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Pragmatic interoperability and translation of industrial engineering problems into modelling and simulation solutions

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Abstract. Pragmatic interoperability between platforms and service-oriented architectures exists whenever there is an agreement on the roles of participants and components as well as minimum standards for good practice. In this work, it is argued that open platforms require pragmatic interoperability, complementing syntactic interoperability (e.g., through common file formats), and semantic interoperability by ontologies that provide agreed definitions for entities and relations. For consistent data management and the provision of services in computational molecular engineering, community-governed agreements on pragmatics need to be established and formalized. For this purpose, if ontology-based semantic interoperability is already present, the same ontologies can be used. This is illustrated here by the role of the “translator” and procedural definitions for the process of “translation” in materials modelling, which refers to mapping industrial research and development problems onto solutions by modelling and simulation. For the associated roles and processes, substantial previous standardization efforts have been carried out by the European Materials Modelling Council (EMMC). In the present work, the Materials Modelling Translation Ontology (MMTO) is introduced, and it is discussed how the MMTO can contribute to formalizing the pragmatic interoperability standards developed by the EMMC.

Keywords: Pragmatic interoperability · materials modelling

1 Introduction

The capabilities of service, software, and data architectures increase greatly if they are able to integrate a variety of heterogeneous resources into a common framework. In general, this requires an exchange of information with a multitude of systems of resources, each of which follows the paradigm and structure, or *language*, favoured by its designers. As the number n of such systems increases, establishing and maintaining a direct 1 : 1 *compatibility* between each pair of standards (e.g., file formats) becomes impractical, considering that $n(n - 1)$ converters would need to be developed and updated as each of the relevant standards is modified; beside the unfavorable scaling of the effort required to develop such an architecture, this would also presuppose that the designers of each system understand all other systems and are interested in ensuring a compatibility with each of them, neither of which can be taken for granted. Instead, $n : 1 : n$ *interoperability* based on a single intermediate standard only requires $2n$ mappings; if the interoperability standard has the approval of a significant community, which can be expected whenever the number of participating systems is large enough, developers have an intrinsic interest in maintaining the interoperability. For this purpose, they merely need to keep track of changes to their own system and the common intermediate standard.

Hence, interoperability is generally the favoured approach to integrating distributed and heterogeneous infrastructures. Since this addresses a problem of languages, the aspects of interoperability can be categorized according to their relation to three major areas of the theory of formal languages: Syntax, semantics, and pragmatics – or how to write correctly (according to a given format or grammar), how to associate a meaning with the communicated content (by which data items become information), and *how to deal with information* and transactions that involve an exchange of information. While well-known and well-established approaches for ensuring syntactic and semantic interoperability exist, *pragmatic interoperability* has not acquired the same degree of attention.

Software and data architectures often neglect to explicitly formulate any requirements at the level of pragmatics, since they are assumed to be guaranteed by institutional procedures (e.g., who is given an account, and who may ingest data). However, this delegation of responsibilities cannot be upheld for *open infrastructures* where anybody is invited to participate and to which a multitude of external tools and platforms connect, each of which may have its own users, roles, service definitions, access regulations, interfaces, and protocols. Accordingly, finding that semantic interoperability cannot reach its goals if it is not supplemented by an agreement on “what kind of socio-technical infrastructure is required,” it has been proposed to work toward a universal *pragmatic web* [33]; in full consequence, this would add a third layer to the world-wide web infrastructure, operating on top of the semantic web and hypertext/syntactic web layers. This raises the issue of requirements engineering (i.e., specifying and implementing requirements) for service-oriented infrastructures, which becomes non-trivial whenever “stakeholders do not deliberately know what is needed” [38]. Previous work has established that ontologies are not only a viable tool for semantic inter-

operability, but also for enriching the structure provided for the semantic space by definitions of entities, relations, and rules that are employed to specify jointly agreed pragmatics [33, 37]; to provide additional procedural information, *workflow patterns* have been suggested as a tool [36], e.g., employing the Business Process Model and Notation (BPMN) [1]. Since BPMN workflow diagrams can be transformed to RDF triples on the basis of an ontology [30], this approach is well suitable for domains of knowledge where ontologies already exist.

The present work follows a similar approach; it intends to contribute to the aim of the European Materials Modelling Council (EMMC) to make services, platforms, and tools for modelling and simulation of fluid and solid materials interoperable at all levels, which includes pragmatic interoperability. The workflow pattern standard of the EMMC is MODA (i.e., Model Data) [7], which as an ontology becomes OSMO, the ontology for simulation, modelling, and optimization; this ontology development [20] constitutes the point of departure for the present discussion. One of the concepts at the core of this line of work is that of materials modelling *translation*, i.e., the process of guiding an industrial challenge toward a solution with the help of modelling [11, 12]. The experts that facilitate this process are referred to as *translators*; they provide a service for companies and can be either academics, software owners, internal employees of a company, or independent engineers. Previous work on data science pragmatics by Neff et al. [26] concludes that it is particularly relevant to “get involved in observing the day-to-day practices of the work of data science” when addressing a scenario that “requires translation across multiple knowledge domains” to “make data valuable, meaningful, and actionable.” This is the case here as well.

The remainder of this work is structured as follows: Section 2 introduces the approach to interoperability established by the EMMC (and associated projects), the relevant definitions of roles and best practices concerning materials modelling translation, and how ontologies can be employed in this context. For this purpose, Section 3 introduces the main contribution from the present work, the Materials Modelling Translation Ontology (MMTO) version 1.3.4, together with OSMO version 1.6.6 which is extended in comparison to the previously published version 1.2 [20]. Section 4 discusses the identification of key performance indicators. Finally, a conclusion is given in Section 5.

2 Interoperability in materials modelling

2.1 Review of Materials Modelling, MODA, and ontologies

Where a physically based modelling approach is followed, physical equations are employed jointly with materials relations that parameterize and complement the physical equations, e.g., for a particular substance. The combination of physical equations and materials relations is referred to as the system of governing equations; on the basis of the Review of Materials Modelling [3], common physical equation types are identified categorized into four groups according to their granularity level: Electronic, atomistic, mesoscopic, or continuum. Subsequent

to the review activity and the agreement on a basic nomenclature as formalized by the Review of Materials Modelling [3], the EMMC developed MODA, a semi-formalized simplified graph representation for simulation workflows [7]; this notation, which is immediately intelligible to human readers, but not immediately machine-processable, was further extended to permit the inclusion of graph elements that represent logical data transfer [20]. In MODA graphs, there are four classes of vertices, which are here referred to as *sections*:

1. Use case, i.e., the physical system to be simulated.
2. Materials model, i.e., the system of governing equations, with one or multiple physical equations and materials relations.
3. Solver, i.e., the numerical solution of the model in terms of the variables that occur in the governing equations explicitly (and nothing beyond this).
4. Processor, i.e., any computational operation beyond the above.

For each section, the MODA standard contains a list of text fields, which are here referred to as *aspects*, where more detailed information can be provided; however, since this is plain text, it is not immediately possible to extract semantically annotated content from this representation automatically. In logical data transfer graphs, additionally, there are vertices for *logical resources* that store *logical variables*, i.e., abstractions of quantities and data structures that are exchanged between sections; the representation of the workflows and the flow of information is conceptual, or *logical*, in the sense that it does not carry any information on how the exchange of data is realized technically [20].

Semantic technology, centered on the use of ontologies as a tool, is increasingly applied to data management in all areas, including computational chemistry and molecular engineering [16, 34]; beside ontologies, other types of semantic assets, such as XML schemas, can be employed [32]. As a feature of the semantic web, semantic assets can link to entity definitions from external sources, facilitating distributed development and complex multi-tier architectures. The highest level of abstraction is usually given by a top-level ontology. These components of the semantic web, such as the Basic Formal Ontology [2], DOLCE [6], ThingFO [27], and the Unified Foundational Ontology [18], are largely domain-independent and reused frequently in very diverse contexts; at the top level, philosophical concerns are at least as significant as the practical demands of research data technology. The EMMC advances its own top-level ontology, the European Materials and Modelling Ontology (EMMO), which is based on the philosophical paradigms of nominalism, merotopology, and semiosis following Peirce [14, 17, 21, 28]. To achieve interoperability within the framework of the projects and infrastructures involving the EMMC community, all lower-level, i.e., domain-specific ontologies need to be aligned with the EMMO.

In particular, for the Virtual Materials Marketplace project, which develops a platform where services and solutions related to computational molecular engineering can be traded, and with which multiple other platforms are expected to interoperate, it is essential to standardize the semantic space, e.g., for the exchange of information during data ingest and data retrieval [22]; this includes the characterization of services, models, documents, data access, etc., and

may involve communication with external resources such as model and property databases. The domain ontologies that are developed by the Virtual Materials Marketplace project for this purpose are referred to as *marketplace-level ontologies* [22, 23]; the marketplace-level ontology OSMO is directly based on the MODA workflow graph standard as well as its logical data transfer extension [20]. Thereby, a section from MODA, e.g., a solver, becomes a `osmo:section` entity, e.g., a `osmo:solver`. However, in MODA, the aspects (entries) of a section can only contain plain text; by using the relation `osmo:has_object_content` from OSMO, it becomes possible to point to semantically characterized content defined anywhere on the semantic web, including individuals and classes from OSMO and other ontologies. Similarly, OSMO formalizes the workflow graph elements and the exchanged logical variables. In this way, the MODA standard becomes machine-processable through OSMO. The materials modelling translation ontology from the present work, cf. Section 3, is based on this approach; it is closely connected to OSMO, and by extending the structure of the accessible semantic space to additionally deal with translation in materials modelling, it explicitly builds on OSMO and implicitly generalizes the MODA standard.

2.2 Specification of roles and processes

The role of the materials modelling *translator* is defined in the EMMC Translators' Guide [12]; a translator needs to be able to bridge the “language gap” between industrial end users, software owners, and model providers who are usually academics. The work of a translator aims at delivering not just modelling results, but a valuable and beneficial solution for a problem from industrial engineering practice. Previous work by Faheem et al. [15] has shown that ontology engineering can support the implementation of a “mapping scheme from the problem domain to the computer domain” with a focus on deployment on high performance computing architectures, which as a challenge is roughly of the same type as translation in materials modelling – in particular, considering potential solutions such as the *translation router* developed by the Virtual Materials Marketplace project [22]. An instance of the translation process, some agreed features of which are codified by the EMMC Translators' Guide [12] and the EMMC TC Template [11], is referred to as a *translation case* (TC). It begins with exploring and understanding the *business case* and the *industrial case*, or multiple relevant business cases and/or industrial cases, which describe the socioeconomic objectives and boundary conditions, cf. Section 3.

Role definitions are known to be helpful in establishing sustainable good practices in data stewardship; e.g., this is illustrated by recent work proposing the position of the *Scientific Data Officer* (SDO), jointly with providing a role definition that is tailor-made for addressing major concerns from research data management in high performance computing [31]. The responsibilities associated with this role relate to technical, organizational, ethical, and legal aspects of data stewardship [25]. One of the most important tasks that an SDO is expected to perform is data annotation; since data can only be curated with the help of metadata, concrete tasks include adaptation of existing metadata models to

a use case and the support of automated metadata extraction. Moreover, the SDO's responsibilities also include a mediation role between different groups of interest, e.g., between scientists and the operators of computing and storage facilities. This mediation role has a high impact for pragmatic interoperability, since many problems arise when different technical languages, terminologies or jargons are conflicting. In this way, the SDO is in a position that shares certain characteristics with that of the materials modelling translator, particularly if metadata are seen as a form of communication as proposed by Edwards et al. [10].

Translation can be a process with multiple iterations. Thereby, the active and regular contact with the end user (i.e., the industrial client of the translator) is a prerequisite for an effective and successful working relationship: The translator needs to be in communication with the client during the whole project duration to discuss regularly the project dynamics, possible changes to the line of work and development, and any other relevant feedback. The level of detail required for a modelling and simulation based contribution to an economic analysis of a value-added chain makes it necessary to go beyond computational molecular engineering in the strict sense, since eventually, key performance indicators of processes and products need to be optimized. The subsequent sections propose a solution for documenting these processes, providing the required business case, industrial case, and translation case descriptions (Section 3) as well as key performance indicators (Section 4).

3 Materials Modelling Translation Ontology

The present release of the MMTO (version 1.3.4) and OSMO (version 1.6.6) is available as free software under the terms and conditions of the GNU Lesser General Public License version 3 [23, 35]. The revision of OSMO generalizes the section structure from MODA by introducing `osmo:application_case` as a new superclass of `osmo:use_case`. Beside use cases, in this way, business cases (`mmto:business_case`), industrial cases (`mmto:industrial_case`), and translation cases (`mmto:translation_case`) become subclasses of `osmo:application_case` and can be dealt with in a similar way as the sections from MODA. The relevant part of the MMTO and OSMO class hierarchy is visualized in Fig. 1, including the relations that are most useful and common in this context.

The TC *aspects*, cf. Tab. 1, directly correspond to the text fields from the EMMC TC Template [11], except that the MMTO permits the provision of semantically characterized content; this follows the approach from OSMO, which delivers the same feature for the text fields from MODA. The aspects by which business cases and industrial cases are described in the MMTO are given in Tabs. 2 and 3. Thereby, a business case can represent any economic problem at the management level, whereas an industrial case refers to an industrial engineering problem or an optimization problem in research and development. Within the translation process, a suitable approach based on modelling and simulation is identified and carried out; subsequently, the outcome is translated back to support an actionable decision at the business case and industrial case levels. The

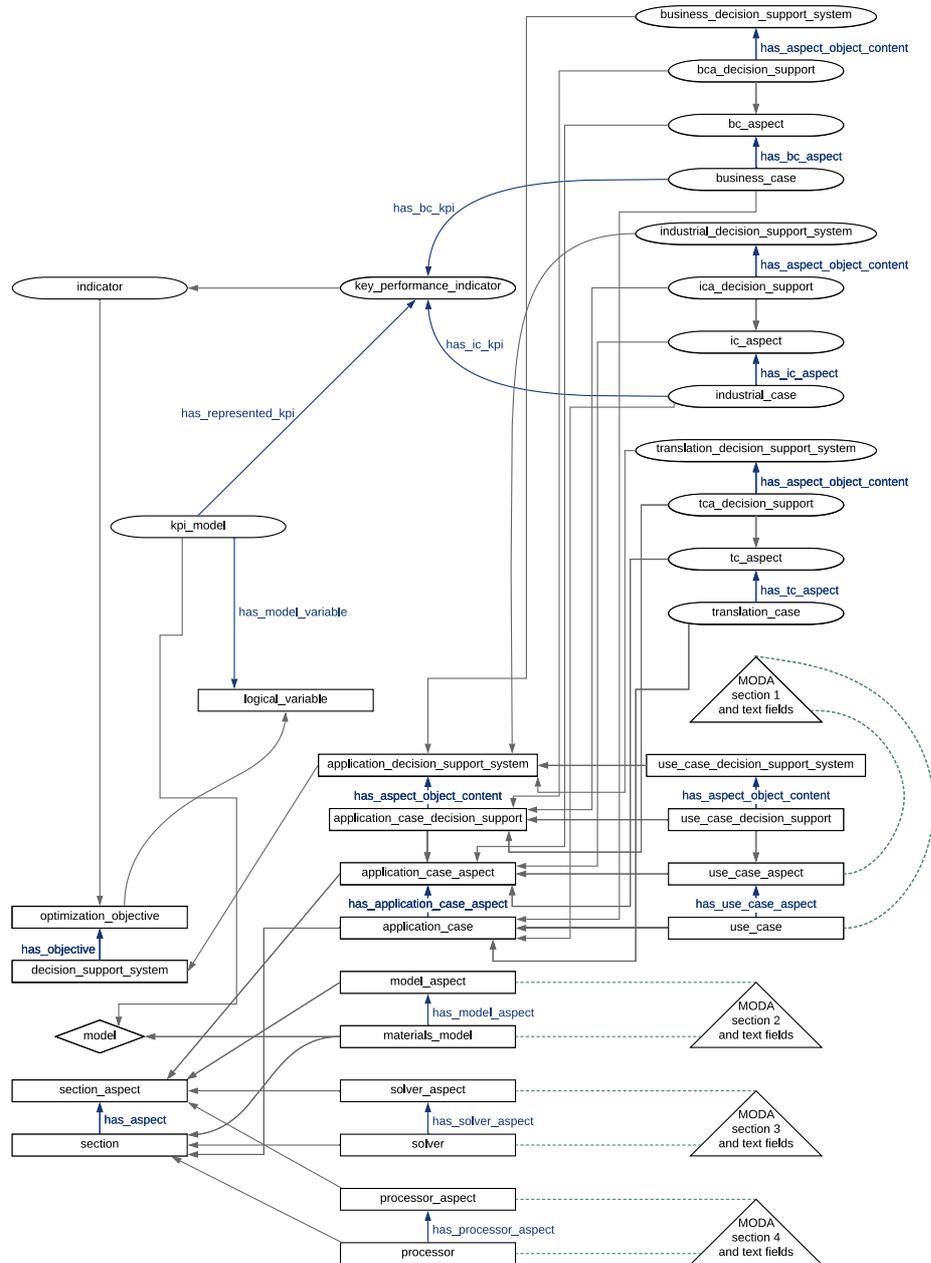


Fig. 1. Entities from MMTO version 1.3.4 (rounded boxes), OSMO version 1.6.6 (rectangular boxes), EMMO version 1.0.0 alpha 2 (diamond), MODA sections (triangles), and a subset of the relations defined by MMTO and OSMO, where grey arrows correspond to the transitive reduction of the `rdfs:subClassOf` relation, blue arrows to relations between individuals as indicated by arrow labels, and green dashed lines to correspondences between elements from MODA and OSMO.

stages of the translation process according to the EMMC Translators' Guide [12], together with the corresponding MMTO entities, are reported in Tab. 4. To show how this would actually be realized on a digital marketplace, an illustrative exchange of communications taking place during a translation process (ordered as a sequence in time from top to bottom) is depicted in Fig. 2, together with the class hierarchy of the relevant branch of the MMTO.

Table 1. Aspects of a translation case (TC), `mmto:translation_case`, specified by the MMTO on the basis of the EMMC TC Template [11].

aspect class name	content description
<code>mmto:tca_translator</code>	<i>translator(s) involved in the TC</i> content type: <code>evmpo:translator</code> [23]
<code>mmto:tca_end_user</code>	<i>involved end user(s), i.e., client(s) of the translator</i> content type: <code>evmpo:end_user</code> [23]
<code>mmto:tca_industrial_case</code>	<i>industrial case(s) associated with the TC</i> content type: <code>mmto:industrial_case</code>
<code>mmto:tca_business_case</code>	<i>business case(s) associated with the TC</i> content type: <code>mmto:business_case</code>
<code>mmto:tca_expected_outcome</code>	<i>expected outcome of the translation process</i> content type: plain text, i.e., <code>xs:string</code>
<code>mmto:tca_pe_type</code>	<i>physical equation type(s) employed for modelling</i> content type: <code>osmo:physical_equation_type</code> [20]
<code>mmto:tca_discussion</code>	<i>summary of discussions with the end user</i> content type: plain text, i.e., <code>xs:string</code>
<code>mmto:tca_kpi_model</code>	<i>employed KPI model(s)</i> content type: <code>mmto:kpi_model</code>
<code>mmto:tca_evaluation</code>	<i>evaluation (assessment) of the TC</i> content type: <code>vivo:translation_assessment</code> [23]
<code>mmto:tca_impact</code>	<i>impact and benefit to the end user; how does the TC contribute to improving processes/products?</i> content type: plain text, i.e., <code>xs:string</code>
<code>mmto:tca_decision_support</code>	<i>employed decision support system(s)</i> content type: <code>osmo:decision_support_system</code>

The MMTO and OS MO are connected to the EMMO through the European Virtual Marketplace Ontology (EVMPO), a module which is developed jointly by the Virtual Materials Marketplace and MarketPlace projects, and the EMMO-VIMMP Integration component for ontology alignment [22, 23]. Additionally, the MMTO employs the ISO 4217 standard for currency descriptions through the Currency Amount Ontology (CAO) module of the Financial Industry Business Ontology [5, 9], cf. Tab. 2; it also refers to entity definitions from two further marketplace-level ontologies from the Virtual Materials Marketplace project [22, 23]: Classes of agents (e.g., `evmpo:end_user` and `evmpo:agent`) and messages (e.g., `evmpo:interlocution` and `evmpo:statement`) from the EVMPO in combination with the VIMMP Communication Ontology, and the description

Table 2. Aspects of a business case, `mmto:business_case`, in the MMTO.

aspect class name	content description
<code>mmto:bca_description</code>	<i>abstract or rough description</i> content type: plain text, i.e., <code>xs:string</code>
<code>mmto:bca_industrial_case</code>	<i>related industrial case(s)</i> content type: <code>mmto:industrial_case</code>
<code>mmto:bca_red_zone</code>	<i>red zone(s), i.e., operational constraint(s)</i> content type: plain text, i.e., <code>xs:string</code>
<code>mmto:bca_context</code>	<i>business-case context; revenue streams, risk management, distribution channels, etc.</i> content type: plain text, i.e., <code>xs:string</code>
<code>mmto:bca_currency</code>	<i>budgeting currency</i> content type: <code>cao:Currency</code> from CAO [5, 9]
<code>mmto:bca_contribution_to_cost</code>	<i>contribution to cost (in budgeting currency)</i> description type: plain text, i.e., <code>xs:string</code> magnitude type: decimal, i.e., <code>xs:decimal</code>
<code>mmto:bca_total_cost</code>	<i>total cost (in budgeting currency)</i> content type: decimal, i.e., <code>xs:decimal</code>
<code>mmto:bca_contribution_to_benefit</code>	<i>contribution to benefit (in budgeting currency)</i> description type: plain text, i.e., <code>xs:string</code> magnitude type: decimal, i.e., <code>xs:decimal</code>
<code>mmto:bca_total_benefit</code>	<i>total benefit (in budgeting currency)</i> content type: decimal, i.e., <code>xs:decimal</code>
<code>mmto:bca_return_on_investment</code>	<i>return on investment</i> content type: decimal, i.e., <code>xs:decimal</code>
<code>mmto:bca_decision_support</code>	<i>employed decision support system(s)</i> content type: <code>osmo:decision_support_system</code>

of marketplace-interaction evaluations (here, `vivo:translation_assessment`) from the VIMMP Validation Ontology (VIVO), cf. Tab. 1.

4 Key performance indicators

Key performance indicators (KPIs) can be used as a vehicle to map industrial problems onto modelling and simulation workflows. In business administration and management, a KPI is understood to be a natural-language description of something which is a selling argument. This reflects the point of view corresponding to organizational roles that are comparably distant from research and development, e.g., in sales or high-level management. In scenarios that arise in the context of such organizational roles, it necessarily appears to be most crucial to address concerns that are immediately relevant to business-to-administration, business-to-business, and business-to-customer relations [4].

We propose to reserve the keyword KPI (`mmto:key_performance_indicator`) to indicators (scalar quantities) that are directly relevant to characterizing, modelling, or optimizing such scenarios. On this basis, from the point of view of a materials modelling translator, two major distinctions need to be made:

Table 3. Aspects of an industrial case, `mmto:industrial_case`, in the MMTO.

aspect class name	content description
<code>mmto:ica_constraints</code>	<i>constraints: production capacity, supply chains, etc.</i> content type: plain text, i.e., <code>xs:string</code>
<code>mmto:ica_data_source</code>	<i>data sources (documents, citations, databases, etc.)</i> content type: <code>iao:information_content_entity</code> [8]
<code>mmto:ica_data_access</code>	<i>data access conditions (licensing, ownership, etc.)</i> content type (description): plain text, i.e., <code>xs:string</code>
<code>mmto:ica_decision-support</code>	employed decision support system(s) content type: <code>osmo:decision_support_system</code>

1. Some KPIs are closely related to human sentience (aesthetics, haptics, taste, etc.). Studies aiming at gaining information on these quantities typically rely on market research and other empirical methods that involve human subjects; such indicators are referred to as *subjective* KPIs (`mmto:subjective_kpi`). Obversely, an *objective* KPI (`mmto:objective_kpi`) can be determined by a standardized process, e.g., a measurement, experiment, or simulation, the result of which (assuming that it is conducted correctly) does not depend on the person that carries it out.
2. An objective KPI is *technological* (`mmto:technological_kpi`) if it is observed or measured within a technical or experimental process, referring directly to properties of the real product or manufacturing process; properties of a model, which are determined by simulation, are *computational* KPIs (`mmto:computational_kpi`).

The distinction between subjective and objective KPIs is similar to that between critical-to-customer and critical-to-quality measures [13, 24, 29]. The formulation given above, however, is more closely related to concepts from the EMMO. Due to its foundation on Peircean semiotics [28], it is straightforward in the EMMO to categorize signs by the way in which their interpretation depends on the subjective impression of an interpreter or observer [14, 21]. In particular, the same distinction is made in EMMO version 1.0.0 alpha 2 [14, 17]. Accordingly, this approach is best amenable to a prospective alignment of the MMTO with the EMMO and the approach to interoperability guided by the EMMC.

The relation between properties accessible to materials modelling and the technological KPIs that are most immediately relevant to real industrial processes and products is necessarily indirect; it requires the mediation through a translation process and a TC as formalized above, which includes modelling KPIs as a function of other quantities, i.e., the creation of KPI models (`mmto:kpi_model`). For the present purpose, a KPI model is given by a condition, correlation, or other formalism containing a set of variables, which can – but need not – be KPIs or other indicators, by which one or multiple KPIs are represented (i.e., here, predicted, correlated, or modelled). In this way, KPI models can represent observables: Mathematical operators that map logical variables to scalar quantities, by which, e.g., computational KPIs determined as the outcome of a

Table 4. MMTO representation of the stages of a materials modelling translation process (subclasses of `mmto:translation_step`), as specified by the EMMC Translators’ Guide [12]. The numbers in the first column, which follow the EMMC Translators’ Guide, are related to the stages by the datatype property `mmto:has_emmc_guide_no`. The considered sections, i.e., individuals of the classes given in the third column without an asterisk, are related to the stages by `mmto:considers_section`. *Remark on no. 4: The relations connecting `mmto:translation_step_modelling` to `osmo:workflow_graph` is `mmto:considers_workflow`; **remark on no. 6: The relations connecting `mmto:translation_step_decision` to `osmo:decision_support_system` and `mmto:kpi_model`, respectively, are `mmto:has_step_decision_support`, and `mmto:considers_kpi_model`.

no.	MMTO class identifier and description	entities connected by relations
1	<code>mmto:translation_step_bc</code> <i>good understanding of the business case</i>	<code>mmto:business_case</code>
2	<code>mmto:translation_step_ic</code> <i>good understanding of the industrial case</i>	<code>mmto:industrial_case</code>
3	<code>mmto:translation_step_data</code> <i>analysis of the data from experiment and simulation available to the end user</i>	<code>osmo:use_case</code>
4*	<code>mmto:translation_step_modelling</code> <i>translation to simulation workflows</i>	<code>osmo:materials_model</code> and <code>osmo:workflow_graph</code> *
5	<code>mmto:translation_step_execution</code> <i>execution and validation strategy</i>	–
6**	<code>mmto:translation_step_decision</code> <i>evaluation of the simulation results to facilitate an actionable decision</i>	<code>osmo:decision_support_system</code> ** and <code>mmto:kpi_model</code> **

complex simulation workflow can be correlated, and a technological KPI can be estimated on the basis of computational KPIs.

5 Conclusion

By developing the MMTO, which extends the *section* concept from OSMO to cover business cases, industrial cases, and translation cases, a formalism was introduced by which translation in materials modelling can be represented in a way that implicitly also extends MODA, the pre-existing EMMC standard for simulation workflows. Just as OSMO is the ontology version of MODA, the MMTO is the ontology version of an implicit generalization of MODA by which, beside the simulation workflow itself, its socioeconomic context can be described. In this way, the MMTO is also a tool for representing the exchange of information during translation processes (e.g., on KPIs) as a workflow, analogous to the formalization of MODA and logical data transfer graphs within OSMO. Since it is given as an ontology, the *aspects* from the MMTO (and from OSMO), which correspond to plain-text form entries in MODA, can contain links to entities defined elsewhere in the semantic web which can be immediately processed computationally, and to which automated reasoning can be applied. Where available, previous

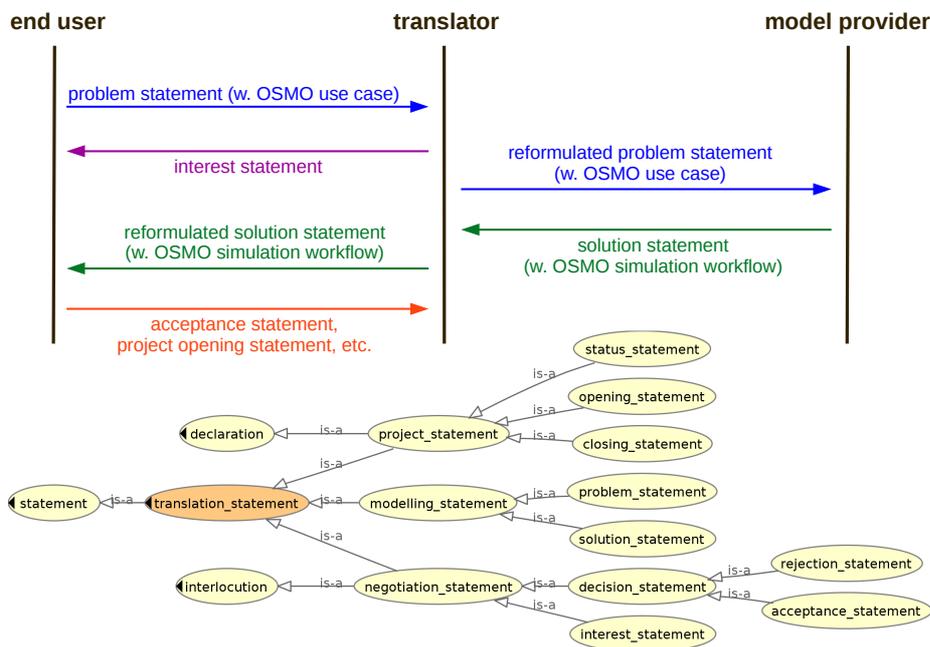


Fig. 2. Top: A possible interchange between participants of a materials modelling marketplace during steps 1 to 4 of a translation process, cf. Tab. 4, expressed in terms of `mmto:translation_statement` entities. Bottom: Diagram showing the transitive reduction of the `rdfs:subClassOf` relation (grey arrows) for the `mmto:translation_statement` branch of the MMTO, wherein `evmpo:declaration`, `evmpo:interlocution`, and `evmpo:statement` are entities from the European Virtual Marketplace Ontology (EVMPO) [23]; this diagram was generated using OWLViz [19].

agreements have been taken into account in the form of the EMMC Translators' Guide and the EMMC TC Template, which are codified by the MMTO. To guarantee pragmatic interoperability between translation-related services and platforms such as materials modelling marketplaces, open translation environments, business decision support systems, and open innovation platforms, substantial further standardization efforts will be required.

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References

1. Allweyer, T.: BPMN 2.0: Introduction to the Standard for Business Process Modeling. BOD, Norderstedt, Germany, 2nd edn. (2016)
2. Arp, R., Smith, B., Spear, A.D.: Building Ontologies with Basic Formal Ontology. MIT Press, Cambridge, Massachusetts, USA (2015)
3. De Baas, A.F. (ed.): What makes a material function? Let me compute the ways. EU Publications Office, Luxembourg (2017), this document is by convention known as the Review of Materials Modelling (RoMM)
4. Barrientos, L.G., Cruz Sosa, E.R., García Castro, P.E.: Considerations of e-commerce within a globalizing context. *Int. J. Manag. Inf. Sys.* **16**(1), 101–110 (2012)
5. Bennett, M.: Reuse of semantics in business applications. In: Guizzardi, G., Pastor, O., Wand, Y., de Cesare, S., Gailly, F., Lycett, M., Partridge, C. (eds.) *Ontologies in Conceptual Modeling and Information Systems Engineering (ONTO.COM/ODISE 2014)*. CEUR-WS, Aachen, Germany (2014)
6. Borgo, S., Masolo, C.: Ontological foundations of DOLCE. In: Poli, R., Healy, M., Kameas, A. (eds.) *Theory and Applications of Ontology: Computer Applications*, pp. 279–295. Springer, Dordrecht, Netherlands (2010)
7. CEN-CENELEC Management Centre: Materials modelling: Terminology, classification and metadata. CEN workshop agreement 17284, Brussels, Belgium (2018)
8. Ceusters, W.: An information artifact ontology perspective on data collections and associated representational artifacts. *Stud. Health Technol. Inform.* **180**, 68–72 (2012)
9. EDM Council: FIBO Primer (2018)
10. Edwards, P.N., Mayernik, M.S., Batcheller, A.L., Bowker, G.C., Borgman, C.L.: Science friction: Data, metadata, and collaboration. *Soc. Stud. Sci.* **41**(5), 667–690 (2011)
11. EMMC Coordination and Support Action: EMMC Translation Case Template. <https://emmc.info/emmc-translation-case-template/> (2017), date of access: 31st December 2019
12. EMMC Coordination and Support Action: EMMC Translators’ Guide. <https://emmc.info/translators-guide-2/> (2018), date of access: 31st December 2019
13. EMMC Coordination and Support Action: Report on business related quality attributes for industry integration of materials modelling. Project deliverable report 6.3 (2018)
14. EMMC Coordination and Support Action: European Materials and Modelling Ontology, version 1.0.0 alpha 2. <https://github.com/emmo-repo/> and <https://emmc.info/emmo-info/> (2020), date of access: 7th April 2020
15. Faheem, H.M., König-Ries, B., Aslam, M.A., Aljohani, N.R., Katib, I.: Ontology design for solving computationally-intensive problems on heterogeneous architectures. *Sustainability* **10**, 441 (2018)
16. Farazi, F., Akroyd, J., Mosbach, S., Buerger, P., Nurkowski, D., Salamanca, M., Kraft, M.: OntoKin: An ontology for chemical kinetic reaction mechanisms. *J. Chem. Inf. Model.* **60**(1), 108–120 (2020)
17. Goldbeck, G., Ghedini, E., Hashibon, A., Schmitz, G.J., Friis, J.: A reference language and ontology for materials modelling and interoperability. In: *Proceedings of the NAFEMS World Congress 2019, Québec*. p. NWC_19_86. NAFEMS, Knutsford, UK (2019)

18. Guizzardi, G., Wagner, G.: Using the Unified Foundational Ontology (UFO) as a foundation for general conceptual modeling languages. In: Poli, R., Healy, M., Kameas, A. (eds.) *Theory and Applications of Ontology: Computer Applications*, pp. 175–196. Springer, Dordrecht, Netherlands (2010)
19. Horridge, M.: OWLViz (2010), <https://protegewiki.stanford.edu/wiki/OWLViz>, date of access: 31st December 2019
20. Horsch, M.T., Niethammer, C., Boccardo, G., Carbone, P., Chiacchiera, S., Chiricotto, M., Elliott, J.D., Lobaskin, V., P. Neumann, P.S., Seaton, M.A., Todorov, I.T., Vrabec, J., Cavalcanti, W.L.: Semantic interoperability and characterization of data provenance in computational molecular engineering. *Fluid Phase Equilib.* **65**(3), 1313–1329 (2020)
21. Horsch, M.T., Chiacchiera, S., Seaton, M.A., Todorov, I.T.: Multiscale modelling and simulation of physical systems as semiosis. Technical report 2020-B, Inprodat e.V., Kaiserslautern, Germany (2020). <https://doi.org/10.5281/zenodo.3902901>
22. Horsch, M.T., Chiacchiera, S., Seaton, M.A., Todorov, I.T., Šindelka, K., Lísal, M., Andreon, B., Kaiser, E.B., Moggi, G., Goldbeck, G., Kunze, R., Summer, G., Fiseni, A., Brüning, H., Schiffels, P., Cavalcanti, W.L.: Ontologies for the Virtual Materials Marketplace. *KI – Künstl. Intell.* (2020). <https://doi.org/10.1007/s13218-020-00648-9>
23. Horsch, M.T., Chiacchiera, S., Seaton, M.A., Todorov, I.T., Toti, D., Goldbeck, G.: Introduction to the VIMMP ontologies. Technical report, EMMC ASBL, Brussels, Belgium (2020). <https://doi.org/10.5281/zenodo.3936796>
24. Machač, J., Steiner, F., Tupa, J.: Product life cycle risk management. In: Oudoza, C.F. (ed.) *Risk Management Treatise for Engineering Professionals*. pp. 51–72. IntechOpen, London, UK (2018)
25. Mons, B.: *Data Stewardship for Open Science*. CRC Press, Boca Raton, Florida, USA (2018)
26. Neff, G., Tanweer, A., Fiore-Gartland, B., Osburn, L.: Critique and contribute: A practice-based framework for improving critical data studies and data science. *Big Data* **5**(2), 85–97 (2017)
27. Olsina, L.: ThingFO: A foundational ontology for things. Technical report (2020). <https://doi.org/10.13140/RG.2.2.11163.21281/1>
28. Peirce, C.S.: *Peirce on Signs: Writings on Semiotic*. University of North Carolina Press, Chapel Hill, North Carolina, USA (1991)
29. Pries, K.H., Quigley, J.M.: *Reducing Process Costs with Lean, Six Sigma, and Value Engineering Techniques*. CRC Press, Boca Raton, Florida, USA (2013)
30. Rospocher, M., Ghidini, C., Serafini, L.: An ontology for the business process modelling notation. In: Garbacz, P., Kutz, O. (eds.) *Formal Ontology in Information Systems: Proceedings of the Eighth International Conference*. pp. 133–146. No. 267 in *Frontiers in Artificial Intelligence and Applications*, IOS Press, Amsterdam, Netherlands (2014)
31. Schembera, B., Durán, J.M.: Dark data as the new challenge for big data science and the introduction of the scientific data officer. *Philos. Technol.* **33**, 93–115 (2019)
32. Schembera, B., Iglezakis, D.: EngMeta: Metadata for computational engineering. *Int. J. Metadata Semant. Ontol.* **14**(1), 26 (2020)
33. Schoop, M., de Moor, A., Dietz, J.: The pragmatic web: A manifesto. *Comm. ACM* **49**(5), 75–76 (2006)
34. Todor, A., Paschke, A., Heineke, S.: ChemCloud: Chemical e-science information cloud. *Nat. Prec.* (2011). <https://doi.org/10.1038/npre.2011.5642.1>
35. VIMMP Project Consortium: *Virtual Materials Marketplace* (2020), <https://vimmp.eu/>, date of access: 15th July 2020

36. Weber, J.H., Kuziemy, C.: Pragmatic interoperability for eHealth systems: The fallback workflow patterns. In: 2019 IEEE/ACM 1st International Workshop on Software Engineering for Healthcare (SEH). pp. 29–36. IEEE, Piscataway, New Jersey, USA (2019)
37. Weidt Neiva, F., David, J.M.N., Braga, R., Campos, F.: Towards pragmatic interoperability to support collaboration: A systematic review and mapping of the literature. *Informat. Software Technol.* **72**, 137–150 (2016)
38. Wiesner, S., Thoben, K.D.: Requirements for models, methods and tools supporting servitisation of products in manufacturing service ecosystems. *Int. J. Comput. Integr. Manuf.* **30**(1), 191–201 (2016)