VIMMP / Semantics in a digital marketplace for materials modelling

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Towards Materials and Manufacturing Commons - the enablers Digital Marketplaces, FAIR Principles and Ontologies
VIMMP is a H2020 project[*] that has developed (Jan 2018-June 2022) a digital marketplace, i.e., a platform to facilitate exchanges between providers and users in the area of materials modelling. Below, we show a graphical summary of the VIMMP concept.

An open platform. The interoperability of components relies on semantic standards (i.e., a set of ontologies).

The VIMMP ontologies

We have developed a system of ontologies, aligned with the EMMO, providing a framework to organize knowledge on virtual material marketplaces.

Are used as metadata in the VIMMP platform, for data ingest, storage, search and browsing.

License: LGPL-v3. Ontology repository:
https://gitlab.com/vimmp-semantics/vimmp-ontologies

Documentation: see "References" slide
(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
A snapshot of the VIMMP metadata-enriched platform, showing an entry for Materials Modelling (MM) Software.

VIMMP ontologies are used, mainly VISO and OSMO in this case.

Other top categories beside Software: Challenges, Computational Resources, Data Sets, People, Training.

The VIMMP platform (based on Zontal Space), its UI and API were run by OSTHUS, the VIMMP platform architect.
Metadata-enriched platform: Ingest example

Creating a record for a “software” on the VIMMP backend (run by Osthus, based on Zontal Space). Fields (left) and dropdowns (right) are related to the VIMMP ontologies.

Note: here “STFC” was a temporary tag in names, to avoid name clash in the development phase.
The VIMMP ontologies in use on Zontal

URIs for properties and for classes for dropdown menus.
Which tools/platforms and ontologies have you been using?

**Tools:** Protégé, OntoFox [1], Owlready2 [2] (for ontologies); Zontal Space [3] (for data and metadata management); Widoco, Matportal and GitLab (documentation and development).

**Ontologies:**
- EMMO (TLO, applied sciences)
- EVMPO (MLO, digital marketplaces)
- VIMMP Ontologies (set of DOs, digital marketplaces for materials modelling)
- Re-use of multiple semantic artefacts (both generic, as SKOS, and specific as SWO)

What benefits did you observe from use of semantic technologies in your use case?

- Better knowledge organization, metadata handling

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[1] https://ontofox.hegroup.org/

TLO = Top-level ontology
MLO = Mid-level ontology
DO = Domain ontology
**FAIRness, access rights and governance**

**FAIRness and Interoperability** (Syntactic, semantic; both within VIMMP and with the wider landscape):
- Ontologies in OWL, TTL format.
- RESTful APIs for the marketplace (for ingest, search, download) exchanging data as JSON-LD.
- Reuse of multiple semantic artefacts (e.g., IAO, SWO) and formalization of knowledge sources (e.g., MODA and concepts from RoMM -> OSMO). Alignment with EMMO. Co-developed EVMPO (with Marketplace project, also used within DOME 4.0).

**Data space:**
- The marketplace has a "data space", with UI and API; entries can be metadata only or have attachments
- **Access levels** to records from the UI: public (open to all) and restricted (visible after login only). Possibility to create private collaborative spaces between users (e.g., to exchange data).
- **How does your system deal with ontology updates?** A workflow for metadata governance was designed (cf. VIMMP D1.6 "Taxonomy editor")
Challenges / difficulties

- Using new technologies without missing out on existing previous approaches and a plethora of available tools
- Finding a right balance between expressivity and usability
- Identifying suitable levels of detail for the descriptions
- Many choices need to be made during ontology development: impossible to combine consensus with wider field and development time constraints
- Finding and evaluating suitability of existing artefacts before re-use, then harmonizing them
Lessons learnt and suggestions

- **Interoperability:** Semantics is an important part of the solution, but not the whole story. Syntactics does matter too (e.g., concrete/technical implementations and the constraints they carry).

- **Human factor:** User-facing components (e.g., dropdown menus) need to be navigable and friendly; annotation and alignment are personnel-intensive (tools welcome, can give partial support).

- Importance of sharing own ontologies (also in early development stages) and **getting feedback** (from peers, end-users, developers of components using the ontologies).

- Importance of in-depth **documentation** of semantic assets (including alignments).
References

- **Development:** on GitLab.com [1]
- **Releases:** on [1] and also on matportal.org [2]
- **Documentation:** Springer Brief [3], KI paper [4], Zenodo technical report [5]
- **VIMMP Project overview:** website [6] and CORDIS (including deliverables) [7]


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Thank you for your attention!

Questions?

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