domain specific concepts.**

- **Detailed level of description** (for interoperability, simulation documentation)

At a lower level, assets for our field have been developed within the NOMAD\(^3\) and SimPhoNy\(^4\) projects.

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