

**Remark:** For information beyond subclass relations, refer to the TTL specification of OTRAS.

#### Referenced external resources and semantic assets

- CCSO: Curriculum Course Syllabus Ontology, version 0.7, by Evangelos Katis.
- EVMPO: European Virtual Marketplace Ontology, internal draft document.
- IAO: Information Artifact Ontology, by Albert Goldfain, Barry Smith, et al.

<sup>1</sup> Confer <a href="https://vkreations.github.io/CCSO/">https://vkreations.github.io/CCSO/</a> for further information.

<sup>2</sup> Confer <a href="http://www.obofoundry.org/ontology/iao.html">http://www.obofoundry.org/ontology/iao.html</a> for further information.

- ICALTZD: Ontology for iCalendars with time-zone datatypes,<sup>3</sup> version 1.6, World Wide Web Consortium (W3C).
- KMK Operator Catalogue: <sup>4</sup> Agreement of the German Federal Conference of State Cultural Ministries (KMK) for English-language learning-outcome operator designations in the natural sciences (Physics, Biology, Chemistry), version 265.

## Normal form of a learning-outcome specification to be used with OTRAS

A normal form of stating a desired learning outcome can be given as follows:

"After successfully completing  $X_1$ , participants can  $X_2$  with respect to  $X_3$  by doing  $X_4$ ; for example,  $X_5$ ." (Note:  $X_4$  and  $X_5$  are not required, and  $X_1$  is not a specifier of the outcome.)

Therein,  $X_1$  is the course or training unit for which a learning outcome is stated. The entities  $X_2$ ,  $X_3$ ,  $X_4$ , and  $X_5$  are the **specifiers** of the learning outcome:

- **X**<sub>2</sub> specifies the **operator** of the learning outcome (class operator\_specifier); a **catalogue of operators**<sup>4</sup> with three-digit operator codes is included.
- X<sub>3</sub> specifies the **operand** of the learning outcome (class operand\_specifier); the operand can, and usually will, be related to one or multiple topics for which the present ontology uses the class topic, equivalent to CCSO:Topic. Within materials modelling, a **taxonomy of topics** (class mm\_topic) with four-digit topic codes will be developed; in the present draft, a generic structure is already included.
- X<sub>4</sub> specifies the **implementation** (class implementation\_specifier), describing the way in which the competency is carried out in practice (e.g., "by writing a C++ code" or "by carrying out an appropriate series of DPD simulations"); this is optional, and no catalogue will be developed.
- X<sub>5</sub> specifies an **example** (class example\_specifier), explaining how the competency might be applied in a particular special case (e.g., "if asked to develop a molecular model for caffeine, the participant might suggest a rigid coarse grained model consisting of six Mie interaction sites"). This sort of specifier is also optional, it is technically only an explanation of the learning outcome.

The difference between  $X_4$  and  $X_5$  is that the implementation is a general statement on the acquired competency, whereas the example can be any arbitrary illustration of it.

<sup>3</sup> Source: https://www.w3.org/2002/12/cal/icaltzd.

<sup>4</sup> Developed for the use at German Schools outside Germany; source: <a href="https://www.kmk.org/fileadmin/Dateien/pdf/Bildung/Auslandsschulwesen/Kerncurriculum/Auslandsschulwesen-Operatoren-Naturwissenschaften-englisch-03-2014.pdf">https://www.kmk.org/fileadmin/Dateien/pdf/Bildung/Auslandsschulwesen/Kerncurriculum/Auslandsschulwesen-Operatoren-Naturwissenschaften-englisch-03-2014.pdf</a>.

# Operator catalogue for competency specification<sup>4,5</sup>

- 1XX Operators to be predominantly used for basic-level competencies: *Generic basic-level operator* (code 100), "to name/label" (code 120), "to outline/present" (code 130), "to list/give" (code 140), "to write a lab report/data log" (code 150), "to sketch" (code 160), "to draw" (code 170).
- 2XX Operators to be predominantly used for intermediate-level competencies: Generic intermediate-level operator (code 200), "to compare" (code 215), "to deduce" (code 220), "to estimate" (code 225), "to analyse and identify" (code 230), "to apply" (code 235), "to calculate" (code 240), "to describe" (code 245), "to find" (code 250), "to explain" (code 255), "to describe and explain" (code 260), "to formulate" (code 265), "to derive" (code 270), "to sort/group/classify" (code 275), "to test/verify" (code 280), "to investigate/examine" (code 285), "to generalize" (code 290), "to summarize" (code 295).
- 3XX Operators to be predominantly used for advanced-level competencies: *Generic advanced-level operator* (code 300), "to propose a hypothesis" (code 320), "to evaluate" (code 330), "to justify/give reasons" (code 340), "to comment on/assess" (code 350), "to prove" (code 360), "to discuss" (code 370), "to interpret" (code 380), "to plan" (code 390).

### Taxonomy of the topics covered by training in materials modelling

The aim here is, by the point at which the VIMMP Marketplace starts to operate, to include two fully elaborated hierarchy levels as classes, and any further categorization that may be helpful below these two levels implemented in terms of individuals. Parallel to the taxonomy, there are four-digit codes characterizing the respective individuals.

At the first hierarchy level, the fields covered by materials modelling training are subdivided as follows (confer the TTL file for further information):

- Class mm\_topic\_basic (codes 1XXX and 2XXX): Basic prerequisites for materials modelling, including contents from undergraduate or secondary education.
- Class mm\_topic\_computational (codes 3XXX): Computational and numerical aspects of materials modelling.
- Class mm\_topic\_data (codes 4XXX): Data science and technology aspects.
- Class mm\_topic\_materials (codes **5XXX**): Topics related to materials, including but not limited to fluids, and their properties.

Refer to the ontology TTL file or the KMK document for a *definition* (i.e., a more detailed description) of these operators; e.g., the operator which is *expressed by* "explain" is *defined by* giving a detailed account of causes and relationships, whereas the operator *expressed by* "describe and explain" has a *definition* that includes giving examples. These definitions, which are not always self-evident from the employed expressions, are a part of the present semantic asset on the basis of the KMK document.

- Class mm\_topic\_social (codes 6XXX): Social, economic, and community aspects of materials modelling.
- Class mm\_topic\_theoretical (codes 7XXX): Non-computational theoretical aspects of materials modelling.
- Class mm\_topic\_interdisciplinary (codes **8XXX**): Topics that are best described as belonging to multiple categories at the first hierarchy level.
- Class mm\_topic\_side (codes 9XXX): Topics from other disciplines that can be included as relevant side interests in materials modelling curriculum design.

### **Suggested future steps**

Beyond the single course description from *Alta Scuola Politecnica*, it will be necessary to evaluate a substantial corpus of courses and syllabi from universities, *CECAM*, and institutions such as the *Hartree Centre*, covering the range of topics that occur in Materials Modelling curricula, in the broadest sense. In this way, we will **complete the catalogue of topics** and topic codes; the present structure is generic enough to facilitate this. To reach this objective, a **survey on training material and course syllabi** should be conducted and evaluated as soon as possible.

For the eventual operation of the VIMMP Marketplace, a **didactics advisory board** should be formed to review proposed syllabi and supporting information for submitted training events and materials, and to assist training providers at properly formulating and assessing learning outcomes where needed.<sup>6</sup> This board should be in charge of maintaining the catalogue of topics and the topic codes; it could be formed jointly with the MARKETPLACE project or as a *EMMC Working Group for Materials Modelling Didactics*.<sup>7</sup> The aim should be to have a state-of-the-art approach to curriculum design in operation at the VIMMP Marketplace. This will allow training providers to properly formulate and communicate interdependencies between courses<sup>8</sup>, to co-design teaching and assessment by constructive alignment, and to **have certificates issued automatically** to the participants who have successfully completed a course.

At the level of tradeable objects in general, a formalism needs to be introduced by which participants can evaluate courses and communicate their assessment on the provider. This **feedback certificate mechanism** could be formalized by EVMPO, VICO, VIVO, VTO, or another marketplace-level ontology or pre-existing external ontology framework.<sup>9</sup>

<sup>6</sup> Intended as a help for training providers to access our marketplace effectively; not to exclude anyone.

<sup>7</sup> Instead of founding a new group, this might also be included within the scope of the EMMC Translation and Training for Companies Working Group if the colleagues agree.

<sup>8</sup> Courses from different providers can only be declared as equivalent (or fulfilling prerequisites of one another) on the basis of an analysis of the learning outcomes, which needs to be carried out by a neutral party, such as the marketplace itself or the EMMC.

<sup>9</sup> Note: VIMMP Translation Ontology (VTO) draft version 0.3.2 already contained such a formalism.