Ontology development for virtual marketplaces in materials modelling
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, monolithic database architecture.)
Ontologies in computational engineering: *Protege* tool
The **VIMMP Marketplace** concept: To serve its participants and facilitate exchange, e.g., between materials **model providers**, industrial & academic client **end users**, and **translators**.

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

Decision Support

Repository

Translation Environment

Simulation Platform 1

Simulation Platform 2

user

Bespoke Functionality
(e.g., “I would like this as an input file for code X”)
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)
Physical equation taxonomy from RoMM and OSMO

<table>
<thead>
<tr>
<th>Electronic</th>
<th>Atomistic</th>
<th>Mesoscopic</th>
<th>Continuum</th>
</tr>
</thead>
<tbody>
<tr>
<td>EL.1: Ab-initio quantum mechanics</td>
<td>A.1: Classical DFT (atomistic)</td>
<td>M.1: Classical DFT (mesoscopic)</td>
<td>CO.1: Continuum solid mechanics</td>
</tr>
<tr>
<td>EL.2: Effective Hamiltonian models</td>
<td>A.2: Molecular statics (atomistic)</td>
<td>M.2: Molecular statics (mesoscopic)</td>
<td>CO.2: Continuum fluid mechanics</td>
</tr>
<tr>
<td>EL.4: Charge transport (statistical)</td>
<td>A.4: Partition function (atomistic)</td>
<td>M.4: Partition function (mesoscopic)</td>
<td>CO.4: Phase field models, DGT</td>
</tr>
<tr>
<td>EL.5: Spin transport (statistical)</td>
<td>A.5: Atomistic spin models</td>
<td>M.5: Mesoscopic spin models</td>
<td>CO.5: Continuum thermodynamics</td>
</tr>
<tr>
<td>EL.7: Processes and devices</td>
<td></td>
<td></td>
<td>CO.7: Electromagnetism</td>
</tr>
</tbody>
</table>

22nd October 2019
Simulation workflows following MODA and OSMO

**OSMO**
- use case
  - 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

**MODA**
- section 1
- section 2
- section 3
- section 4

**OSMO**
- “sections”
- “aspects”
- “graphs”

**VIMMP**
- Virtual Materials Marketplace

---

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

<table>
<thead>
<tr>
<th>Aspect</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1 ASPECT OF THE USER CASE TO BE SIMULATED</td>
<td>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 (as 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 can be documented here.</td>
</tr>
<tr>
<td>1.2 MATERIAL</td>
<td>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.</td>
</tr>
<tr>
<td>1.3 GEOMETRY</td>
<td>Size, form, picture of the system (if applicable) Note that computational choices like simulation boxes are to be documented in chapter 3.</td>
</tr>
<tr>
<td>1.4 TIME LAPSE</td>
<td>Duration of the case to be simulated. This is the duration of the simulation to be run. This is not the same as the computational time to be done in chapter 3.</td>
</tr>
<tr>
<td>1.5 MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS</td>
<td>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 loading forces. Please note that these must appear as terms in the PDE or as boundary conditions and this will be documented in the relevant chapters. Note: These conditions will be expressed in physics relations in chapter 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.</td>
</tr>
<tr>
<td>1.6 PUBLICATION ON THIS DATA</td>
<td>Publication documenting the simulation with this single model (if available) and if not already included in the overall publication.</td>
</tr>
</tbody>
</table>
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

arXiv:1908.02335 [cs.DC]

Ontology for Simulation, Modelling, and Optimization

http://www.vimmp.eu/semantics/osmo/osmo.ttl
European Materials and Modelling Ontology¹

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*)

European Materials and Modelling Ontology¹

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”

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

Information Artifact Ontology
ICALTZD (W3C calendar)
KMK operators
Course Curriculum & Syllabus Ontology
CAS RN, EINECS, ELINCS, NLP List, etc.

EMMO
EVMPO
OEMO
VICO
VIVO
VOV
VISO
CVII & MACRO
MMTO
QUDT
EDAM
SWO
MODA
RoMM terminology
MolMod DB nomenclature

17 | 22nd October 2019
Molecular model nomenclature and database

Z-matrix formalism for the site coordinates of multi-site models\textsuperscript{1,2}

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

Molecular Model Database (MolMod DB)

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

pair potentials for over 150 molecular fluids

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

end user

problem statement (w. OSMO use case)

interest statement

reformulated problem statement (w. OSMO use case)

translator

reformulated solution statement (w. OSMO simulation workflow)

solution statement (w. OSMO simulation workflow)

model provider

acceptance statement, project opening statement, etc.

VIMMP Translation Ontology

MMTO
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.

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.

Enabling Transfer Platform
Market Place, Translators, Training, Validated Software

Underpinning Foundations
Data Repositories, Integrated Open Simulation Platform, Interoperability and Metadata Schema, Models and Methodologies

Novel Market Products
Decision Support, Application Cases, Impact Metrics

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 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.

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.).
Significant collaboration acknowledged:

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- **Cambridge**  —  Gerhard Goldbeck, Gabriele Mogni
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- **Stuttgart**  —  Christoph Niethammer

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