EMMC-CSA

European Materials Modelling Council

Documentation

on

Materials Modelling Ontology in UML

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1. Executive summary

1.1 Description and objectives

Document and describe the European Materials Modelling Ontology (EMMO)

Less focus has been placed on using UML in the description of EMMO. UML is a widely used standard for designing class diagrams for actual code implementations. But with the development of EMMO we have moved to a higher level of abstraction. Since W3W Web Ontology Language (OWL) is the de facto standard for describing ontologies we have chosen it instead of UML. OWL is a language specifically designed for ontologies and is much better suited than UML for this task. However, some syntactic rules of the graphical representation of EMMO has been taken from UML.

1.2 Major outcome

The outcome of this deliverable includes:

- Documentation of EMMO generated from OWL file using the Python package that is a part of the documentation on “Design and Implementation of metadata schema for syntactic and semantic interoperability”.
- Communication with and involvement of more than 100 experts in the development process of EMMO.

2. Progress report (main activities)

2.1 Documentation of EMMO

The EMMO is provided in the form of OWL definitions in machine readable RDF/XML format. It is building upon and formalising the Review of Materials Modelling [1], the CEN Workshop Agreement [2] and the MODA template [3]. It is currently hosted on a private github [4] repository, until it will be published and made publicly available.

However, since this deliverable is a documentation, we will here provide a human readable documentation and reference description of all relations and classes defined in EMMO. This documentation is the real deliverable and is included as an annex to this report.

The documentation has been generated with a Python package `emmo` and the open source software `pandoc` [5]. Input is the OWL definition of EMMO, a set of markdown files, a yaml file with metadata (title, version, authors, date, …) and templates for html and pdf output. This `emmo` package can represent EMMO in a natural way as a set of related Python classes. Individuals are represented as instances of these classes. On top of this package, we have created a tool called `emmodoc` that generates the actual documentation including graphical representations of the different branches and subbranches. The markdown input includes an introduction and titles and ingresses for the automatically documented branches and subbranches. The introduction describes the primitive elements in EMMO, its theoretical foundations, some important concepts and how to read the generated graphs and documentation. This way, we will be able to easily maintain a human readable documentation of EMMO for any version of EMMO.

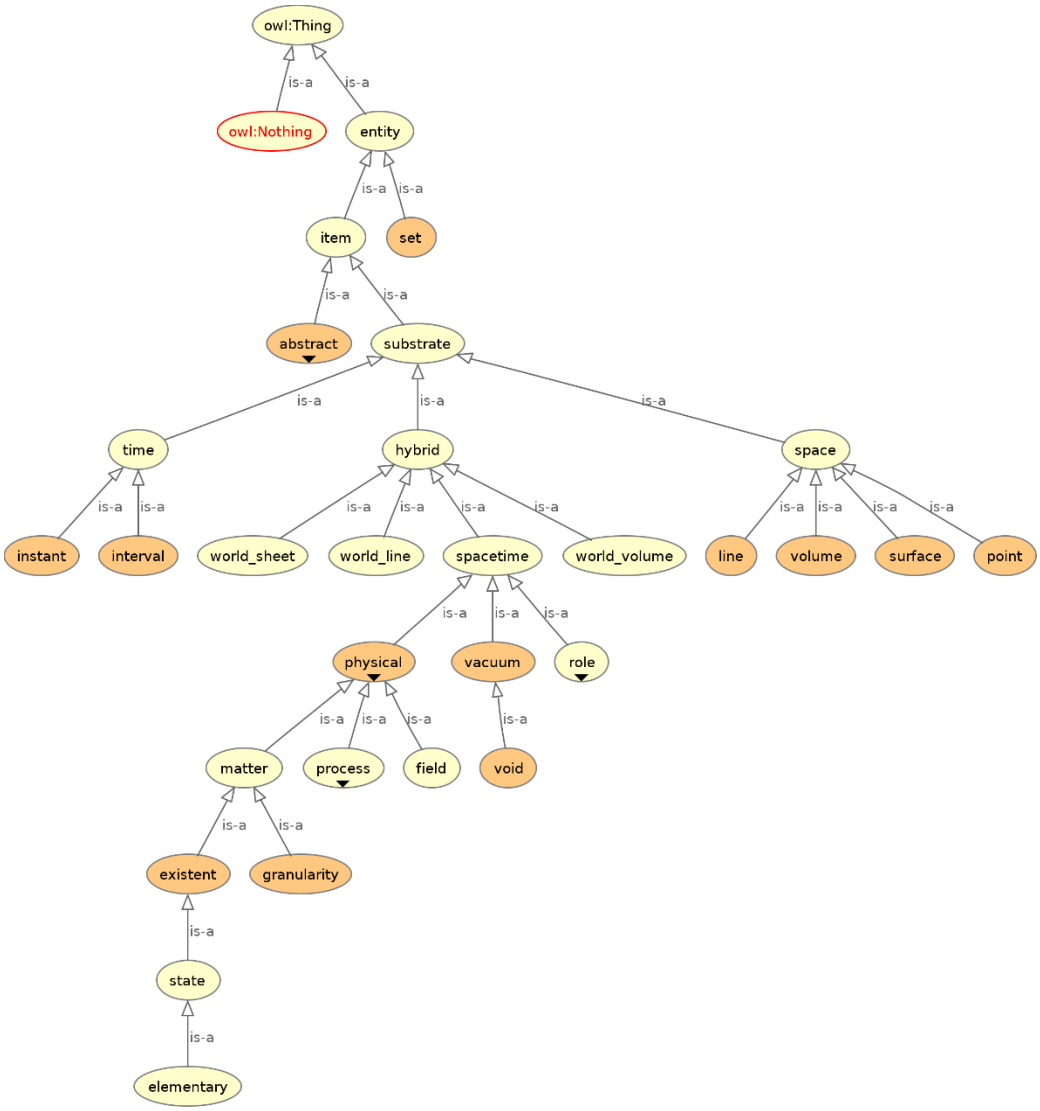

Figure 1 – The base branch of EMMO showing the *elementary* that constitutes all matter. All real materials will be defined in the *state* branch while natural laws, models and properties will be defined in the *abstract* branch.

2.2 Communication and community involvements

The communication and involvement of experts has taken place at the following events:

- Expert Meeting at SINTEF in December 2016
- IRAG meeting, Jan 2017
- Sessions at International Workshop in Vienna, Feb 2017
- A number of exchanges by email and telecon with a.o. Barry Smith and Hedi Karray
- Cambridge IntOp Workshop Nov 2017
- CWA finalised Jan 2018
- EC Materials Ontology Workshop June 2018
- IRAG online meeting and webinar July/August 2018
- IRAG workshop on EMMO Sept 2018

3. Conclusions

A wide community of experts has been approached during the development of EMMO. This input has been formalised in OWL, the language used to define EMMO. Based on the OWL sources, a controlled vocabulary has been extracted from which an annotated and complete documentation of EMMO has been generated.

4. References

[1] https://publications.europa.eu/en/publication-detail/-/publication/ec1455c3-d7ca-11e6-ad7c-01aa75ed71a1
[2] https://www.cen.eu/news/workshops/Pages/WS_2016-013.aspx
[3] https://emmc.info/moda-workflow-templates/
[4] https://github.com/nanodome/emmo/
[5] https://pandoc.org/

5. Annex

Documentation of the European Materials Modelling Ontology (EMMO) in pdf and html formats (emmodoc.pdf, emmodoc.html)

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Consortium		
TU WIEN	Technische Universität Wien	Austria
FRAUNHOFER	Fraunhofer Gesellschaft	Germany
GCL	Goldbeck Consulting Limited	United Kingdom
POLITO	Politecnico di Torino	Italy
UU	Uppsala Universitet	Sweden
DOW	Dow Benelux B.V.	Netherlands
EPFL	Ecole Polytechnique Federale de Lausanne	Switzerland
DPI	Dutch Polymer Institute	Netherlands
SINTEF	Stiftelsen SINTEF	Norway
ACCESS e.V.	ACCESS e.V.	Germany
HZG	Helmholtz-Zentrum Geesthacht Zentrum für Material- und Küstenforschung GMBH	Germany
MDS	Materials Design S.A.R.L	France
QW	QuantumWise A/S	Denmark
GRANTA	Granta Design LTD	United Kingdom
UOY	University of York	United Kingdom
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