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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 serviceoriented 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 associated roles and processes, substantial previous standardization efforts have been carried out by the European Materials Modelling Council (EMMC ASBL). 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 EMMC ASBL.

Keywords: Pragmatic interoperability · applied ontology · process data technology · European Materials Modelling Council (EMMC ASBL)

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* [38]; 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" [42]. Previous work has established that ontologies are not only a viable tool for semantic interoperability, 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 [38, 41]; to provide additional procedural information, *workflow patterns* have been suggested as a tool [40], *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 [34], 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 ASBL) 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 endorsed and developed by EMMC ASBL is MODA (*i.e.*, Model Data) [7], which as an ontology becomes OSMO, the ontology for simulation, modelling, and optimization; this ontology development [21] 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 [13, 25, 32]. 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 [26]. Previous work on data science pragmatics by Neff et al. [29] 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 EMMC ASBL (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 1.3.7, together with OSMO version 1.7.5 which is extended in comparison to the previously published version 1.2 [21]. 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 [9], common physical equation types are identified categorized into four groups according to their granularity level: Electronic, atomistic, mesoscopic, or continuum. doi = 10.1080/0951192X.2015.1130243lowing RoMM, the discrete objects Subsequent to the review activity and the agreement on a basic nomenclature as formalized by the Review of Materials Modelling [9], the EMMC coordination and support action 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 [21]. 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 [21].

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, 39]; beside ontologies, other types of semantic assets, such as XML schemas, can be employed [37]. 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 [30], and the Unified Foundational Ontology [19], are largely domain-independent and reused frequently in very diverse contexts; at the top level, philosopical concerns are at least as significant as the practical demands of research data technology. EMMC ASBL advances its own top-level ontology, the European Materials and Modelling Ontology (EMMO), cf. Francisco Morgado et al. [17], which implements the ontological paradigms of mereosemiotics [23], combining mereotopology [3] with semiotics following Peirce [31]. 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.q., for the exchange of information during data ingest and data retrieval [24]; 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, 24]; the marketplace-level ontology OSMO is directly based on the MODA workflow graph standard as well as its logical data transfer extension [21]. Thereby, a section from MODA, e.g., a solver, becomes a osmo:section entity, e.q., 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 [25]; 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 [26]. 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 [24]. An instance of the translation process [32], some agreed features of which are codified by the EMMC Translators' Guide [25] and the EMMC TC Template [13], 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 [36]. The responsibilities associated with this role relate to technical, organizational, ethical, and legal aspects of data stewardship [28]. One of the most important tasks that an SDO is expected to perform is data annotation, reducing or eliminating dark data [35]; 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.q., 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. [11].

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 most recent updates of the MMTO (presently,⁵ version 1.3.7) and OSMO (presently,⁶ version 1.7.5) are available as free software under the terms and conditions of the GNU Lesser General Public License version 3. Compared with the previously published version of OSMO [21], its present version 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 case (mmto:translation_case) become subclasses of osmo:application_case and can be dealt with in a similar way as the sections from MODA. The

⁵ URL: http://www.molmod.info/semantics/mmto.ttl, as of 11th May 2021.

⁶ URL: http://www.molmod.info/semantics/osmo.ttl, as of 11th May 2021.

TC aspects, cf. Tab. 1, directly correspond to the text fields from the EMMC TC Template [13], 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 stages of the translation process according to the EMMC Translators' Guide [25], 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. 1, 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 [13].

aspect class name	content description
mmto:tca_translator	translator(s) involved in the TC
	content type: evmpo:translator [22]
mmto:tca_end_user	involved end $user(s)$, i.e., $client(s)$ of the translator
	content type: evmpo:end_user [22]
mmto:tca_industrial_case	industrial $case(s)$ associated with the TC
	content type: mmto:industrial_case
mmto:tca_business_case	business $case(s)$ associated with the TC
	content type: mmto:business_case
mmto:tca_expected_outcome	expected outcome of the translation process
	content type: plain text, <i>i.e.</i> , xs:string
mmto:tca_pe_type	physical equation type(s) employed for modelling
	content type: osmo:physical_equation_type [21]
mmto:tca_discussion	summary of discussions with the end user
	content type: plain text, <i>i.e.</i> , xs:string
mmto:tca_kpi_model	employed KPI model(s)
	content type: mmto:kpi_model
mmto:tca_evaluation	evaluation (assessment) of the TC
	content type: vivo:translation_assessment [22]
mmto:tca_impact	impact and benefit to the end user; how does the
	TC contribute to improving processes/products?
	content type: plain text, <i>i.e.</i> , xs:string
mmto:tca_decision_support	$employed \ decision \ support \ system(s)$
	content type: osmo:decision_support_system

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

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

The MMTO and OSMO 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, 24]. 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], cf. Tab. 2; it also refers to entity definitions from two further marketplace-level ontologies from the Virtual Materials Marketplace project [22, 24]: 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 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 [10]. In business administra-

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

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

tion 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:

- 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 [14, 27, 33]. The formulation given above, however, is more closely related to concepts from the EMMO. Due to its foundation on Peircean semiotics [31], 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 [17, 18, 23]. In particular, the same distinction is made in EMMO version 1.0.0 beta [12]. Accordingly, this approach is best amenable to a prospective alignment of the MMTO with the EMMO and the approach to interoperability guided by EMMC ASBL.

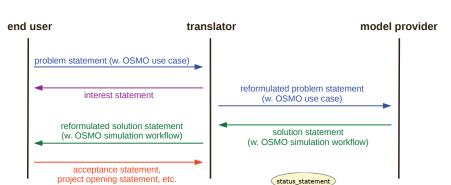
Table 4. MMTO representation of the stages of a materials modelling translation process (subclasses of mmto:translation_step), as specified by the EMMC Translators' Guide [25]. The numbers in the first column, which follow the EMMC Translators' Guide, are related to the stages by the datatype property 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	mmto:translation_step_bc	mmto:business_case
	good understanding of the business case	
2	mmto:translation_step_ic	mmto:industrial_case
	good understanding of the industrial case	
3	mmto:translation_step_data	osmo:use_case
	analysis of the data from experiment and	
	simulation available to the end user	
4^{\star}	mmto:translation_step_modelling	osmo:materials_model
	translation to simulation workflows	and osmo:workflow_graph*
5	mmto:translation_step_execution	_
	execution and validation strategy	
6**	mmto:translation_step_decision	osmo:decision_support_system**
	evaluation of the simulation results to	and mmto:kpi_model**
	facilitate an actionable decision	*

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 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



oject statement

modelling statement

negotiation statement

declaratio

ranslation statement

Interlocution

statement

opening_statement

closing_statement

olution_statemer

decision statement

interest statement

rejection_statement

acceptance statement

Fig. 1. 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) [22]; this diagram was generated using OWLViz [20].

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 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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